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IOP Institute of Physics

Plenary Speakers

Progress Towards the Digital Twin for Plasma Microelectronics Fabrication

Mark Kushner[1]
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Plenary Talk: Prof. Mark J. Kushner, June 18, 2024, 09:00 - 10:00

The rapid advancement in microelectronics fabrication and device capability – Moore's Law – is being challenged by those devices approaching atomic dimensions. Increasing device performance is now relying on more complexity and new materials as limits are being reached in the ability to shrink devices. The transition to 3-dimensional devices (e.g., 3D-NAND memory) reflects the trend to improve performance by stacking devices as opposed to shrinking. With the majority of manufacturing steps involving plasmas (etching, deposition, cleaning, implantation) this added complexity is stressing both developing new plasma processes and the economics. An industry wide effort to address these challenges is the digital twin – conceptually, a computational representation of the entire fabrication process, from delivery of blank wafers to packaging of final devices. Digital twins for plasma processing would address equipment scale production of fluxes of reactive species (radical, ions, electrons, photons) delivered to the wafer and the nanoscale evolution of features in response to those fluxes; and so be tools used in process development. Digital twins would also track the state of the reactor predicting, for example, erosion of components or coatings on plasma facing surfaces, and recommending when preventative maintenance is necessary. In this talk, the status of one aspect of the digital twin, computational models for plasma etching, will be discussed. The current status of reactor and feature scale modeling for plasma etching will be reviewed, with assessments of progress needed to achieve digital twin status. The roles of fundamental physics-based modeling and that of machine learning in the digital twin will be discussed

Accessing non-equilibrium at the intrinsic scales of molecules

Jascha Repp[1]
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Plenary Talk: Prof. Jascha Repp, June 21, 2024, 12:00 - 13:00

While scanning probe microscopy (SPM) has revolutionized our understanding of the atomistic world it is usually too slow to capture non-equilibrium excitation processes. Two complementary approaches that allow accessing non-equilibrium phenomena with SPM will be presented.
Accessing ultra-fast phenomena is enabled by combining lightwave electronics with scanning tunneling microscopy (STM), allowing for combined femtosecond and sub-angstrom resolution in observing matter (1). Lightwave STM also provides access in the control of matter by utilizing localized electric fields to exert atom-scale femtosecond forces (2). Further, we show how lightwave STM can be extended to its ultrafast spectroscopy variant (3). The corresponding ultrafast and atomically resolved tunnelling spectra reveal transient energy shifts of a single selenium vacancy in a WSe2 monolayer on gold.

Another approach gives us access to intermediate timescales that are relevant for spin precession and relaxations. We exploit the high sensitivity of atomic force microscopy (AFM) to perform STM and spectroscopy on molecules in absence of any conductance of the underlying substrate. Thereby, we gain access to out-of-equilibrium charge states (4) that are out of reach for conventional STM. Extending this technique by electronic pump-probe spectroscopy, we measured the triplet lifetime of individual molecules and its quenching by nearby oxygen molecules (5). Combined with radio-frequency magnetic-field driving we introduce AFM-based electron spin resonance and spin manipulation showing long spin coherence in single molecules (6).

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Combinatorial synthesis and high-throughput characterisation of thin film materials libraries for the accelerated discovery of materials

Prof. Dr. Alfred Ludwig[1]
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Plenary Talk: Prof. Alfred Ludwig, June 19, 2024, 09:00 - 10:00

Discovery of new materials is a key challenge in materials science. New materials for sustainable production/storage/conversion of energy carriers are necessary to improve existing and to enable future energy systems. Compositionally complex materials, frequently called high entropy materials, offer a vast multidimensional search space, which provides opportunities for discovering new materials. However, efficient methods for the exploration and exploitation of this search space are necessary. Here, the integration of high-throughput thin-film combinatorial materials science methods with simulation and materials informatics (1) is presented as an effective means to produce large datasets on new materials, which enables mastering of the search space. The approach combines theoretical predictions from high-throughput computations with production of large, consistent and complete experimental datasets, which are used for materials informatics. Thin-film materials libraries are fabricated by combinatorial sputter deposition and optional post-deposition treatments, followed by high-throughput characterization, and finally the organization of the acquired multi-dimensional data in adequate databases as well their effective computational analysis and visualization, e.g., of quinary systems in the form of composition-processing-structure-function diagrams, interlinking compositional data with structural and functional properties. The talk will discuss examples of combinatorial discoveries (2, 3) and the targeted development of new compositionally complex materials for electrocatalysis (4) where compositional complexity offers a new design principle (5). This includes also a new type of microscale thin film materials libraries (6). Furthermore, a new approach (7) to accelerate atomic-scale measurements for complex alloys is presented as well as applications of materials informatics to accelerate and improve the materials discovery process (8, 9).

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Surface structure from machine learning

Prof Bjørk Hammer[1]
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Plenary Talk: Prof. Bjork Hammer, June 21, 2024, 09:00 - 10:00

In recent years, machine learning interatomic potentials (MLIPs) have been developed to a stage, where they are replacing Density Functional Theory (DFT) in e.g. molecular dynamics calculations [1]. For structure determination it remains, however, a challenge to formulate active learning protocols, where new DFT training data are provided to improve the MLIPs, while the searches progress and discover new atomic motifs [2]. In this work, strategies for how to collect the training data and for how to construct the MLIPs will be presented. The training data may e.g. be constructed using the same technology as in image generation (diffusion models) [3] while the construction of the MLIPs may involve neural networks and Gaussian Process Regression methods [4]. Examples of surface structures solved will include complex ultra-thin surface oxides on Ag(111) [5] and Pt3Sn [6]. Our computer codes are available as an open-source python package, AGOX [7, 8].

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OrbiSIMS – high resolution mass spectrometry imaging with simultaneous chemical identification and localisation with high confidence

Professor Ian Gilmore[1]

[1] *National Physical Laboratory, United Kingdom*

Plenary Talks: Prof. Ian Gilmore (EPS Invited Lecture) and Prof. Zhaofeng Chen, June 20, 2024, 08:30 - 10:30

Since the origins of secondary ion mass spectrometry (SIMS), almost nine decades ago, the field has evolved along distinct pathways where a process of natural selection has seen the emergence and decline of techniques as they, in turn, are superseded by new innovations. This has resulted in today's powerful SIMS instruments that are having extraordinary impact in almost every area of materials science and increasingly in the life-sciences [1]. However, independent evolutionary lineages have led to segmentation of the community. Recent advances in instrumentation and advances in fundamental understanding are now beginning to show prospects for evolutionary convergence.

To put this in context, recent developments driven by a fundamental analytical challenge will be discussed. Techniques, like nuclear magnetic resonance, provide high confidence in identification but with limited information on localisation. Whilst techniques like electron microscopy, give high confidence in localisation but low confidence in identification. This has been termed the "molecular uncertainty principle" [2]. In 2017, NPL introduced the OrbiSIMS technology [3] with an objective to simultaneously provide molecular identification and localisation as close to this limit as possible. Since then, the number of OrbiSIMS instruments around the world has increased significantly and the community of users and range of applications has grown. In this presentation, we briefly introduce the OrbiSIMS and use examples of the applications in advanced materials [4] and life-sciences [5] to highlight a convergence of "static SIMS" and "dynamic SIMS" as some of the traditional barriers begin to disappear. In a look to the future, further advances in mass spectrometers are expected, for example multiple reflection Time of Flight analysers, ion mobility and other novel hybrid analysers as well as improved sensitivity using quantum detection.

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Vacuum insulation panel and its application in the field of building

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Plenary Talks: Prof. Ian Gilmore (EPS Invited Lecture) and Prof. Zhaofeng Chen, June 20, 2024, 08:30 - 10:30

Energy used for heating, ventilation, and air conditioning in commercial and residential buildings contributes 30% of the total energy consumed in many countries. Energy consumption in buildings is becoming the main carbon reduction target for carbon peak and neutrality. In vacuum insulation panel, a core material is vacuum sealed in a membrane material to eliminate gas convection, thus having the lowest thermal conductivity (0.0015W/m×K) than other thermal insulations. Vacuum insulation panel found extensive use in the construction and industrial sectors. The core material serves three purposes: first, it can support the soft film to preserve the structure; second, it can block infrared radiation; and third, it stops gas from diffusing after a tiny quantity of gas incursion. The core materials are of three types: fiber, foam, and powder. The membrane serves to ensure the integrity of the vacuum insulation panel, prevents penetration of outside air and moisture, and provides a simple ultra-thin shape. The membrane material are of three types: plastic for low temperatures such as in building, metal for intermediate temperatures, and ceramic for high temperatures. Vacuum insulation panel offers thin but highly effective insulation solutions to reduce thermal losses for both new and renovated buildings. This study presents a comprehensive review of the vacuum insulation panel comprising glass fibre/fly ash core and laminated aluminium foil membrane materials, used as building envelopes in China. Characterization of the material composition, installation method procedures, and future outlook have been investigated and discussed. The outer barrier layer of fibreglass cloth protects vacuum insulation panel from localized alkaline cement and mechanical stress. Insulation assembly debonding from building walls was curbed by a combination of reinforced fibreglass mesh and a plastic spacer. Besides, elongated slots were made in small gaps between the vacuum insulation panel and a wall against unanticipated moisture conditions. Furthermore, the bolt could pass through the peephole in vacuum insulation panel to improve its adherance to the wall, and prevented it from loosening or falling off.

Feature Talks

Integration of ultrafast switches into a single-molecule vacuum electronics

Hirofumi Yanagisawa[1]
[1] *Shizuoka University, Japan*

Electronic Materials, Energy Reduction and Carbon Reduction 2, June 21, 2024, 10:30 - 12:00

A switch in vacuum nanolectronics consists of a sharp metallic needle and a counter electrode, as depicted in Figure 1(a). Irradiating such a needle with femtosecond light pulses generates electron emissions from the apex[1]. This situation is equivalent to a transistor switch with an optical gate, as shown alongside. Since electron emissions occur on a time scale of femtoseconds to attoseconds, this kind of switches significantly surpasses the speed of current computer switching devices by three to six orders of magnitude. Concurrent plasmonic effects that appear upon illuminating the tip enable precise spatial control of electron emission on a 10-nm scale[2]. Leveraging this phenomenon allows the selection of emission sites A or B in Figure 1(b). This situation is equivalent to two switches, whose gates can independently be controlled by light, as shown in the accompanying diagram. Consequently, this site selectivity aids switch integration. However, further miniaturization of such an electron source through plasmonics poses challenges. Here, we discuss the possibility of achieving subnanometric emission site control by utilizing the quantum nature of a single molecule. In this setup, fullerene molecules are positioned on a metallic substrate[3], as illustrated in Figure 1(c). Electrons, supplied from the substrate, are emitted from the single molecules after traversing specific molecular orbitals (MOs). Depending on the involved MOs, the emission sites vary at subnanometric scale. Our research demonstrates the optical control of the MOs that electrons pass through, thus realizing an electron source with subnanometric emission site-selectivity[4]. This technique facilitates the integration of switches into a single molecule.

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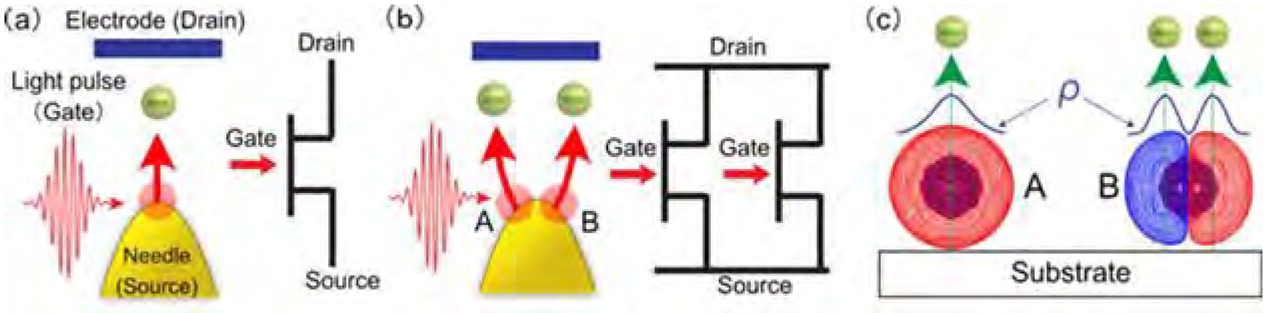

The Einstein Telescope beampipe vacuum

Carlo Scarcia[1,2], Giuseppe Bregliozzi[1], Paolo Chiggiato[1], Manjunat Dakshinamurthy[1], Gilles Favre[1], Jose Antonio Ferreira[1], Cedric Garion[1], Jan Hansen[1], Leonel Marques Antunes[1], Ana Teresa Perez Fontenla[1], Gregory Pigny[1], Luigi Scibile[1], Stefano Sgobba[1], Mauro Taborelli[1], Ivo Wevers[1]

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Large Vacuum Systems, June 17, 2024, 11:00 - 12:35

Building upon the success of the LIGO and Virgo experiments in gravitational wave (GW) detection, the GW community is now setting its sights on new laser interferometers capable of detecting GWs from cosmological events spanning a much larger volume of the universe and occurring in its early phases. In pursuit of this objective, the European community has proposed the construction of the Einstein Telescope (ET), a complex comprising six interferometers arranged within a triangular tunnel spanning 10 km on each side. To mitigate noise stemming from statistical pressure fluctuations, the laser beams necessitate Ultra-High Vacuum (UHV) conditions within a 1-meter diameter beamtube, extending across a total vacuum length of 120 km. However, the projected cost of the ET vacuum system, based on previous-generation GW detectors, is notably high, second only to that of the civil engineering. To address this challenge, CERN, in collaboration with other institutes, has launched a study to explore alternative and more cost-effective technological solutions. This investigation includes assessing the UHV compatibility of various steels, with the potential elimination of high-temperature degassing treatments, reducing bakeout temperatures, designing and implementing thin-walled pipes, and optimizing vacuum layouts and tunnel integration logistics. To validate these optimizations, a 36-meter-long pilot sector will be constructed at CERN.

Confined epitaxy of Sn-induced structures beneath epitaxial graphene hosting correlated electronic properties

Dr Zamin Mamiyev[1], Chitran Ghosal[1], Niklas Witt[2,3], Siheon Ryee[2], Tim Wehling[2,3], Christoph Tegenkamp[1]
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Carbon Materials 2, June 19, 2024, 10:30 - 12:35

Manipulation of graphene properties using proximity interaction is one of the sophisticated approaches for enhancing its capability and device performance. To form and investigate such interactions, confined epitaxy of atomically flat materials beneath high-quality epitaxial graphene (EG) has been shown as a promising route. In particular, high-Z elements (e.g., Sn, Pb, Bi, etc.) enable the forming of correlated electronic states in proximity to graphene relativistic electron gas.

In this study, we utilize high-resolution electron energy loss spectroscopy, low-energy electron diffraction, scanning tunneling microscopy, and spectroscopy, along with density functional calculations, to investigate Sn-induced interfaces and graphene sandwich structures. Intercalated Sn atoms form various phases, including disordered and ordered 1×1, dilute and long-range ordered $(\sqrt{3}\times\sqrt{3})$R30° relative to SiC substrate.[1] Notably, the interaction of EG with these phases varies; while EG on the Sn(1×1) phase is charge neutral, EG on the Sn$(\sqrt{3}\times\sqrt{3})$ phase is doped to ~8×10^{12} 1/cm^2. The observed sheet plasmons on EG/Sn/SiC heterostructures exhibit similar dispersions, albeit with variations due to interface metallicity. Multipole plasmonic excitations, whose frequency is predominantly influenced by electronic distribution and hybridization across the interface, further confirm this trend.[2]

Atomically-resolved STM showed that the strong local interaction of Sn(1×1) with atop EG forms a $(\sqrt{3}\times\sqrt{3})$R30° interference pattern revealing Kekule' bond order. On the other hand, the Sn$(\sqrt{3}\times\sqrt{3})$ with respect to SiC is strongly hybridized with EG. Further improving the interface Sn$(\sqrt{3}\times\sqrt{3})$ periodicity enabled the detection of the interband transition corresponding to the Mott gap. This observation was confirmed by local spectroscopy, providing insights into this transition. With detailed DFT modeling, we found the magnitude of this gap is sensitive to the shift of surface potential, which in turn affects the degree of hybridization.

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Experimental Characterization of Defect-Induced Phonon Lifetime Shortening

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Advances in Experimental and Theoretical Methods 1, June 17, 2024, 11:00 - 12:35

We present the first direct experimental measurement of defect-induced lifetime shortening of acoustic surface phonons. Defects are found to contribute a temperature-independent component to the linewidths of Rayleigh wave phonons on a Ni(111) surface. We also characterized the increase in phonon scattering with both surface defect density and phonon wave vector. A quantitative estimate of the scattering rate between phonon modes and surface line defects is extracted from the experimental data for the first time.

How the 2nd coordination sphere affects the reactivity of “single-atom” catalysts

Gareth Parkinson[1], Ali Rafsanjani Abbasi[1], Faith Lewis[1], Matthias Meier[1], Florian Buchner[1], Georg Madsen[1], Michael Schmid[1], Ulrike Diebold[1]

[1]Tu Wien, Austria

Catalysis and Electrocatalysis including Single Atom and In Operando Studies 2, June 19, 2024, 16:00 - 17:30

So-called „single-atom“ catalysis (SAC) is currently a hot topic in catalysis research. While the initial aim was to minimize the amount of precious metals required in reactions, it quickly became clear that the coordination of the single atom affects its electronic structure and thus its reactivity. The heterogeneity of powder-supported catalysts makes it difficult to study structure-function relationships, and this motivates research on model systems where the atomic-scale structure can be precisely defined. In this talk, I will compare how O2 interacts with Pt atoms supported on two model surfaces; Fe3O4(001) [1,2] and Fe2O3(012) [3]. At first glance, the single atoms seem similar. In both cases the Pt are two-fold coordinated to oxygen and slightly oxidized. However, the Pt1/Fe2O3(012) reacts strongly with O2 at room temperature, whereas the Pt1/Fe3O4(001) does not. Using a combination of scanning probe data, XPS, and density functional theory-based calculations, I will show that the location of the 2nd nearest neighbour Fe cations is the deciding factor in whether dissociative adsorption can occur on these model catalysts. These results demonstrate how careful control of the atom/support can have a significant impact on the reactivity of SAC systems.

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Planar Niobium Oxide Clusters on the Au(111) Surface

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Metal Surfaces - Adsorption, Desorption and Reactions 2, June 17, 2024, 14:00 - 15:30

Supported oxide ultrathin films are attractive systems for the investigation of catalytic mechanisms in inverse catalysts, where the low oxide dimensionality and the nature of the interaction with the metal substrate play an important role. Moreover, at submonolayer coverages, oxide boundaries and finite size effects give rise to a variety of unique local atomic environments which are absent in continuous films [1].

Beyond the pristine epitaxial honeycomb Nb_2O_3 monolayer [2], we report a joint experimental and theoretical investigation on the atomic structure and stabilization mechanisms of small oxide clusters on the Au(111) surface [3]. A large variety of such objects, composed of four-, five-, and six-membered rings, were grown by thermally driven oxidation of metallic Nb and characterized on the atomic scale in high-resolution STM experiments. With the help of DFTB-aided genetic algorithms we were able to determine the chemical compositions and atomic structures of alternative isomers, identify the most stable ones under the experimental conditions, and convincingly demonstrate their oxygen-rich character. We argue that the oxygen excess is stabilized by a particularly strong interaction between the oxide clusters and the Au(111) substrate, which is accompanied by large interfacial electron transfer and an increase of the Nb oxidation state. We show that the interaction with the Au substrate, which narrows down the formation energies of particles consisting of threefold coordinated cations, is also responsible for the observed coexistence of such wide range of cluster structures and compositions.

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The Diamond-II Vacuum System

Dr Matthew Cox[1], Mr Toby Lockwood[1], Mr Timothy Darby[1], Mr Hugo Shiers[1], Mr Richard Howard[1], Dr Christopher Burrows[1], Dr Neil Warner[1]

[1] *Diamond Light Source, United Kingdom*

Large Vacuum Systems of Particle Accelerators, June 18, 2024, 10:30 - 12:30

Diamond Light Source is the UK's national synchrotron. Currently underway is the Diamond-II upgrade programme, an in-place upgrade for the storage ring, which will reduce beam emittance, increase brightness, and enable three new beamlines.

For the Diamond-II upgrade, almost the entire 562 m circumference Diamond storage ring vacuum system has to be replaced. The target vacuum performance is 1E-9 mbar at 300 mA of beam current after 100 A.h conditioning time. The small aperture of the electron beam channel (typically 20 mm diameter), and the resultant conductance-limited design, requires the use of distributed pumping which is provided by non-evaporable getter (NEG) coatings, supplemented by ion pumps. Mechanical stability, photon extraction routes, heat load management, beam impedance, operational reliability and limiting the user beam dark period to 18 months are also crucial. As part of the machine upgrade, the entire 162 m circumference booster ring also has to be replaced and many of the front ends upgraded along with installation of some new front ends.

This paper will present the Diamond-II accelerator vacuum system designs, outlines the challenges and how these have been resolved.

Quantum-based realizations of the pascal in Europe

Dr. Dr. Tom Rubin[1]
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Vacuum Metrology, June 20, 2024, 11:00 - 13:00

Accurate pressure measurements are a key technology for important applications in a variety of currently relevant areas, such as climate, energy, and medicine. It has already been shown that quantum-based methods of pressure measurement by determining gas density enable faster calibration of pressure sensors and lead to an improvement in uncertainties. Accordingly, the current EU project "MQB-Pascal" presented here deals with the implementation of a metrological infrastructure for an SI-traceable quantum-based Pascal between 1 Pa and 1 MPa.
Following the successful completion of the previous "QuantumPascal" project, which focused on the gases helium and argon, this time the focus is on nitrogen.
In particular, instruments and quantum-based methods are being developed and evaluated with regard to practical applications in order to meet the needs of the interest groups. The MQB-Pascal project started in June 2023, has a duration of three years and aims to further develop the technologies and enable the development of corresponding products and services everywhere (also outside metrology institutes) in the future.

Ångström-Scale Topography in Neutral Helium Microscopy: Evaluating Thin-Film Coatings over Large Areas

Dr Sabrina Eder[2], Dr Adam Fahy[1], Dr Matthew Barr[1], Prof Jim Manson[3], Prof Bodil Holst[2], **Prof Paul Dastoor**[1]

[1]University Of Newcastle, Australia, [2]University of Bergen, Norway, [3]Clemson University, United States of America

Advanced Thin Film Characterisation, June 19, 2024, 16:00 - 17:30

Nanoscale thin film coatings and surface treatments are ubiquitous across industry, science, and engineering; imbuing specific functional or mechanical properties (such as corrosion resistance, lubricity, catalytic activity and electronic behaviour). Non-destructive nanoscale imaging of thin film coatings across large (ca. centimetre) lateral length scales, crucial to a wide range of modern industry, remains a significant technical challenge. By harnessing the unique nature of the helium atom–surface interaction, neutral helium microscopy images these surfaces without altering the sample under investigation. Since the helium atom scatters exclusively from the outermost electronic corrugation of the sample, the technique is completely surface sensitive. Furthermore, with a cross-section that is orders of magnitude larger than that of electrons, neutrons and photons, the probe particle routinely interacts with features down to the scale of surface defects and small adsorbates (including hydrogen). Here, we highlight the capacity of neutral helium microscopy for sub-resolution contrast using an advanced facet scattering model based on nanoscale features. By replicating the observed scattered helium intensities, we demonstrate that sub-resolution contrast arises from the unique surface scattering of the incident probe. Consequently, it is now possible to extract quantitative information from the helium atom image, including localised ångström-scale variations in topography.

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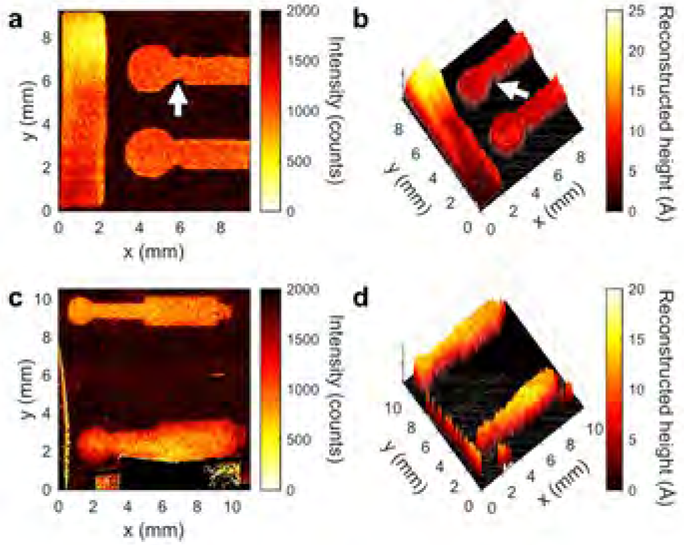

Can tunnel current fluctuations accurately track molecular diffusion?

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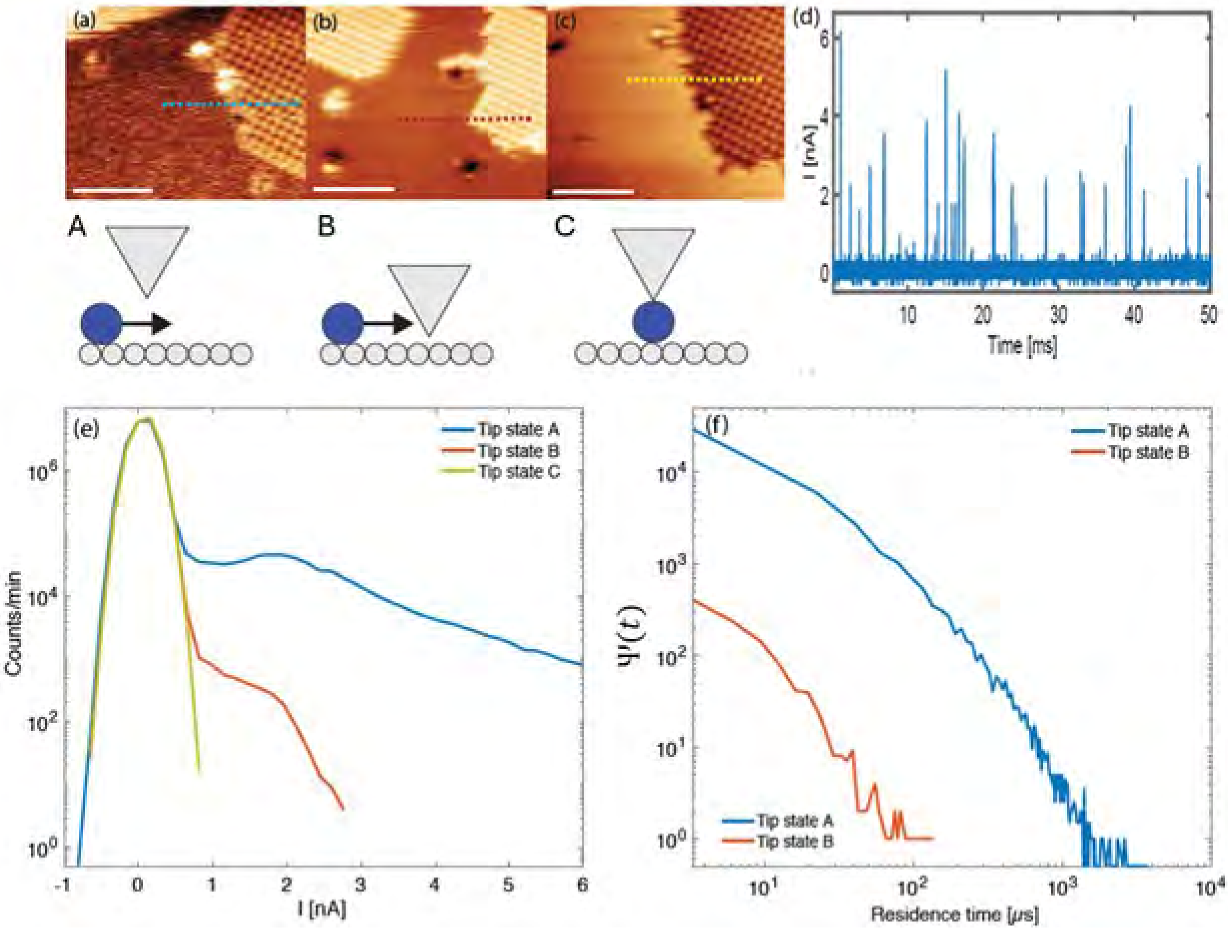
Advances in Experimental and Theoretical Methods 3, June 17, 2024, 16:00 - 17:35

Although scanning tunnelling microscopy (STM) has long been used to image the motion of adsorbates on surfaces by acquiring sequential images, this strategy is limited to the rather low bandwidth (typically ~ hundreds of mHz at best) associated with imaging. An alternative, higher bandwidth approach is to use atom tracking to follow the diffusive motion of an individual adsorbate -- Swartzentruber [Phys. Rev. Lett. 76 459 (1996)] demonstrated a 1000-fold increase in temporal resolution via this method.

Even higher improvements in bandwidth (by many orders of magnitude) are possible by monitoring fluctuations in the tunnel current as molecules diffuse underneath a fixed STM tip. Nonetheless, a key issue arises: to what extent does the mesoscopic and atomistic structure of the tip influence the diffusion dynamics? Indeed, might it be possible to turn the invasive nature of the measurement to our advantage in order to determine the tip-sample interaction potential [Schiel et al, J. Electrochem. Soc. 169 096515 (2022)]?

We have explored these questions using the 3,4,9,10-perylene-tetracarboxylicdianhydride (PTCDA)-on-Ag(110) system as a model platform. Using a combination of variable temperature STM measurements, atom-tracking for drift correction (down to a level of ~ 10 pm/min during acquisitions at 300 K), and a tunnel current pre-amp bandwidth of 80 kHz, we acquire a series of tunnel current fluctutation events (typically numbering of order 1E6 per run) arising from molecular diffusion. As can be seen from Fig. 1, the state of the tip has an exceptionally strong influence on the tunnel current fluctuation statistics. We shall discuss the potential of machine learning architectures for the classification of tip states on this basis.

Fig. 1(a),(b),(c): STM images of PTCDA islands acquired with different tip states (A,B,C); (d) example of current fluctuation trace; (e), (f) tip-dependent histograms and residence time distributions, respectively.


(a)
(b)
(c)
(d)
A
B
C
I [nA]
Time [ms]
(e)
Tip state A
Tip state B
Tip state C
Counts/min
I [nA]
(f)
Tip state A
Tip state B
$\Psi(t)$
Residence time [μs]

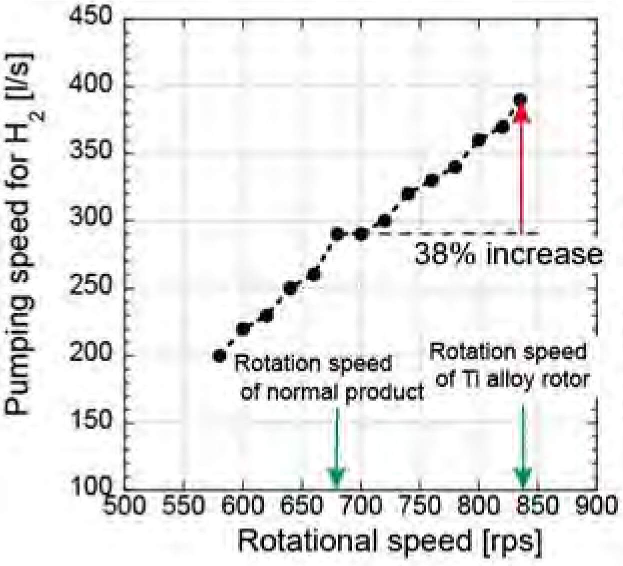
High performance turbomolecular pump with titanium alloy rotor blades

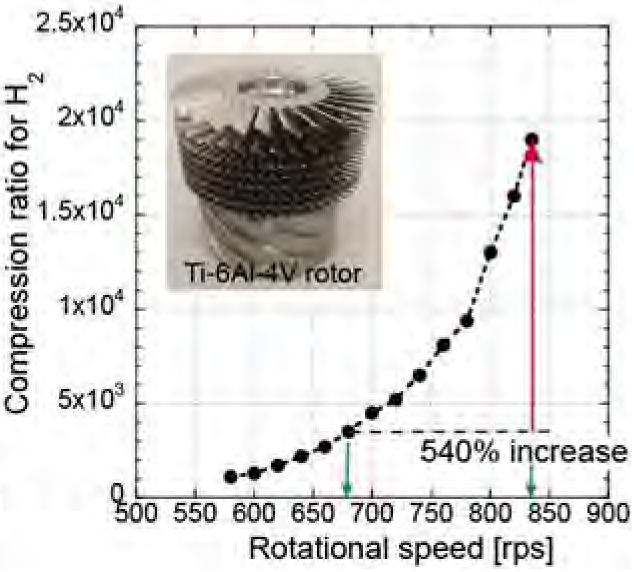
Junichiro KAMIYA[1], Kaoru Wada[2], Nang Nang Tin Tin Htwe[3]
[1]Japan Atomic Energy Agency / J-PARC center, Japan, [2]Tokyo Electron Ltd, Japan, [3]Osaka Vacuum Ltd, Japan

Vacuum pumps, June 21, 2024, 10:30 - 12:00

J-PARC 3 GeV rapid cycling synchrotron (RCS) is one of the highest beam power proton accelerators. Turbo molecular pump (TMP) is used as main pump in the RCS because TMP can evacuate the additional outgassing by the beam induced desorption with large pumping speed in wide pressure range. For the higher beam power upgrade in the future, the development of higher performance TMP of the same size is very important. Pumping speed and compression ratio of existing TMP are limited by the rotational speed, which is derived from the specific strength limit of rotor material; aluminum alloy. We focused on Ti-6Al-4V because of its high specific strength and easy availability. Since the specific strength of Ti-6Al-5V is 1.47 times that of aluminum alloy, the rotational speed of the rotor blade can be increased by more than 1.2 times.

The rotational speed of the developed TMP was successfully increased to 835 rpm compared to 680 rpm of the existing TMP. By increasing the speed of the rotor blades, the pumping speed for hydrogen increased by 34% and the compression ratio increased by 540% compared to the existing TMP. Since hydrogen remains in an ultra-high vacuum chamber, this is a significant achievement that will lead to the ultra-high vacuum technology necessary for the advancement of accelerators, semiconductors, and analytical equipment.





The oxidation of diamond surfaces at near-ambient pressure

Doctor Simon Astley[1], Doctor Kerry Hazeldine[1,2], Doctor Alex Walton[3], Doctor Gruffudd Willliams[4], **Professor Andrew Evans**[1]

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Carbon Materials 1, June 18, 2024, 16:00 - 17:30

Control of the surface is critical in realising sensing and quantum applications of single-crystal, polycrystalline and nano-diamond [1]. In synthetic diamond manufacture, the surface is usually hydrogen-terminated; subsequent treatment is required to produce other terminations such as oxygen-termination. This can be achieved by wet chemical treatment or exposure to gases or plasmas, but variation in carbon-oxygen surface bonding poses a challenge in reproducing optimised surfaces. Surface science methods are widely used for characterisation but are often limited to samples and measurement conditions that do not reflect the application environment. X-ray Photoelectron Spectroscopy (XPS) in gaseous environments has been applied to monitor the oxidation of H-terminated diamond and nanodiamond (ND) surfaces and these O-terminated surfaces are compared to acid-etched and plasma-treated surfaces. The conductivity of diamond substrates can significantly influence the measurement; this effect has been identified by varying the doping and experimental parameters such as the temperature and the x-ray energy and flux [2]. Identifying surface and bulk regions is particularly challenging for nanoparticles where the dimensions are comparable to the XPS probing depth (1-10 nm) and where a large number are sampled in each measurement. Single-layer films of H-terminated NDs were prepared on metal substrates using vacuum drying of monodispersed NDs and their in-situ exposure to molecular oxygen was compared to H-terminated bulk diamond surfaces. XPS measurement at pressures from ultrahigh vacuum to 20 mbar, and at temperatures between 20 °C and 900 °C, revealed the various stages of adsorbate attachment and removal. Different x-ray energies were used to excite photoelectrons with different mean free path and the size and shape of the nanodiamonds were confirmed using Dynamic Light Scattering (DLS) and Transmission Electron Microscopy (TEM).

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Temperature-dependent selectivity and detection of hidden carbon deposition in methane oxidation

Ulrike Küst[1,3], Weijia Wang[2], Changda Wang[4], Helena Hagelin-Weaver[5], Johan Gustafson[1], Andrey Shavorskiy[2], Jason F. Weaver[5], **Jan Knudsen**[1,2,3]
[1]Division Of Synchrotron Radiation Research, Lund University, Sweden, [2]The MAX IV Laboratory, Lund University, Sweden, [3]NanoLund, Lund University, Sweden, [4]National Synchrotron Radiation Laboratory, University of Science and Technology of China, China, [5]Department of Chemical Engineering, University of Florida, United States of America

Catalysis and Electrocatalysis including Single Atom and In Operando Studies 1, June 19, 2024, 14:00 - 15:30

Reaction products in heterogeneous catalysis can be detected either on the catalyst surface or in the gas phase after desorption. However, if atoms are dissolved in the catalyst bulk, reaction channels can become hidden. This is the case if the dissolution rate of the deposits is faster than their formation rate. That might lead to the underestimation or even overlooking of reaction channels such as e.g. carbon deposition during hydrocarbon oxidation reactions which is problematic as carbon can have a significant influence on the catalytic activity[1].

In this contribution[2], we discuss and demonstrate how such hidden deposition channels can be uncovered by carefully measuring the product formation rates in the local gas phase just above the catalyst surface with time-resolved Ambient Pressure X-ray Photoelectron Spectroscopy. As a case study, we investigate methane oxidation on a polycrystalline Pd catalyst in oxygen-lean conditions at a few millibar pressure. By ramping the temperature between 350 °C and 525 °C we follow how mass transfer limitations change the selectivity between the different possible reaction pathways: Complete combustion forming CO_2, partial combustion forming CO, and carbon formation leading to subsurface or surface carbon deposition. Outside the oxygen mass transfer limit (O-MTL) CO_2 is the only reaction product observed in the gas phase above the catalyst surface, while CO formation only is observed within the O-MTL. Further we use the localized water signal as a measure of the conversion rate of methane together with the balanced reaction equations to reveal that carbon deposition surprisingly takes place also outside the O-MTL.

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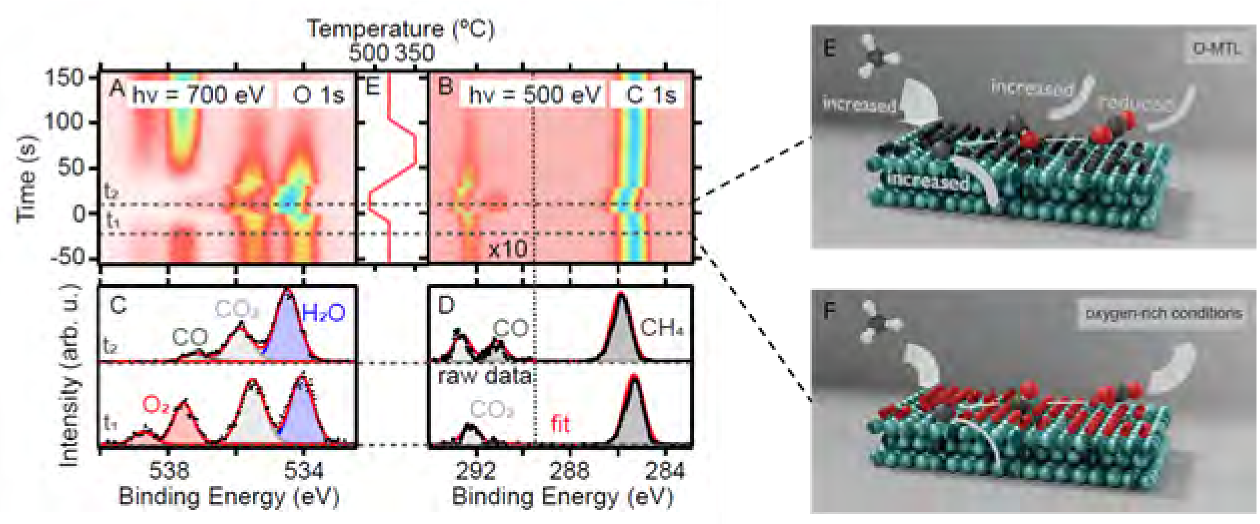

Recent Progress of Diamond Semiconductors: Two-Inch Diamond Wafer and High-Power Diamond MOSFETs

Professor Makoto Kasu

[1]*Saga University, Japan*

MS-5: Electrochemical MEMs Sensing for Environmental and Biological Monitoring, June 19, 2024, 14:00 - 15:30

Diamond possesses a wider bandgap (5.47 eV), higher breakdown electric field (>10 MV/cm), higher thermal conductivity (22 W/cmK), and higher electron and hole mobilities (4500 and 3800 cm2/Vs, respectively) than GaN and SiC. Therefore, diamond is considered to be the most capable candidate for the power semiconductor device application [1].
So far, diamond single-crystal substrates have been limited to sizes of 4 mm. Recently, we demonstrated diamond wafers with a two inch-diameter was grown on Ir/ misoriented sapphire (□-Al2O3) $(11\bar{2}0)$ substrate [2]. This wafer exhibited the highest crystal quality, with an XRC (004) FWHM of 98 arcsec.

We then fabricated diamond p-channel MOSFETs on CVD diamond wafers [3]. We have established two semiconductor fundamental technologies of p-type doping with NO2 and surface passivation/ gate insulator with an Al2O3 layer. We successfully fabricated diamond power MOSFETs. In the drain current–voltage (ID–VDS) characteristics, the maximum ID was 0.68 A/mm [Fig. 1(a)]. A low ON resistance of 50 Ω·mm was obtained. The off-state drain current characteristic of the MOSFET at VGS = 7 V indicates a high breakdown voltage (VBR) of −2568 V [Fig. 1(b)]. The specific on-state resistance, (RON,spec) was determined to be 7.54 mΩ·cm2. Consequently, the BFOM (= VBR2/RON,spec) — where VBR, LSD, and 2LT were −2568 V, 13.6 μm, and 1.48 μm, respectively — was determined to be 874.6 MW/cm2, the highest ever in diamond and comparable to GaN.

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Niloy Chandra Saha, Makoto Kasu et al., IEEE Electron Device Letters 43, 777 (2022).

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Plasmonic nanoalloys. Manufacturing with properties tuned by the assistance of machine learning method

Mr Marcin Lapinski[1], Mr Pawel Syty[1], Mr Jozef E. Sieniewicz[1], Mr Wojciech Sadowski[1], Ms Barbara Koscielska[1]
[1] *Gdansk University Of Technology, Poland*

Plasmonics and Excited States at Surfaces, June 19, 2024, 10:30 - 12:35

As-deposited metallic films with a nanometric thickness can be meta- or unstable. It leads to disintegration (so called dewetting, rupture, self-organization, agglomeration) of the continuous layer into isolated nanoislands [1]. That process can be observed at temperature well below the melting point of nanolayer, even at room temperature [2]. The transformation mechanism is driven by thermally accelerated diffusion that leads to the minimalization of surface free energy in the system [3].
The thermal dewetting of a metallic multilayers could be used for the preparation of nanoalloys or nanocomposites. Properties of manufactured nanostructures depend not only on its size, but most of all its nanostructure and chemical composition. Therefore, a wide knowledge about kinetics and nanostructures formation parameters play key role from practical applications point of view.
In this work, we would like to present an experimental method for manufacturing the plasmonic nanostructures based on gold-silver, gold-copper and silver-copper nanoalloys and nanocomposites. We would also like to illustrate the potential of the machine learning method for controlling optical properties of bimetallic nanostructures.

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Acknowledgements
Financial support of these studies from Gdańsk University of Technology by the DEC-11/1/2022/IDUB/I3b/Ag grant under the ARGENTUM–'Excellence Initiative–Research University' program is gratefully acknowledged.

Residual Gas Analysis using a membrane inlet

Professor Stephen Taylor[1], Mr Robin Hathaway[2]
[1]University Of Liverpool, United Kingdom, [2]SS Scientific Ltd, United Kingdom

MS-6: RGA User Meeting 1, June 19, 2024, 10:30 - 12:35

Residual Gas Analysers (RGA) using quadrupole mass analysers are widely used for contamination monitoring in vacuum systems, for process control in chemical and environmental monitoring, and for a range of other uses. Typically the sample inlet to the RGA is by direct gaseous leak or via a capillary (which may be heated) into an ion source which may be open (OIS) or closed (CIS). The use of a membrane inlet either instead or alongside a capillary inlet greatly extends the application space by allowing direct sampling from liquids and vapours as well as direct gas sampling. In this talk some applications of membrane inlet RGA will be highlighted and considered including use for monitoring of drugs, hidden persons, oil-in-water (OiW) monitoring and volatile organic compounds (VOCs) including breath analysis for healthcare applications. As well as being immersible in liquids, the membrane inlet has the advantage of being faster in operation than typical capillary inlets. This which allows membrane inlet RGA to be used for online analysis of individual analytes or mixtures in real time.

Invited Speakers

Understanding the structure of two dimensional films using X-ray standing waves

Dr David Duncan[1]
[1]University of Nottingham, United Kingdom

Advances in Experimental and Theoretical Methods 2, June 17, 2024, 14:00 - 15:30

X-ray standing waves has been used to determine the structure of over 15 two dimensional graphene-like films (e.g. graphene, boron nitride, silicene, transition metal dichalcogenides). This work has provided the beginnings of insight into how these 2D films interact with their growth substrates from films that basically free-standing on the growth substrate [1], to those that are effectively alloyed with it [2]. Much of this work has been performed in close collaboration with theoretical collaborators. However, due to often small mismatches between the lattice parameters of the substrate and the two dimensional film, the overlayer unit cell can be quite large and, in some cases, non-unique. This problem can quickly become intractable for accurate density functional theory (DFT) calculations. As a result, much of the simulations present in the literature are for artificially strained overlayer unit cells [3,4,5], but this may be an unhelpful approximation for many two dimensional films [5]. In this talk I will introduce the X-ray standing waves measurements that have been performed for these films, discussing the variation in results that have been observed and how they have been interpreted. I will then address the performance DFT calculations to precisely model these structures, with a focus on the limitations of these overlayer unit cells and the need to perform fuller, more expensive calculations to gain meaningful results.

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[5] M. A. Stoodley, et al. Physical Review Letters just accepted

Characterisation of sodium ion batteries - from post-mortem to operando analysis

Prof. Marcus Rohnke[1]
[1]Justus Liebig University Giessen, Center for Materials Research, Germany

Biomaterials 2 and Bioengineering, June 18, 2024, 14:00 - 15:30

Lithium-ion batteries (LIBs) have been at the forefront of energy storage technology since the early 1990s due to their relatively high energy density (260 Whkg−1), reasonable cost ($153/kWh), and long lifespan.[1]However, the high demand, lack of raw material availability, poor ecological, political and working conditions in the mining countries require new battery concepts. Despite their lower energy density (~150 Whkg−1) compared to LIBs, sodium ion batteries (SIBs) appear to be an interesting alternative, especially for non-portable applications where weight is secondary. SIBs could be used for stationary storage of excess energy from renewable sources such as wind or solar power. Moreover sodium is the 6th most abundant element on earth and is more evenly distributed throughout the globe than lithium.

Researchers around the world are working on concepts for SIBs with liquid and solid electrolytes, so-called solid-state sodium ion batteries.[2]In most cases, the interface properties between the materials used determine the battery kinetics and long-term cycling behavior. Here surface analytical methods such as time-of-flight secondary ion mass spectrometry (ToF-SIMS) or X-ray photoelectron spectroscopy (XPS) play a key role, in combination with 3D analysis and cross-section preparation.[3]They offer the opportunity to learn more about interfacial processes taking place. This knowledge is essential for continuously improving the performance of batteries.

Within this talk we will give insights in our ongoing work on SIBs with liquid as well as solid electrolytes. We will highlight how SIMS, XPS, SEM and TEM can be used in combination with classical electrochemical methods to learn more about electrode and decomposition reactions in SIBs. The first example focuses on the interfacial kinetics in solid state Na batteries with the solid electrolyte NASICON (Na3.4Zr2Si2.4P0.6O12). In the second example classical hard carbon electrodes from electrochemical cells with liquid electrolytes are characterized in 3D with a special focus on the so called solid electrolyte interface (SEI). Here a decomposition layer is formed, which has a significant impact to the cellular kinetics.

Funding was received through POLiS Cluster of Excellence – Post Lithium Storage.

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Advantages and challenges of graphene transistors for biosensing

Mr Pedro ALPUIM[1]
[1]Braga, Portugal

Biointerfaces/Biophysics/Biosensers, June 19, 2024, 10:30 - 12:35

Biosensing graphene transistors, with their promising potential, are a significant area of research. Their inherent 2D nature, high carrier field-effect mobility and ambipolar transport, chemical inertness and robustness, and the possibility of surface functionalization make them a compelling choice. When operated as liquid-gate transistors (LGFET), they open a new era in label-free device sensitivity and limit of detection, reaching concentration values inaccessible to other technologies [1]. Their integration with microfluidic platforms or other sample-delivering methods enables point-of-care and point-of-use platforms with unprecedented sensitivity in low power consumption real-time measurements.
The sensing principle, local gating by analyte molecules whenever they attach to the graphene channel, modulates its Fermi energy (EF), causing a shift in the transistor transfer curve, typically detected by measuring the Dirac point voltage, the point of minimum conductance in the curve [1]. However, electronic devices based on polycrystalline 2D materials often suffer from electrical instability due to the interaction of their charge carriers with the defects in the surrounding insulator layers [2]. In LGFETs, the charges trapped in the SiO2 layer underneath the graphene channel can provoke hysteresis and drift in the transistor output due to uncontrolled doping [2], hindering biodetection at low analyte concentrations. Here, we present a complete model for the response of an LGFET, showing that, at the transistor operating voltages, the graphene E¬F sits within the oxide bandgap and between the two SiO2 defect bands [3]. The electron capture and emission rates from and to the defect bands depend on the energy barrier between the graphene E¬F and the defect, the distance of the defect from the surface, and the strength of the electron-phonon coupling. The model is validated against experiments with devices immersed in a 10 mM phosphate buffer solution. We also show that operating the LGFET in AC mode is another way to minimize the drift. Examples of neurotransmitter detection in the brain of animal models will be shown.

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Light-matter interaction probed at the atomic scale

Dr. Anna Roslawska[1]
[1]MPI Stuttgart, Germany

Plasmonics and Excited States at Surfaces, June 19, 2024, 10:30 - 12:35

Light-matter interaction is essential for mechanisms such as luminescence, photosynthesis, and energy harvesting, defining the emission characteristics of molecular systems and governing the conversion of energy between photons and electrons. While these processes are intensively studied and employed, little is known about their dependence on atomic-scale properties since reaching such precision in optics is extremely demanding. This challenge is nowadays overcome thanks to the combination of optical spectroscopy approaches with scanning probe microscopy. In my talk, I will discuss how mapping optical properties of single molecules with nearly atomic precision [1,2] is enabled by the extreme field enhancement provided by the tip and show its application to induce and probe resonant energy transfer [3] and photochemical reactions [4] with sub-nm precision.

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Identification of chirality of the organic molecular domains in the reciprocal space

Grażyna Antczak[1], Thorsten Wagner[2], Dorota Wilgocka-Ślęzak[3], Błażej Gołyszny[2], Nika Spiridis[3]
[1]University of Wrocław, Poland, [2]Johannes Kepler University, Austria, [3]Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Poland

Spectroscopy and Microscopy of Nanostructures Modelling Nanostructure Properties, June 20, 2024, 11:00 - 13:00

The properties of the molecule-substrate interface are important for the performance of devices with an active layer of organic molecules. By co-adsorption of different organic molecules, so called bimolecular or binary monolayers are formed, which have interesting properties such as modulation of charges at the interface on the nm scale. In our study, we focus on the molecular layer composed of phthalocyanines adsorbed on the metallic surface. Phthalocyanine (Pc) molecules are a group of molecules that have been intensively studied due to their interesting properties for applications in optoelectronics. We study the combination of phthalocyanines by mixing molecules on the surface with opposite influence on the work function of the substrate. For this we use low energy electron microscopy (LEEM). The subject of this talk are the bimolecular domains composed of cobalt phthalocyanine (CoPc) and perfluorinated copper phthalocyanine (F16CuPc) adsorbed on Ag(100) surfaces at room temperature and subsequently annealed at 470 K. The CoPc up to monolayer coverage decreases the work function of the silver surface while F16CuPc increases it. Due to the electrostatic interaction between the partially negatively charged fluorine atoms of F16CuPc and the partially positively charged hydrogen atoms of the CoPc, the first monolayer of the mixed phase in a 1:1 ratio is arranged in a checkerboard-like superstructure [1]. The individual phthalocyanine (Pc) molecules are adsorbed in this molecular structure in such a way that their molecular axis is rotated by 27o with respect to the <011> directions of the substrate [2, 3]. This leads to the development of two mirror domains with opposite chirality. In this talk we will show that the structure factor of the constituent molecules allows the identification of these domains using the micro-diffraction mode (µLEED) of the LEEM apparatus. Furthermore, when the µLEED mode is applied to the dilute 2D molecular gas formed by about 0.5 ML of F16CuPc on the surface, it allows a direct imaging of the molecular structure factor and, hence, the identification of the adsorption geometry of the molecule.

The authors gratefully acknowledge the financial support from program 'Excellence initiative research university' for years 2020-2026 for University of Wrocław.

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Hexagonal boron nitride monolayers on metals and alloys: relevance for templating and model catalysis

Dr László Óvári[1,2]
[1]HUN-REN-SZTE Reaction Kinetics and Surface Chemistry Research Group Szeged, Hungary, [2]Extreme Light Infrastructure ALPS, Hungary

Supported Nanostructures, June 17, 2024, 14:00 - 15:30

Surface templating is a highly promising route towards designing large-scale artificial atomic and molecular nanostructures with tailored chemical, quantum or spin functionalities. From the manifold of procedures, surface templating by electrostatic potentials is the least invasive way to steer the growth of adsorbates on surfaces. As an example, the templating ability of a periodically undulating hexagonal boron nitride (h-BN) monolayer on Rh(111) stems from the local surface potential difference between the closer pore and farther wire regions. Recently we demonstrated that it is possible to enhance the local work function nanopatterning by using Au/Rh(111) surface alloys as a substrate. Beside the electronic tuning, structural parameters of h-BN can also be controlled by the amount of gold. While corrugated h-BN monolayers are known templates for molecules and clusters adsorbed on top of them, we extend this functionality towards the subsurface. Moreover, by changing the chemical nature of the substrate metal, we can also influence other properties of h-BN: with an interfacing gold layer between h-BN and Rh(111), the thermal stability of boron nitride can be significantly improved. Metal clusters supported by h-BN are increasingly used as non-oxidic model catalysts. Thereby it is important to reveal thermally induced processes of the model catalyst itself. The observed behavior differs significantly for admetals of different reactivity. While for gold nanoparticles sintering, intercalation and desorption are the dominant phenomena on h-BN/Rh(111), the more reactive Rh nanoparticles are able to disrupt the BN bonds as well, allowing the diffusion of BN fragments on top of Rh clusters. Examples for model catalytic studies related to the transformation of ethanol and acetaldehyde will also be presented. The applied methods span core level and angle resolved valence band photoemission (momentum microscopy), other electron and ion spectroscopic methods, STM and DFT calculations.
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NEG as an multifunctional coating: pro & cons, present limitations & possible developments/applications for future machines

Reza Vakizadeh[1]

[1]Science and Technology Facilities Council (STFC), United Kingdom

Non-evaporable getter coatings, June 18, 2024, 14:00 - 15:30

Thin film Non Evaporable getter (NEG) is used in particle accelerators around the globe for the past two and half decades. Its primary function is to provide a barrier layer for inhibiting hydrogen diffusion from the wall of the vessel into the vacuum. It second function is to provide an active sorption surface to provide a very effective and distributed pumping for residual gas species (i.e., H_2, H_2O, CO, N_2, O_2, CO_2) through the formation of stable chemical bonds. Once activated it provide a surface which significantly reduces thermal outgassing low secondary electron yield, with electron and photon stimulated desorption yield.

The ternary alloys NEG (TiVZr) which has been used extensively in particle accelerators has an activation temperature of 180°C while the quaternary alloy NEG (TiVZrHf) introduced by ASTeC has an activation temperature of 140°C due to its even smaller grain size as compared to ternary alloy. NEG morphology plays an important role in its combined properties. A columnar and porous structure will provide an efficient pumping surface, as a dense structure it provides an effective semi-surface barrier, acting as reservoir for hydrogen diffusion from the chamber's wall into the vacuum system. On the other hand, NEG in nitride form will perform as true barrier for hydrogen diffusion. Hence at ASTeC we devised a triple layer structure starting with a nitride layer followed by a thick dense layer terminated by a highly columnar structure.

As the new generation of particle accelerators aims to achieve the lowest emittance and highest luminosity possible there is a push to reduce the beam pipe dimension to as low as few mm in diameters. This brings new challenges in term of coating of long narrow tubes, which is needed to be solved in order to achieve the goals set by the new generation of particle accelerator. Surface impedance of vacuum chambers play an important role in accelerator facilities instabilities. It can significantly effect on budget of total impedance of machine and therefore degrade the beam emittance. The surface resistance of traditional ternary NEG is several of magnitude higher than copper, which can be an inhibiting factor in choosing NEG as active surface of the vacuum vessel. To address this problem, a conductive NEG has been proposed and tested to reduce the surface resistance of the NEG comparable to copper but keeping its all other combined properties. The conductive layer is consist of traditional NEG with added high conductive elements of Au, Ag, Al, or Cu. We report on the activation temperature, activation procedure, pumping speed and sticking probability of CO, CO_2, H_2, secondary electron yield (SEY), photon electron yield (PEY), photon and electron stimulated desorption (PSD, ESD), surface resistance and film structure, morphology and composition of all different type of NEG thin film.

The bulk composition of the film is determined with Rutherford back scattering (RBS), Secondary Ion Mass Spectroscopy (SIMS) and the surface composition and chemical bonding are determined by X-ray photo-electron spectroscopy (XPS). The surface topography is determined with scanning electron microscope (SEM) and scanning tunnelling microscope (STM) and the film grain size is calculated by X-ray diffraction (XRD) and electron back scattered diffraction (EBSD).

Novel 2D materials stabilized on surfaces

Yukiko Yamada-Takamura[1]

[1]Japan Advanced Institute of Science and Technology, Japan

Nanoparticles, June 18, 2024, 14:00 - 15:30

To realize group IV two-dimensional (2D) materials which lack “layered host materials”, one has to grow them epitaxially on single-crystalline substrates. Such novel materials have to be characterized thoroughly by complementary surface characterization methods, and first-principles calculation is indispensable to understand their crystal and electronic structures since they are very different from their bulk counterparts. One of such materials is “silicene”, which is a honeycomb structure made of Si atoms. We have demonstrated, in 2012, by a combination of scanning tunnelling spectroscopy (STM), core-level and angle-resolved photoelectron spectroscopy (ARPES), and first-principles electronic structure calculations, that on epitaxial ZrB2(0001) films grown on Si(111) substrates, Si atoms from the substrate segregate to the film surface and crystallize in a honeycomb structure [1,2].

In this talk, I would like to introduce a 2D Ge lattice having a “bitriangular” structure, which was synthesized on ZrB2(0001) film surface using similar method. Our theoretical study on freestanding bitriangular lattice demonstrated that the flat band of a kagome lattice can be embedded in this 2D structure [3]. We have found out by combing STM observation, total reflection high energy positron diffraction, photoelectron spectroscopy, and first-principles calculations, Ge atoms segregate and crystallize into such a bitriangular lattice on the surface of ZrB2(0001) films grown epitaxially on Ge(111) substrates [4]. The electronic structure measured by ARPES at room temperature reveals “nearly” flat band at Fermi level which is evidence of the metallic nature of this 2D Ge layer. Moreover, at temperature lower than 150 K, the in-plane unit cell of this 2D Ge layer becomes 3 times larger, indicative of a transition to charge density wave phase. The detail of the structural change and the possible mechanism will be discussed.

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The Role of Vacuum Gas Dynamics in the Particle Exhaust of Stellarator and Tokamak Fusion Devices

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Vacuum Gas Dynamics, June 18, 2024, 16:00 - 17:30

The particle exhaust of a nuclear fusion reactor is one of the major problems that significantly affects the plasma conditions and is related to a wide range of operational and safety aspects. The effective control of the exhaust process provides a route to high-density regimes required for high performance and hence high-energy gain.

The main components that determine the particle exhaust of a fusion device, are the divertor and the associated vacuum systems. Their main goal is to remove efficiently gas fuel, namely deuterium and tritium, the helium ash, which is a product of the fusion reaction, as well gas impurities, as Argon, Neon, Xenon etc. The design and optimization of such a system requires the exploitation of a simulation tool capable of dealing with very complex geometries and of describing the vacuum flow conditions, in the whole range of the Knudsen number.

The most effective numerical tool, which is capable of dealing with the above-mentioned challenges, is the Direct
Simulation Monte Carlo (DSMC) method [1], which is currently the main numerical approach, within the European
Fusion program, for modelling the vacuum gas dynamics in the particle exhaust of tokamak [2,3] and stellarator fusion
devices [4].

The focus of the present talk is mainly twofold. First, the 3D simulations of the particle exhaust of the Wendelstein 7-X stellarator, will be highlighted. This modelling activity is characterized by high geometrical complexity and high1computational effort. The implementation of the DSMC method allowed for quantifying all the macroscopic parameters i.e. pressure, number density, temperature etc, as well as overall quantities i.e. pumped fluxes and gas leakages in the divertor area. Additionally, comparisons between numerical and experimental results, have been performed. Moreover, based on the 3D simulations, design optimization strategies of the particle exhaust configuration, have been identified.

The second part of this talk is devoted to the modelling and optimization of the divertor pumping system of a tokamak type demonstration power plant (DEMO) [5], which represents conceptually the first commercial fusion
reactor for wide energy production. By applying the DSMC method coupled with corresponding plasma codes, the optimal position of the pumps is investigated for various operational conditions (plasma scenarios) and pumping speeds. The presented results include the estimation of all macroscopic quantities of practical interest as well as the qualitative behavior of the gas flow inside the DEMO divertor region.

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Energy level alignment and fundamental processes at interfaces between monolayer transition metal dichalcogenides and organic semiconductors

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2D Materials and Van der Waals Heterostructures 2 and Ferroelectric Behaviour, June 20, 2024, 11:00 - 13:00

The combination of two different semiconductors enables enhanced functionality of electronic and optoelectronic devices. This correspondingly holds for 2-dimensional transition metal dichalcogenide (TMDC) monolayers (MLs) and their amalgamation with organic semiconductors (OS), which are also excitonic materials that feature strong light-matter coupling. Depending on the electronic energy level alignment at ML-TMDC/OS interfaces, useful phenomena can arise, such as energy transfer and ground or excited state charge transfer, as well as hybrid excitations. For knowledge-based ML-TMDC/OS structure formation, the energy level alignment at the interfaces must be unraveled. That is a challenging task, because of the many degrees of freedom of such systems and their dependence on many environmental parameters. Employing photoemission spectroscopy, the primary method to study electronic properties, for ML-TMDC/OS structures is, however, non-trivial. Here, it will be shown how photoemission spectroscopy can be used to determined the energy level alignment at interfaces between ML-MoS2 or ML-WS2 and a range of different OSs. In turn, this then allows identifying key processes at these interfaces, including resonance energy transfer, excited state charge transfer, as well as doping.

PtSe2/metal interfaces: electronic and eletronic transport properties, and the access to the topological gap in PtSe2[VSe] monolayer

Roberto Miwa[1], Rafael L. H. Freire[2], Felipe Crasto de Lima[2], Caio H. Lewenkopf[3], Adalberto Fazzio[2]
[1]Universidade Federal de Uberl ˆandia, Brazil, [2]Brazilian Center for Research in Energy and Materials, Brazil, [3]Universidade Federal Fluminense, Brazil

Electronic Structure of Materials, Surfaces and Interfaces, June 18, 2024, 10:30 - 12:30

Among the two-dimensional materials, platinum diselenide (PtSe2) has been the sub1ject of several studies addressing applications in different areas, for instance, the development of electronic devices like 2D transistors and sensors. One important feature to take advantage of in nanoelectronics is (i) the tickness dependency of the bandgap of the few-layer systems of PtSe2. Meanwhile, (ii) recent theoretical study predicted the emergence of (topological) Quantum Spin-Hall phase in PtSe2-ML mediated by the presence of selenium vacancies, PtSe2[VSe]-ML [Nano Letters 21, 9398 (2021)]. Here, based on the density functional theory, in (i) we performed first-principles calculations of the structural, electronic, and electronic transport properties of the monolayer (ML), bilayer (BL) and trilayer (TL) of PtSe2 lying on the Au(111) surface, PtSe2-X/Au (X = ML, BL, and TL). We found the emergence of chemical interaction between the PtSe2 adlayer and the Au(111) surface, resulting in an ohmic contact, and the hole doping of PtSe2. The semiconductor PtSe2-ML becomes metallic in PtSe2-ML/Au, whereas, in PtSe2-BL/Au, the topmost PtSe2 layer, which is not in contact with the Au(111) surface, remains semi conductor. Further electronic transport calculations unveiled the tickness dependence of the electronic transmittance and the Schottky barriers along the PtSe2-X channels in contact with PtSe2-X/Au(111) leads. Based on the (present) atomistic understanding of the electronic properties of PtSe2-X/Au, we propose a heterostructure composed of PtSe2-TL intercalated by metallic contacts Au(111), Au/PtSe2-TL/Au, in which the metal-to-semiconductor transition can be carried out through mechanical strain. In (ii), we show that through a suitable choice of the metal contact, it is possible to control the access of the non-trivial gap in PtSe2[VSe]-ML. We believe that these findings are timely, bringing important contributions to the applicability of few-layer PtSe2 for developing 2D electronic devices.

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Novel inorganic-organic materials through ALD/MLD as enablers of next-generation energy and nanotechnology applications

Maarit Karppinen[1]
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Advanced Thin Film Fabrication, June 19, 2024, 10:30 - 12:35

The combined ALD/MLD (atomic/molecular layer deposition) thin-film technique allows us to fabricate novel hybrid materials not readily accessible through any other fabrication route.1 These include exciting in-situ crystalline metal-organic framework (MOF) materials,2 and inorganic-organic interfaces and superlattice structures in which ultra-thin organic layers are introduced periodically between nm-scale metal oxide layers to e.g. enhance mechanical flexibility, provide electrical doping, block phonon conduction, or bring photoactivity. In this presentation, I will briefly discuss exciting examples of properties/functionalities realized for these materials: (i) electroactive lithium-organic thin films for battery components,3 (ii) luminescent lanthanide-organic layers for white-light phosphors and bioimaging,4-6 and (iii) ε-Fe2O3:azobenzene superlattice films for flexible and photo-responsive room-temperature magnets.7,8

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Single-atom alloy catalysts: born in a vacuum, tested in reactors, and understood in silico

Charles Sykes[1]
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Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 3, June 20, 2024, 11:00 - 13:00

In this talk I will discuss a new class of heterogeneous catalysts called Single-Atom Alloys in which precious, reactive metals are utilized at the ultimate limit of efficiency.1-6 These catalysts were discovered by combining atomic-scale scanning probes with more traditional approaches to study surface-catalyzed chemical reactions. This research provided links between atomic-scale surface structure and reactivity which are key to understanding and ultimately controlling important catalytic processes. In collaboration with Maria Flytzani-Stephanopoulos these concepts derived from our surface science and theoretical calculations have been used to design Single-Atom Alloy nanoparticle catalysts that are shown to perform industrially relevant reactions at realistic reaction conditions. For example, alloying elements like platinum and palladium with cheaper, less reactive host metals like copper enables 1) dramatic cost savings in catalyst manufacture, 2) more selective hydrogenation and dehydrogenation reactions, 3) reduced susceptibility to CO poisoning, and 4) higher resistance to deactivation by coking. I go on to describe very recent theory work by collaborators Stamatakis (Oxford University) and Michaelides (Cambridge University) that predicts reactivity trends for a wide range of Single-Atom Alloy combinations for important reaction steps like H-H, C-H, N-H, O-H, and CO2 activation. Overall, I hope to highlight that this combined surface science, theoretical, and catalyst synthesis and testing approach provides a new and somewhat general method for the a priori design of new heterogeneous catalysts.

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Charles Sykes Abstract.docx (could not be inserted)

Modification of the surface properties of a Pt(111) surface by ionic liquids

Prof. Hans-Peter Steinrueck[1]
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Metal Surfaces - Adsorption, Desorption and Reactions 1, June 17, 2024, 11:00 - 12:35

Ionic liquids (ILs) are salts with melting points below 100 °C, which are characterized by an extremely low vapour pressure. Their physical and chemical properties can be tailored over a wide range, and they therefore represent a fascinating class of liquid materials with interesting applications in catalysis. One important example is the Solid Catalyst with Ionic Liquid Layer (SCILL) approach, which is already used in large-scale for hydrogenation reactions. In SCILL, a heterogeneous catalyst, immobilized on a solid support, is impregnated with an IL layer to enhance selectivity and product yields. To further improve this approach, a molecular level understanding of the specific IL/catalyst interactions is required, which can be obtained from UHV-based surface science studies of model systems. This knowledge then allows for tailoring the interface in real SCILL systems. We recently characterized the adsorption of ultrathin layers of the IL 1,3 dimethylimidazolium bis(trifluoromethanesulfonyl) imide ([C1C1Im][Tf2N]) on Pt(111) by XPS and STM [1]. Moreover, using molecular beam methods and MD calculations we demonstrated how the adsorption dynamics of 1,3-butadiene and 1-butene on Pt(111) can be modified by a thin IL film [2]: We observed that increasing the IL coverage leads to an increased blocking of adsorption sites for both olefins. Interestingly, a smaller amount of IL is needed to prevent 1-butene adsorption as compared to 1,3-butadiene adsorption, which we propose to be directly related to the IL's influence on selective hydrogenation in SCILL catalysis.

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Ionization of sputtered material in high power impulse magnetron sputtering plasmas

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Plasma Science 2, June 19, 2024, 14:00 - 15:30

The high degree of ionization among sputtered species is the reason for the favorable properties - like improved adhesion and increased hardness - that are often observed in films deposited using high power impulse magnetron sputtering (HiPIMS). However, where this ionization occurs within the discharge is not really understood. In this contribution, the ionization of sputtered species in HiPIMS of titanium, chromium, and aluminum targets is analyzed using Abel-inverted spectroscopic imaging. From the spatial emission of neutrals, it is deduced that most of the sputtered titanium particles become ionized within 0.5 mm distance from the target, whereas sputtered aluminum or chromium can travel much further through the discharge before ionization occurs. Probe measurements reveal the reason for this difference to be the unusually high electron temperature of around 4.5 eV for titanium compared to 2.6 eV and 1.5 eV for aluminum and chromium as the target material, respectively. This difference between the three discharges can be traced back to be mostly caused by the sputter yield. Thus, we propose that ionization in discharges with low-yield materials should generally be expected to occur closer to the target surface, leading the ions to be affected more strongly by the electric field across the magnetic trap region, resulting in a more severe deposition rate loss compared to high-yield materials.

This work was supported by the DFG as part of the SFB TR-87.

Unprecedented insights into microstructure-property relations of Ti(Al)SiN coatings by combinatorially applied advanced characterization methods

Nina Schalk[1], Yvonne Moritz[1], Ganesh Kumar Nayak[1], David Holec[1], Christoph Hugenschmidt[2], Vassily Vadimovitch Burwitz3[2], Lucian Mathes[2], Maximilian Schiester[1], Christoph Czettl[3], Markus Pohler[3], Christian Mitterer[1], Michael Tkadletz[1]

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Thin Film and Particle Deposition, 2D, June 18, 2024, 14:00 - 15:30

Coating systems used to protect cutting tools are becoming increasingly complex, which necessitates the combination of several advanced characterization methods to establish synthesis - structure - property relationships. Here, TiSiN was chosen as model system to demonstrate the necessary insight into the coating structure on the nanoscale. Literature on the formed phases in TiSiN is controversial; while there are reports on the formation of a single-phase TiSiN solid solution, the majority of publications reports the formation of a nanocomposite structure. However, the phase composition of the nanocomposite is equally controversial. Commonly, the formation of Si-free TiN nanocrystals, accompanied by either a crystalline or an amorphous Si-containing phase is reported, but there are also works suggesting the formation of a TiSiN solid solution instead of the Si-free phase. To illuminate the formation of a nanocomposite structure versus a TiSiN solid solution, a series of TiSiN model coatings was synthesized. By the combination of (high temperature) X-ray diffraction, transmission electron microscopy, atom probe tomography and Doppler broadening spectroscopy of the positron annihilation lines as well as annealing treatments and differential scanning calorimetry, the structure of these model coatings was investigated in detail. In addition, the experimental studies were complemented by density functional theory calculations, shining light on the effect of the Si content, defects and the deposition atmosphere on the formed phase(s). The combination of these experimental and simulation methods allows to gain a novel and previously not accessible insight into the complex correlation of deposition conditions and structure of TiSiN coatings, providing answers to open questions under debate for almost three decades, i.e. nanocomposite versus solid solution formation in TiSiN coatings. The presented approach enables the establishment of a solid basis for the development of coatings with outstanding properties.

A new facility for growth and study in UHV of two-dimensional semiconductors

Professor Amalia Patane[1]
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2D Semiconductors, June 18, 2024, 14:00 - 15:30

For several decades, silicon-based devices have dominated modern technologies. However, existing silicon-based technologies are reaching physical limits that could halt further advances. Two-dimensional semiconductors (2SEM) present an opportunity to overcome these challenges. Here, I will review my research on 2SEM and present a bespoke facility (EPI2SEM) for the EPitaxial growth and In situ analysis of 2SEM. By integration of growth, advanced microscopy and spectroscopy in UHV, we can create atomically-thin semiconductors with engineered physical properties beyond the current state-of-the-art.

Pd-cyclometallated complexes at Ag(110): from self-assembly to the synthesis of new compounds

Dr Letizia Savio[1]
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Self-Assembly, Characterisation and Reactivity of 2D Structures of Molecules at Surfaces, June 21, 2024, 10:30 - 12:00

Among possible organometallic compounds, complexes of the Group 10 elements are attractive due to their widespread use in numerous applications such as catalytic synthetic processes, biological chemistry and material science. In particular, many palladium complexes have been extensively studied as catalysts in several cross-coupling reactions. Their coupling to a metal surface is interesting, since it could lead to a major impact in catalysis and sensoristic, but research in this field is still limited.
Cyclometallated complexes are good candidates for this kind of studies since they are thermally stable and can be sublimed in vacuum conditions. However, only few studies have been reported in literature [1,2], mainly concerned to the use of Ir(III)- and Pt(II)-containing molecules of interest as light emitters.

Based on our previous experience on surface-assisted polymerization of aromatic hydrocarbons [3,4], we deposited Pd cyclometallated compounds - relevant especially for catalytic applications [5,6] - on Ag(110). Their self-assembly at the surface may lead to the formation of a C-based layer with Pd atoms acting as active centers in well-defined positions. The deposition and the thermal evolution of these complexes was followed by scanning tunnelling microscopy and X-ray photoemission spectroscopy, while the initial and final configurations are validated by ab-initio calculations.
However, Pd-cyclometallates reveal a surface chemistry much more complex than expected. Different self-assembled geometries are observed depending on experimental conditions, but in all cases the molecules dissociates, Pd atoms diffuse below the Ag surface and new compounds can form via cross coupling between the two organic fragments.
In my talk I will present our recent results on this system and a preliminary comparison with similar experiments performed on HOPG, on which molecular dissociation does not occur.

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Letizia Savio.doc (could not be inserted)

Advances in traceable vacuum and outgassing rate measurements

Matthias Bernien[1], Annas Bin Ali[1], Thomas Bock[1], Claus Illgen[1], Tom Rubin[1], Janez Šetina[2], Perrin Waldock[3], Kirk Madison[3], Karl Jousten[1]
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Vacuum Metrology, June 20, 2024, 11:00 - 13:00

The reliability of quantitative pressure and outgassing rate measurements in vacuum is a prerequisite for many industrial and scientific applications. The accuracy of a measurement result is ensured through a chain of calibrations relating it to a primary standard at a national metrology institute. The presentation will provide an overview on the advances of PTB's Vacuum Metrology Group both in reducing the uncertainty of primary pressure realizations in the vacuum regime and in improving the reliability of transfer standards for pressure and outgassing rates.

In the pressure range from 10 mPa to 130 Pa, a fully automated static expansion system made of aluminum has been set up and validated. The principle of static expansion is based on the transfer of a fixed amount of gas from a small volume to a larger volume. Thereby, a well-known lower pressure is generated if the initial pressure and the ratio of the two volumes are known precisely. To reduce the uncertainty in gas temperature the system is built from vacuum components made of aluminum, whose thermal conductivity and diffusivity is higher by more than one order of magnitude compared to stainless steel. The temperature is measured by a total of 90 Pt100 sensors. As a result, relative standard measurement uncertainties between 0.8‰ and 0.12‰ are achieved.

For the high vacuum range from 10-6 Pa to 10-2 Pa a new type of ionization vacuum gauge has been developed. Unlike conventional Bayard-Alpert and extractor gauges, the new gauge features well-defined electron trajectories and mechanically robust electrodes. It exhibits excellent stability and linearity resulting in a measurement uncertainty of 1%, a reduction of one order of magnitude compared to the conventional gauges. The gauge can be used as reference or transfer standard. The essential parameters of the gauge geometry and electrode voltages are published in ISO/TS 6737:2023. By adhering to the standard, manufactures can produce gauges with predictable gauge sensitivity and relative gas sensitivity factors without the need for metrological characterization.

Primary standards based on cold atom traps promise a new route to the realization of the pascal in the ultra-high vacuum range by measuring the loss rate induced by collisions with gas molecules. To establish such standards, comparisons with conventional standards must be carried out in order to validate their working principle. The University of British Columbia and the PTB have performed a comparison of a mobile standard based on cold atoms and a continuous expansion system. The comparison covered N2, Ar and H2 in the pressure range from 3×10−8 Pa to 1×10^−6 Pa. The obtained values of the collision cross sections are compared with values obtained by NIST.

In the semiconductor industry, outgassing from components in vacuum must be well controlled. These contaminants are monitored by quadrupole mass spectroscopy. However, a quantitative measurement of the amount of contamination is challenging as quadrupole mass spectrometers (QMSs) inherently lack stability of their sensitivity. This is particularly problematic when maximum levels of contaminants must be agreed between manufacturers and suppliers. To improve the comparability of outgassing rate measurements, PTB together with IMT and industrial partners has developed outgassing rate reference samples for dodecane and water. By means of an in-situ calibration of QMS, traceable outgassing rate measurements can be achieved.

Amorphous solid water: from the laboratory to the interstellar medium

Jenny Noble[1]
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Water and Environmental Surfaces, June 19, 2024, 16:00 - 17:30

Amorphous solid water has been studied in the laboratory for decades, not only as a model for liquid water, but also due to its interest for astrophysics. Ice mantles grow on dust grains in the coldest and densest regions of the interstellar medium, the process beginning in molecular clouds, with icy grains evolving on their journey through cores and protostars, to disks and, eventually, planets. The first observations of solid water in the interstellar medium were made around half a century ago and, ever since, the study of molecular solid analogues in the laboratory has been key to interpreting astronomical data. Measurement of the infrared absorption spectra of water-dominated icy analogues under cryogenic UHV conditions is critical for direct comparison to spectra obtained with telescopes, while physical chemical characterisation of the reactivity of these molecular solids when subjected to heating or to irradiation by photons, electrons or atomic ions builds up a picture of the mechanisms at play during star and planet formation. In this talk, I will give an overview of the techniques used to study amorphous water ices in the laboratory and the knowledge gained thereby on interstellar ice composition and evolution. I will go on to present some examples of how laboratory studies are being used to interpret observations as we enter the era of the James Webb Space Telescope.

Imaging and tracking polarons in Fe2O3 and SrTiO3 by atomic force microscopy

Martin Setvin[1]
[1]Charles University, Czech Republic

Oxide Surfaces and Nanomaterials - Spectroscopy, Imaging and Physicochemical Processes, June 18, 2024, 10:30 - 12:30

Noncontact atomic force microscopy (nc-AFM) has recently proven to be a powerful tool for manipulating and imaging single electrons at surfaces. Single electrons could be localized at trapping sites such as Au atoms on thin NaCl films [1], small molecules on oxide surfaces [2], or larger organic molecules on thicker NaCl films [3].

This talk will focus on the possibilities of investigating polarons in materials: Polarons are electrons or holes that self-localize in ionic lattices due to electron-phonon interaction [4]. Such charge carriers can move to adjacent lattice positions, provided they are given certain activation energy. Polarons play a key role in many applications and materials properties, such as electrical conductivity, optical properties, catalysis and photocatalysis, and they stand behind exotic properties such as colossal magnetoresistance or high-temperature superconductivity. The successful imaging of polarons in hematite Fe2O3 and SrTiO3 will be shown, and the new possibilities offered by this technique will be discussed.

The work was supported by projects MSMT CZ.02.01.01/00/22_008/0004572 and LL2324.

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Development of new structured-core transparent vacuum insulation panels contributing to insulation retrofit of existing buildings

Takao Katsura[1]
[1] Hokkaido University, Japan

Electronic Materials, Energy Reduction and Carbon Reduction, June 19, 2024, 16:00 - 17:30

Reducing the energy consumption of buildings, factories, and other facilities is essential to achieving decarbonization. In order to reduce the energy consumption in the residential houses and commercial buildings, Zero Energy Buildings (ZEB) and Houses (ZEH) have been defined in Japan. Then efforts are underway to make buildings ZEB or ZEH. However, energy-saving technologies have not been introduced in existing buildings, especially insulation performance is insufficient. In order to retrofit the insulation of existing buildings, new, low-cost transparent vacuum insulation panels (TVIPs) using structured cores for the windows of existing buildings are proposed. The TVIP is produced by inserting the structured core, the low emissivity film, and the adsorbent into the transparent gas barrier envelopes. The outlines, the design and thermal analysis method, the performance evaluation (test) method are introduced. In addition, the challenges to realizing TVIPs and the research that has been carried out to solve them will be presented.

Surfaces of cleaved aluminosilicates at the atomic scale

Dr. Giada Franceschi[1]
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From Nanostructured thin films to nanoparticles. Reactions at nanostructures, June 18, 2024, 16:00 - 17:30

Aluminosilicates are ubiquitous and play integral roles in many essential processes such as weathering, soil formation, CO2 sequestration, and atmospheric ice nucleation. A fundamental understanding of these processes requires detailed knowledge about the surfaces of these minerals.

However, accessing the surface details of aluminosilicates is challenging due to their insulating nature. The hurdle has been recently overcome thanks to developments in non-contact atomic force microscopy (ncAFM) in ultra-high vacuum (UHV).

Here, we discuss the insights obtained on UHV-cleaved aluminosilicate surfaces leveraging ncAFM and ab-initio theoretical calculations. We focus on potassium feldspars (KAlSi3O8)—widely regarded as efficient ice nucleators in the atmosphere [1]—and explore how their surface chemistry influences their atomic-scale interaction with water [2]. We interpret the results in the context of the available literature on ice nucleation.

This work is supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 883395, Advanced Research Grant 'WatFun').

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Porous nanocolumnar thin films deposited at glancing angles: fundamentals and applications

Dr. Rafael Alvarez
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Thin Film Growth Simulation, June 18, 2024, 10:30 - 12:30

The magnetron sputtering technique operated at oblique geometries has recently emerged as an invaluable tool for the deposition of porous thin films. Not only has it managed to reproduce similar film morphologies as those obtained by classical evaporation methods at glancing angles, but, by fine tuning the plasma conditions during deposition, it has also widened the variety of available nanostructures, e.g. well-isolated nanocolumnar arrays, sponge-like structures or even compact films that embed porous networks with different connectivity. Furthermore, the use of patterned substrates has broadened even more the nanostructuring possibilities of the technique, allowing the direct growth of well-ordered arrays of pillars or hole structures in scales of about 100 nm, among many other possibilities (see figure 1). In this presentation, an up to date description of its fundamentals and possibilities are shown, along with numerous potential applications in different fields. Their use in the development of sensors devices, in which the high specific surface of these coatings optimizes the interaction with an external gas or liquid, or in biomedicine, where a nanocolumnar biocompatible antibacterial thin film has been recently reported, will be specifically addressed in this presentation.
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Functional coatings for aerospace applications

Jolanta Klemberg-sapieha[1]
[1] *Polytechnique Montréal, Canada*

Functional Coatings 1, June 17, 2024, 14:00 - 15:30

Materials exposed to demanding environments in applications such as aerospace continue to face increased technological, environmental and economic challenges, especially since the performance of systems and components is frequently pushed to and beyond their limits. This is particularly valid for aircraft engine parts exposed to harsh operation conditions that can vary widely from severe erosive wear to exposure to hot oxidative gases, extreme thermal loads, corrosion, or even instant ice accretion on critical surfaces leading to material deterioration that gives rise to increased operation and maintenance costs, decreased efficiency, premature failure, and compromised safety. This calls for a better understanding of the material deterioration mechanisms and for developing appropriate strategies to protect technologically relevant substrate materials and their surfaces.

In this context, our Functional Coating and Surface Engineering Laboratory (FCSEL, www.polymtl.ca/larfis) has proposed a comprehensive approach to surface engineering challenges. This is based on a simultaneous action of the following key elements: (i) in-depth analysis of the technological problem, (ii) availability of the appropriate metrology tools (testing methods) that allow one to validate suitable solutions, (iii) development of nanostructured coating materials, and (iv) their integration in specific coating architectures while applying (v) relevant fabrication processes.

In this presentation, the global approach described above will be illustrated by examples pertinent to different sections of the aircraft engine and related to the development of protective coating systems against ice accumulation, solid particle erosion, and high-temperature oxidation, as well as for the next-generation low-emissivity thermal barrier coatings.

Plasma diagnostics in various configurations of reactive pulse magnetron sputtering systems used for thin film deposition of semiconductors

Dr Zdeněk Hubička[1], A Kapran[1], A Písaříková[1], I Venkrbcová[1], H Krýsová[1], J Olejníček[1], M Čada[1], R Hippler[1]
[1] *Institute of Physics Czech Academy of Sciences, Czech Republic*

Plasma Science 2, June 19, 2024, 14:00 - 15:30

Recently, pulsed reactive sputtering has emerged as an increasingly promising deposition technology for the production of semiconductor thin films. A major advantage of this approach is its good compatibility with industrial mass production. Various semiconductor thin film binary and ternary oxides have recently been intensively investigated for gas sensors, photonic sensors and photoelectrochemical cells for solar water splitting and hydrogen production. Plasma parameters in the reactive sputtering process play a key role in the final quality of the semiconductor material. The most critical parameters are the electron temperature, the plasma density, the energy distribution function of the positive and negative ions and the degree of ionization of the sputtered particles. A reactive magnetron sputtering systems operating in different pulse modes (HiPIMS, MF) have been used for the deposition of various semiconducting oxides such as ZnO, WO3, Fe2O3:Sn, CuxWO4 and CuFeO2. The plasma parameters during the deposition of these films were determined by means of an RF probe, magnetized QCM with biased electrode, optical emission spectroscopy and measurement of the energy distribution function of positive and negative ions at the substrate using an energy resolved ion mass spectrometer and an RFA analyzer with a magnetic filter. The semiconducting properties of these films were determined by measurements in a photoelectrochemical cell, Mott-Schottky analysis and conductivity and photoconductivity measurements. High quality oxide semiconductor films such as ZnO, WO3 and Fe2O3:Sn, CuxWO4, CuFeO2 were deposited under specific conditions of pulsed reactive magnetron sputtering. Optimum conditions were found for each material studied. The influence of the obtained plasma parameters such as electron temperature, ion density and the nature of the energy distribution function of positive and negative ions on the semiconductor parameters was demonstrated. It was found that the measured plasma parameters have a significant influence on the resulting semiconductor parameters.

Remote RGA Operation up to 100m, with a novel Radiation Resistant Extender Cable

William Roger Fletcher[1], Daniel RioPousa[1], Jonathan Leslie[1], Stuart Johnson[1], George Jennings[1], **Dr Farnoush Salarzaei**[1], Mark Aitken[1]
[1]MKS, United States of America

MS-6: RGA User Meeting 2, June 19, 2024, 14:00 - 15:30

Residual gas analyzers (RGA) are regarded as essential gas-composition monitoring instrumentation for both high and ultra-high vacuum processes. High Energy Physics vacuum installations often place RGA sensors within ionizing radiation environments, which can degrade the semiconductor and other components of their control/analysis modules. Radiation sensitive electronics components can be protected from such harsh radiation exposure, positioning the electronics control unit (ECU) at a remote location - away from the quadrupole mass filter (QMF) subsystem - and through an extender cable connection between both modules. Extender cables include mixed connection paths for conveying (1) mass spectrometry signals (mass setting and ion currents), (2) control signals (electrode biases), (3) power lines (filament current supply) and (4) high-amplitude radiofrequency signals for mass selection (coaxial transmission line.) Critical to the operation is the delivery of precisely controlled dual-phase RF supply signals to the QMF assembly, as required to achieve repeatable mass spectra. The RF supply signal amplitude is of the order of hundreds of volts peak-to-peak (Vpk) and its frequency is typically a few MHz. With modern vacuum installation projects demanding cable lengths exceeding 50 meters, our engineering team recently developed a patented methodology for (1) conveying a time-varying voltage signal from ECU to QMF including (2) monitoring and adaptively controlling the amplitude of the time-varying voltage signal at the QMF. A physical length of the transmission line configured to correspond to an electrical length substantially equal to a positive integer multiple of one-half wavelength of the time-varying voltage signal allows the transmission line to operate resonantly and adaptively control the amplitude of the time-varying voltage signal from the ECU for cable lengths exceeding 100 meters. Ultra-long extender cables, specifically designed to match customer specified lengths, are presently a reality and the preferred solution for the operation of RGA under hard radiation environments.

Electrical properties of crystalline MoO3 monolayers

Dr. Maciej Rogala
[1]*University of Lodz, Poland*

2D Materials and Van der Waals heterostructures 1, June 19, 2024, 14:00 - 15:30

Within the broad group of two-dimensional materials, it is the transition metal oxides that can find commercial applications relatively quickly. This is related to the fact that they allow to take the already proven functionalities of their three-dimensional counterparts from the fields of catalysis, batteries, sensors and optoelectronics to a whole new level in a simple and effective way. This is particularly true for flexible electronics and thin-film systems.

Here we present a monolayer (1L) of MoO3 which is a single layer of the octahedral net with the thickness of 6.9 Å. In contrast to the previously available results, we present highly stable 1L α-MoO3−x which uniformly covers the graphite (HOPG) substrate. We chose such substrate to analyze the growth process on a near perfect, defect- and contamination-free graphene-like layer. This allows for precise scanning probe microscopy characterization performed under the UHV conditions and gives direct information about fundamental physical properties essential for further applications in organic electronic devices such as OLED and OPV and additionally in resistive random-access memories (ReRAM) systems. By a combination of ultraviolet and x-ray photoelectron spectroscopy (UPS and XPS), we investigate the chemical composition of α-MoO3−x /HOPG and the interface-induced defects states. Using scanning tunnelling microscopy and spectroscopy, we investigate the electronic properties of MoO3−x at the nanoscale and prove the ability of nanomanipulation and local electromodifications.

This work was supported by the National Science Centre, Poland, grant 2020/38/E/ST3/00293.

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High entropy proton conducting perovskites for solid oxide fuel cells

Dr Rebecca Clulow[1]
[1]Uppsala University, Sweden

Low-dimensional Thin Film Materials, June 17, 2024, 11:00 - 12:35

Materials with multiple principle elements have attracted significant interest in recent years particularly as high entropy alloys. Many of these materials are known to possess improved properties including hydrogen sorption and tensile strength as well as giving rise to interesting magnetic properties1. In addition, the flexibility of possible compositions will lead to a high degree of tunability in the properties of these materials and allow for multiple functionalities. Whilst, this approach has already been extensively utilised in alloys, it has only more recently been applied to perovskites.2

One significant application for high entropy perovskites is as proton conducting materials in solid oxide fuel cells (SOFCs). SOFCs convert chemical energy directly to electrical energy with very high efficiencies and few emissions however, they are currently limited by their high operating temperatures.3 Proton - conducting solid oxide fuel cells (PC-SOFCs) provide a potential solution, though materials with the necessary properties still need to be developed. High entropy perovskites could overcome the current limitations of proton conducting materials allowing for the design of novel compounds with high ionic conductivity, stability and tunability.

In this talk, a new family of high entropy perovskites based on the n = 2 and n = 1 Ruddlesden-Poppers will be presented. Their general formulae are La0.5Sr2.5(M)2O7-□ (n = 2) and La2-xSrx(M)O4-□ (n = 1) where M is a combination of four or more transition metals.4,5 The compounds have been studied using a combination of neutron diffraction, X-ray diffraction, thermal analysis and magnetometry. The n = 2 compounds are oxygen deficient and exhibit unusual spin glass behaviour whilst the n = 1 materials absorb water from the air under ambient conditions which is a prerequisite for proton conduction.

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Understanding complex features of partially-magnetized deposition plasmas

Professor Sedina Tsikata[1]
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Plasma Science, June 18, 2024, 16:00 - 17:30

Crossed-field plasma discharge configurations give rise to complex features, including various types of instabilities created by the relative drifts of ions and electrons, and large-scale self-organization. Devices where such phenomena arise include planar magnetrons, widely-used for plasma-assisted deposition in direct current and pulsed high power impulse sputtering regimes. Although the connection between such features and macroscopic device performance still requires clarification, such features are associated with anomalous transport and heating of charged species. Understanding such features requires advanced numerical modeling, theory, and experiments. In recent work, information on the highly-dynamic electron properties and drifts, and electron density fluctuations associated with different instabilities, has been obtained using coherent and incoherent Thomson scattering. This talk focuses on the new understanding gained from such studies and future directions of study.

Engineered surfaces for biotribological applications: a soft solution for a hard problem?

Professor Michael Bryant[1]
[1]University of Birmingham, United Kingdom

Biomaterials 2 and Bioengineering, June 18, 2024, 14:00 - 15:30

This talk will highlight some of the recent advanced in surface engineering at the University of Birmingham, focussing on the current and future needs for total joint replacement and technologies for earlier intervention. Attention will be paid to advances in PVD coatings for wear-corrosion application and the advanced preclinical testing that enables translation to clinic. Looking forward to emerging technology demands, recent development of entangled polymer surfaces that emulate the natural lubrication mechanisms of cartilage will be discussed. These bio-inspired solutions not only replicate the superlubricity found in healthy synovial joints but also promote the integration of the engineered surfaces with the body's natural systems. Such innovations are setting new standards in the biotribological performance of orthopedic devices, offering a 'soft' solution to the 'hard' problems of wear and corrosion in joint replacements.

The high-luminosity large hadron collider vacuum system

Vincent Baglin[1]
[1]CERN, Switzerland

Large Vacuum Systems of Particle Accelerators, June 18, 2024, 10:30 - 12:30

The High-luminosity Large Hadron Collider presently under construction at CERN will deliver an integrated luminosity of 3 000 fb-1 by the 40ies. To this aim, 1.2 km of long straights around ATLAS and CMS will be rebuilt and their final focussing triplets will be upgraded to a more powerful version with larger aperture allowing the desired increases of luminosity. By mitigating beam induced pressure rise, the vacuum system will grant a reasonable background to the experiments. Using tungsten shielded beam screens inserted into the 1.9 K cold bore of the 60 m long cold mass string, the vacuum system will also provide a protection of these superconducting magnets against radiation damage originating from energetic debris escaping out of the luminous collision point. The presentation will discuss the challenges, design choices, construction status and installation plan of the HL-LHC vacuum system.

Diamond surface science for quantum and electronics applications

Prof Alastair Stacey[1]
[1]RMIT University, Australia

Carbon Materials 1, June 18, 2024, 16:00 - 17:30

Diamond materials possess superlative properties, ideal for room temperature quantum and various electronics applications. However, realization of devices in such applications inevitably requires development of a toolbox of surface and interface science and functionalities. While diamond's lack of solid-state oxide is a boon in this regard, it has shown to be an otherwise challenging surface material to control. In this presentation I will detail our efforts to identify crystallographic defects at the diamond surface [1], how these relate to epitaxial growth processes and the potential impact of such defects on electronic device parameters, such as band bending [2] and Fermi level pinning. I will describe our efforts to control the surface chemistry of diamond, to create novel surface termination chemistries and to fabricate quantum electronic and electron emission devices, including for medical diagnostic imaging applications [3].

I will describe our efforts to develop a toolbox of diamond surface chemistries and interfaces, including silicon [4] related terminations, interfacing with cubic silicon carbide [5], and the development of extreme electron affinity surfaces [6]. To support these surface chemistry studies we have established a protocol for quantification of oxygen terminated species on the diamond surface, showing that traditional x-ray photoelectron spectroscopy assignments do not apply [7] and detailing how a combination of x-ray photoelectron and absorption spectroscopies can be used to robustly identify and quantify otherwise problematic surface moieties. This expanding toolbox of surface terminations and control suggests that potentially stable surface transfer doping is possible [8], as well as the development of record ultra-low work-function surfaces.

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Cell electrospinning: revolutionising tissue engineering and regenerative medicine

Professor Suwan Jayasinghe[1]
[1]University College London, United Kingdom

Biomaterials 1, June 18, 2024, 10:30 - 12:30

Electrospinning, a century old technology has recently seen its applicability to many areas of research and development. This technology has entered commercial exploitation for the creation of face masks, filters to the clothing industry to name a few. Under the remit of research and development the technology has been investigated for nearly 30 years, as an approach for generating scaffolds for growing and proliferating both specialised and unspecialised cells. Although those studies have contributed to an increased understanding of the utility of such scaffolds in biomedical sciences, its translation to the clinic has been seldom, as the scaffolds have been demonstrated to limit cell infiltration. Cell electrospinning, reimagined the technology where the electrospinning solution would be a biocompatible polymer (hydrogel) accommodating living cells, as a living cell suspension. In 2005 cell electrospinning was discovered and demonstrated to have no negative effects brought on the post-cell electrospun cells from a molecuklar level upwards. Thus, opening the technology for directly handling living cells for forming cell bearing fibres from which living scaffolds are generated for the reconstruction of three-dimensional, fully cellularised scaffolds. Such scaffolds have widespread applicability ranging from the repair, replacement to rejuvenation of damaged and/or aging tissues/organs, biological models, to having implications outside our healthcare, in areas such as our evolving food industry. The talk will introduce the discovery, its capabilities to date and its future.

Hide and seek in the electron’s world

Federico Mazzola[1]
[1]University of Venice and CNR IOM, Italy

Spin Physics, June 17, 2024, 16:00 - 17:35

For many years, since the beginning of the 19th century, the existence of magnetism in low dimensions has been both desired and controversial. It was long thought, that magnetic orders in low dimensional systems could not be realized at temperatures different from zero. At least, this was what the Mermin-Wagner theorem stated for isolated Heisenberg spins. The scarcity of low-dimensional materials with magnetic properties, and the partial understanding of the role of spin-anisotropy have supported this picture for several decades.

In three-dimensions, magnetism has revolutionized our everyday life, enabling familiar technologies which are of common use. A few examples include computers’ memories, RAM, hard-disks, key cards, credit cards, electric batteries, light, and distance sensors. This relentless pace of development has motivated the search for magnetism in systems with increasingly smaller sizes.

With cooperation of experimental and theoretical physics, researchers discovered that spin-anisotropy can stabilize low-dimensional magnetism. In this, spin-orbit coupling plays an important role. Surface experimental probes, such as angle-resolved photoelectron spectroscopy provide researchers access to the electronic structure of solids. Despite the advances in the field, recently, new forms of surface local magnetism completely different from standard descriptions have appeared.

Here, I aim to give an overview of a new powerful methodology to uncover hidden phases of electrons, including spins, and magnetism which was so fare elusive. I will do this by showing two of my research achievements.

Investigating Biointerfaces using Integrative ToF-SIMS Imaging

Dr. Sebastiaan Van Nuffel[1]
[1]Maastricht University, Netherlands

Biointerfaces/Biophysics/Biosensers, June 19, 2024, 10:30 - 12:35

Dr. Sebastiaan Van Nuffel is presenting various examples of the ongoing research in his group using Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) imaging. ToF-SIMS is an ultra-high vacuum (UHV) technique capable of analyzing the top 1-3 monolayers of a surface. For the past two decades, ToF-SIMS imaging in particular has successfully answered various research questions, because it can visualize the spatial distribution of small molecules (< 2000 Da) in 2D with a spatial resolution comparable to that of a light microscope. Through ion beam sputtering, it is also possible to depth profile and create 3D image stacks with a depth resolution down to 5-10 nm. ToF-SIMS imaging can be used to simultaneously investigate the elemental composition, the metabolome and the lipidome of single cells and tissue sections as well as their interaction with non-native compounds such as drugs or toxins. Furthermore, as ToF-SIMS can observe inorganic and organic compounds, it is also eminently suited for research involving biointerfaces.

Although ToF-SIMS allows for label-free detection, ambiguity always remains with regards to structural identification of compounds given the secondary ions of the different compounds present in the sample are all formed together after the impact of the primary ion. Consequently, a typical ToF-SIMS mass spectrum can be considered a summation of the spectra of the individual compounds present and spatial colocation does not necessarily mean that these mass peaks all originate from one compound. Luckily, the creation of ToF-SIMS instruments with MS/MS capabilities makes unambiguous identification finally possible. Regardless, the data generated is very complex, especially in the case of biological systems, and its integration with multivariate analysis techniques for image segmentation and more advanced machine learning approaches for biomarker discovery will be covered as well. In addition, it is difficult to detect large molecules such as intact proteins with a typical ToF-SIMS instrument. It is therefore necessary to integrate ToF-SIMS with other techniques such immunohistochemistry in order to establish a spatially resolved multi-omics atlas. However, there are several issues still hampering its widespread application. In order to become truly competitive with immunofluorescence microscopy, the same field of view needs to be achieved at a similar throughput rate. Ongoing research efforts developing SIMS-IHC methods in combination with novel stigmatic SIMS imaging instrumentation will be discussed.

Contributed Oral Talks

Progress in Vacuum System Design for Thailand's New Light Source

Thanapong Phimsen[1], Supan Boonsuya[1], Acting Sub Lt. Sarawut Chitthaisong[1], Prapaiwan Sunwong[1], Siriwan Jummunt[1], Porntip Sudmuang[1], Prapong Klysubun[1]
[1] *Synchrotron Light Research Institute, Thailand*

Large Vacuum Systems of Particle Accelerators, June 18, 2024, 10:30 - 12:30

The vacuum system of Siam Photon Source II (SPS-II), Thailand's first 4th generation light source, is positioned to significantly enhance the country's local manufacturing capabilities and strengthen the Thai industrial community through technology transfer by domestically fabricating most of the main components in the system. Utilizing existing Thai expertise, conventional pumping technology is chosen. However, Design adaptations are needed to overcome the challenges posed by the dense Double-Triple Bend Achromat (DTBA) magnet lattice with limited aperture. Strategic positioning of pumps is required to achieve optimal pumping efficiency. Lump pumps are being strategically distributed throughout the system. A combined approach is employed for pressure profile evaluation, using 1D iteration for the overall pressure profile with conductance values calculated from 3D Molflow+ simulation, enabling optimization of the pump distribution strategy. To minimize cost and impedance, bellows are eliminated between chambers in both upstream and downstream arc sections. Finite element analysis is ongoing to ensure the modified design can withstand operational stresses. The paper concludes by outlining the overall progress and future plans for the SPS-II vacuum system design.

Ultra-thin metal oxide superstructures grown on Pd(001) as passivation interlayers at the metal/porphyrin interface

Dr. Isheta Majumdar[1], Dr. Francesco Goto[1], Prof. Alberto Calloni[1], Prof. Lamberto Duò[1], Prof. Franco Ciccacci[1], Prof. Gianlorenzo Bussetti[1]
[1] *Department of Physics, Politecnico di Milano, Italy*

Metal Surfaces - Adsorption, Desorption and Reactions 1, June 17, 2024, 11:00 - 12:35

In organic electronics, the evaluation of the molecule-substrate interaction poses a major challenge for the correct preparation of metal electrode/organic molecule heterojunctions. In our previous studies, we focused on the cobalt tetraphenylporphyrin (CoTPP)/Fe(001) interface, demonstrating a molecule-substrate decoupling effect on the O passivated Fe surface Fe-p(1×1)O, where the ultra-thin metal oxide (UTMO) decoupling layer had a formal 1:1 Fe:O stoichiometry, or 100% O coverage [1, 2]. A strong interaction with the Fe(001) surface was detected in the absence of O passivation. At present, it is not clear whether it is possible to tune this decoupling effect as a function of the surface O density.

In this work, we considered Pd(001) and their different UTMO layers to check the O decoupling effect. This has been investigated by CoTPP deposition on well-known O superstructures: p(2×2)O and p($\sqrt{5}\times\sqrt{5}$)R27°O, with 25% and 80% O coverages, respectively. Electron diffraction showed a clear molecular ordering only on the p($\sqrt{5}\times\sqrt{5}$)R27°O surface, that we attribute to the higher mobility of CoTPP molecules in the absence of a strong interaction with the substrate. X-ray photoelectron spectroscopy revealed the presence of buried O atoms at the CoTPP/Pd(001)-p($\sqrt{5}\times\sqrt{5}$)R27°O interface but not at the CoTPP/Pd(001)-p(2×2)O interface, thus solidifying the effectiveness of the Pd(001)-p($\sqrt{5}\times\sqrt{5}$)R27°O superstructure as a functional passivation interlayer. The CoTPP molecular features, Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) were detected by ultra-violet photoelectron and inverse photoemission spectroscopies, respectively, only at the CoTPP/Pd(001)-p($\sqrt{5}\times\sqrt{5}$)R27°O interface (see Figure).

Our results clearly show that there is a minimum O coverage at the metal/organic interface to enable a full passivation effect, and that a UTMO layer can indeed act as passivation interlayer even without 100% O coverage of the metal substrate.

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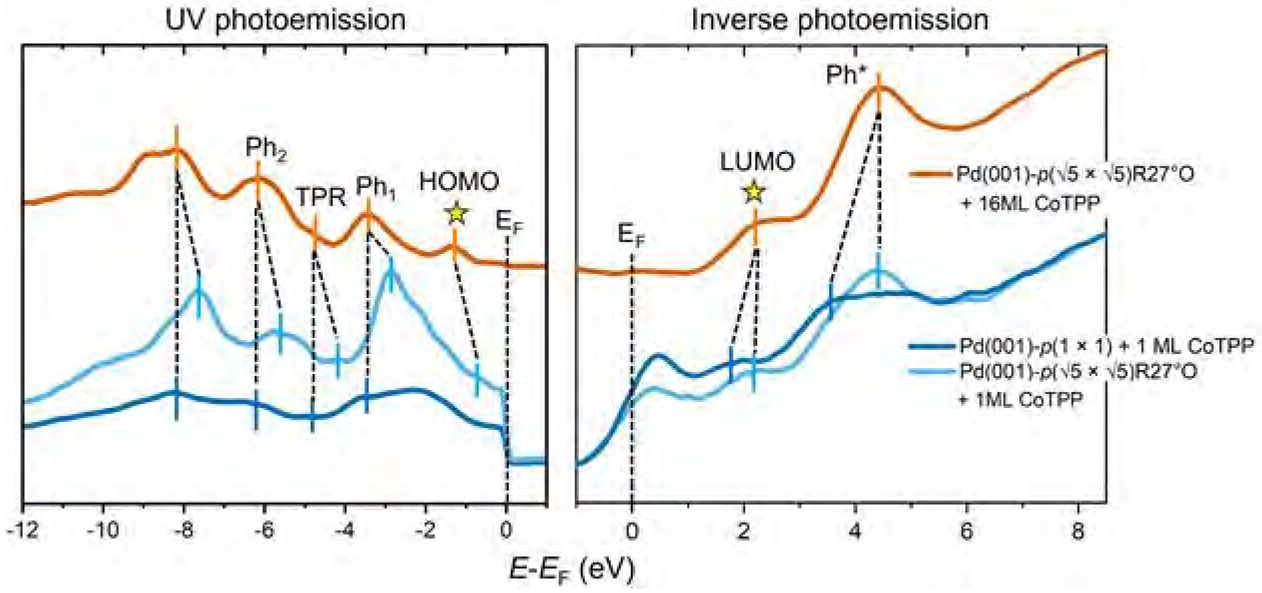

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Selective hydrogenation of butadiene by single metallic atoms anchored on graphene-based catalysts

Safouan Ziat[1], Theo Becquet[1], Clovis Lapointe[1], Luc Moreau[1], Bertrand Kierren[1], Emilie Gaudry[1]

[1]*Jean Lamour Institute, Lorraine University, France*

Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 3, June 20, 2024, 11:00 - 13:00

Petroleum cracking processes yield highly unsaturated hydrocarbons, which likely poison reactions widely used in the chemical industry. Effective removal of such unsaturated hydrocarbons is crucial, commonly achieved through catalytic hydrogenation. Traditional noble metals are efficient, but lack the desired selectivity. Single metallic atoms anchored on graphene-based catalysts have recently shown excellent performances for such reactions, but a deep understanding of the mechanisms involved has not yet been achieved. In this work, we focus on butadiene hydrogenation because of its practical relevance in industrial processes and the relative simplicity of its mechanism, which is expected to be smoother than that involving more complex molecules, potentially containing oxygen.

In this work, using Density Functional Theory, we have systematically computed adsorption energies of hydrogen, butadiene and butenes on 32 structural models of single atom catalysts consisting of isolated atoms anchored on N-doped graphene systems. Both the support and the active site are modified, by tuning the nitrogen content and the transition metal, and their impact are discussed in relation to the adsorption strength and adsorbate conformation, paving the way to a better understanding of the catalytic activity. Additionally, barriers for hydrogen dissociation have been determined for a reduced number of catalyst models.

These results aim to help the analysis of surface science experiments planned in the group, with scanning tunneling microscopy (STM) and spectroscopy (STS), using samples elaborated by Molecular Beam Epitaxy (MBE). This approach aims to advance our understanding via the comparison of computational results with experimental measurements.

Computational Modelling of CO2 Reduction to Ethylene over Doped Copper Catalysts

Dr Moyahabo Hellen Chuma[1], Toby Joe Hodges[2], Saurav Chandra Sarma[2], Elena Cristina Corbos[2]
[1]Johnson Matthey, United Kingdom, [2]Johnson Matthey, United Kingdom

Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 3, June 20, 2024, 11:00 - 13:00

The electrochemical reduction of CO2 presents a promising opportunity to decarbonize the chemical industry by targeting feedstock molecules, such as ethylene, that are currently produced from fossil sources in large volumes. Additionally, multi-carbon products can be oligomerized to produce longer hydrocarbons, which could play a crucial role in decarbonizing the shipping and aviation industries. This route from CO2 to fuels offers increased energy efficiency compared to established processes, such as Fischer-Tropsch synthesis.

In this study, we employed computational modelling techniques based on Density Functional Theory (DFT) to guide materials synthesis and provide a deeper understanding of the reaction pathways of CO2 reduction to ethylene over doped Copper catalysts. A reaction pathway was proposed over a doped Cu(111) surface, followed by an in-depth study of key intermediate steps, including C-C coupling and the selectivity-determining step for ethylene formation. A series of dopants were introduced to the surface to investigate their effects on selectivity and activity of the catalyst.

The activation energy barrier (Ea) of the C-C coupling step via *OCCHO species formation was calculated over various doped Cu(111) surfaces. Overall, the studied dopants tune the reactivity of the surfaces differently. This shows the need to balance the effect on the activation energy barriers of C-C coupling step, as well as adsorption energies for CO and H species. Our study suggests that a compromise may be necessary to balance selectivity towards desired products and minimize hydrogen evolution.

Comparison of SRG transducer technology to Ion gauge technology in process applications

Martyn Green[1], Peter Hofmann[1]
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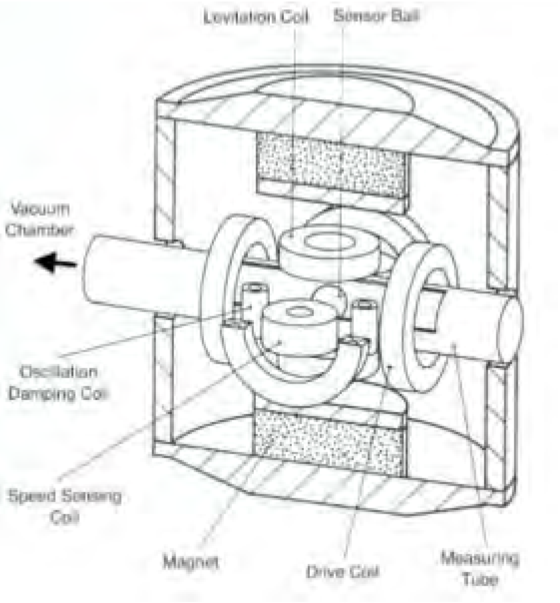
Vacuum Metrology, June 20, 2024, 11:00 - 13:00

Due to their simplicity, accuracy and long term stability, Spinning Rotor Gauges (SRGs) were widely used as references in vacuum calibration laboratory applications (10-2 to 10-6mbar range, 1% of rdg. etc.).

Additional strengths of SRF such as like corrosion resistance, deposition insensitivity, free of altering effects and a ultraclean/simple design make them an ideal soluton for semiconductor process applications and vacuum similation tools.

The new generation of SRG transducers enable autonomous use, has a compact design and is intended as a process manometer, working under harsh conditions, where widely used Ion gauges are not accurate enough, constantly drift and have short lifetimes to failure.

The topic of this lecture is to present the history of SRG development and compare its strengths and weaknesses with the prevalent Ion Gauge.



Correlation of mass spectrometry and pressure in ultra-high vacuum systems

Mareen Czech[1], Mr Marvin Warner[1], Mr Jaka Perovšek[1], Dr.-Ing. Jens Grosse[1]
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MS-6: RGA User Meeting 2, June 19, 2024, 14:00 - 15:30

For experiments with ultra-cold atoms, background gases should be removed as far as possible to avoid collisions. Hence, an Ultra-High Vacuum (UHV) is required. Such a UHV system is demonstrated in a prototype for the ISS project Bose-Einstein Condensates and Cold Atom Laboratory (BECCAL) at the Center of Applied Space technology and Microgravity (ZARM) in Bremen. The Space Technologies team works on several systems using UHV for ultra-cold atom research in space, mainly being responsible for systems engineering and vacuum design.

This contribution shall give an introduction of the prototype set-up and performed tests. An analysis of how the mass spectrometry data of the UHV prototype correlates to pressure data and what conclusions can be drawn from these correlations shall be presented. It shall be discussed if these correlations can help improve vacuum quality.

Optimising high integrity vacuum viewport design and manufacture

Dr Chris Peters[1]
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Large Vacuum Systems, June 17, 2024, 11:00 - 12:35

United Kingdom Atomic Energy Authority has a long history of building and operating large-scale vacuum devices for use in fusion energy research. Its Special Techniques Group (STG) was established to develop and manufacture first of a kind and prototype components to support fusion research.

In the early 1970s STG took interlayer diffusion bonding techniques and developed them to provide high-integrity joins from ceramics and glasses to metals. This has application to the manufacture of vacuum viewports for in-vessel diagnostics. STG has designed and manufactured viewports for JET and ITER as well as other demanding customers around the world.

Applications for viewports, particularly in areas such as quantum research, are increasingly demanding on optical quality. This presentation will discuss the development and use of a predictive finite element modelling tool to predict surface deformation due to thermal stresses, helping to optimise viewport design.

Data presented will compare predicted and measured characteristics of the optical windows and cast light on the scope for further optimisation.

Extrinsic activation of 2D polymerization on inert surfaces using atomic clusters

Dr Leonardo Forcieri[1], Dr Qingqing Wu[1], Mr Alessio Quadrelli[1], Dr Sonjun Hou[1], Prof Neil Champness, Dr David Buceta, Prof Arturo Lopez-Quintela, Prof Colin Lambert, **Dr Samuel Jarvis**[1]
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MS-3: On-Surface Synthesis of 1D and 2D Functional Graphitic Materials, June 19, 2024, 10:30 - 12:35

Developing atomically precise surface polymers on inert and insulating substrates is essential to fully realize many of their applications, but has proven to be exceptionally challenging [1]. The most common method for surface polymerization is thermal activation, however, in the absence of a surface catalyst covalent coupling reactions become energetically unfavorable. This results in the so-called 'desorption problem' [2], where molecules desorb from inert surfaces before they can polymerize. A number of alternative strategies have been designed to address this problem, including recent reports of photoactivated polymerization with exceptionally high quality [3]. However, such strategies typically rely on specific molecular designs and substrates that place limits on the structures that can be realized. The more general and, in principle, predictable method of thermal activation therefore remains an attractive option for surface polymerization.

Here we report on-surface polymerization on bulk inert surfaces using atomic quantum clusters (AQCs) [4] as extrinsic catalysts. Using temperature-controlled X-ray photoelectron spectroscopy (TP-XPS) and high-resolution atomic force microscopy (AFM), we show that Cu and Ag AQC catalysts, as small as five atoms in size, reduce the activation temperature for on-surface polymerization by as much as 150±30 °C, resulting in stable surface covalent structures on both metallic and inert surfaces that survive ambient conditions. We report a strong dependence between the catalytic activity of AQCs and their stabilizing oxygen layer, highlighting the potential to further tune the catalytic activity of these atomic scale catalysts.

Figure 1. (a) Schematic of surface polymer activation on inert substrate. 2D TP-XPS plot of the Br3p region for Br4TPP (b) in the absence, and (c) in the presence atomic quantum clusters, respectively.

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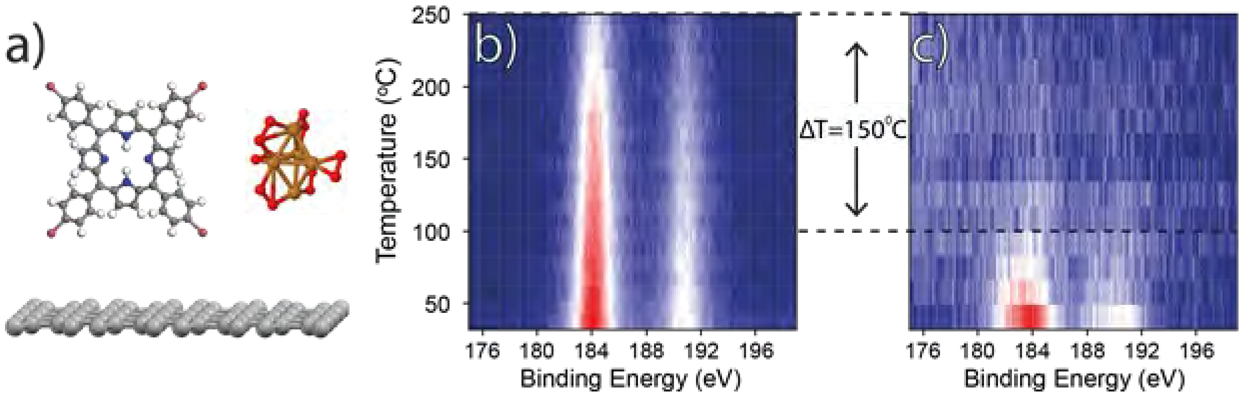

The adsorption and reactivity of N-heterocyclic carbenes on ultrathin films of reactive metals on Au(111)

Miss Ines Bertaso[1,2], Dr Federico Grillo[1,2], Dr. Stephen M Francis[1], Mark D Aloisio[2,3], Prof. Cathleen M Crudden[2,3,4], Prof. Christopher J Baddeley[1,2]
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Metal Surfaces - Adsorption, Desorption and Reactions 1, June 17, 2024, 11:00 - 12:35

The involvement of metal adatoms in determining the adsorption geometry of N-heterocyclic carbenes (NHCs) on coinage metal surfaces has been previously studied(1-3), however work on more reactive metal surfaces such as Ru are relatively unknown.
Herein, the desorption of benzannulated N-heterocyclic carbenes onto thin films of Ru or Cu over Au(111) have been investigated in an ultra-high vacuum environment in order to characterise the binding, self-assembly and reactivity of these organic molecules on these surfaces. Temperature programmed desorption (TPD) revealed that the binding of the NHC molecules is influenced by adsorbate–substrate interactions and nature of the wingtip substituents. Scanning Tunnelling Microscopy (STM) studies were used to determine the energetically favoured adsorption geometries and characterise any ordered domains that form for the NHC when adsorbed on metallic thin films on Au(111).

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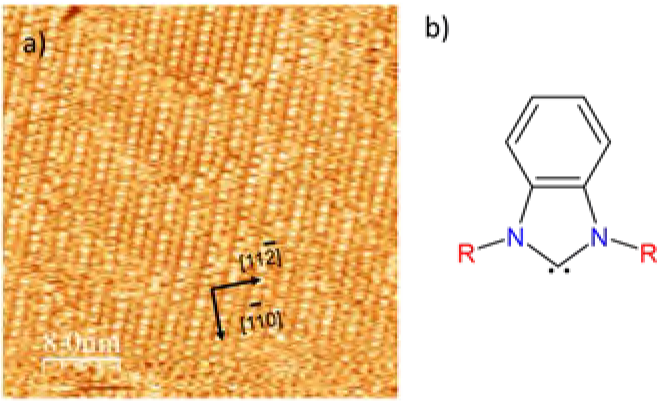

Figure 1: (a) STM topography of Au (111) after 1 hour of Cu deposition at 4.0 A, 30 minutes of NHC^{iPr} deposition and annealing to 453 K 40 × 40 nm^2 , 1.4 V, 0.11 nA) (b) General structure of NHC molecule, with wingtip groups marked as R

Identification of defects on CVD-grown hydrogen-terminated diamond using scanning tunnelling microscopy

Yi-Ying Sung[1], Dr. Lachlan Oberg[2], Dr. Rebecca Griffin[1], Alex Schenk[1], Dr. Henry Chandler[3], Dr. Tetiana Sergeieva[4], Dr. Santiago Corujeira Gallo[3], Dr. Marcus Doherty[3], Dr. Cedric Weber[2], prof. Chris Pakes[1]
[1]La Trobe University, Australia, [2]The Australian National University, Australia, [3]Quantum Brilliance Pty Ltd, Australia, [4]Quantum Brilliance GmbH, Germany

Carbon Materials 1, June 18, 2024, 16:00 - 17:30

Impurity centres in diamond, such as the nitrogen-vacancy (NV-) centre, provide a platform for the development of robust and portable devices for quantum information processing and sensing. For device schemes in which near-surface impurity centres are desirable, the quality of the surface plays a critical role in realising the capability of the technology. Surface defects are important both in fabrication schemes for precision engineering of multi-qubit devices, and in the operation of engineered devices where surface defects may act to degrade performance. Wide-field spectroscopy has been employed for the study of diamond surface defects which are candidates for electron trapping and noise sources.1 However, these techniques cannot conclusively identify which defects are present nor do they offer the spatial resolution required to probe the structure and position of the defects on the surface.

The present study uses ultra-high vacuum Scanning Tunnelling Microscopy (STM) to identify several distinct surface defects on the H:C(100)-2x1 surface of boron-doped samples prepared by chemical vapour deposition. By comparing high-quality STM images with state-of-the-art first-principles simulations, we determine the atomic structure of the observed defects (Figure 1), including surface adsorbates which play a role in accepted models for CVD diamond growth. Tip-based manipulation of the structure of some of the observed defects is demonstrated, providing an avenue to engineering their electronic and magnetic properties.

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Atomically dispersed cobalt atoms embedded in a bilayer of C60

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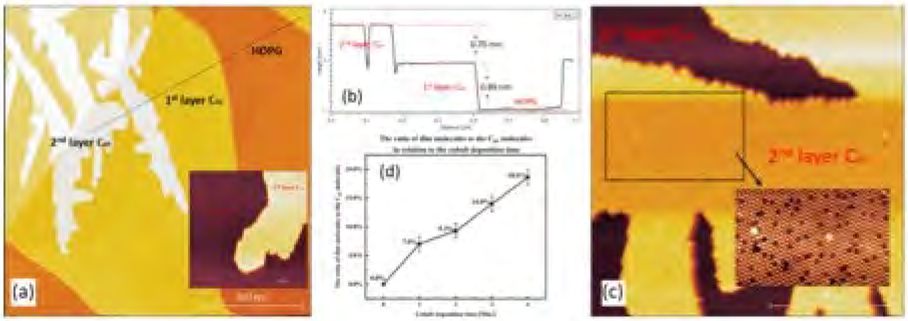
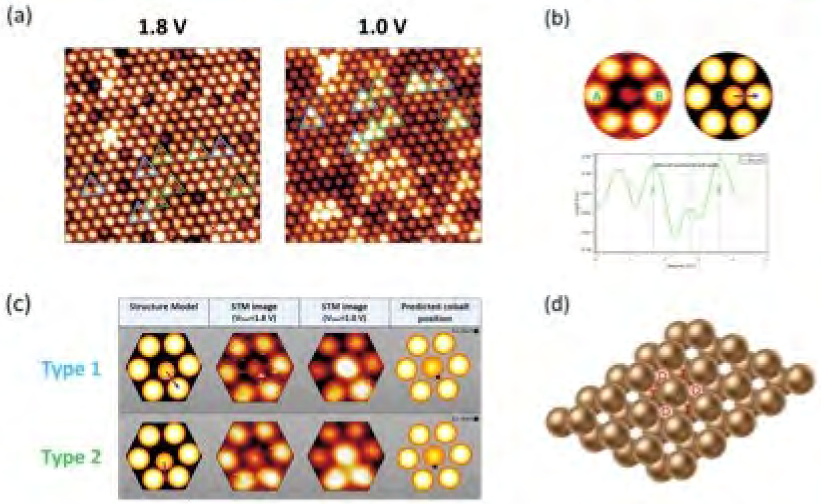
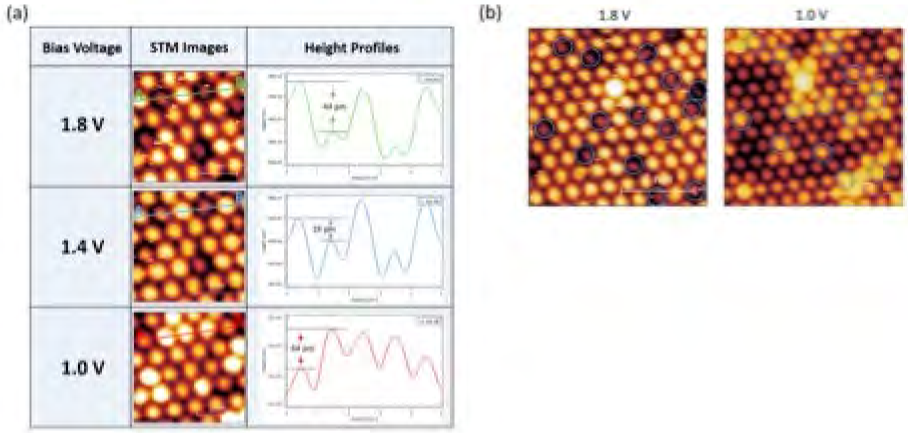
[1]University of Birmingham, United Kingdom

Carbon Materials 2, June 19, 2024, 10:30 - 12:35

In this study, the scanning tunnelling microscopy (STM) was used to investigate the capability of C60 templates in controlling the distribution and localization of single cobalt atoms or cobalt clusters at the nanoscale. The C60 template is in the form of a closed-packed monolayer and/or multilayer supported by a graphite substrate. The cobalt atoms from the evaporator seem to follow mostly a land-and-stick route with very limited lateral diffusion. Co atoms or small Co clusters are found to occupy the interstitial site within the C60 layers. Therefore, the C60 layers provide some guiding effect on the location of trapped atoms/clusters. The limited volume associated with the interstitial site prevents the formation of large clusters. The charge-transfer between cobalt and C60 molecules was then revealed by the dim and bright features in the STM images. The effectiveness of C60 template in directing the formation of size-controlled cobalt clusters was thus demonstrated at the atomic level. The cobalt-doped C60 networks were stable even after annealing the sample at a temperature much higher than that required for C60 desorption.


(a)
HOPG
1st layer C60
2nd layer C60
(b)
0.75 nm
0.89 nm
The ratio of dim molecules to the C60 molecules in relation to the cobalt deposition time
(d)
(c)
2nd layer C60


(a)
1.8 V
1.0 V
(b)
A
B
(c)
Structure Model
STM image (Vbias=1.8 V)
STM image (Vbias=1.0 V)
Predicted cobalt position
Type 1
Type 2
(d)


(a)
Bias Voltage
STM Images
Height Profiles
1.8 V
44 pm
1.4 V
19 pm
1.0 V
64 pm
(b)
1.8 V
1.0 V

Investigation of the effect of fabrication of SrTiO3 doped thin film samples on a silicon substrate and the experimental techniques used on surface cracking and destruction

Mr. Zdenek Jansa[1], Mrs. Štěpánka Jansová[1], Mrs. Lucie Nedvědová[1], Mr. Pavel Calta[1], Mr. Ján Minár[1]
[1] Univesity of West Bohemia, New Technologies Research Centre, Czech Republic

Advanced Thin Film Fabrication, June 19, 2024, 10:30 - 12:35

The present work is part of a larger body of work devoted to the use of strontium titanate SrTiO3 (STO) in visible light applications. This work addresses the problem of surface cracking of STO thin films on a silicon substrate. STO material belongs to the group of perovskites. It is an ionic compound of known formula ABX3. In their original composition, perovskites are dielectrics with a large gap in the valence band. The use of dopants, preferably transition metals, affects the physical properties in the sense of exploiting the favorable original properties. Overall, the work is devoted to the assessment of the effect of these transition metals on various physical properties, including the utilization of the electromagnetic spectrum of visible radiation. In this work, the influence of nickel (Ni), yttrium (Y), and iron (Fe) was considered.
STO samples were prepared by magnetron pulse deposition. Several methods were used to investigate the structural and electronic properties of the SrTiO3 material under consideration. XRD analysis methods including high-temperature experiments, scanning electron microscopy - SEM, and X-ray photoemission spectroscopy - XPS were used for all the samples evaluated. After performing the individual experiments, the data obtained were evaluated and further procedure was determined. Finally, all data were analyzed together.

The problem discussed in this work is the surface cracking of thin films. The conclusion of the work mentions as probable causes of cracking both the critical thickness of the thin film of 150 nm and the visco-elastic behavior of the thin film during heat treatment and subsequent relaxation. The conclusion of this paper is consistent with the findings of the experimental results. That is, surface cracking occurs after annealing during relaxation. Thus, there is a need to determine the ideal procedure for sample preparation and further processing to avoid this undesirable phenomenon.

Low-temperature heterogeneous hydrogenation of carbonyl compounds: molecular systems for reversible hydrogen storage

Prof. Dr. Swetlana Schauermann[1], Carsten Schröder, Jan Smyczek, Philipp Haugg, Jessica Wulfes
[1]*Institute Of Physical Chemistry, Kiel University, Germany*

Electronic Materials, Energy Reduction and Carbon Reduction, June 19, 2024, 16:00 - 17:30

Hydrogenation of carbonyl compounds to alcohols is an important step in many technological applications, including the emerging molecular systems for reversible hydrogen storage. This class of reactions is challenging as it requires the activation of a stable C=O bond, typically occurring under harsh conditions. There is an ongoing discussion on an alternative theoretically predicted pathway, comprising two consecutive steps: keto-enol tautomerization of the carbonyl compound to its enol counterpart followed by hydrogen insertion into the C=C bond. Both steps were predicted to proceed via significantly lower barriers than for direct hydrogen insertion into the C=O bond. The major challenge of this mechanism is the low stability of enols that – if not stabilized – readily convert back to ketones.
In this study, we present our recent investigations on formation of enol species from carbonyl compounds acetophenone and butanal and their stabilization via hydrogen bonding with neighboring carbonyls.1, 2
By employing a combination of IRAS, STM and molecular beam techniques, we demonstrate the proof-of-principles experiments confirming the possibility of their low-barrier hydrogenation proceeding via keto-enol tautomerization as a first step. The enol species become stabilized on surfaces in form of ketone-enol dimers or ketone-enol-enol trimers via strong hydrogen bonding between the C=O group of the ketone form and the OH-group of the enol species. The enol species in the ketone-enol dimer can be hydrogenated already at the surface temperatures of 240 K, suggesting drastically reduced activation barrier as compared to direct hydrogenation of the carbonyl group. The stabilization of enols in form of ketone-enol dimers or ketone-enol-enol trimers turns out to be the crucial reaction step, allowing the enol-containing reaction intermediate to enter the second reaction step – hydrogenation of the olefinic bond.

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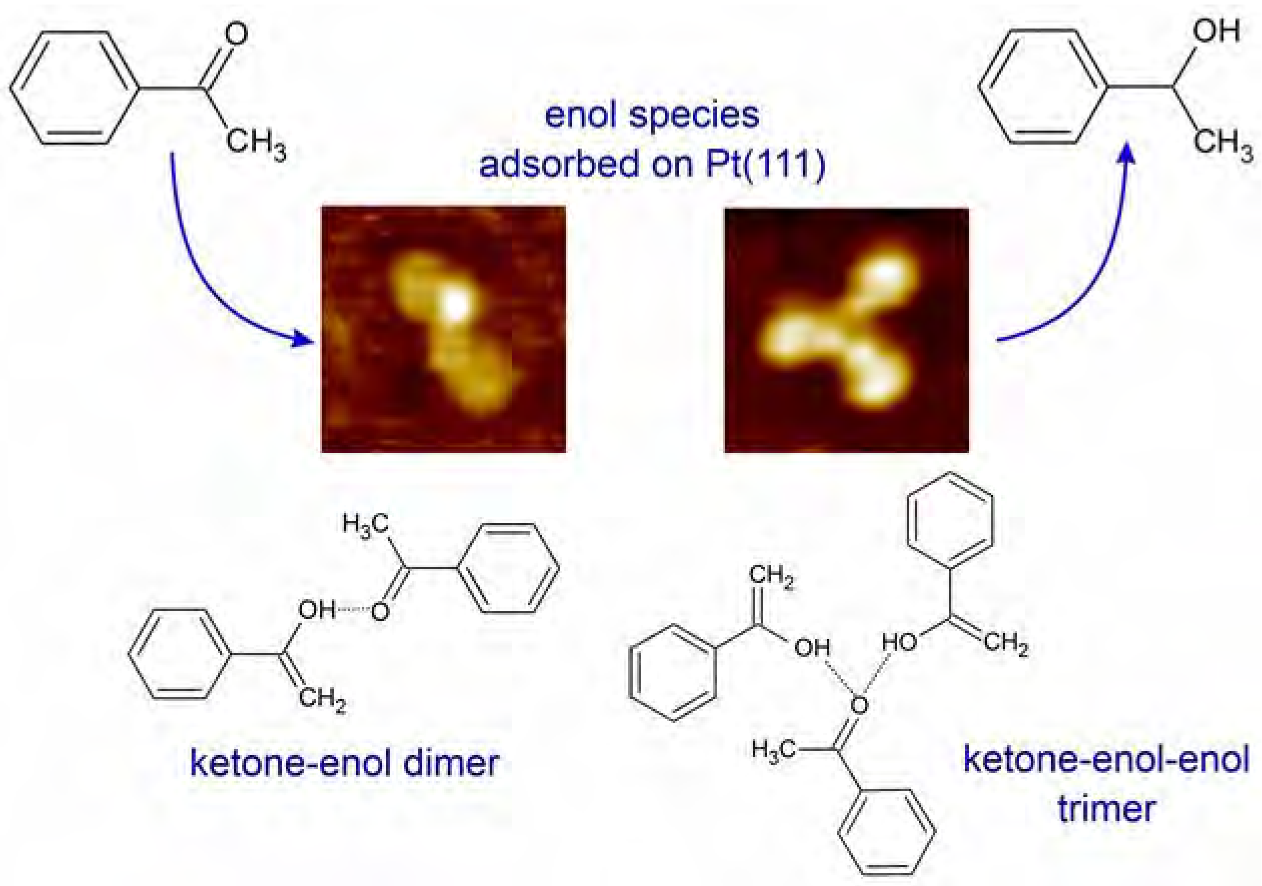
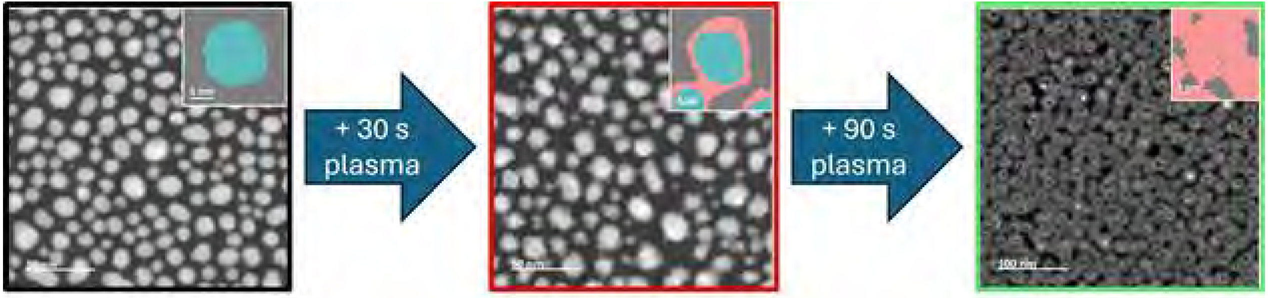

enol species
adsorbed on Pt(111)
ketone-enol dimer
ketone-enol-enol
trimer
O
CH_3
OH
H_3C
CH_2
HO

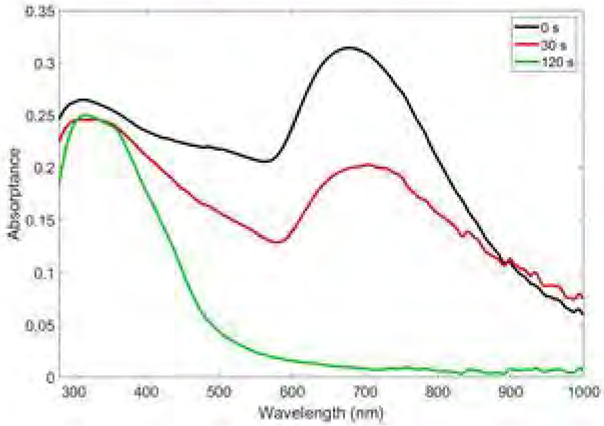
Influence of air plasma treatments on plasmonic properties and composition of Cu nanoparticles

Eleonora Spurio[1,2], Giovanni Bertoni[2], Sergio D'Addato[1,2], Samuele Pelatti[1,2], Paola Luches[2]
[1]Università di Modena e Reggio Emilia, Italy, [2]CNR - Istituto Nanoscienze, Italy

From Nanostructured thin films to nanoparticles. Reactions at nanostructures, June 18, 2024, 16:00 - 17:30

Nanostructures of Cu and corresponding oxides are promising candidates for photocatalytic applications, thank to their unique optical properties. Copper tends to oxidize in atmosphere, forming stable oxides like CuO and Cu2O, that are interesting for photocatalysis. The oxidation of Cu thin films and nanoparticles (NPs) has been demonstrated to depend on the temperature and pressure conditions, and the oxygen exposure influences the position and the shape of their plasmonic resonance. We investigated the morphology and composition evolution of Cu NPs as a function of the exposure to air plasma, and their spectral response in the ultraviolet-visible region following the shift of the plasmonic resonance. We found that the NPs, after 30 s exposure to air plasma, change their composition, forming core-shell NPs, with a metallic core and a thin CuO shell, while the NPs dimensions and the substrate coverage remain unmodified. After 90 s of plasma treatment, no more Cu(0) is observed: the metallic core turns into Cu2O, while the CuO shell is thickened. Some of the NPs start to exhibit the internal voids typical of the nano-Kinkerdall effect, while the surface coverage by CuO is enhanced and the separation between NPs diminishes. After 120 s of plasma, almost all NPs present a hollow structure surrounded by a CuO shell. The morphological results are compatible with the optical absorptance spectra measured at the different steps: after 30 s of plasma treatment, the optical spectra still show the absorptance band ascribed to the plasmonic excitation of the NPs, red-shifted with respect to the initial situation, compatibly with the numerical simulations for core@shell Cu@CuO NPs. After 90 s, only a weak plasmonic band is present, and this completely disappears when the NPs are treated for 120 s with plasma. The research in this work was funded by the PNRR MUR project ECS_00000033_ECOSISTER.





Functionalizing GaN surfaces for enhanced soft tissue integration in biomedical applications

Dr. Monu Mishra[1], Dr. Jitendra Sharan[2], Prof. Manish Kumar Kashyap[3], Prof. Govind Gupta[4]
[1]Department of Physics, Dyal Singh College, University Of Delhi, India, [2]Department of Dentistry, All India Institute of Medical Sciences Bhubaneshwar, India , [3]School of Physical Sciences, Jawaharlal Nehru University, India, [4]Sensors Devices Metrology, CSIR – National Physical Laboratory, India

Biomaterials 1, June 18, 2024, 10:30 - 12:30

Biomedical implants have become a routine treatment these days which serve to recover the functional difficulties in humans for a better quality of life. Biomedical implants have wider applications in rebuilding and healing damaged areas of human body i.e., hip/knee replacement, maxillofacial reconstruction, dental/orthopaedic implants etc. However, due to the cyto-toxic nature and higher young modulus of elasticity, commercial medical grade Titanium based biomedical implants (i.e., Ti-6Al-4V) are often failed due to poor soft tissue integration. Gallium Nitride (GaN) being a biocompatible, aqueous and chemical stable material has potential in the field of optoelectronics, photonics, chemical and biological sensors. GaN offers enormous opportunities to modulate the fundamental material properties and surface chemistry to promote adhesion of targeted biomolecules for its efficient utilization in biomedical implants. Here, we report a new three step process for the functionalization of GaN surfaces to promote the attachment/growth of human periodontal ligament fibroblast cells and reduce soft tissue integration related failures in dental implants. We have modified the morphology and surface chemistry of GaN thin films using sodium hydroxide (NaOH) and 3-aminopropyltriethoxy silane (APTES) followed by its bioconjugation with type 1-human collagen (T1HC). Further, changes in chemical states, morphology, wettability, pH, and aqueous stability of surface functionalized films have been investigated. Finally, the cell culture studies analysing cell proliferation and adhesion/survivability studies at different time intervals have been performed using MTT Assay and SEM evaluation. The studies divulge that chemically functionalized T1HC bio-conjugated GaN surfaces display excellent cell culture properties with a cell viability of ~ 95%. It demonstrates that GaN films can be useful in various procedures where integrating soft tissues with biomedical implant is highly desirable.

On-surface synthesis of porphyrin-graphene nanoribbons

Dr Alex Saywell[1]
[1] *University of Nottingham, United Kingdom*

MS-3: On-Surface Synthesis of 1D and 2D Functional Graphitic Materials, June 19, 2024, 10:30 - 12:35

Graphene nanoribbons (GNRs) possess fascinating electronic properties with the potential for application within (opto)electronic devices [1], and therefore there is significant interest in achieving doped and heterostructured GNRs to facilitate bandgap and fermi-level engineering. Studies of GNRs often focus upon the on-surface synthesis of extended graphitic polymers formed from the Ullmann-type coupling of halogen functionalised bianthracene units [2], and in common with many on-surface synthesis protocols, the initial, intermediate and product states can be studied by scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) to provide sub-molecular insights into reaction pathways and resultant structures [3].

Here I will detail the use of electrospray-based deposition (ESD) to deposit a polymeric precursor species onto a Au(111) substrate held under ultra-high vacuum (UHV) condition (utilising methodologies from our previous work [4-7]) and characterise the on-surface synthesis of a porphryin-graphene nanoribbon using a combination of scanning tunnelling microscopy (STM) and photoelectron spectroscopy-based techniques (including XPS, NEXAFS, and NIXSW). Our proposed methodology is to utilise the atomic precision of solution phase chemistry to form highly regular polymeric precursor species, and to employ on-surface protocols to enable reaction steps which are not often facile in solution (e.g. the dehydrogenative-cyclisation reaction step required to produce conjugated graphitic materials). Our focus is on the inclusion of porphyrin species within the graphene nanoribbons; giving rise to porphyrin-fused graphene nanoribbons (PGNRs).

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A systematic approach for contamination control

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[1]TNO, Netherlands

MS-6: RGA User Meeting 3, June 19, 2024, 16:00 - 17:30

As the demand for smaller, faster, and more energy efficient microchips continues, there is an ever-increasing complexity during manufacturing. Contamination concerns that use to be not a concern now suddenly are.

To ensure that products are reasonable priced the production yield needs to be as high as possible. To ensure a high yield a systematic approach is needed with respect to contamination.

A systematic approach for contamination control starts at the design of the product. The design must enable an end result that meets the cleanliness requirements.

During the manufacturing and the assembly process the cleaned products need to stay clean, or have a process in place to be cleaned after assembly.

Finally, in most cases a proof is needed that the product is clean before acceptance. With the decrease of allowed contamination levels it is becoming harder and harder not only to meet the requirement but also to proof that the product meets the requirement.

In the above paragraphs a common V-model in systems engineering approach is described. Within contamination control the product lifetime cycle model could be better used. The product lifetime cycle model also incorporate the “in use” of the product. Using the product lifetime cycle model also incorporated recovery, or cleaning actions during use of the product

The semiconductor industry is one of the front runners in contamination control and this knowledge can be very useful for other industries, however other industries also have very use-full processes implemented of which the semiconductor industry could benefit.

During this presentation I will discuss why a systematic approach is needed and beneficial to reach stringent contamination requirements at acceptable cost, and I will make cross links between several technology domains and what methodology developed in one domain could be useful for another domain.

Probing the mechanism of facile water dissociation on oxygen covered Cu(111) by Reflection Absorption Infrared Spectroscopy (RAIRS)

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[1]École Polytechnique Fédérale de Lausanne, Switzerland

Water and Environmental Surfaces, June 19, 2024, 16:00 - 17:30

The presence of oxygen atoms on a Cu(111) surface strongly reduces the activation barrier for water dissociation, as compared to bare Cu(111). In this work, we present a direct experimental observation of the hydrogen abstraction mechanism for H_2O dissociation on a O/Cu(111) surface using reflection absorption infrared spectroscopy (RAIRS)[1]. By dosing $^{18}O_2(g)$ onto a Cu(111) single crystal, we create a partially oxidized ^{18}O/Cu(111) surface, which is subsequently exposed to a flux of $H_2{}^{16}O$ molecules, resulting in the detection of two RAIRS peaks assigned to ^{18}OH(ads) and ^{16}OH(ads). We also observe that chemisorbed hydroxyl species produced by water dissociation on O/Cu(111) undergo an efficient hydrogen atom transfer from trapped water molecules, leading to the rapid replacement of the initial oxygen isotope coverage and the detection of only a single hydroxyl isotopologue on the surface, in apparent contradiction with the hydrogen abstraction mechanism.

Figure 1. RAIR spectra of UHV background $H_2{}^{16}O$ exposure to Cu(111) pre-covered with 0.07ML of ^{18}O(ads); a)-f) were taken with UHV background pressure of $P(H_2O) < 2\times10^{-11}$ mbar; g)-i) – after the introduction of $P(H_2O)$ ~ 7×10^{-10} mbar; one can clearly observe both peaks are present initially but ^{18}OH disappears immediately after the leak valve is opened

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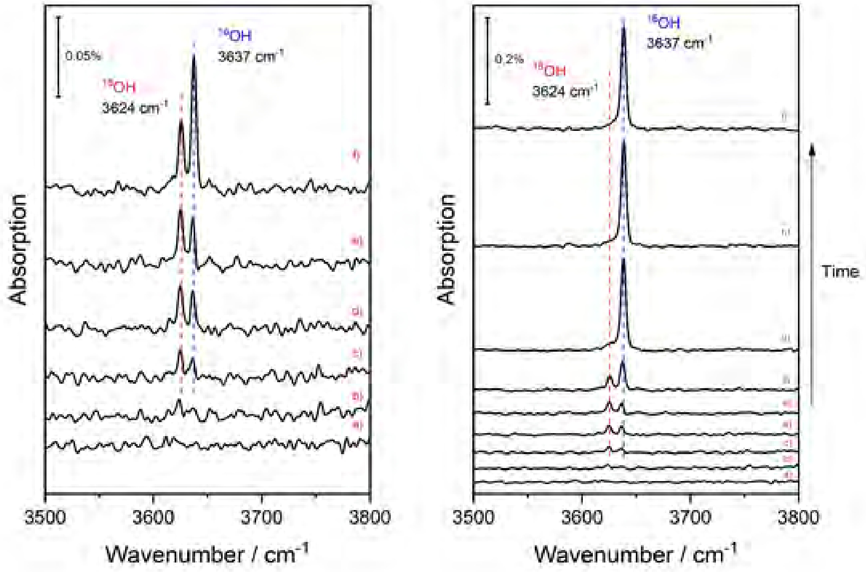


Structure formation in miscible and immiscible thin binary alloy films synthesized by temporally modulated vapor fluxes

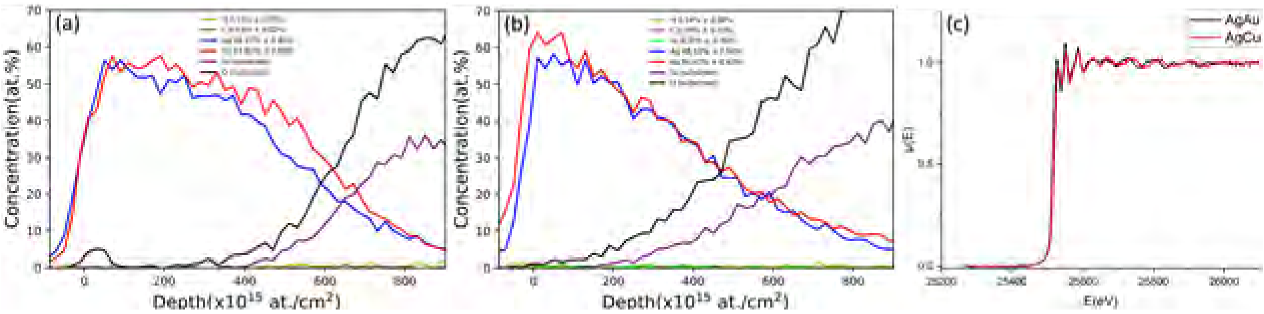
Spyridon Korkos[1,2], Antti-Jussi Kallio[1], Ryan Trevorah[1], Rene Bes[1], Kenichiro Mizohata[1], Simo Huotari[1], Kostas Sarakinos[1,2]
[1]University Of Helsinki, Finland, [2]KTH Royal Institute of Technology, Sweden

Advanced Thin Film Fabrication, June 19, 2024, 10:30 - 12:35

The physical attributes of multicomponent thin films are defined by chemical composition and atomic arrangement across different length scales. The atomic arrangement is predominantly influenced by the complex interplay among thermodynamics either allowing or impeding miscibility and compound formation, kinetic conditions affecting the rates of atomic-scale structure-forming processes, and the arrival pattern of vapor species at the film growth front. In this study, AgAu and AgCu thin films are deposited using vapor fluxes modulated with sub-monolayer (ML) and microsecond resolution [1] by applying electrical power to spatially separated magnetron sources in the form of unipolar pulse trains. This allows flux temporal profiles from co-deposition to fluxes where 4 ML of Ag and Au or Cu vapors are deposited in an alternating fashion. Power is adjusted to deposit equimolar samples, as determined by time-of-flight elastic recoil detection analysis (ToF-ERDA) and Rutherford backscattering spectrometry (RBS). X-ray diffractometry (XRD) show a Face-Centered cubic (FCC) structure at different synthesis conditions, while superlattice structure is formed after deposition of 4 ML per pulse train. The atomic arrangement of neighboring atoms for different synthesis conditions is revealed by extended x-ray absorption fine structure (EXAFS) measurements at European synchrotron radiation facility.

Fig. 1: (a), (b) ToF-ERDA depth profiles of 100 nm AgCu and AgAu, respectively, deposited on SiO_2/Si substrate using 100 alternate pulses, and (c) their normalized EXAFS spectra.

[1] Method of coating a substrate so as to provide a controlled in-plane compositional modulation, PCT/EP2014/052831, granted (Inventors: K. Sarakinos and D. Magnfält).



Temperature dependent disassembly analysis of a molecular adlayer reveals molecule-molecule and molecule-surface interaction energies separately

Dr. Thiruvancheril Gopalakrishnan Gopakumar[1], Ms. Richa Arjariya[1]
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Metal Surfaces - Adsorption, Desorption and Reactions 2, June 17, 2024, 14:00 - 15:30

Understanding the energetics of self-assembled molecular nanostructures on the surface at a molecular level is of great importance in tuning its microscopic patterns on surface. These molecular nanostructures are stabilized by a delicate balance between the intermolecular and molecule-surface interactions. In this work we show that using temperature dependent AFM micrographs of the assembled phases of 1,2,4,5-Tetrakis (4-carboxylphenyl) benzene, the energy required to dissemble different assembled phases (disassembly enthalpy) can be quantitatively calculated. Furthermore, it is demonstrated that one can determine molecule-molecule and molecule-surface interaction energies separately. These are the component energies of disassembly enthalpy of an assembled adlayer and is directly related to the desorption energy. While desorption energy is determined experimentally, its component energies (molecule-molecule and molecule-surface interaction energies) are so far only extracted using theoretical methods.

Reversibility in aligned step direction on an on-axis Si (110) 16×2 single-domain surface

Hidehito Asaoka[1], Masahiro Yano[1], Tomo-o Terasawa[1], Satoshi Yasuda[1]
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2D Semiconductors, June 18, 2024, 14:00 - 15:30

Tuning of surface stress is a powerful strategy for tailoring self-assembled nanostructures at the atomic scale. This is because tuning of surface stress has an immense potential to modify not only physical properties but also chemical ones. The stress magnitude, direction, and symmetry on the surface alter, for example, electronic performance, surface bond strength, and the surface diffusion of adatoms. The unique reconstruction on silicon surface is known to be based on dangling bond reduction and adatom formation. Although the rearrangement of the surface atoms largely reduces the electronic energy of the surface by reducing the number of surface dangling bonds, the surface reconstruction increases the surface stress and the surface energy as well. Among the silicon surfaces, a reconstructed Si(110)-“16×2” has a chiral structure (L or R) with one-dimensional mono-atomic steps and pentagon pair rows along [1-12] and/or [-112] directions. The chiral structure exists as a double domain on the surface, with the two combinations in equal proportions. It is known that the domain orientation on the surface is determined the direction of the monatomic steps pre-existing on the off-axis Si(110) plane, however, no method has yet been established to reproducibly and selectively control the homochirality on the on-axis Si (110) one.
Here we show that an externally uniaxial stress-driven Si(110)-“16×2” structure controls the chiral one-dimensional reconstruction. We found the Si(110)-“16×2” reconstruction has anisotropic tensile stress intrinsically on the bulk Si(110)-1×1 structure. The anisotropic Si(110)-“16×2” structure has the potential to be tailored to self-assembled nanostructures by using uniaxial extrinsic stress. Furthermore, as expected, we were able to find selectively the chiral reconstructed structure. Our results demonstrate how to form homochirality on the Si surface, which consists of a one-dimensional chiral structure.

Machine-learning-augmented simulation of thin metal film growth on weakly-interacting substrates

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Thin Film Growth Simulation, June 18, 2024, 10:30 - 12:30

Deposition of thin metal films on 2D-material, insulating, and semiconducting substrates is relevant in many applications, such as photovoltaics, low-emissivity windows, catalysers, and sensors. Such films are typically synthesized via condensation from the vapor phase, whereby device functionality crucially depends on film morphology. Achieving morphology control is, however, not trivial, as metal atoms may exhibit weak interaction with the substrate leading to agglomeration of three-dimensional islands. [1]

Experiments have shown that metal film morphology can be manipulated in a non-invasive fashion by deploying minority gaseous [2,3] or metal species [4,5] (surfactants) at the film growth front. In the present work, we seek to unravel atomic-scale mechanisms by which surfactants affect morphological evolution of thin-metal films on weakly-interacting substrates by means of kinetic Monte-Carlo (kMC) simulations. Multielemental thin-film growth poses a considerable modelling challenge: atomic interactions must be described accurately in the complicated chemical environments of the growth front, while maintaining computational efficiency to reach microsecond or longer timescales.

To address this challenge, we are developing a machine-learning (ML) augmented kMC model for Ag thin film growth on weakly-interacting substrates in the presence of Cu and Au surfactants. The migration barriers are calculated on-the-fly and used to concurrently train a ML model that will eventually replace the relatively slow barrier calculations. The model builds on earlier work where we utilized neural networks in simulating Cu surface diffusion. [6]

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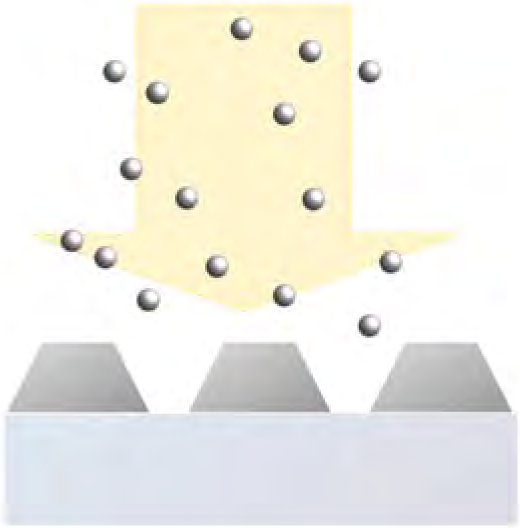

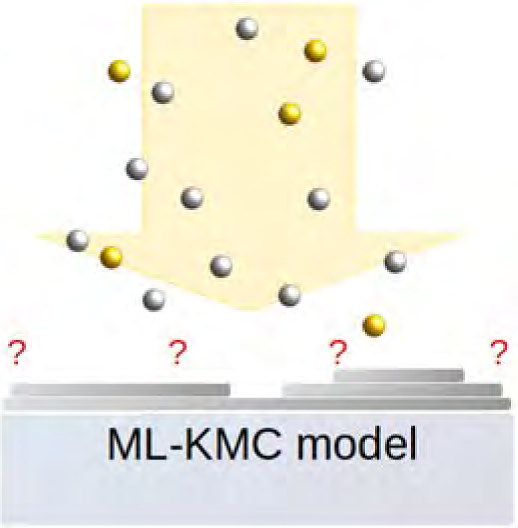

Automated Classification of the State of a Scanning Probe Tip without Machine Learning

Mr Dylan Barker[1]
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Advances in Experimental and Theoretical Methods 3, June 17, 2024, 16:00 - 17:35

Atomic resolution scanning probe microscopy (SPM) provides a critical tool for studying the chemical and electronic structure of surfaces at the single atom scale, however, practically these techniques require a large amount of experimental time to manually prepare the scanning probe tip in-situ, usually via controlled indents into the surface. This apparently simple, but time-consuming process, is potentially an ideal candidate for automation using machine learning and computer vision techniques.

Previous attempts to automate the classification of probe tips from topographical images have been made using machine learning methods [1-2], however using prior knowledge of the system in question we find it is also possible to classify the tip state using computationally simple image analysis methods involving template matching.

In this work I will present a comparison between "template matching" image analysis methods and machine learning approaches for tip state classification [3]. I will also address the known issue of small sample sizes for training ML techniques for SPM image classification, via an automated (scripted) data generation approach, as well as a practical example of the template matching method being used to automate tip state classification.

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Exploring Spinterface Formation of Sexithiophene (6T) on Fe3O4: Insights into Interface Engineering for Enhanced Functionalities

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Spin Physics, June 17, 2024, 16:00 - 17:35

Organic semiconductors (OSCs) have become a dynamic field of research and innovation, encompassing physics, materials science, engineering, and technology [1]. The notable benefits of the integration of OSCs in spintronic devices lie in their physical properties, adaptable chemistry, and economical nature. Therefore, OSCs, including conjugated small molecules, hold the potential for mass production and the creation of fully flexible devices [2]. Concurrently, interfaces between organic molecules and ferromagnetic materials play a key role in various spin-related effects [3]. To utilise these spin interfaces, or spinterfaces, for next-generation molecular spintronic devices, it is essential to characterise and control these spin effects, introducing an additional layer of complexity to the field. Here, we have investigated the controlled deposition of sexithiophene (6T; $C_{24}H_{14}S_6$) monolayers on a ferromagnetic oxide, Fe_3O_4, with a specific focus on coverages from 0.25 monolayers (ML) to 1 ML to allow this prototypical spinterface to be studied as it forms. Advanced spectroscopic and microscopic techniques were used to characterise spinterfacial properties with atomic force microscopy (AFM) revealing that a 0.25 ML coverage leads to forming edge-on 6T orientation, while with an increased thickness of 1 ML, island formation occurs. X-ray photoelectron spectroscopy (XPS), and ultraviolet photoelectron spectroscopy (UPS) data contribute further valuable insights. As we will discuss, the findings highlight the essential role of adsorption geometry, molecular packing, and surface reconstruction in shaping the spinterfacial electronic structure and associated device performance. Comparisons will also be made to 6T adsorption on Fe [4] revealing the differences between spinterface formation at ferromagnetic metal and ferromagnetic oxide surfaces.

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Determination of the actual valence band of Bi2Se3

Mr. Yuki Higuchi[1], Ph.D. Ryota Itaya[1], Mr. Harutaka Saito[1], Mr. Yuichiro Toichi[1], Ph.D Takahiro Kobayashi[1], Ms. Mito Tomita[1], Prof. Kenta Kuroda[2], Prof. Fumihiko Matsui[3], Prof. Shigemasa Suga[1], Prof. Hitoshi Sato[2], Prof. Katsuhiro Suzuki[4], Prof. Kazunori Sato[1], Prof. Kazuyuki Sakamoto[1]

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Electronic Structure of Materials, Surfaces and Interfaces, June 18, 2024, 10:30 - 12:30

Owing to its unique physical properties, topological insulators (TIs) are promising candidates for next-generation spintronic devices, and a topological p-n junction (TPNJ) is an important concept to realize them. To actualize a TPNJ, an accurate understanding of the binding energy (EB) of bulk valence band maximum (BVBM) is essential together with tuning the Fermi level above and below the Dirac point (DP) [1-3], which can make n-type and p-type regions on TI. However, even in the case of Bi2Se3, a typical n-type TI, different results on the EB of the BVBM have been reported, i.e., a EB lower than DP in [4,5], which means that it is not possible to make a p-type Bi2Se3 and thus a TPNJ, and a EB higher than the DP in [6,7]. In this paper, we present detailed experimental and theoretical studies on the location of BVBM of Bi2Se3. No trace of BVBM was observed at EB lower than DP in the angle-resolved photoemission spectroscopy (ARPES) measurements providing in a wide momentum range that covers several Brillouin zones. The theoretical calculations performed using a quasiparticle self-consistent GW (QSGW)-DFT, which can quantitatively evaluate the band gap by self-consistently incorporating the effects of electron-electron interactions and thus provides a qualitative and quantitative assessment of the bulk band structure, supports our experimental results. The obtained results indicate that Bi2Se3 is a good candidate for making a TPNJ.

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Ti-Nb-Zr Ternary Alloy Coatings Produced by Magnetron Sputtering

Mrs Ana Garcia[1], Mr Angelo Gobbi[2], Professor Valmor Mastelaro[3], Professor Conrado Afonso[1], **Professor Pedro Nascente**[1]

[1]Federal University of Sao Carlos, Brazil, [2]Brazilian Center for Research in Energy and Materials, Brazil, [3]University of Sao Paulo, Brazil

Biomaterials 1, June 18, 2024, 10:30 - 12:30

The absence of toxic elements and a low modulus of elasticity are two important criteria in the development of metallic materials for producing prosthetic devices. Ti, Nb, and Zr are non-toxic and non-allergenic biocompatible metals, and the addition of Nb and Zr to Ti favors the stabilization of the β (body-centered cubic – BCC) phase. This phase is more adequate for biomedical applications since it presents a lower elastic modulus, a shape memory effect, and superelastic characteristic. However, bulk β-Ti-Nb-Zr alloys are much more costly than stainless steel and Co-Cr alloys that are commonly used as implants. An interesting option to overcome this problem would be to coat an implant with a β-Ti-Nb-Zr thin film having adequate composition in order to enhance the material biocompatibility. Nevertheless, the ideal amounts of the constituent elements in the Ti-Nb-Zr ternary system are undetermined. Combinatorial strategies allow for the production and characterization of many alloys simultaneously, and magnetron sputtering is suitable to produce ternary alloy coatings having various compositions. In this work, Ti, Nb, and Zr targets were positioned in a triangular configuration below a Si(100) wafer substrate, and a composition gradient was formed over all the substrate area by magnetron co-sputtering. Five samples were cut from different patches of the coated wafer with the following compositions (at.%): Ti67Nb21Zr12, Ti49Nb13Zr38, Ti43Nb42Zr15, Ti36Nb59Zr5, and Ti22Nb58Zr20, measured by EDS. XRD analysis revealed that all coatings presented mainly the β phase, with a minor contribution of the α (hexagonal close-packed – HCP) phase. AFM analysis showed that the coating grain sizes were in the range of 52 to 84 nm. XPS analysis indicated that the coating surfaces were oxidized, and the predominant phases were TiO2, Nb2O5, and ZrO2. These oxidized surface layers provide better corrosion protection and are beneficial for biomedical applications.

Heterostructures based on 2D-Bi and van der Waals layers as an effective method to protect 2D materials against oxidative degradation

Mrs Klaudia Toczek[1], Mr Maciej Rogala[1], Mr Paweł Krukowski[1], Mr Maxime Le Ster[1], Mr Iaroslav Lutsyk[1], Mr Paweł Dąbrowski[1], Mr Michał Piskorski[1], Mr Rafał Dunal[1], Mrs Aleksandra Nadolska[1], Mr Przemysław Przybysz[1], Mr Wojciech Ryś[1], Mr Paweł Kowalczyk[1]

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2D Materials and Van der Waals heterostructures 1, June 19, 2024, 14:00 - 15:30

Two-dimensional materials are of growing interest due to their unique chemical, physical, electronic, and optical properties. [1] The less understood ones are in group 15th of the periodic table, and among them are those based on bismuth (Bi). Bi is a semimetal with minimal radioactivity.

It has been shown that bismuth-based 2D structures can be fabricated. Atypical electron states appear at its edges to provide electron flow without electrical resistance, while the interior remains a semiconductor. [2,3]. Thus, the fabrication of electronic devices based on Bi could contribute to advances in electronics, optoelectronics, spintronics and catalysis. However, Bi nanostructures are known to degrade rapidly in air. Therefore, it is extremely important to understand the growth and degradation pathways of this new material.

In this work, we will present the properties and morphology of heterostructures based on epitaxially grown bismuth and van der Waals materials - highly oriented pyrolytic graphite (HOPG) and hexagonal boron nitride (hBN).

The growth of bismuth thin films and the fabrication of heterostructures was carried out in ultra-high vacuum. X-ray photoelectron spectroscopy (XPS), Raman spectroscopy and atomic force microscopy (AFM) were used to characterize the samples. XPS was used to analyze the chemical composition of metallic and oxidized surfaces. Raman spectroscopy (in an inert atmosphere) was also used to identify the oxidized phase on the sample surface, and the surface topography of the oxidized layers was also studied in the atmosphere using atomic force microscopy.

The above research is supported by the National Science Center under the project no. 2019/35/B/ST5/03956.

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Heat Assisted Ferroelectric Reading for High Speed SNDM Ferroelectric Probe Data Storage

Yasuo Cho[1]
[1]Tohoku University, Japan

2D Materials and Van der Waals Heterostructures 2 and Ferroelectric Behaviour, June 20, 2024, 11:00 - 13:00

We previously proposed ferroelectric probe data storage that uses scanning nonlinear dielectric microscopy (SNDM), called SNDM probe memory, as a next-generation ultrahigh-density information recording method. We confirmed an extremely high recording density and high-speed writing using $LiTaO_3$ single crystal media.

However, since reading is based on the detection of very small nonlinear dielectric constants of ferroelectric materials using SNDM technique, slow playback speed (actually 2Mbps) hinders the practical use of SNDM probe memory.

To solve this problem, a material with a large nonlinear dielectric constant is required. Our basic experiments revealed that a nonlinear dielectric constant has an extremely large temperature dependence and is proportional to $(T_0\text{-}T)$^-3.5 where T is the medium temperature and T_0 is the Curie temperature. This means that an increase in the nonlinear dielectric constant, which would enable ultrahigh-speed reading (Gbps or faster), can be easily obtained even in $LiTaO_3$ crystal by making T close to T_0. However, simply increasing the medium temperature closer to the Curie temperature under thermal equilibrium degrades the polarization retention characteristics.

Therefore, we propose a heat-assisted ferroelectric reading (HAFeR) method that increases the reading speed while maintaining the polarization retention characteristics. This is achieved by locally heating the medium for a very short time at the data reading position using laser pulse irradiation. We conducted a basic experiment and confirmed that laser pulse irradiation increased the SNDM signal strength much more.

We also discuss the relationship between the maximum number of laser irradiation pulses and the optical pulse width for a medium heated to 550 °C (equivalent to a reading speed of 5 Gbps).

The proposed method overcomes the fundamental problems of next-generation ultrahigh-density ferroelectric scanning probe data storage.

LEEM and PEEM investigation of structural and electronic properties of F16CuPc thin films on Ag (100) surfaces.

Błażej Gołyszny[1], Thorsten Wagner[2], Dorota Wilgocka-Ślęzak[3], Nika Spiridis[3], Grażyna Antczak[1]
[1]University of Wrocław, Faculty of Physics and Astronomy, Poland, [2]Johannes Kepler University, Institute of Experimental Physics, Austria, [3]Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Poland

Advanced Thin Film Characterisation, June 19, 2024, 16:00 - 17:30

Thin films of metal phthalocyanines are being investigated due to their promising applications in molecular electronics devices. This study focuses on the structural and electronic properties of thin films composed of perfluorinated phthalocyanine F16CuPc deposited on silver (100) surfaces. The structural properties were investigated using Low Energy Electron Microscope (LEEM) operating in diffraction mode. An electron beam with energy of 12 eV was employed to observe molecular growth during the continuous deposition at rate of 0.1 monolayer (ML)/min. The sample was maintained at room temperature, and the deposition was carried out until reaching a coverage of 2.5 ML. At the initial stage of deposition, diffraction patterns suggest a presence of 2D molecular gas on the surface. The characteristic disc around the (0,0) spots and four leaves could be observed, originating from the incoherent superposition of the diffraction patterns of individual F16CuPc molecules, adsorbed randomly on the silver in well-defined geometries. Above 0.8 ML the appearance of sharp diffraction spots due to molecular layer condensation was detected, and their intensity increased until the completion of first ML. The dark field LEEM investigations at monolayer regime suggested the coexistence of two mirror domains of F16CuPc. The evolution of the film morphology was studied in real space and time by Photoemission Electron Microscopy (PEEM). For investigations a mercury lamp, with a spectral line of photon energy 4.9 eV was used to excite the photoelectrons. During deposition continuously images were taken allowing to track changes of the electron yield induced by the organic molecules on the surface. The sequence of PEEM images provides insight into the evolution of the local work function via Fowler-DuBridge theory.

The authors gratefully acknowledge the support from the program „Excellence Initiative - Research University" for years 2020 - 2026 for University of Wrocław.

Atomic force microscopy and Raman spectroscopy combined to in-situ and real time investigation of graphite anion intercalation

Marco Menegazzo[1], Gianlorenzo Bussetti[1], Lamberto Duò[1], Chiara Castiglioni[2], Matteo Tommasini[2], Andrea Lucotti[2], Luca. Magagnin[2], Valeria Russo[3], Andrea Li Bassi[3], Martina Siena[4], Alberto Guadagnini[4], Samuele Grillo[5], Davide Del Curto[6], Sergey Mitko[7]

[1] Department Of Physics, Politecnico Di Milano, Italy, [2] Department Of Chemestry Materials and Chemical Engeneering and, Politecnico Di Milano, Italy, [3] Department of Energy, Politecnico di Milano, Italy, [4] Department of Civil and Environmental Engineering, Politecnico di Milano, Italy, [5] Department of Electronics, Information and Bioengineering, Politecnico di Milano, Italy, [6] Department of Architecture and Urban Studies, Politecnico di Milano, Italy, [7] NT-MDT BV Hoenderparkweg 96 b, Netherlands

Carbon Materials 2, June 19, 2024, 10:30 - 12:35

An innovative and versatile set-up for in-situ and in-operando measurements, coupling micro-Raman spectroscopy and atomic force microscopy (AFM) in an electrochemical cell, is described.
We present the results obtained on the basal plane of a HOPG in H_2SO_4 1M solution, characterizing the process of ion intercalation across basal plane defects. During and after cyclovoltammetry we can control and characterize the process of intercalation and deintercalation of ions within the HOPG. Due to the process, both morphological and spectroscopic changes related to structural modifications are detected in the basal plane of graphite. Figure 1 depicts the correlation between the change in intensity of the graphite Raman D peak (Figure 1b), linked to the density of the defects, with the morphology (Figure 1a), documenting the presence of areas where the basal plane has been corroded by the action of the acid.[1] The coupling between Raman and AFM measurements during the electrochemical process is more versatile with respect to other approaches, e.g. tip-enhanced Raman spectroscopy (EC-TERS), allowing us to adapt to samples with differing roughness and to study processes that occur outside the water stability region.

Figure 1 a) AFM morphology after 1 CV, b) D peak intensity map, c) Single Raman spectra acquired on different position of the map, as is it possible to see with the cross in panel b.

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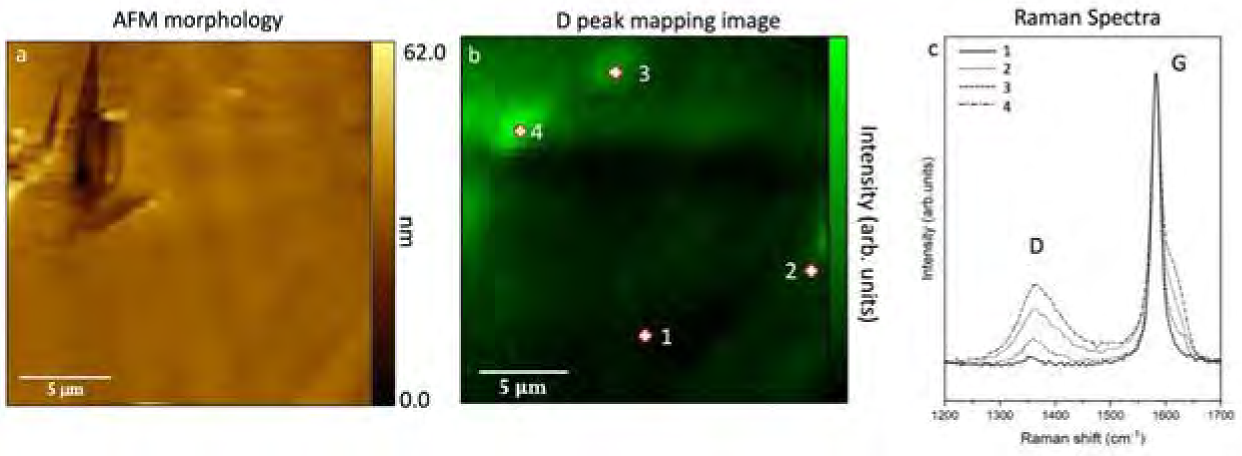
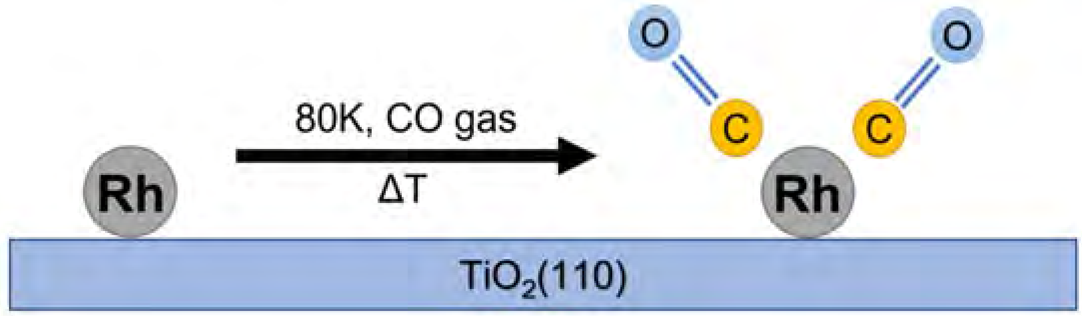


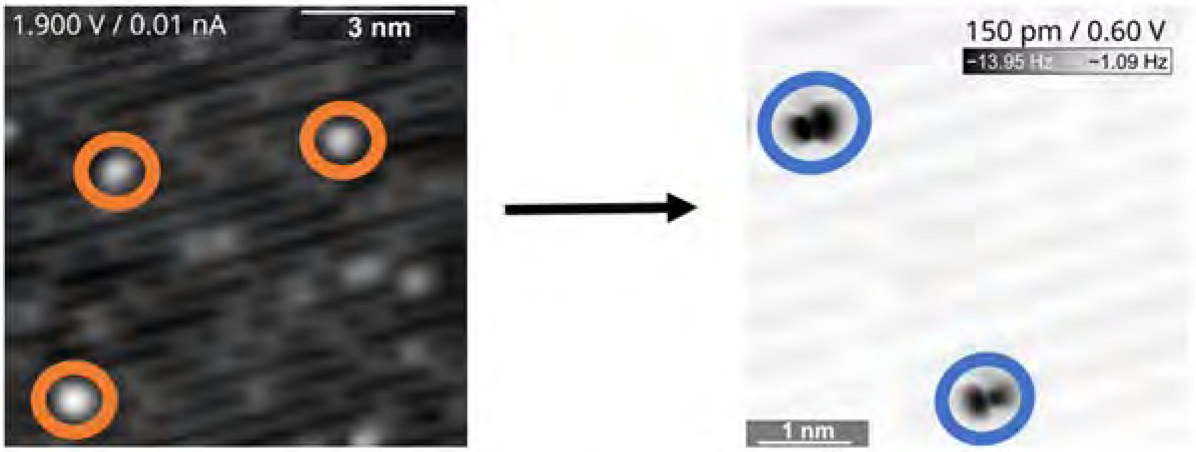
Multi-technique characterization of rhodium single atoms on TiO2(110)

Dr. Moritz Eder[1], Faith J. Lewis[1], Johanna I. Hütner[1], David Rath[1], Jiri Pavelec[1], Gareth S. Parkinson[1]
[1]*TU Wien, Austria*

Catalysis and Electrocatalysis including Single Atom and In Operando Studies 1, June 19, 2024, 14:00 - 15:30

Single atom catalysts (SACs) have emerged as a very prominent research topic in the last decade. The goal is to minimize the noble metal content on metal oxide surfaces down to isolated atoms. A persistent challenge in the field is the characterization of these single atoms on the surface, and showing that they are indeed the dominant sites, since there are but few suitable analytical techniques for this on powder catalysts. Hence, transmission electron microscopy (TEM) and infrared (IR) spectroscopy using adsorbed CO are often the only characterization techniques in many studies, but their informative value is limited. In this contribution, we will show a comprehensive surface science approach to the problem. Using isolated rhodium carbonyls on titania as an example, we characterize these single sites using XPS, TPD, STM, AFM, and a newly designed IR reflection absorption spectroscopy setup to get the complete picture. We compare the results to studies on powder catalysts in the literature and discuss similarities and differences. Our results illustrate that multi-technique approaches are virtually imperative for characterizing SACs adequately and pose a prerequisite for understanding their reactivity.





Monitoring Chamber Health with an Optical Plasma Gauge

Martin Wüest[1], Stefan Kaiser[1]
[1] *INFICON AG, Liechtenstein*

MS-6: RGA User Meeting 3, June 19, 2024, 16:00 - 17:30

Leak testing is a common task in the daily laboratory routine. There are simple but lengthy procedures available to test for leaks, for example the rate-of-rise method. To check if a gas such as water or oxygen is below a certain concentration is often done just by waiting for a time that has been determined by experience. More powerful methods are also available such as mass spectrometers, in particular residual gas analyzers, or dedicated leak detectors. However, they tend to be expensive, are often not very easy to operate, and operate at low pressures. Alternative methods exist such as optical emission spectrometer. They tend to be bulky and extracting robust information is not that easy and below a certain pressure there is not enough light available to analyze.

We have now developed a compact optical plasma gauge to address the questions and shortcomings mentioned above. It combines a gas type monitoring optical plasma sensor with a total pressure sensor. Its design is optimized to allow a gas detection measurement in the range between 10E-7 and 5 hPa. The gauge allows for the detection of gases such as oxygen, nitrogen, hydrogen or argon in–situ or in a rate of rise leak testing. Above 20 hPa the plasma generation is switched off in order to prevent plasma damage in the sensor. The total pressure sensor operates from 10E-5 Pa to atmosphere. Discharge pressure is known to play a substantial role in the various competing collisional excitation and de-excitation processes that occur in the plasma. The measured optical spectrum is convoluted with the independent total pressure data to provide higher accuracy. The intelligence implemented directly on the gauge automatically configures the optimal measurement setting in order to ensure easy integration and optimized signal-to-noise ratio. Impurities > 10 ppm can be detected.

Lifetime and Activation Effect of Non Evaporable Getter Coatings

Miss Eleni Marshall, Dr Oleg B. Malyshev, Dr Reza Valizadeh
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Non-evaporable getter coatings, June 18, 2024, 14:00 - 15:30

Non-evaporable getter (NEG) coatings are thin film, transition metal coatings used in vacuum for two keys reasons. Firstly, they provide a good diffusion barrier, preventing gasses, in particular hydrogen, from degassing from the bulk material into the vacuum. Secondly, they provide a pumping effect, absorbing residual gasses, H2, CO, CO2 etc, out of the vacuum as they stick to the active metals (Ti, Zr, V) in the walls. They additionally exhibit lower electron and photon stimulated desorption yield, and reduced secondary electron yield as well. This makes the very useful in charged particle accelerators. However, NEG coatings can be used in many applications, wherever low distributed pumping is desired, with reduced external pumping requirement.

As the NEG coating is exposed to sorbing gas species, its available sorbing sites become filled with these molecules/atoms, and it loses its pumping capability. The speed of this saturation process depends on the presence of sorbing species and their partial pressures, in atmosphere, this effect is instantaneous. To restart pumping after saturation, the NEG coating must be activated, restoring the oxide surface layer that forms over saturation to its metallic and pumping state. Activation is usually done by heating to temperatures between 160 – 300 ˚C for 24 hrs, with higher temperatures generally leading to increased pumping capabilities. However, lower temperature activations provide more sustainability, and a greater flexibility in the material and design of the component to be coated.

This study discusses the consequence of repeated activation and saturation cycles on the lifetime of the NEG coating. Two samples were investigated, with over 20 repetitions of activation, one at 160 ˚C and the other at 200 ˚C. As well as this, the effect of longer time activation on the pumping properties of NEG coatings is discussed.

Comparison of Residual gas analyser calibration coefficients across in high- to extreme high- vacuum

Miss Eleni Marshall[1], Dr Oleg Malyshev[1], Miss Rebekah Luff[1]
[1]STFC, United Kingdom

MS-6: RGA User Meeting 2, June 19, 2024, 14:00 - 15:30

In vacuum processing, it is critical to know the presence of any gas species within a system. Residual gas analysers (RGAs) are used to monitor the gas spectrum, allowing users to know what is left in their vacuum chambers, allowing leaks to be found, reactions to be tracked, and ensure any changes to a vacuum environment can be analysed.

However, RGAs are very sensitive instruments, and as a result of this, each instrument requires calibration to achieve accurate quantitative gas analysis. There has been shown to be no linear relationship between pressure and the calibration coefficient, and for relationship can be drastically different from one RGA to another [1], this is due to the sensitivity of each RGA to its composition, the electronics and environment it is in can change the readings it provides.

In this study we have used a gas injection method to calibrate RGAs over a range of ~1 × 10-9 to 3 × 10-6 mbar against a UHV ionisation gauge. Calibration was performed with N2, CO, CO2, H2, CH4 and in some cases Ar. Calibration coefficients were normalised to nitrogen and plotted against the pressure. We have performed this calibration technique with 10 RGAs (mostly from MKS, but some HIDEN models were tested), some repeated to calibrate them for new arrangements in vacuum systems. This study collects the calibration coefficients of all the devices and compares them to each other to show the range of variation and prove the importance of in situ calibration for accurate quantitative analysis.

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Reliable Aluminum Vacuum Components for Miniaturized Quantum Technology Applications

Florian Löwinger[1], Andreas Trützschler[1], Jan Hertel[1], **Klaus Bergner**[1]
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Special Vacuum Chambers and Components, June 17, 2024, 16:00 - 17:35

Second generation quantum technology aims for the manipulation of single quantum objects to control specific quantum processes or states. This enables the use of quantum technology for a multitude of applications like information processing, metrology and secure information transmission. In order to ensure access to these promising applications for a wide range of users, a variety of technological and economic challenges are to be overcome.

Regarding the vacuum systems employed in quantum system physics packages, desired requirements include low form factors, low weight, robust and economic design. However, first demonstrators often rely on costly and space consuming wide-range equipment, as well as fragile craft solutions. The commercialization of second-generation quantum systems calls for miniaturization of the enveloping architecture as well as for increased reliability of employed vacuum systems and components. In addition, optimization and up-scaling of manufacturing processes is key to single out competitive technologies.

The focus of this talk is to explain the demands of quantum technology for vacuum systems and components, as well as how these demands are met through commercially viable solutions. By the example of AluVaC® aluminum vacuum CF components, we show how robust and durable aluminum vacuum components are used in publicly funded projects to promote the development of quantum technology.

Mastering Clean Vacuum: Overcome Contamination for science and industrial applications

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MS-6: RGA User Meeting 3, June 19, 2024, 16:00 - 17:30

In the realm of vacuum technology, a pivotal focus is shifting towards different stages of clean vacuum products, with an emphasis on overcoming the adverse effects stemming from particulate and filmic contamination. This shift holds significant importance for accelerators, advancing lithography, quantum technology, and vacuum based analytics for biological and pharmaceutical purposes. This change in focus sets the stage for future applications in diverse fields such as cancer treatment, communication, personalized vaccination and consumer electronics.

As a result, different scientific and industrial sectors are increasingly coming into contact with vacuum technology - along with their different perspectives on issues and compliance with specific regulations.

This challenge becomes especially pronounced in the context of ultra-clean vacuum systems, where meticulous attention is paramount throughout the entire lifecycle – from design and production to cleaning, assembly, and maintenance. The risk of failure due to contamination necessitates a comprehensive approach to address and mitigate potential pitfalls. In this evolving landscape, the pursuit of excellence in clean vacuum technology becomes not just a goal but a prerequisite for ensuring the reliability and success of cutting-edge applications in various industries.

We show how surface contamination can be reduced from a double-digit µg/cm2 value to a single-digit ng/cm2 value and ensure stable processes. We highlight the most essential steps in the design phase, the right choice of cleaning technologies, appropriate analyze methods and constant process monitoring.

In summary, we provide a decided insight into process chain for the realization of ultra-clean vacuum components in all stages of "cleanliness". True to the motto: Design clean, Plan clean, Make clean, Prove clean, Keep clean.

Photon-stimulated desorption studies of TiZrV non-evaporable getter coatings at the Diamond Light Source

Chris Burrows[1], Matthew Cox[1], Reza Valizadeh[2], Eleni Marshall[2], Zhengwei Mei[1], Oleg Malyshev[2]
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Non-evaporable getter coatings, June 18, 2024, 14:00 - 15:30

Diamond Light Source is the UK's national synchrotron. Currently underway is the Diamond-II upgrade programme, an in-place upgrade for the storage ring, which will reduce beam emittance, increase brightness, and enable three new beamlines.

The majority of the Diamond-II storage ring will be coated with a nominally 1 µm thick TiZrV non-evaporable getter (NEG) layer. The well-known distributed pumping effect, along with the reduced outgassing [1], of the NEG layer is necessary to compensate for the limited vacuum conductance of the small-diameter vacuum vessels. Furthermore, the reduced electron- and photon-stimulated desorption of NEG [2] compared to common vacuum vessel materials positively impacts the design and operating behaviour of the storage ring.

In preparation for the upgrade, a photon-stimulated desorption (PSD) beamline has been designed and installed on the existing Diamond storage ring. The PSD beamline resides entirely within the storage-ring vault and is based on the 'three-gauge method' [3] for PSD yield determination.

We present an overview of the experimental arrangement, and outline both its operation and data analysis methods. We also show a comparison of the measured PSD yields for the uncoated and coated stainless-steel vessels. In the case of the TiZrV-coated vessel, PSD yields have been determined for the non-activated, thermally activated, and high-purity N2 saturated states.

The measurements show that the non-activated NEG coating has a higher initial PSD yield than the uncoated vessel. Following activation of the TiZrV layer, a reduction in PSD yield is observed. The N2-saturated coating displays improved PSD yields relative to the non-activated NEG layer and uncoated vessel, while remaining higher than the activated coating PSD yields.

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Investigation of the X-type metal seal for future fusion reactor

Professor Qingxi Yang[1], phD Qingzhou Yu[1,2], Mr. Hao Xu[1], phD Zhaoxi Chen[1], Mr. Genmu Shi[1,2]
[1]Institute of Plasma Physics, Hefei Institutes of Physical Science, Chinese Academy of Sciences, China, [2]University of Science and Technology of China, China

Large Vacuum Systems, June 17, 2024, 11:00 - 12:35

Tokamak as the main fusion device, is being world-wide employed to carry out fusion research, exploring fusion energy for the human-being. Cryostat as the tokamak important sub-system, is provided approximate 1E-4 Pa vacuum to insulate heat loads from atmosphere to superconducting magnet coils due to convection. Hundreds of sealing interfaces, especially for the large-size diameter sealing interfaces are the main factors affecting ultimate vacuum of the cryostat. For the fusion reactor, the metal seal will be used instead of fluororubber O ring due to radiation environment which make fluororubber material Crosslinking and cleavage accelerating to fail in sealing within a short time. The diameter of metal seal for the cryostat of China Fusion Engineering Test Reactor (CFETR) will reach up to ⌀38m, which bring big challenge to design and manufacture feasibility metal seal. This paper focuses on the exploration new-type metal seal for fusion reactor cryostat. Based on the leakage rate lower than 1E-9 $Pa \cdot m^3/s$, high resilience for better sealing performance and simple manufacturing requirements, two novel types of metal seal ring are raised, one is the lip-type metal seal formed and sealed by welding, the other X-type metal seal formed and sealed by welding and pre-tightening respectively. Investigation on the contact stress, resilience performance and leakage rate for them have been carried out, manufacturing process also are assessed. The X-type metal seal has much better advantages by comparison, which has higher resilience rate of exceeding 90%, lower leakage rate of lower 1E-9 $Pa \cdot m^3/s$ and simpler manufacturing process. Moreover, R&D for X-type metal seal is carried out, and results show that X-type seal has satisfactory sealing performance and low leakage rate on the order of 1E-10 $Pa \cdot m^3/s$, which lays the technical foundation for the future application of this metal seal in fusion reactor.

Research and development of high-performance screw vacuum pump rotor

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Vacuum pumps, June 21, 2024, 10:30 - 12:00

Screw vacuum pump (SVP), as a newly emerged dry pump, has been widely used in advanced fields such as semiconductors, aerospace, and nuclear energy due to its simple and compact structure, no contact between rotors, wide range of suction pressure (1E5~1E-1 Pa), and oil free. With the industrial upgrading, more demanding requirements have been placed on SVPs in such aspects as noise, energy conservation, ultimate vacuum and others. Therefore, it is crucial to optimize and innovate the technology of SVPs. The screw vacuum pump rotor (SVPR) , as the core of the SVP, directly determines overall performance of the pump. This study focuses on the research and development of high-performance SVPRs, exploring the key technical difficulties in terms of optimizing rotor profile, designing complex and irregular new shapes and self-balancing. As to profile optimization, a comprehensive study is conducted on the influence of basic profile parameters on the rotor area utilization coefficient, equivalently unbalanced mass on the end face, contact line length and machining feasibility. It is found that when the profile parameters satisfy $\kappa \in [0.3, 0.4]$ and $\alpha \geq 120°$, the rotor gives better overall performance. Additionally, this study tries to establish a general theoretical mathematical model and propose a three-dimensional solid generation method for irregularly conical rotor with energy conservation and low inter-stage leakage, and then the effectiveness of the method is verified. Finally, the new self-balancing rotors including fixed/variable screw patch without theoretical unbalanced mass are developed to reduce the operating noise of the SVPs and avoid damage of the SVPRs caused by traditional dynamic balancing treatment. This study systematically optimizes and analyses the SVPR, the research methods and results can provide practical references for the design of high-performance SVPRs, which contributes to overall performance and reliability of the pump.

Simulations of alternative forms of the Bessel box electron energy analyser

Dr Christopher Walker[1], Mr Yousuf Alharbi[1], Dr. Andrew Pratt[1], Prof. Steven Tear[1], Prof. Mohamed El Gomati[2]

[1]University Of York, United Kingdom, [2]York Probe Sources Ltd, United Kingdom

Advances in Experimental and Theoretical Methods 1, June 17, 2024, 11:00 - 12:35

The Bessel box electron energy analyser (BBA) has recently been used to acquire electron energy spectra in a scanning electron microscope (SEM) and in ultra high vacuum (UHV) experiments [1-3]. Spectra acquired over the elastic peak (at an energy in the range 30-60 eV) were also used to obtain images of a domain wall in scanning field emission microscopy (SFEM) [4]. The BBA is compact enough that it will fit on a DN40CF (2.75" OD) flange and is suitable for use in instruments requiring a small footprint. It can be used, for example, in the acquisition of Auger electron spectra (AES) as we have previously demonstrated [1,2]. However, at the primary beam energies needed for AES, the BBA suffers from internal scattering resulting in a background under the Auger peaks. We explore via simulation using CPO [5] and SIMION [6] alternative forms of the BBA which could reduce or eliminate internal scattering providing a route to a more sensitive BBA for AES. We determine the effects of changing the geometry of the BBA on energy resolution showing that the energy resolution worsens for a longer entrance cone.

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How to calculate an oxide sputter yield?

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Thin Film Growth Simulation, June 18, 2024, 10:30 - 12:30

An existing semi-empirical model to calculate the compound sputter yields is used to fit a large set of literature data on oxide sputter yields which consists of data for 21 different materials, and 65 datasets. The dedicated fitting procedure enables to link the surface binding energy of the metal and oxygen atoms with the oxide cohesive energy. This approach resolves a long standing problem in the research community on the accurate prediction of oxide sputter yields.

Structure and Dynamics of Chirality-Transfer Complexes on Pt(111)

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[1]*Laval University, Canada*

Metal Surfaces - Adsorption, Desorption and Reactions 2, June 17, 2024, 14:00 - 15:30

Control of enantioselection is an especially demanding challenge in heterogeneous catalysis and its study explores phenomena ranging from ligand-induced rate-enhancement to the interplay between chemisorption and intermolecular forces in determining the structure and dynamics of chirality transfer complexes. In this study, a combination of STM, DFT and reflectance-IR data is used to define the structure of individual chirality transfer complexes, the intermolecular interactions involved, the activation of prochiral functional groups, and complexation state changes within isolated complexes. Although the studies are carried out on model systems under vacuum conditions, the observed phenomena are largely consistent with the operando heterogeneous asymmetric catalysis literature. Emphasis will be placed on the three most important insights gained from studies of single complexes formed by (R)-(+)-1-(1-naphthyl)ethylamine and activated ketones on Pt(111): (i) complexation is driven by multiple attractive non-covalent interactions; (ii) weak non-covalent interactions play a determining role in stereodirection; (iii) precursor state dynamics are key to forming privileged complexation structures. It will also be shown that DFT calculations perform well in predicting the structure and dynamics of individual chemisorbed chirality transfer complexes.

Temperature dependent initial sticking probability of Mg on Si and SiO2 surfaces and possible applications in microlitography.

Ulrich Hagemann[1,2,3], Miriam Fritscher[1,2], Hermann Nienhaus[1,2]
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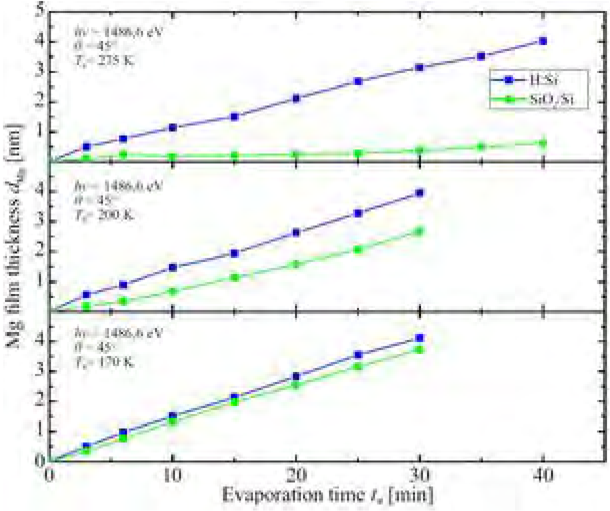
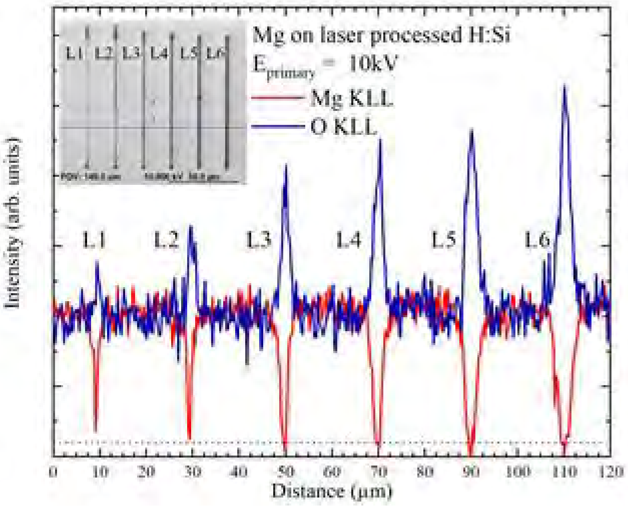
Metal and Oxide Single Crystal Surfaces - Growth, Preparation, and Characterisation, June 18, 2024, 16:00 - 17:30

The growth rate of thin magnesium films on hydrogen passivated silicon (H:Si) and silicon dioxide (SiO2:Si) surfaces is strongly dependent on the temperature of the substrate. Mg is evaporated from a Knudsen cell onto both samples simultaneously and X-ray photoelectron spectroscopy (XPS) is used to determine the magnesium thickness. Below < 210K the growth rate of the magnesium film and hence also the initial sticking probability is not distinguishable between the two surfaces. At higher temperatures the initial sticking probability is close to zero for SiO2:Si and non-zero for H:Si surfaces. This reduction in initial sticking probability seems to be independent on the thickness of the oxide layer. Using a 532 nm Laser with a maximum laser power of 650 mW two different kind of structures were written onto the H:Si surface at different laser writing speeds and laser powers. The first kind of structures were squares of roughly 100 µm², which could be measured in a microfocus XPS. The second kind of structures were sets of 6 individual lines written at different speeds and powers. The laser writing locally removes the hydrogen passivation of the silicon surface and leads to thin layer silicon oxide growth. The thickness of these oxide layers was measured in XPS to be around 0.2 nm to 0.3 nm. Magnesium was then evaporated onto the prepared substrate at RT leading to an Mg film thickness of about 2 nm on the hydrogen passivated areas. The laser structured areas were investigated in detail using scanning auger microscopy and show in detail the strong effect of ultrathin oxide films on the initial sticking probability.





Dynamics and self-organization of HiPIMS plasma during individual pulses

Dr. Matjaž Panjan
[1]*Jožef Stefan Institute, Slovenia*

Plasma Science 2, June 19, 2024, 14:00 - 15:30

Plasma in high-power impulse magnetron sputtering (HiPIMS) discharges is not azimuthally homogenous instead it is organized in dense regions known as spokes [1]. These structures typically exhibit triangular shape, form periodic or semi-periodic patterns and rotate with velocities of several km/s. The spoke phenomenon is not exclusive to HiPIMS discharges, it also occurs in classical DCMS [2] and RFMS [3] discharges.

In this study, we used a high-frame-rate camera with microsecond time resolution to systematically investigate plasma dynamics and self-organizatoin at different Ar pressures (0.25-2 Pa) and peak currents (10-400 A). The experiments show three distinct stages in the plasma evolution during HiPIMS pulses. From the current onset and up to around 25 A, spoke dynamics is similar to the one observed in DCMS discharges. Spokes display an elongated triangular shape and rotate in the -E×B direction with velocities in the 4-15 km/s range. The velocity depends on the current growth rate, pressure and the number of spokes. In the 25-50 A range, plasma undergoes chaotic reorganization, displaying irregular patterns and propagation in the -E×B and E×B directions. At higher currents, periodic patterns begin to form. Spokes exhibit characteristic triangular shape and rotate in the E×B direction with velocities in the 6-9 km/s range. The velocity depends on the pressure but is not affected by the discharge current or the number of spokes.

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The research was financially supported by the Slovenian Research Agency (project J2-2509).

Contact electrification monitored with ultra-high sensitivity and microsecond time-resolution

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Advances in Experimental and Theoretical Methods 1, June 17, 2024, 11:00 - 12:35

The charge transfer between two surfaces in short contact is measured with a custom-made charge amplifier exhibiting a sensitivity of approximately 1 fC and a temporal resolution of better than 1 µs. In the experiment a free falling sphere of 1 mm in diameter bounces on a metallic or insulating surface. As shown in the figure, the experimental setup comprises a horizontal parallel plate capacitor in a stainless steel chamber which can be evacuated to ultrahigh vacuum. Each plate is connected to an individual charge amplifier. The spheres are dropped into the capacitor through a small orifice and bounce several times onto the lower plate. The impact velocity is below 1 m/s. The charge on the sphere as well as the position between the plates can be precisely monitored by measuring the induced charge. Various combinations of materials are studied. Significant charge transfer is observed for metal spheres (Au, Cu) contacting a CuBe plate. The amount of transferred charge depends on the impact velocity and is surprisingly larger than expected from contact potential estimations. This is explained by the steep capacitance increase during the few µs lasting mechanical deformation of the contacting surfaces [1]. The high temporal resolution of the charge detection enables us to resolve a shift of the center of charge on the sphere in close proximity to the plate before and after the collision. This is due to the electron motion caused by the electrical induction field. On insulating spheres (ruby, Al2O3, quartz) the charge saturates after several contacts and has much higher values than on metal spheres.

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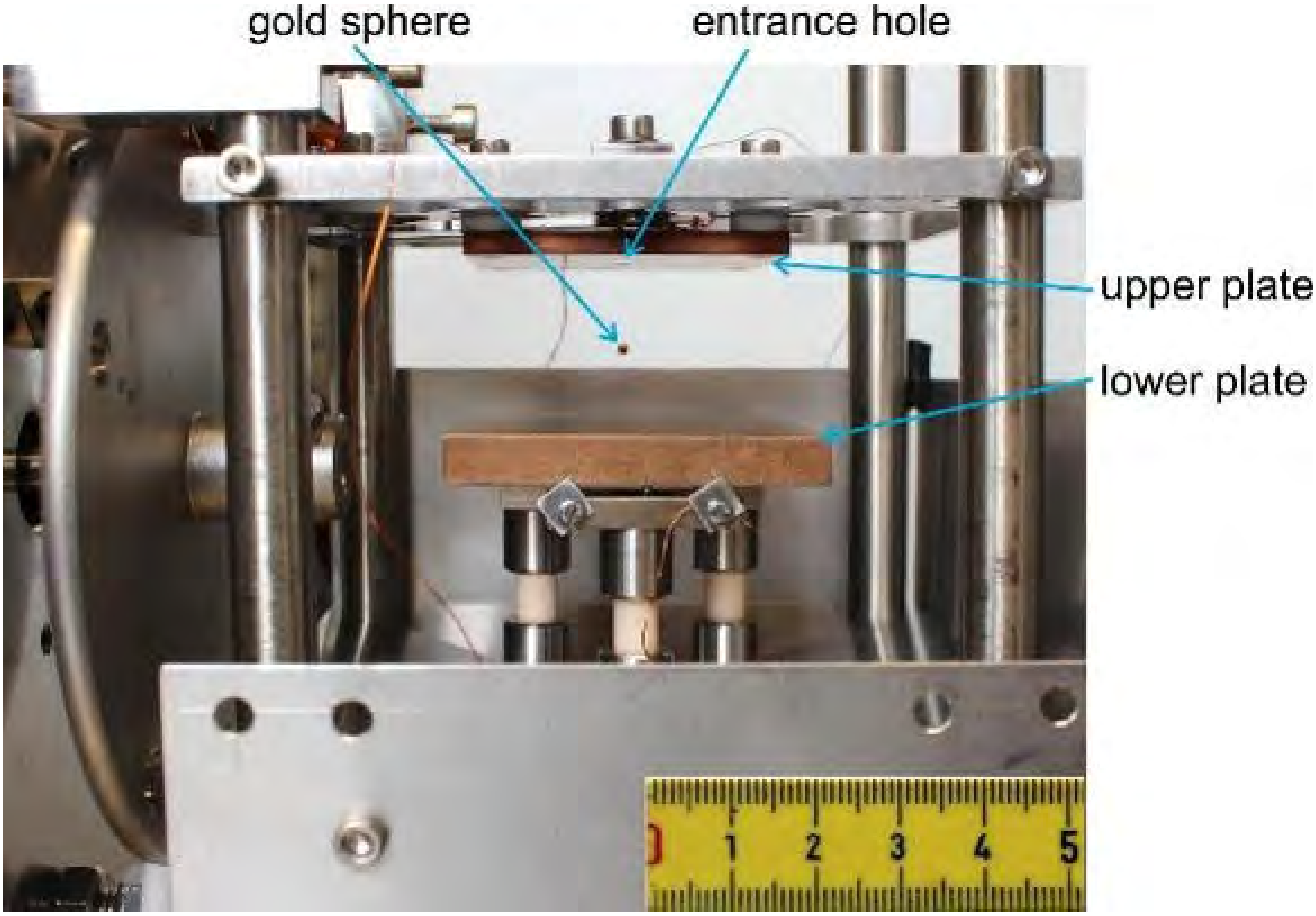
gold sphere
entrance hole
upper plate
lower plate
0
1
2
3
4
5

Generating Antiaromaticity: Thermally-selective Skeletal Rearrangements at Interfaces

Dr. Ana Barragán[1], Elena Pérez-Elvira[1], Qifan Chen[2,3], Dr. Diego Soler-Polo[2], Dr. Ana Sánchez-Grande[1,2,4], Diego J. Vicent[5], Dr. Koen Lauwaet[1], José Santos[5], Dr. Pingo Mutombo[2], Dr. Jesús I. Mendieta-Moreno[2], Dr. Bruno de la Torre[6], Dr. José M. Gallego[7], Prof. Rodolfo Miranda[1,4], Prof. Nazario Martín[1,5], Prof. Pavel Jelínek[2,6], Dr. José I. Urgel[1], Prof. David Écija[1]

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MS-3: On-Surface Synthesis of 1D and 2D Functional Graphitic Materials, June 19, 2024, 10:30 - 12:35

On-surface synthesis is a promising strategy for the design of novel nanomaterials complementary to solution-based chemistry. The chemical structure of the final products depends on the reaction mechanism followed by the precursor upon sublimation onto the selected surface. For instance, ring-rearrangement reactions are recently gaining increasing attention as a possible alternative toward the generation of novel nanostructures1-2. However, controlling such reaction mechanisms remain challenging due to the enormous amount of possible skeletal rearrangements. Here, we show the sublimation of dibromomethylene-functionalized molecular precursors on a pristine Au (111) substrate held at high temperature, which results in a novel intra- and intermolecular reaction affording a skeletal ring-rearrangement (Scheme 1). Such reaction pathway differs from the covalent polymerization of the same species upon deposition on Au(111) at room temperature followed by subsequent annealing3. Combined scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) investigations unveil the chemical structures of the obtained compounds, showing the formation of antiaromatic subunits within the molecular backbones. We envision that the control of ring-rearrangement reactions of carbon-based compounds on surfaces may open new routes toward the design of electron-rich low dimensional materials with prospects in molecular optoelectronics.

Scheme 1. On-surface generation of antiaromatic subunits in PCHs and 1D polymers by a) Intramolecular thermal rearrangement and organometallic polymerization of dibromomethylene-functionalized p-quinoid-based precursors, and b) Intramolecular thermal rearrangement and subsequent homocoupling polymerization.

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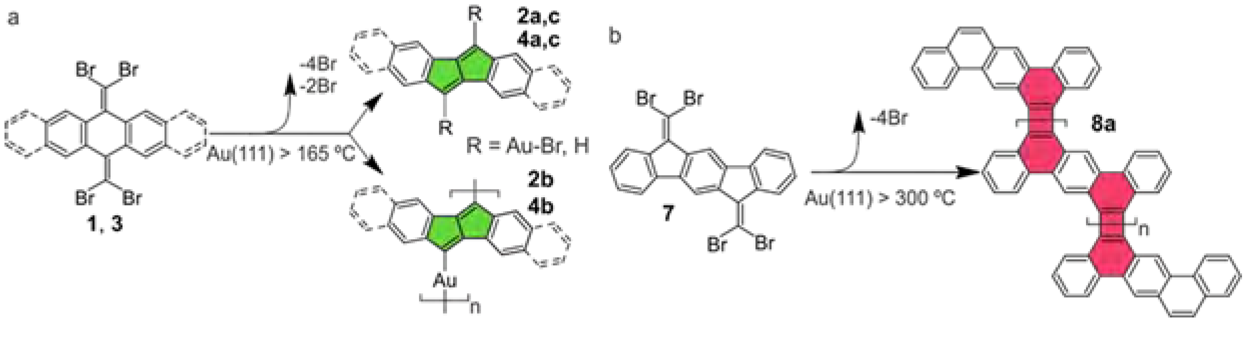

Designing VO2 films with variable transition temperatures: effect of chemical strain

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Advanced Thin Film Fabrication, June 19, 2024, 10:30 - 12:35

Strain in thin films can significantly affect their structural, mechanical, and opto-electronic properties. While lattice mismatch between the film and the substrate is utilized during the mechanical straining, chemical straining involves the intrinsic or extrinsic (dopants) defects to cause the strain in the material. Chemical straining is often preferred due to its applicability in both thin and thick films, unlike mechanical straining, which strains the lattice till the film thickness is below the critical value. In this regard, the chemical straining of bulk VO_2 could tune its transition temperature (Tc) to the desired value for a given application. VO_2 displays an interesting reversible switching from the M_1 (Monoclinic) phase at room temperature to the R (Rutile) phase at higher temperatures, but the Tc being slightly higher limits the applications for pure VO_2. In this work, VO_2 thin films with varying doping concentrations of W+6, Mo+6, Nb+5 and Ta+5 have been fabricated using a single-step process in RF magnetron sputtering. Compound sputtering targets are prepared in-house using the oxides of these dopants (1-3 wt.%) with V_2O_5. The chosen dopants would substitute some V+4 species, thus not only chemically straining the lattice but also introducing extra charge carriers. Overall, structural distortion as well as electronic changes, cause the lowering of the Tc in these doped-VO_2 systems. Additionally, an electrical stimulus is applied to the deposited films to cause SMT, and a correlation between the stimuli, temperature and electrical current, has been established. To complement the experimental work, ab initio (DFT) calculations have been performed to calculate the structural stability, electronic properties, and phase transition behaviour of the pure and doped VO_2 systems. Thermodynamic analysis is then carried out to estimate the reduction in Tc per at.% of doping and the results obtained from both experimental and theoretical work have been correlated.

Operando Nanobeam Soft X-ray Microscopy: Unveiling the Energy Landscape of Nanocrystal-Based Devices

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Advances in Experimental and Theoretical Methods 2, June 17, 2024, 14:00 - 15:30

Due to their broadly tunable optical properties, colloidal nanocrystals (NCs) have become essential components in various optoelectronic devices, ranging from display light sources to infrared imaging devices [1].

The design and optimization of such devices require a thorough understanding of the electronic structure of NCs, not only in their pristine state but also within their operational environment, which includes surrounding transport layers, electrodes, and applied electric fields.

In this presentation, I will discuss a scanning soft X-ray photoemission microscopy investigation aimed at elucidating the energy landscape of nanocrystal-based devices during operation, achieving a spatial resolution of less than 1 µm. This method offers exceptional versatility, enabling its application across a broad spectrum of device geometries, including Field Effect Transistors (FETs) [2]., photoconductive devices [3]., photodiodes [4]., and complex focal plane arrays (FPA) [5].

Using this technique, we can reveal the effects of applied drain and gate electric fields, visualizing a complete 3D reconstruction of the device energy landscape. Additionally, thanks to the high spatial resolution, a map of the electric field vectoral distribution can be obtained, elucidating the current flow paths within the NC film.

This breakthrough in nanobeam soft X-ray microscopy significantly enhances our capability to study nanocrystal-based devices in operando conditions, leading to a deeper understanding that can inform better design and performance improvements.

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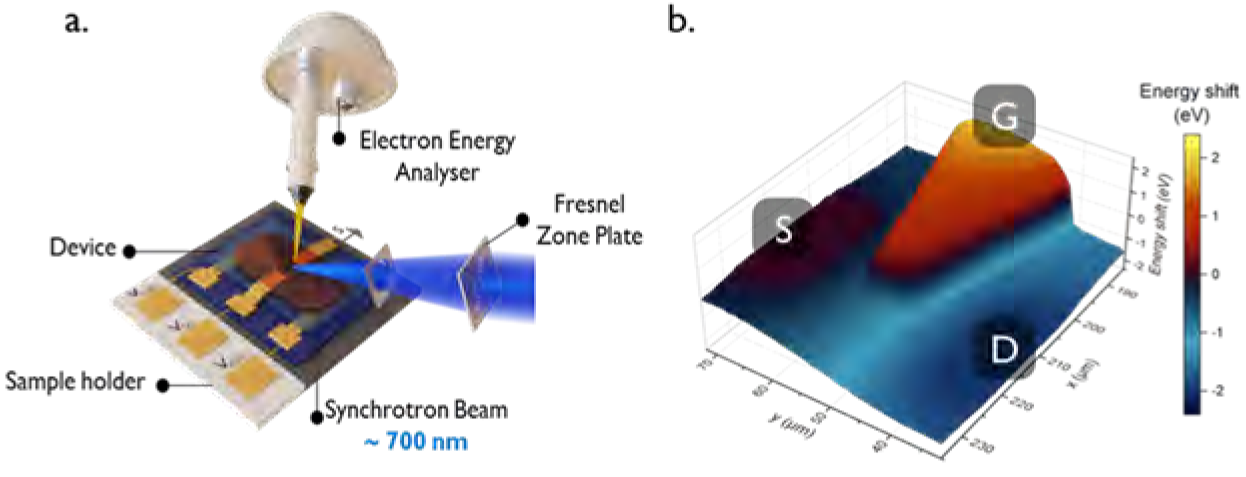


Figure 1. a. Schematic of the X-ray photoemission microscopy setup. b. 3D mapping of the energy shift in a NC-based FET under drain and gate bias application.

Defect-induced Anatase Phase Stability in TiO2-based Thin Films: Role of Tantalum and Oxygen

Mr Shivam Shukla[1], Mr Soham Shirodkar[1], Dr Emila Panda[1]

[1]*Department of Materials Engineering, Indian Institute of Gandhinagar, India*

Electronic Materials, Energy Reduction and Carbon Reduction, June 19, 2024, 16:00 - 17:30

The anatase TiO_2 thin films, when engineered using intrinsic and extrinsic defects, have steered a wider range of applications in the areas of water treatment, gas sensors, self-cleaning, antimicrobial surfaces, affordable optoelectronic, photovoltaic devices, and flat panel displays. However, the anatase phase is metastable and undergoes an irreversible structural transformation to a thermodynamically stable rutile crystal structure at a range of temperatures, thereby limiting its applicability. Hence, to ensure the stability of the metastable anatase phase, it is crucial to understand defect-induced structural transformation in TiO_2 thin films. In this context, this study investigates the role of Ta solubility and lattice oxygen towards the anatase-rutile phase transition (ART) in Ta:TiO_2 thin films. These films have been synthesized using an industrially viable magnetron sputtering where Ta and O content in the films have been modulated by varying the target composition and deposition environment. The detailed chemical composition, constitution, and phase of post-annealed thin films have been correlated with their electrical and optical properties to understand the disparity between impurity concentration in these films and actual impurity substitution into the host lattice sites. Results indicate that Ta substitution in Ti lattice sites and/or reduction in oxygen vacancies inhibit the ART in TiO_2 thin films. Experimental observations suggest that Ta, below its solubility limit (5 at. %), gets incorporated as a substitutional donor impurity and stabilizes the anatase phase, consequently improving the electrical conductivity of Ta:TiO_2 thin films. However, higher Ta and O concentrations promote the formation of impurity-rich oxides, leading to reduced film crystallinity and insulating properties. Additionally, Nb substitution is also found to be an anatase phase stabilizer similar to Ta. Moreover, the understanding developed through this study can be helpful in tuning the impurity and oxygen content in a thin transparent layer for diverse applications.

Ag Micromesh/TTO Hybrid Transparent Conductors: Understanding Ag/TTO Electronic Interface

Mr Shivam Shukla[1], Dr. Jeremy Fleury[2], Dr Krishna Manwani[2], Dr Andreas Schueler Schueler[2], Dr Emila Panda[1]

[1]Department of Materials Engineering, Indian Institute of Technology Gandhinagar, India, [2]Solar Energy and Building Physics Laboratory, EPFL, Switzerland

Electronic Structure of Materials, Surfaces and Interfaces, June 18, 2024, 10:30 - 12:30

Transparent conductors (TCs) are among the most critical components of high-demand optoelectronic devices like large-area displays, solar photovoltaic arrays, and touch panels. TiO_2-based TCs like Nb:TiO_2 (NTO) and Ta:TiO_2 (TTO) are being extensively studied over the conventional TCs like Sn-doped In_2O_3 (ITO) and F-doped SnO_2 (FTO) on account of their low-cost and environment-friendly nature. However, despite their high visible and near-infrared (NIR) transparency, polycrystalline TTO films fabricated using the industrially viable magnetron sputtering on glass substrates exhibit higher sheet resistance (RS, in KΩ range). In this context, this study focuses on the development of a hybrid structure comprising Ag mesh (of a few microns thickness) stacked upon the existing TTO films using a scalable metal aerosol jet printing technique. For improved optoelectronic properties, the linewidth and thickness of these micro-meshes have been optimized by tuning the printing parameters. This hybrid structure is found to induce a 3-order reduction in RS while compromising only 5-8% visible and NIR transparency. Furthermore, the elemental makeup, as well as the interfacial and bulk electronic properties of this Ag/TTO structure, has been analyzed using in-situ XPS and UPS characterizations. The electronic band alignment along the Ag/TTO interface has been explained through detailed energy band diagrams, which demonstrated the variations in the density of states and fermi-level positions as a function of film thickness. Finally, the evolution of the electronic structure along the Ag/TTO interface has also been correlated with the compositional variations and compared with that of the bulk polycrystalline TTO. Moreover, this study provides a deeper understanding of the electron transport mechanism responsible for n-type conductivity in both TTO and Ag/TTO systems, which can be helpful for the development of low-cost metal/metal-oxide hybrid transparent conductors.

Outgassing rate behaviour of selected polymers used in vacuum systems of particle accelerators

Ivo Wevers[1], Giuseppe Bregliozzi[1], Paolo Chiggiato[1], Sergio Sammartano[1,2]
[1]CERN, Switzerland, [2]MAX IV, Sweden

Special Surfaces and Outgassing, June 17, 2024, 14:00 - 15:30

The outgassing of polymers in a vacuum system is very often the limiting factor in achieving low ultimate pressures. In this study, the outgassing behaviour in function of time, thickness and conditioning of two polyimides, Kapton® and Vespel®, as well as polyether-ether-ketone (PEEK) and a polyethylene terephthalate (Mylar) is presented and discussed. Samples of five different thicknesses for each material were investigated after exposure to normal levels of humidity present in the lab air (30-65% R.H.). The residual gas analysis revealed that all tested polymers release high quantities of water vapour and carbon dioxide; in addition, Vespel® and Mylar released significant quantities of atmospheric gas species such as nitrogen, oxygen and argon. The initial pump down of the samples showed the typical t-1/2 diffusion-limited behaviour and then, an exponential decay followed by a deviation from the Fickian model. An empirical model to predict outgassing rates of polymers in high vacuum is presented and discussed.

Surface reactivity of Weyl semimetal Co3Sn2S2 from vacuum to water splitting conditions

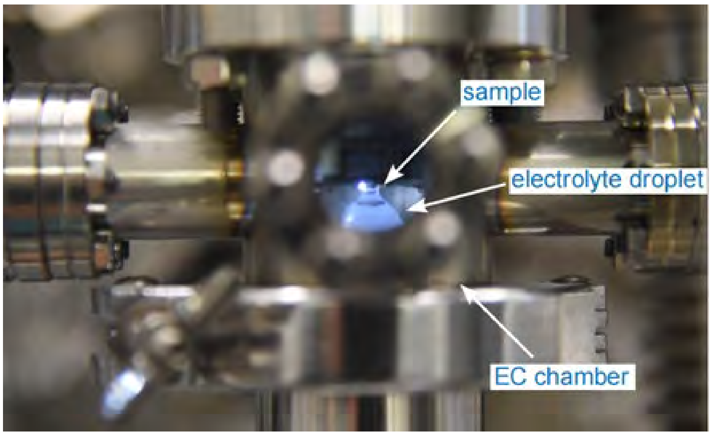
Dr Li Ma[1], Nikolaos Antonios Nemet[2], Martin Bremholm[2], Zhaozong Sun[1], Anders Koldby Vestergaard[1], Zheshen Li[3], Jeppe V. Lauritsen[1]

[1]iNANO, Aarhus University, Denmark, [2]Department of Chemistry, Aarhus University, Denmark, [3]Department of Physics and Astronomy, Aarhus University, Denmark

2D Materials and Van der Waals Heterostructures 2 and Ferroelectric Behaviour, June 20, 2024, 11:00 - 13:00

Weyl semimetals, such as $Co_3Sn_2S_2$, are gaining attention as potential electrocatalysts for water splitting due to their metallic properties in contrast to topological insulators. This study explores whether the topologically protected surface of $Co_3Sn_2S_2$ that enhance its robustness against environmental perturbations. Despite the significance of the natural surface terminations in influencing catalytic activity, their specific impact remains unclear. We have investigated the surface compositional evolution of $Co_3Sn_2S_2$ single crystal from ultra-high vacuum (UHV) to catalytic reaction conditions, using synchrotron X-ray spectroscopy (XPS). After evaluating the reactivity of the pristine surface, we studied the impact of surface oxidation on the oxygen evolution reaction (OER) activity.

At room temperature, the surface cleaved in ambient air undergoes complete oxidation, resulting in the formation of Co oxides and Sn oxides/hydroxides. The overpotential needed to achieve a current density of 10 mA/cm^2 for OER is 503 mV/RHE. In contrast, the UHV-cleaved surface preserves the pristine features of $Co_3Sn_2S_2$, displaying notably sluggish kinetics compared to the air-cleaved sample. Under UHV conditions, Sn demonstrates reactivity towards oxygen and water vapor, while increased environmental pressure promotes Co oxidation, leading to the significant formation of Co oxides in atmospheric air. An increase in catalytic activity is associated with the enrichment of Co. Below the Curie temperature, Sn primarily forms hydroxides which are reducible by photons with low energy (e.g., 20 eV), indicating its potential for high photosensitivity and worthy of further study. Despite encountering adverse evidence regarding surface robustness, this study provides crucial insights into the surface reactivity of $Co_3Sn_2S_2$.



Van der Waals epitaxy of a magnetic transition metal dihalide

Daniel Rothhardt[1,2,3], Zuned Ahmed[1,2], Christopher Penschke[4], Hao Liu[1,2], Regina Hoffmann-Vogel[3], Peter Saalfrank[4], Hans Hug[1,2], **Amina Kimouche**[3]

[1]EMPA, Switzerland, [2]Department of Physics, University of Basel, Switzerland, [3]Institute of Physics and Astronomy, University of Potsdam, Germany, [4]Institute of Chemistry, University of Potsdam, Germany

2D Materials and Van der Waals heterostructures 1, June 19, 2024, 14:00 - 15:30

In recent years, van der Waals materials have emerged as a new platform for studying low-dimensional quantum phenomena. In recent years, the introduction of a new class of two-dimensional (2D) materials like transition metal dihalides (TMHs) are expected to open a wide range of possibilities for quantum applications. These materials have shown promising potential to not only study 2D magnetism where spin fluctuations are expected to be strongly enhanced but also to investigate the growth mechanism in these magnetic crystals. Up to now only few publications show the growth of monolayer transition metal dihalides however, their local magnetic visualization is still lacking. Here, low temperature Multimodal Scanning Probe Microscopy (SPM) imaging combined with Kelvin Probe Force Microscopy (KPFM) and Magnetic Force Microscopy (MFM) revealed a ferromagnetic ground state persisting even in the monolayer regime. Various phases have been formed giving rise to a reach variety of electronic structures as revealed by KPFM.

Smart VO2-based coatings for energy-saving windows

Mr. Michal Kaufman[1], prof. Jaroslav Vlček[1], doc. Jiří Houška[1]

[1]Department of Physics and NTIS – European Centre of Excellence, University of West Bohemia, Czech Republic

Electronic Materials, Energy Reduction and Carbon Reduction, June 19, 2024, 16:00 - 17:30

Vanadium dioxide (VO2) exhibits a reversible phase transition from a low-temperature monoclinic VO2 (M1) semiconducting phase to a high-temperature tetragonal VO2 (R) metallic phase at a transition temperature of approximately 68 °C for the bulk material. The automatic response to temperature and the abrupt decrease of infrared transmittance without attenuation of luminous transmittance in the metallic state make VO2-based coatings a promising candidate for thermochromic smart windows reducing the energy consumption of buildings.

The paper deals with a scalable sputter deposition technique for the preparation of strongly thermochromic YSZ/W and Sr co-doped VO2/SiO2 coatings on standard soda-lime glass at a relatively low substrate surface temperature (320 °C) and without any substrate bias voltage. The W and Sr co-doped VO2 layers were deposited using a controlled high-power impulse magnetron sputtering of a V-W target combined with a simultaneous pulsed DC magnetron sputtering of a Sr target in argon-oxygen gas mixtures. The bottom antireflection Y-stabilized ZrO2 (YSZ) layers were deposited using a controlled reactive high-power impulse magnetron sputtering of a Zr-Y target, while the top antireflection SiO2 layers were deposited using a reactive mid-frequency bipolar dual magnetron sputtering of two Si targets.

The fundamental principles of this technique, and the design, structure and optical properties of the thermochromic coatings are presented. The coatings exhibit a transition temperature of 22-25 °C with an integral luminous transmittance up to 64 % (at almost the same luminous transmittance above the transition temperature) and a modulation of the solar energy transmittance over 11 %. Such a combination of properties, together with the relatively low deposition temperature (320 °C), has not yet been published by other teams for thermochromic VO2-based coatings prepared by a scalable deposition technique compatible with the existing magnetron sputter systems in glass production lines and in large-scale roll-to-roll deposition devices.

On-surface induced fitting and mobility of conformationally flexible molecules inside nano confinements

Dr Aisha Ahsan[1], Dr. Luiza Buimaga-Iarinca[2], Dr. Thomas Nijs[1], Dr. Sylwia Nowakowska[1], Dr. SK Rejaul[1], Dr. Fatemeh Mousavi[1], Dr. Mehdi Heydari[1], Prof. Meike Stöhr[3], Dr. Sameena Zaman[5], Prof. Cristian Morari[2], Prof. Lutz Gade[4], Prof. Thomas Jung[6]
[1] University of Basel, Switzerland, [2] National Institute for Research and Development of Isotopic and Molecular Technologies, Romania, [3] Zernike Institute for Advanced Materials, University of Groningen, The Netherlands, [4] Universität Heidelberg, Germany, [5] Habib University, Pakistan, [6] Paul Scherrer Institute, Switzerland

Self-Assembly, Characterisation and Reactivity of 2D Structures of Molecules at Surfaces, June 21, 2024, 10:30 - 12:00

Host-guest architectures provide ideal systems to investigate site-specific physical and chemical effects. Condensation events in nanometer sized confinements are particularly interesting for the investigation of inter-molecular and molecule-surface interactions. As objects of study we have chosen a series of non-planar, conformationally flexible cyclo-alkanes (c-alkanes) to study their site-specific condensation in the confinement provided by 1.6 nm sized pores in a surface supported coordination network. Adsorption of these molecules is observed to be accompanied by conformational adjustments which resemble the 'induced-fit' model proposed for site-specific molecular assembly and recognition in molecular life-sciences. Also, we report that the symmetry of small clusters formed upon condensation, their registry with the substrate and their lateral packing as well as their adsorption height is characteristically modified by the confined packing of the cycloalkanes. While cyclopentane and cycloheptane display cooperativity upon filling of the hosting pores, cyclooctane and to a lesser degree cyclohexane diffusively re-distribute to more favoured adsorption sites. Also we observe an unexpected dynamic behaviour of cyclooctane in the full, four-fold occupied pore at 5K. This is in significant contrast to the melting point of cyclohexane lying very close to room temperature. The c-alkane system at hand showcases the site-specific modification of the interactions and the cooperative behaviour of adsorbates in confinements as it plays a crucial role in many applications of 3D porous materials as gas storage agents or catalysts/bio-catalysts.

References

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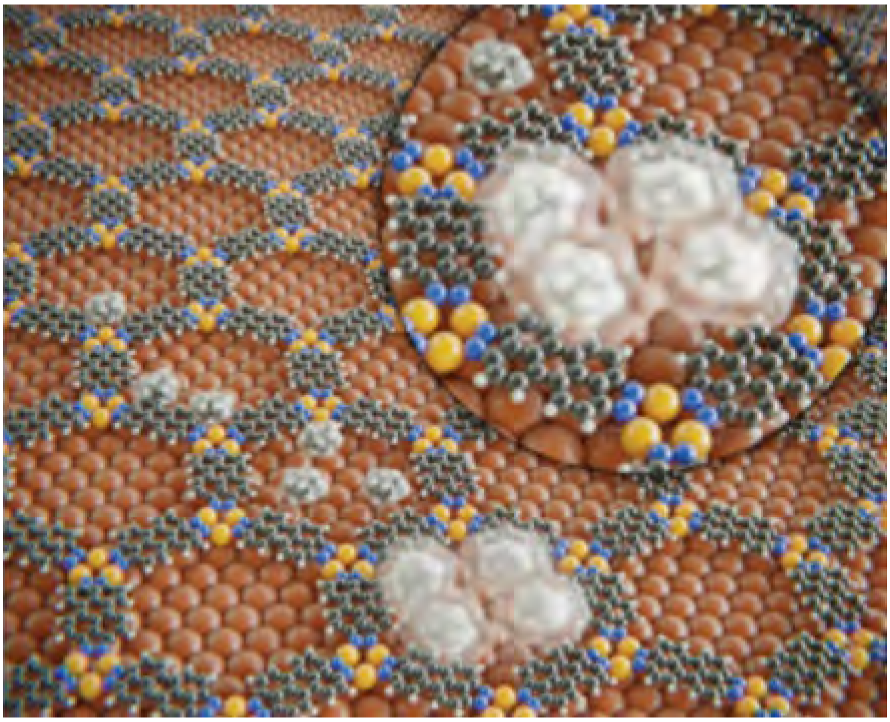

Tuning the electronic structure of nanoporous graphene by chemical adsorption.

<u>Dr. Andrea Tonelli</u>[1], Dario Marchiani[2], Carlo Mariani[2], Maria Grazia Betti[2], Roberto Biagi[1], Deborah Prezzi[3], Elisa Molinari[1], Valentina De Renzi[1]

[1]Physics, Informatics and Mathematics Department, University of Modena and Reggio Emilia, Italy, [2]Physics Department, Sapienza University of Rome, Italy, [3]Istituto Nanoscienze (NANO-S3), Consiglio Nazionale delle Ricerche (CNR), Italy

Carbon Materials 2, June 19, 2024, 10:30 - 12:35

Chemical adsorption represents a powerful strategy to tune the electronic band structure of graphene and obtain new carbon-based materials with radically different properties and functionalities. Nanoporous graphene (NPG) is a 3D graphene arrangement formed by few weakly interacting layers [1], representing an excellent candidate to investigate chemical adsorption on free-standing graphene.
In this work, we investigate how chemical adsorption modifies the electronic structure of NPG, by means of High-Resolution Electron Energy-Loss Spectroscopy (HREELS) and state-of-art ab-initio simulations. In particular, we consider the opposite effects, induced by deuteration [2] and alkali metal doping [3], on the electronic properties of the system.
In deuterated NPG, the frequency of the C-D stretching modes depends on the specific structural configuration of D adsorption; comparison between HREELS spectra and DFT calculations allows to prove that the deuterated structure is 2-side (Fig.1a). Furthermore, HREELS reveals the onset of the electronic transition upon deuteration, demonstrating the opening of a semiconducting gap at 3.25 eV (Fig.1b). Comparison with ab-initio GW and Bethe-Salpeter equation calculations suggests the relevant role of excitons (Fig.1c).
In potassium-doped NPG, the K-induced conduction band occupation leads to a Dirac plasmon excitation, observed as an asymmetric peak in the HREEL spectra (Fig.1d). Upon K-dose, the plasmon loss blue-shifts and shows a marked broadening, associated to the increased damping due to the increased probability of π* electron and π hole pair excitations. The plasmon energy dependence on n-carrier density is evaluated by combining HREELS and Ultraviolet Photoelectron Spectroscopy (UPS) data.

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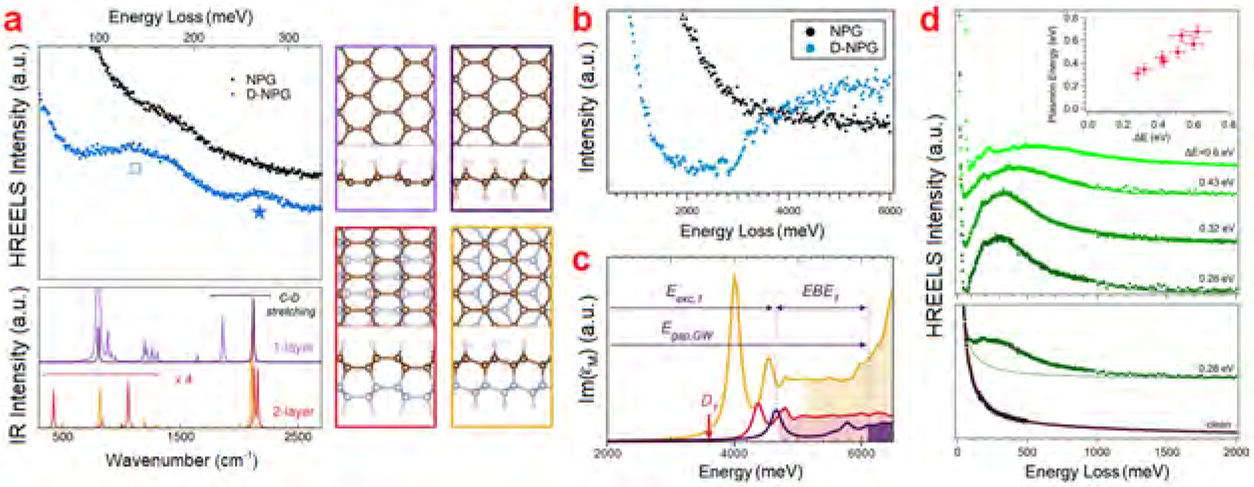

Directional picoantenna behavior of tunnel junctions in the presence of atomic-scale defects.

David Mateos Roncero[1], Óscar Jover[2], Miguel Varea[2], Koen Lauwaet[2], Daniel Granados[2], Rodolfo Miranda[1,2], Antonio Isaac Fernandez-Dominguez[3], Alberto MartIn-Jimenez[2], Roberto Otero[1,2]
[1]Departamento de Física de la Materia Condensada (IFIMAC), Universidad Autónoma de Madrid, Spain, [2]IMDEA Nanociencia, Spain, [3]Departamento de Física teórica de la Materia Condensada (IFIMAC), Universidad Autónoma de Madrid, Spain

MS-2: Light-matter Interaction at Atomic Scales, June 17, 2024, 16:00 - 17:35

Plasmonic nanoantennas, metallodielectric structures with engineered size and shape, have attracted much attention lately as they make the control of the directionality and temporal characteristics of light emitted by fluorophores possible. Nanoantennas exploit light-matter interactions mediated by Localized Surface Plasmon Resonances and, so far, have been demonstrated using metallic nanoparticles or other metallic nanostructures. Plasmonic picocavities could act as antennas to mediate light-matter interaction even more efficiently than their nanoscale counterparts due to their extreme field confinement, but the directionality on their emission is difficult to control. In this work, we show that the plasmonic picocavity formed between the tip of a STM and a metal surface with a monoatomic step shows directional emission profiles and, thus, can be considered as a realization of a picoantenna. Comparison with electromagnetic calculations demonstrates that the observed directionality arises from light emission tilting of the picocavity plasmons. Our results, thus, pave the way to exploiting picoantennas as an efficient way to control light-matter interaction at the nanoscale.

Figure 1. a) Experimentally obtained radiative PhDOS along the 1 and 2 steps. This is obtained normalizing the STML spectra by the Rate of inelastic tunnelling 1. Line spectra height profile shown below b) STM image of a Ag(111) surface with steps at different orientations. Inset: EM simulations of the PhDOS when the tip is placed atop a step (black), and over the terrace (blue), as a function of the azimuthal angle. c) Measured angular distribution of the emitted light. The dots correspond to the integrated PhDOS on the steps, referred to each step's frame of reference. The cyan line is a fitting of our experimental data to a cardioid-like function.

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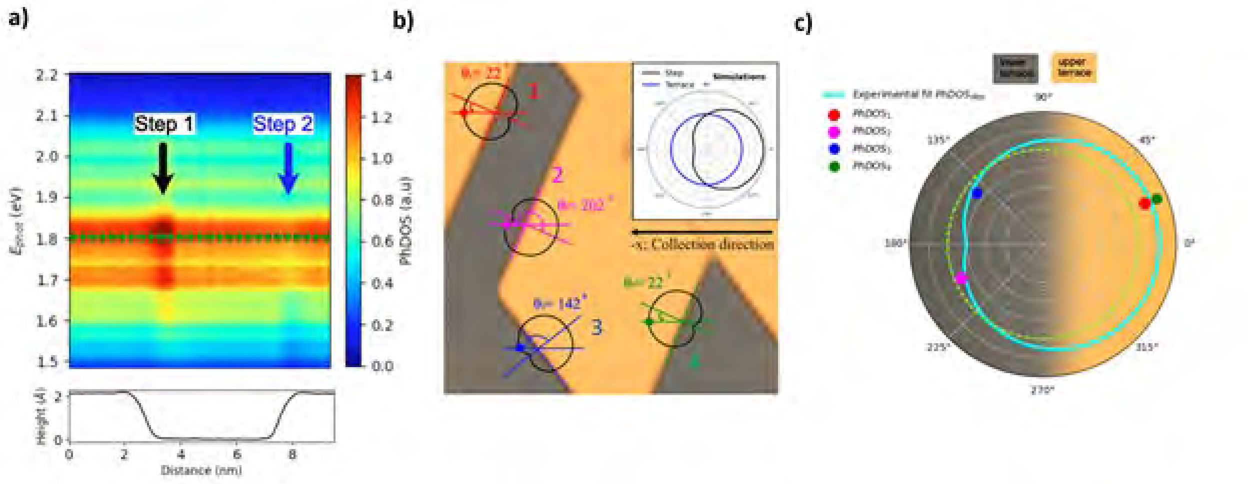

Simulations of strained films evolution: extending accessible timescales through Convolutional Neural Networks

Daniele Lanzoni[1], Fabrizio Rovaris[1], Luis Martín-Encinar[2], Andrea Fantasia[1], Roberto Bergamaschini[1], Francesco Montalenti[1]
[1]L-NESS and Dept. of Materials Science, University of Milano-Bicocca, Italy, [2]Dpto. de Electricidad y Electrónica, E.T.S.I. de Telecomunicación, Universidad de Valladolid, Spain

Thin Film Growth Simulation, June 18, 2024, 10:30 - 12:30

The evolution of the surface morphology of strained films has been the object of several studies since decades. Continuum models tracing material transfers driven by local chemical potential gradients have been widely exploited to study the film instability and islanding dynamics in heteroepitaxy [1]. Despite the macroscopic scale of such models, the simulation on large domains and for long times is a computationally intensive task. In particular, the evaluation of the elastic contribution to the chemical potential is typically a bottleneck as requiring to recalculate mechanical equilibrium at each of the several hundred thousand time-integration steps. Indeed, while semi-analytical approximations can be exploited for small-slope profiles, a full numerical solution via Finite Element Method (FEM) is needed to tackle realistic morphologies. To speed-up such simulations we here propose an approach based on the use of a Convolutional-Neural Network [2] by-passing the explicit strain calculation by directly predicting the map of elastic chemical potential for a given surface profile, at much lower computational cost. The simpler case of a two-dimensional profile with isotropic surface energy is considered and parameters matched to the technologically relevant case of Ge epitaxial films on Si substrates. We show that a dataset of ~70000 FEM evaluations on randomly generated surface profiles provides a sufficient basis for the training of a NN model providing reliable predictions of surface elastic chemical potential for arbitrary morphologies. The NN performances in extrapolating the solution on large domains, even hundreds of times larger than the training one, as well as the approximation errors on different geometries are investigated. The trained model is then used to perform surface evolution simulations reproducing the dynamics of strained films, including island formation and coarsening.

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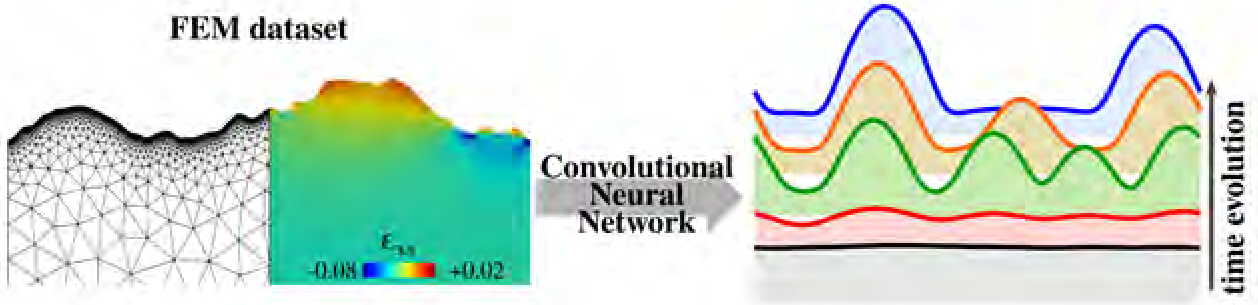

Interplay of crystal faceting, wetting interactions and substrate geometry in solid-state dewetting and selective-area growth: a phase-field approach

Emma Radice[1], Leo Miglio[1], Francesco Montalenti[1], **Roberto Bergamaschini**[1]
[1] L-NESS and Dept. of Materials Science, University of Milano-Bicocca, Italy

Advances in Experimental and Theoretical Methods 3, June 17, 2024, 16:00 - 17:35

The advancing of nanotechnologies toward quantum devices is pushing the research to the realization of complex material architectures at the nanoscale, with high demands on the crystal quality and uniformity. The use of lithographic masks for driving the self-assembly of nanostructures by dewetting dynamics and selective-area epitaxy is one of the most promising strategy to such a goal. Isolated dots, nanowires, ring-like structures as well as interconnected networks can be achieved by a suitable design of growth and annealing processes. Here we analyse how the definition of the substrate/mask, non-planar geometry, returning variable contact boundaries relative to the crystallographic orientations of the deposited material, impacts on its surface evolution and stability. To this goal, a phase-field growth model [1] dealing with both deposition and surface diffusion dynamics and comprising both surface energy and kinetic anisotropy of crystal facets is extended to include the wetting interaction with an arbitrary-shaped substrate. The local consistency of the approach with the Young-Herring contact angle boundary condition is shown. Then, the solid-state dewetting of thin layers and nanoparticles deposited on curved substrates is inspected by full three-dimensional simulations, as a function of the wetting parameter and crystallographic orientation. Finally, the model is applied to the technologically relevant case of selective growth of PbSnTe nanodots and nanowires [2], in close relation to dedicated experiments. It is found that nanostructures grown on (111) substrates develop smooth crystalline fronts when aligned along the <110> in-plane directions while <112>-oriented ones are unstable against refaceting.

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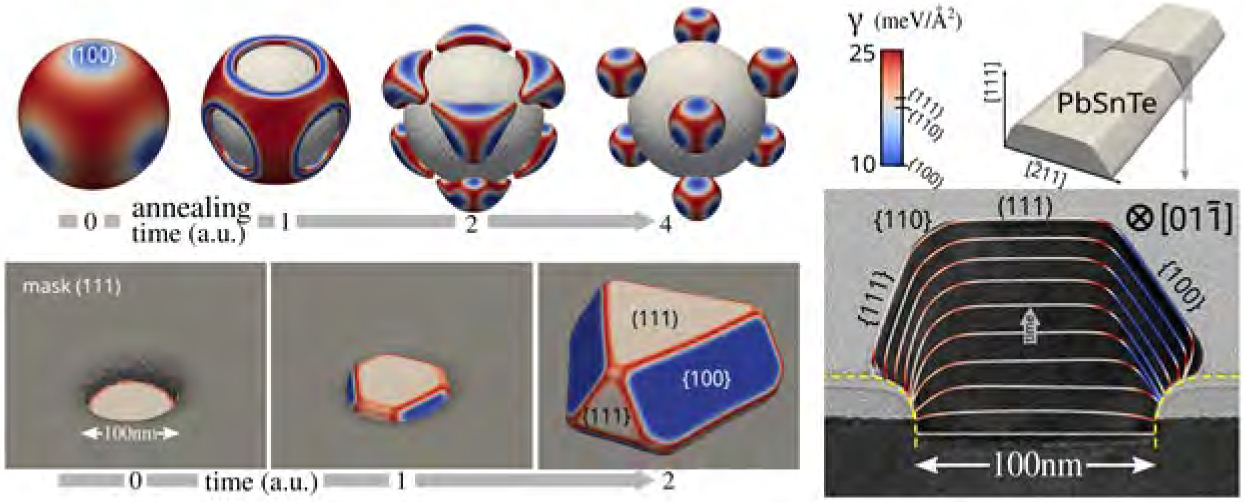

Machine Learning Aided Simulation of Complex Gas Distribution Systems Operating under any Vacuum Conditions

Professor Dimitris Valougeorgis[1], Dr. Serafeim Misdanitis[1]
[1] University Of Thessaly, Greece

Vacuum Gas Dynamics, June 18, 2024, 16:00 - 17:30

Gas distribution systems operating in low, medium, high and ultra-high vacuum conditions are crucial across applications like semiconductor technology, gaseous microfluidics, vacuum metallurgy and nuclear fusion. The typical hydrodynamic approach is not valid and mesoscale kinetic modeling must be employed. In this framework, an in-house ARIADNE code for modeling gas distribution systems under any vacuum conditions has been developed and successfully implemented to model the gas exhaust system of fusion reactors [Vasileiadis et al, 2016]. This code integrates a robust kinetic database into a network solver, ensuring accurate flow rate predictions across rarefaction regimes.

To further address computational challenges, machine learning (ML) techniques, namely symbolic regression (SR), has been employed in an attempt to extract equations from the kinetic database, offering computational efficiency. The application of SR leads to the extraction of relatively simple and accurate closed-form expressions of the flow rate in a pipe element, circumventing the need of computationally demanding kinetic modeling and simulations [Sofos et al, 2023].

In the present work, the developed network solver circumvents the use of the kinetic data base and incorporates the closed form expressions derived by ML in its core. The feasibility of the approach is demonstrated on a micro-distribution network in the whole range of gas rarefaction and it is accordingly benchmarked by comparison with the solver, utilizing the kinetic data base. Machine learning-predicted data hold promise for engineering applications in gaseous microfluidics and vacuum technology, offering a practical solution to computationally expensive kinetic modeling.

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 - EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission.

Spatially resolved surface X-ray diffraction on polycrystalline surfaces

Hanna Sjö[1], Anatoly Shabalin[2], Ulrich Lienert[2], Johan Hektor[3], Andreas Schaefer[4], Per-Anders Carlsson[4], Johan Gustafson[1]
[1]Lund University, Sweden, [2]Deutsches Elektronen-Synchrotron DESY, Germany, [3]Malmö University, Sweden, [4]Chalmers University of Technology, Sweden

Advances in Experimental and Theoretical Methods 2, June 17, 2024, 14:00 - 15:30

Polycrystalline surfaces are of interest when studying, for example, catalytic reactions since they are more realistic model catalysts than single crystals and allow us to measure more than one surface orientation at once. There are tools, such as electron backscattering diffraction, that can be used to study polycrystalline surfaces, but these are limited to low-pressure environments. Surface X-ray diffraction (SXRD) can measure long-range atomic structures, even in high-pressures and liquids. SXRD is, however, limited to simple samples, such as single crystals, due to the long beam footprint, caused by the grazing incidence angle. We are developing spatially resolved SXRD to complement the operando surface science toolbox. One part of this project is grain mapping polycrystalline surfaces using an SXRD setup. By using tools from 3D-XRD[1,2], adapted to a SXRD setup, and the near-surface Bragg reflections, spatially resolved maps are achieved, comparable to maps from electron backscatter diffraction (see Figure 1a). The surface structures can also be studied by following where CTRs or superstructure rods are detected, providing spatially resolved maps of surface structures. This is a method we are calling tomographic surface X-ray diffraction.

For in situ studies, we can make faster measurements by rotating the sample around the surface normal of the now-known grains. This enables us to follow the surface diffraction from grains during reactions. Figure 1b shows the CTR intensity-change relative to the metallic surface during methane oxidation. 1c-d compares the diffraction pattern of two grains. Similarly to a classic SXRD measurement, the method can provide information about surface structures and changes.

In this presentation, we will give an update on the progress of both tomographic surface x-ray diffraction and in situ measurements of polycrystalline surfaces.

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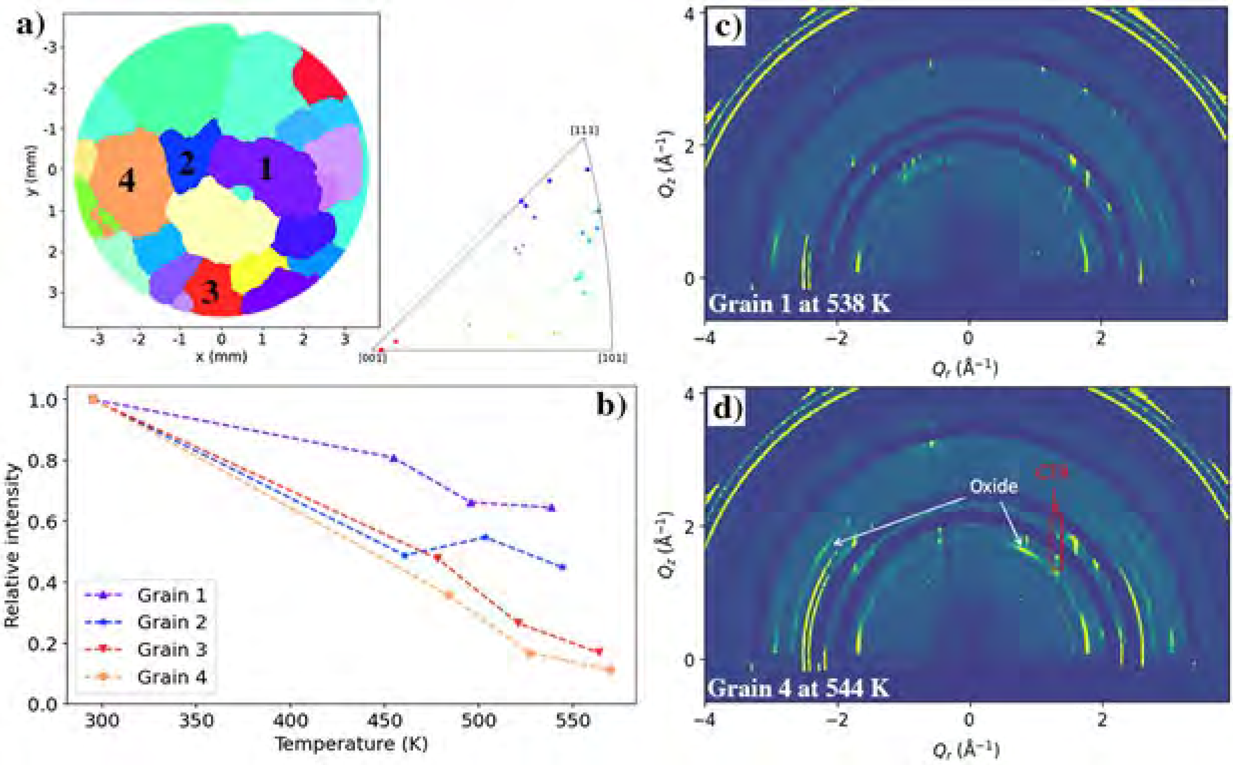
a)
y (mm)
x (mm)
-3
-2
-1
0
1
2
3
4
2
1
3
[111]
[001]
[101]
b)
Relative intensity
Temperature (K)
1.0
0.8
0.6
0.4
0.2
0.0
300
350
400
450
500
550
Grain 1
Grain 2
Grain 3
Grain 4
c)
Grain 1 at 538 K
Q_z (Å^{-1})
Q_r (Å^{-1})
-4
-2
0
2
4
d)
Grain 4 at 544 K
Oxide
CTR

Carrier gas in Helium leak detection – application to conductance-limited devices

Mr Laurent Ducimetiere, Mr Rudolf Konwitschny
[1]*Pfeiffer Vacuum, Germany*

MS-6: RGA User Meeting 1, June 19, 2024, 10:30 - 12:35

Helium leakage testing is a non-destructive test method that offers both high sensitivity and a wide dynamic range. However, in some applications the geometry of the tested part introduces limitations in gas dynamics and conductance resulting in a significant performance loss for this technique. This is especially true for long and thin gas lines as used for gas supply lines or tubular heat exchangers.
A helium spray test involves evacuation of the part to be tested, connection to the helium leak detector and spraying of helium around the outer surfaces of the part. Helium will penetrate through leaks in the wall and be transported to the analyser.

The response time of the analyser is dependent on the volume of the part to be tested and the effective helium pumping speed of the test set-up. The effective helium pumping speed depends upon the helium pumping speed of the leak detector and the conductance of the part and the pipe work connecting it to the leak detector. A typical commercially available leak detector has its maximum sensitivity at comparatively low pressures in the range of 10-2 to 0.5 mbar. When long thin tubes are pumped down to the ultimate pressure of the leak detector, gas flow is in the molecular flow regime. In this flow regime the conductance of the tube is much smaller than for laminar flow which results in extended measuring times. Signal intensity can be drastically reduced by a very broad gas velocity distribution.

In order to achieve fast response time and high sensitivity the leak test is best performed in the laminar flow regime. Introduction of a carrier gas provides a fast and active gas transport through the gas line to the leak detector.

Energy-efficient vacuum applications

Mr Laurent Ducimetiere, Mr Dirk Budelmann
[1]*Pfeiffer Vacuum Sas, Germany*

Vacuum pumps, June 21, 2024, 10:30 - 12:00

Sustainability is becoming increasingly important due to the global climate situation and rising energy prices.
As a manufacturer of vacuum solutions, Pfeiffer Vacuum has set itself the goal of keeping energy consumption and CO_2 emissions as low as possible - both in product manufacturing and in customer applications.
When defining or upgrading a vacuum application, high-efficiency vacuum pumps, such as the HiScroll, are an important key element in reducing the plant's energy consumption.
In addition, there are now new intelligent pump and equipment features that offer even more possibilities for designing an energy-efficient vacuum system.
Pure pumping performance is therefore no longer the only parameter to be taken into account.

Surface Chemistry of Trimethylaluminum and its Implications for Atomic Layer Deposition

Leonhard Winter[1], Francisco Zaera[1]
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Oxide Surfaces and Nanomaterials - Spectroscopy, Imaging and Physicochemical Processes, June 18, 2024, 10:30 - 12:30

Atomic Layer Deposition (ALD) is a chemical method used to grow thin films by sequentially employing complementary, self-limiting half-reactions. ALD offers the possibility to grow high-quality films on geometrically challenging substrates with sub-monolayer thickness control. An important development in ALD research is the ability to perform the growth selectively on specific areas.[1] For example, in the microelectronics industry, an ALD film often needs to be grown only on the dielectric (often SiO_2) or only on the electric contacts (often Cu) while avoiding the other material. Therefore, it is important to understand the surface chemistry of the ALD precursors on the competing surfaces. There has been some progress towards this goal,[2] but more mechanistic details are needed to tailor the selective ALD chemistry.

We have set to first study and contrast the surface chemistry of trimethylaluminum (TMA), a precursor commonly used to deposit Al_2O_3 films, on SiO_2 versus Cu surfaces by using X-ray photoelectron spectroscopy (XPS) and temperature-programmed desorption (TPD). On SiO_2, we have observed high chemical reactivity of this precursor at unexpectedly low temperatures and exposures, below the cryogenic temperatures required for multilayer condensation. This low-temperature chemistry appears to be complex, with desorption of Al-containing fragments being accompanied with changes in the relative Al/C atomic ratio on the surface. It was also determined that the initial sticking coefficient at room temperature is approximately 4-5 times smaller than at cryogenic temperatures, and that the TMA uptake is self-limiting. This high TMA reactivity on SiO_2 surfaces will need to be compared with that on Cu substrates, as the differences are expected to have significant implications for the selectivity of the ALD and for strategies to control it.

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Spectro-microscopy in the scanning field emission microscope

Oskar Fossberg[1], Dr Andrew Pratt[1], Prof Steve Tear[1], Prof Danilo Pescia[2]
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Advances in Experimental and Theoretical Methods 2, June 17, 2024, 14:00 - 15:30

Erbium, amongst other rare-earth metals, proposes an attractive application for nanotechnology where a focus on self-assembled silicide nanostructures formed on crystalline silicon surfaces could be key as device dimensions continue to reduce. Growth modes on silicon surfaces are dependent on crystal orientation. Low-dimensional metallic nanowires of different rare-earth silicides grow successfully on Si(100) [1] whilst two-dimensional films form on Si(111) [2]. Each system is unique, and understanding the growth mechanisms to produce structures of different dimensionalities is far from resolved.

Our work utilises both the tunnelling and field emission regimes of a scanning tunnelling microscope (STM) in a system known as a scanning field-emission microscope (SFEM) [3]. In SFEM mode, the metallic tip is retracted from the sample, up to hundreds of nanometres, such that tunnelling between the tip and sample is entirely suppressed. A negative potential applied between the tip and sample can generate a source of primary electrons through field emission. In this regime, the ejected electrons represent a unique electronic system that can be analysed in the macroscopic environment by an electron analyser [4]. This gives the SFEM a unique advantage over a standard STM with the possibility of secondary electron imaging and spectroscopy.

We present the interaction of erbium deposited onto Si(111) at various coverages, in addition to studies of iron and erbium on W(110) showing complementary STM and STS results. Utilising these surfaces to explore the field emission regime of our microscope, we present energy-filtered imaging and spectroscopy to refine the energy analysis of low-energy electrons.

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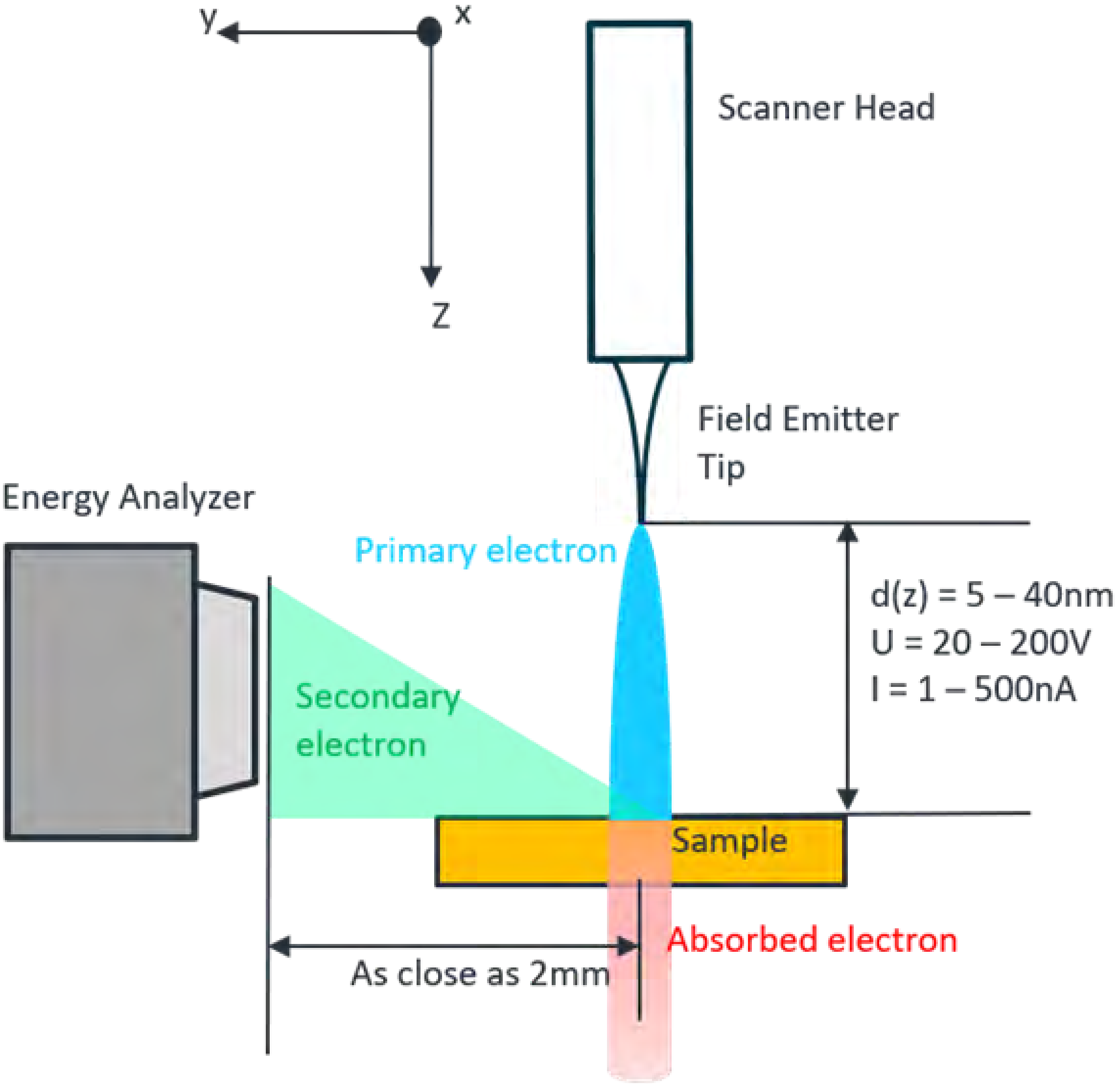
y
x
z
Scanner Head
Field Emitter Tip
Energy Analyzer
Primary electron
d(z) = 5 – 40nm
U = 20 – 200V
I = 1 – 500nA
Secondary electron
Sample
Absorbed electron
As close as 2mm

Oxygen capture and storage in the Nb2O3 (2x2) Honeycomb lattice on Au(111)

Michael Furlan[1], Shuqiu Wang[1], Yuhan Zhu[1], Jacek Goniakowski[2], Claudine Noguera[2], Martin Castell[1]
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Metal Surfaces - Adsorption, Desorption and Reactions 2, June 17, 2024, 14:00 - 15:30

Two-dimensional transition metal oxides (TMOs) supported on metal substrates form an exciting class of materials with potential applications in catalysis, electronics, and energy storage [1]. Due to the strong epitaxial interaction between metal substrates and TMO films, many of the observed lattices are unique and only exist in two dimensions. A subset of TMOs crystalize into a honeycomb (2 × 2) monolayer; for example V2O3 on Pd(111) [2] and Ti2O3/Nb2O3 on Au(111) [3,4].

The Nb2O3 monolayers are grown by Nb deposition and subsequent annealing in a low-pressure oxidizing atmosphere. Scanning tunnelling microscopy (STM) images show that the films form a well-ordered honeycomb lattice with a (2 × 2) periodicity with respect to the $[1\bar{1}0]$ directions Au(111) substrate [4]. Density Functional Theory (DFT) demonstrates the existence of a strong interfacial interaction characterized by a large electron transfer towards the Au substrate, an increase of the Nb oxidation state, and substantial film rumpling [4].

Treating the Nb2O3 honeycomb in increasingly oxygen rich environments we demonstrate additional oxygen uptake into the Nb oxide film. The additional oxygen is stored in the form of a close-packed layer which is in co-existence with the Nb2O3 honeycomb, under-coordinated edge sites in the form of four-fold coordinated Nb atoms, and finally in a novel honeycomb structure with a (2 x 2) periodicity along the $[1\bar{1}\bar{2}]$ directions of the Au(111) substrate.

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Femtosecond time-resolved spectroscopy at the atomic scale

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MS-2: Light-matter Interaction at Atomic Scales, June 17, 2024, 16:00 - 17:35

Many fundamental physical and chemical processes occur on extremely fast time scales (femtoseconds to picoseconds) and at very small length scales (picometers to nanometers), such as energy transfer and charge transfer processes in molecules and semiconductor materials. The precise characterization and manipulation of these processes at their intrinsic time and length scales are crucial for understanding microscopic mechanisms and advancing the development of novel materials. To reach this goal, we have combined femtosecond time-resolved spectroscopic techniques with scanning tunnelling microscopy (STM) [1,2] to facilitate the probing and controlling of electronic and vibrational dynamics in nanoscale systems with simultaneously high spatial (Ångström), temporal (femtoseconds), and energy (meV) resolutions. Specifically, we investigate hot electron dynamics in the plasmonic nanocavity of the STM utilizing pump-probe spectroscopy to detect anti-Stokes emission. Furthermore, we observe nonlinear four-wave mixing (FWM) signals generated by laser pulses, which exhibit high sensitivity to atomic-scale structures. The FWM process at the STM junction also enables the tracking of atomic motions within single molecules through coherent anti-Stokes Raman scattering (CARS). These approaches offer new perspectives for exploring ultrafast light-driven dynamics at the atomic scale.

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Thermal evolution of the metal/PtSe2 systems studied by Raman Spectroscopy

Msc Eng. Jan Raczynski[1], Eng. Jakub Nowaczyk[1], PhD Wojciech Koczorowski[1]
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Low-dimensional Thin Film Materials, June 17, 2024, 11:00 - 12:35

The discovery of graphene and its physical properties started a new era in the investigating of thin layer materials[1,2]. Today, these materials also include Transition Metal Dichalcogenides(TMD), which provide a wide range of physical properties, such as the values of charge carrier mobility and bandgap energy, which depend on the layer thickness[3,4]. One of the most promising TMD materials is PtSe2 with predicted high charge carrier mobility at room temperature(RT). In that case, it is crucial to determine the physical properties of the thin layer as an active channel in the planar sensor device. To fully understand of the formed interface metal/PtSe2 interface, it is necessary to perform measurements to give insight in to the active channel and interface physical properties both at RT and during thermal treatment. In that case, one of the most crucial methodologies is Raman spectroscopy allow analyze of the characteristic mods' position transform it into the change of the doping and stress level in the sample PtSe2[5,6].
The properties of the active layer of PtSe2, especially the changes in the stress and doping type levels at RT and during elevated temperature(up to 473K) will be discussed in this presentation. Simultaneously emphasis will be placed on the properties of the metal(eg.Ti,Ni,Pt)/PtSe2 interfaces and the impact of the deposited metallic layer and thermal treatment on the PtSe2 bulk transformation. The application of the temperature dependent correlation plots allows the determination of the temperature range work of PtSe2 based system for a potential planar device will be presented and discussed.

Acknowledgments: The study reported in this presentation has been partially financed by the National Science Centre, Grant No.2019/35/O/ST5/01940, NAWA grant No.PPN/STA/2021/1/00043 and Ministry of Education and Science(Poland) under Project No.0512/SBAD/2420.

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Diffusion studies of Pb on Si(111)-(7x7) using SFM and KPFM

Paul Philip Schmidt[1], Felix Hartmann[1], Lea Faber[1], Janet Anders[1,2], Regina Hoffmann-Vogel[1]
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Spectroscopy and Microscopy of Nanostructures Modelling Nanostructure Properties, June 20, 2024,
11:00 - 13:00

The diffusion of metals on semiconductors offers a wide range of technical applications, e.g. in the semiconductor industry. This study focuses on the diffusion behaviour of Pb/Si(111)-(7x7). It is known that Pb grows on Si in the Stranski-Krastanov mode. Previous research has shown that this system exhibits explosive island growth and abnormal fast diffusion [1][2]. Based on the structure of the system, it is clear that the diffusion rate must be related to the behaviour of the Pb in and on top of the wetting layer. We have evaporated 5 monolayers of Pb at a Si(111)-substrate temperature of 120 K. After increasing the sample temperature to room temperature we chose an island which showed neither growth nor decay over several hours. We forced a local disequilibrium by contact between the tip and this island. Diffusion was analysed by non-contact scanning force microscopy (NC-SFM) and simultaneous Kelvin probe force microscopy (KPFM). While the topography data essentially confirms the abnormal diffusion on island growth, the KPFM shows significant changes in the local contact potential difference (LCPD). Despite the low time resolution of an SFM measurement, it was possible to determine the time scales of a mass transport in this way. Our KPFM data suggests that the variation in the wetting layer could be explained by the change of the density of Pb.

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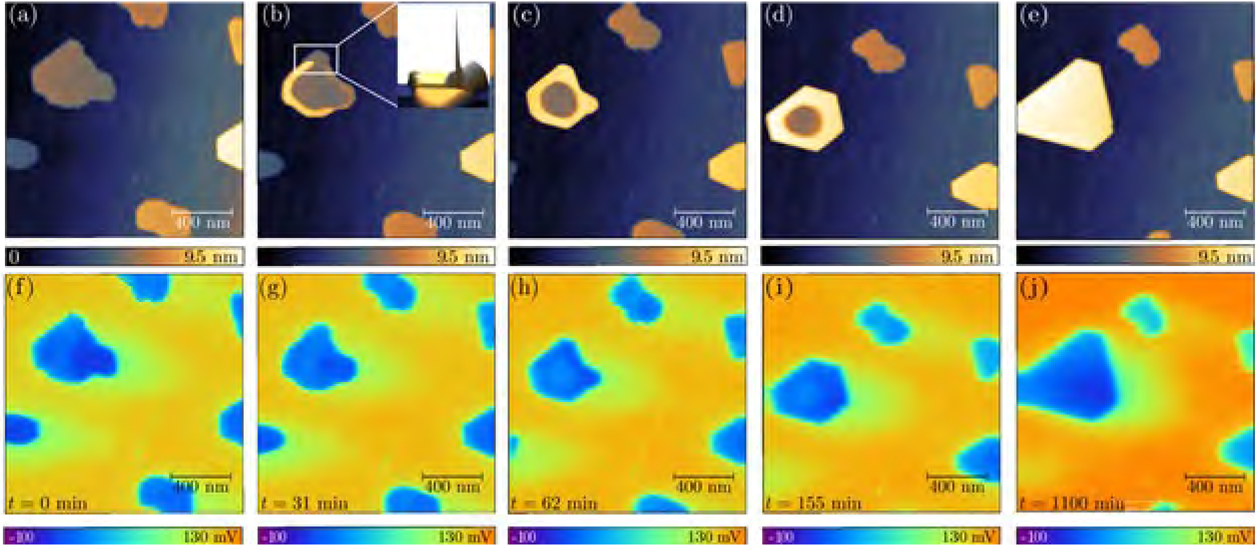

Tracking Sub-millisecond Compositional Changes During CO Oxidation Using Ambient Pressure X-ray Photoelectron Spectroscopy

Calley Eads[1], Weijia Wang[1], Ulrike Küst[2], Julia Prumbs[2], Robert Temperton[1], Mattia Scardamaglia[1], Jan Knudsen[1,2], Andrey Shavorskiy[1]

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Metal and Oxide Single Crystal Surfaces - Growth, Preparation, and Characterisation, June 18, 2024, 16:00 - 17:30

Historically, steady state operation dominates in situ investigations of catalytic reactions which can lead to an incorrect assignment of active species due to its possible overlap with spectator species when analyzing time-averaged spectra. We demonstrate the impact of discerning mechanistic details down to 40 us time resolution in the CO oxidation of Pt(111) to determine the active species at the height of catalytic activity. Using time-resolved ambient pressure X-ray photoelectron spectroscopy with chemical perturbations in the gas composition, we observe that chemisorbed oxygen is actively consumed in the production of CO2 in parallel with the growth of a Pt surface oxide. Thus, resolving the ongoing debate surrounding the role of Pt surface oxide in the CO oxidation of Pt.

Surface chemistry of methyl acetoacetate and aspartic acid on Cu(111) – a model for enantioselective hydrogenation reactions

Dr. Burcu Karagoz[1], Mr Henry Hoddinott[1,2], Dr Alex Large[1], Prof Georg Held[1]
[1]Diamond Light Source, United Kingdom, [2]Swansea University, United Kingdom

Metal Surfaces - Adsorption, Desorption and Reactions 2, June 17, 2024, 14:00 - 15:30

Developing enantioselective chemical processes is essential for the manufacture of pharmaceuticals because the undesired enantiomer of a chiral pharmaceutical can have catastrophic effects on the human body when ingested [1,2]. Heterogeneous metal catalysts can be modified to produce enantiomerically pure compounds by adsorbing chiral molecules such as amino acids. One of the most studied examples of enantioselective catalysis is the hydrogenation of β-ketoesters, e.g. methyl acetoacetate (MAA) into methyl-3-hydroxybutyrate, on chirally modified metal catalysts [3-7]. In this study, we investigated the surface chemistry and adsorption geometry of aspartic acid (Asp), an amino acid widely used as a modifier, MAA, and their coadsorption on the Cu(111) single crystal surface using synchrotron-based X-ray photoelectron spectroscopy (XPS) and angle-resolved near edge X-ray absorption fine structure (NEXAFS). The latter technique enables determining changes in molecules' orientation and bond order. Angle-resolved NEXAFS exhibits that Asp, and MAA bond to the surface in a tilted geometry. Furthermore, O- K edge and C K-edge NEXAFS of adsorbed MAA show the characteristics of C=C, and C=O bond which suggest that the molecule is in its enolate configuration [8]. By coadsorbing Asp and MAA in varying ratios, we gain insights into the effects of the chiral modifier on the orientation of the adsorbed MAA, and, therefore, the stereochemistry that drives enantioselectivity in the hydrogenation reaction.

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Impedance spectroscopy studies on diamond-based nanomaterials and nanostructures

Ruoying Zhang[1], **Professor Haitao Ye**[1]
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MS-5: Electrochemical MEMs Sensing for Environmental and Biological Monitoring, June 19, 2024, 14:00 - 15:30

Diamond based nanomaterials and nanostructures have gained significant interest across various scientific and industrial fields due to their exceptional electronic, thermal, mechanical properties. This talk delves into the application of impedance spectroscopy as a non-destructive analytical technique to investigate the electrical characteristics and behaviour of these materials and structures at the nanoscale. We will discuss the synthesis and structural characterization of various diamond nanomaterials, including nanodiamonds thin films, powders and electronic devices. The focus will be on understanding their impedance spectra in relation to their intrinsic properties such as grain interiors and grain boundaries, and the influence of factors such as defects, surface modification, and interface. Through detailed impedance measurements, we aim to elucidate the charge transport mechanisms, dielectric properties, and potential interface effects that govern the performance of these diamond-based nanostructures. This study not only enhances the fundamental understanding of diamond nanomaterials but also provides insights into their prospective applications in nanoelectronics devices.

Study of the formation of silicon nanoribbons on the Au(110) surface

Ekaterina Tikhodeeva[1], Paola De Padova[2], Guy Le Lay[3], Marina Baidakova[4], Evgeniya Lobanova[4,5], Jaime Sanchez-Barriga[6], Dmitrii Smirnov[6], Serguei Molodtsov[1], Manuel Izquierdo[1], María E Dávila[7]
[1]European XFEL, Germany, [2]Consiglio Nazionale delle Ricerche-ISM, Italy, [3]Aix-Marseille Université, France, [4]Ioffe Institute, Russia, [5]ITMO University, Russia, [6]Helmholtz-Zentrum Berlin, Germany, [7]Spanish National Research Council, Spain

Metal and Oxide Single Crystal Surfaces - Growth, Preparation, and Characterisation, June 18, 2024, 16:00 - 17:30

Silicon nanoribbons (SiNRs) are highly prospective 1D structures for application in nanoelectronics. They self-assemble during silicon deposition on (110) surfaces of fcc metals. Although they have been studied for decades, there are still open questions regarding the specific atomic and electronic structure on different substrates. Especially perplexing is the path from the clean substrate to the SiNRs: the main stages of their development and factors affecting their final structure remain unknown. This contribution reveals insights into the formation of the SiNRs on Au(110), a promising surface for optimal SiNRs growth. The transition from a clean gold single crystal to ordered SiNRs was investigated. Sub-monolayers of Si were deposited on the 2x1-reconstructed Au(110) surface. Low-energy Electron Diffraction (LEED) patterns, angle-resolved photoemission spectra (ARPES) and core-level X-ray Photoelectron spectra (XPS) were recorded at various steps of SiNRs growth. All three techniques revealed the recovery of Au(1x1)-reconstruction during the Si deposition. From detailed XPS analysis a preliminary concept of SiNRs growth on Au(110) can be formulated: at early steps of Si deposition an interface Si/Au-alloy is formed. Upon subsequent Si evaporation SiNRs are formed. Unlike in other metals, like silver, we have realized that the SiNRs grow on top of the alloy. This observation challenges the models proposed to explain the atomic arrangement of the SiNRs and adds complexity to the modelling process. Furthermore, it explains an essential difference between the properties of SiNRs on gold and silver: on silver, the SiNRs are individual, confined within the substrate missing row formed during Si deposition and detachable from the substrate. On gold, Si deposition destroys the intrinsic missing row and leads to the formation of a different structure, which cannot be easily removed from the substrate. This aspect is critical for the applications of these materials.

Studying 2D materials with spatially resolved atom diffraction in scanning helium microscopy

Dr Matthew Bergin[1]
[1]University Of Newcastle, Australia

MS-1: Recent Developments in Surface Microscopy, June 18, 2024, 10:30 - 12:30

Scanning helium microscopy uses a low energy (<100meV) beam of neutral helium atoms as a non-destructive, exclusively surface sensitive tool. It has recently been shown to be possible to use the wave-like nature of the helium to form diffraction patterns from spatially resolved regions of atomically ordered surfaces to determine the local lattice type, orientation, and size [1,2]. Here, recent work is presented that outlines new instrumentation that has been developed to enable moving the detector to directly collect 2D diffraction patterns from a stationary sample. The detector stage has facilitated the study of a range of samples, including MoS2 and MoTe2, where novel imaging modalities can be used to probe the local lattice properties.

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Durable Slippery Liquid Porous Surfaces for drug reduction application

Maria Caruso[1]
[1]Issmc-cnr, Italy

Biointerfaces/Biophysics/Biosensers, June 19, 2024, 10:30 - 12:35

Due to climate change and rising fuel costs, it was necessary to design vehicles that would reduce fuel consumption and gas emissions. The design of marine vehicles for energy efficiency improvement has been a subject of enormous interest in recent years. Inspired by the natural world, where multiple aquatic species have developed systems to reduce friction resistance in underwater conditions. Many researchers have developed water-repellent surfaces where a lubricating liquid is present that allows to maximize the speed of slips and reduce friction resistance when there is a continuous water flow1,2. These surfaces called Slippery Liquid Porous Surfaces (SLIPS) present a microstructured surface, with a low surface energy (<23mN/m) in which a lubricating oil has been infused and stabilized by capillary forces and chemical affinity with the underlying coating 3. In this work, we present, different SLIPS-type coatings, in which we will deposit ceramic nano oxides on alumina obtained by sol-gel and hydrothermal route. Also after depositing a fluorine-free organic layer and infused into lubricating oil, we will check the persistence of the oil in a static way in underwater conditions with measurement of static and dynamic contact angle. Rheometric tests will be carried out for the evaluation of hydrodynamic resistance, immersing the rotor suitably coated with SLIPS surfaces, in a water bath measuring the torque at different angular speeds. The same test will be conducted after immersion of the SLIPS in water for extended periods, to assess the possible degradation of the performances.

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Work Function Dependent Reduction of Transition Metal Nitrides (TMNs) in Hydrogen Environments

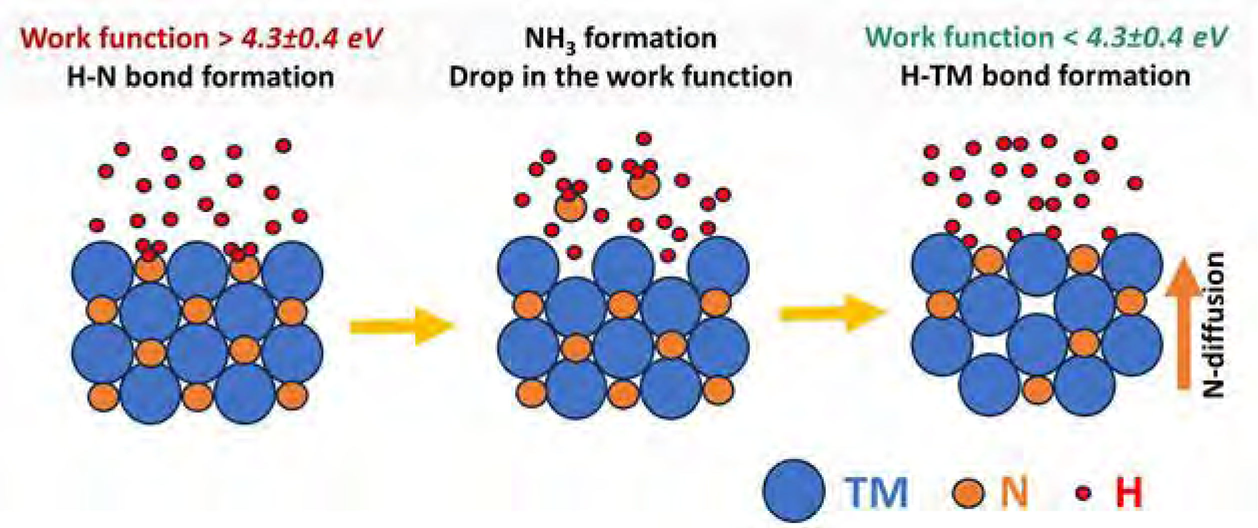
Abdul Rehman[1], Robbert van de Kruijs[1], Wesley van den Beld[1], Marko Sturm[1], Marcelo Ackermann[1]
[1] *University of Twente, Netherlands*

Metal Surfaces - Adsorption, Desorption and Reactions 1, June 17, 2024, 11:00 - 12:35

Hydrogen and its chemistry are highly relevant for applications from green energy (fusion, energy storage, transport) to advanced lithography (plasma, buffer gas, reducing agent). Nevertheless, its proclivity to react with and diffuse into surrounding materials poses a challenge, from degrading sensitive components (sensors, optics) to selective etching of surfaces or metal embrittlement. Hence, it is critical to develop coatings that protect sensitive system components in reactive hydrogen environments. However, predicting the chemical stability of coating materials in hydrogen is not fully understood.

Group IV-V transition metal nitrides (TMNs) are potential candidates for hydrogen-protective coatings due to their exceptional physical properties, yet their chemical stability in hydrogen is less investigated. Based on the change in Gibbs free energy, TMNs would be expected to undergo complete reduction (de-nitridation) in hydrogen radicals (H*) at standard pressure and elevated temperature. However, their reduction reaction spontaneously stops upon reaching a certain reduced state. We show that the reduction of TMN thin films in H* effectively stops when their work functions drop below 4.3±0.4 eV. This value aligns with the value (4.4 ± 0.2 eV) reported by Van de Walle et al. (Nature. 2003), where H+ and H- have equal formation energies in semiconductors and insulators. We propose that the reduction of TMNs in H* depends on whether H* binds to TM-atoms (H+) or N-atoms (H-), determined by the work function of the TMN system. When the work function is below 4.3 ± 0.4 eV, H* preferably bind to TM-atoms, rather than N-atoms. Hence, making it chemically stable as no volatile species form from binding H* to TM-atoms.

We also hypothesize that our model holds for a wider range of transition metal compounds, like carbides and oxides, using the work function as a key parameter for predicting chemical stability of TM compounds in hydrogen environments.



Dioxygen activation at a biomimetic 2D single metal atom catalyst beyond ultra-high vacuum

Stefania Baronio[1], Michela De Col[1], Davide Bidoggia[1], Danilo Comini[2], Dr Mattia Scardamaglia[3], Prof Erik Vesselli[1,4]

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Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 3, June 20, 2024, 11:00 - 13:00

The investigation of 2D metal organic frameworks (MOFs) at surfaces is a hot topic in surface science due to their potential applications also as single atom catalysts (SACs) [1]. Our work focuses on the in situ spectroscopic characterization of a bimetallic MnTPyP-Co framework self-assembled on Gr/Ir(111) and structurally similar to previously investigated Fe- and Co-based systems active towards the oxygen evolution and reduction reactions (OER-ORR) [2,3].

By means of a combined approach exploiting Sum Frequency Generation Spectroscopy (SFG) and Ambient Pressure XPS (AP-XPS), we show how the tetra-coordination of Co ad-atoms by adjacent MnTPyPs affects the overall electronic and vibrational structure of the layer, including the oxidation state of the Mn centers. The bimetallic system is extremely reactive towards O_2: while dioxygen weakly ligates at room temperature and under UHV conditions, at close-to-ambient pressure the molecule undergoes activation and dissociation at the Co sites, and CO oxidation becomes then possible.

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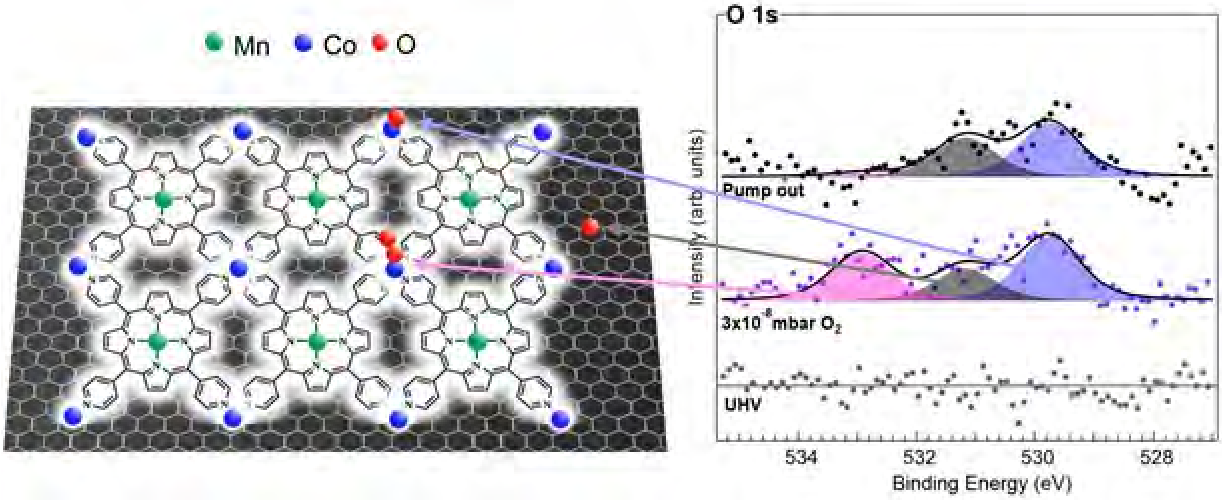

A generic green chemistry surface biofunctionalization cascade; an enzyme activated antibacterial coating

Prof. Miguel Manso Silván[1], Dr. José Ramón Martínez Huerta[1], Dr. John Jairo Aguilera Correa[2], Dr. Jaime Esteban[2], Dr. Juan Rubio Zuazo[3], Dr Rodrigo Calvo Membibre[1]

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Biomaterials 1, June 18, 2024, 10:30 - 12:30

Biofunctionalization is an industrially demanded process requiring organic solvents and crosslinking molecules. The biofunctionalization of substrates with enzymes through greener processes is thus highly demanded. We propose a process based on titanate assisted organosilanized films and genipin as a natural cross-linking agent. The different stages of surface functionalization were characterized using XPS and FTIR. Elemental and molecular fragment identification were consistent with the silane-genipin-enzyme immobilization cascade. The efficiency of the bacterial proliferation was evaluated using a Clostridium perfringens strain on lysozyme-functionalized surfaces, as well as by evaluating the disaccharide degradative activity of α-amylase biofunctionalized surfaces. The microbiology evaluation protocol determined significant differences in the concentration of bacteria adhered to the surface with lysozyme (LZ) and the rest of the surfaces ($P < 0.05$). The concentration of bacteria present in the medium was also estimated, determining that there were no significant differences between the supernatants of each sample, consequently stating that the proposed biofunctionalization process does not affect the concentration of planktonic bacteria in the medium ($P > 0.05$). Furthermore, the biochemical evaluation of the surfaces functionalized with α-amylase determined significant differences in the concentration of D-glucose ($P < 0.05$). In conclusion, the protocol shows favorable results, facilitating the possibility of obtaining biofunctionalized surfaces in a simple way with satisfactory yields.

Structural and electronic properties of ultrathin Sn deposited on Pt(111) studied by low energy electron microscopy

Ewa Mlynczak[1], Dorota Wilgocka-Ślęzak[1], Ewa Madej[1], Ardra Surendran[1], Smibin Shaju[1], Nika Spiridis[1]
[1]Jerzy Haber Institute Of Catalysis And Surface Chemistry Polish Academy Of Sciences, Poland

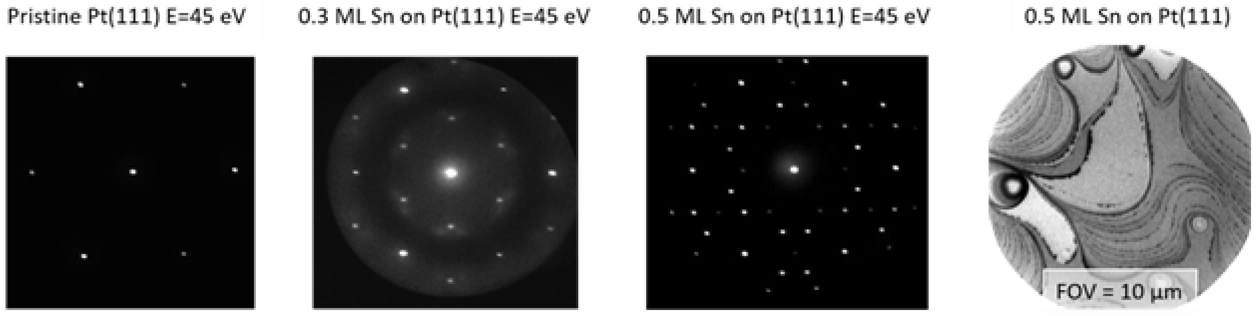
Metal and Oxide Single Crystal Surfaces - Growth, Preparation, and Characterisation, June 18, 2024, 16:00 - 17:30

Sn films grown on Pt(111) have been the subject of considerable scientific interest thanks to their interesting catalytical properties. Platinum is a well-known catalyst, with the drawbacks of its use related to the high cost of the material and fast self-poisoning. It is known, that adding Sn to Pt results e.g. in improved stability, much higher selectivities for isomerisation and aromatisation in hydrocarbon conversion reactions [1] as well as improved performance in the CO oxidation [2]. However, the mechanism responsible for such beneficial effects is not clear yet, with the effects of strain and modification of the electronic structure suggested to play a role [3].

We have performed an investigation of the Sn growth on Pt(111) at room temperature using low energy electron microscopy (LEEM) tracking changes in the sample structure with the amount of deposited material. The observed superstructures varies between $\sqrt{3}$ x $\sqrt{3}$ (R 30°), c(4x2) and $\sqrt{5}$ x $\sqrt{5}$ (R 26.6°) when the coverage increases between 0.3 ML to 0.8 ML. For the coverage between 0.3ML and 0.5 ML we have observed a c(4x2) LEED pattern and a corresponding intriguing real space image, with strong contrast differences between particular atomic terraces of Pt(111) (Fig.). We analyze this peculiar structure with the help of the spatially resolved I(V) curves measured for the structure of interest as well as for the few reference structures. We will discuss the growth mechanism that leads to the different phases forming on separate atomic terraces of Pt(111), being uniform within a single terrace.

[1] R. Burch and L.C. Garla J. Catal. 71, 360 (1981)
[2] H. J. Wallander et al. J. Phys. Chem. C 126, 6258 (2002)
[3] J. R. Kitchin et al. Phys. Rev. Lett. 93, 156801 (2004)

This research was funded by National Science Centre, Poland (NCN), grant number 2022/46/E/ST3/00184.


Pristine Pt(111) E=45 eV
0.3 ML Sn on Pt(111) E=45 eV
0.5 ML Sn on Pt(111) E=45 eV
0.5 ML Sn on Pt(111)

Self-Organised Nanostructuring of Solid Surfaces by Ion Beam Irradiation

Mr Mogtaba Mekki[1,2], **Dr Michael Hunt**[1]
[1]Department of Physics, University of Durham, United Kingdom, [2]Department of Physics, College of Engineering and Physics, King Fahd University of Petroleum and Minerals, Kingdom of Saudi Arabia

Supported Nanostructures, June 17, 2024, 14:00 - 15:30

The removal of species from a solid surface under irradiation with ions of relatively low energy (0.5 – 10 keV) can lead not only to surface roughening but also self-organization of quasi-periodic nanostructures (ripples, dots and holes) under appropriate conditions [1]. Such self-organized structures have potential for a broad range of application including anti-reflective surfaces, opto-electronics and information storage. However, greater understanding of their formation is required for widespread application to be realized.

We report and compare self-organization of nanometre-scale ripple-like structures at the surface of Si(111), polycrystalline Ni and polycrystalline Au films induced by irradiation with a broad Ar ion beam. The evolution of surface topography with ion beam flux, global incidence angle, and fluence was studied using ex-situ atomic force microscopy. The development of these structures was reproduced by numerical solution of a continuum equation describing the evolution of surface morphology under ion irradiation modified from that introduced by Makeev, Cuerno and Barabasi [2], using realistic coefficients derived from material properties.

We demonstrate that differences observed in pattern formation on the two metal surfaces under the conditions studied, such as wavelength stability and exponential growth of interface width compared with wavelength coarsening and interface width saturation on Si(111), can be understood in terms of a cross-over between linear and non-linear behaviours. The global transition of the interface width from smoothing to roughening and associated variation of the structural kinetic amplification rate factor have been captured and explained. Our analysis demonstrates that initial surface interface width is crucial as it seeds the development of the quasi-periodic structures. These results may, in future, be utilised to controllably tailor quasi-periodic surface nanostructures by a straightforward single-step process.

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Langmuir-Hinshelwood Kinetics in Atmospheric Pressure CVD Growth of Few-Layer MoS2 on Silicon

Dr Taghreed Alsulami[1], Professor Lidija Siller[2], Dr Michael Hunt[1]
[1]Department of Physics, University of Durham, United Kingdom, [2]School of Engineering, University of Newcastle, United Kingdom

Spectroscopy and Microscopy of Nanostructures Modelling Nanostructure Properties, June 20, 2024, 11:00 - 13:00

Since the first production of monolayer and few-layer MoS_2 by micromechanical exfoliation there has been an enormous amount interest in this material due to a band gap which is tunable with thickness [1], opening up many potential applications in nanoscale opto-electronics. Atmospheric Pressure Chemical Vapour Deposition (AP-CVD) [2] is a highly attractive route for the growth of MoS_2 thin films and therefore a complete understanding of the growth process is desirable.

In this work, AP-CVD was used to synthesise MoS_2 layers on silicon substrates using MoO_3 and S precursors, and the influence of S vapour pressure (p(S)) on morphology and composition is investigated at substrate temperatures between 550 and 700ºC. Ex-situ Atomic Force Microscopy (AFM) and Raman Spectroscopy indicate that MoS_2 islands and thin films were typically around 2-3 monolayers thick. Scanning Electron Microscopy (SEM) was used to determine global surface coverage and, for a given growth time, we observe a very strong variation in coverage with p(S) at each substrate temperature, with MoS_2 coverage decreasing steeply with increasing sulphur pressure. The observed variation of coverage can be successfully fitted by the Langmuir-Hinshelwood model of growth kinetics, usually applied to reactions on well-defined crystalline surfaces. Suppression of MoS_2 growth with increasing p(S) can then be understood in terms of increasing site-blocking by adsorbed sulphur.

X-ray Photoelectron Spectroscopy (XPS) was used to determine MoS_2 composition as a function of p(S) and provided clear evidence of increasing sulphur vacancy concentration with decreasing p(S). Hence, the conditions of high p(S) which produced the most stoichiometric MoS_2 were associated with the slowest growth kinetics, indicating a tension between coverage and perfection in AP-CVD of MoS_2.

[1] K.F. Mak et al., Phys. Rev Letts. 105 (2012) 136805
[2] S. Wang et al., Nanotechnology 27 (2016) 085604.

Cobalt oxide based model system - growth and structure studies

Karel Mašek[1], Oleksandr Leiko[1], Josef Myslivečk[1], Viktor Johánek[1]
[1]Charles University, Czech Republic

Thin Film Growth Simulation, June 18, 2024, 10:30 - 12:30

Our experiment showed that cobalt oxide layers exhibit interesting catalytic properties in methanol to hydrogen conversion [1]. Fundamental physico-chemical properties are often performed on model well-defined systems. Here we present the growth and structure studies of well-ordered CoO and Co3O4 ultra-thin films supported on copper and iridium single crystals by repeated cycles of metallic cobalt deposition, RF plasma oxidation, and temperature annealing. The films were investigated by Reflection High-Energy Electron Diffraction (RHEED), X-ray Photoelectron Spectroscopy (XPS) and other surface sensitive techniques. The diffraction patterns revealed CoO cubic and Co3O4 spinel structures with (111) epitaxial plane parallel to the substrate surface. The homogeneous chemical state of the layers and different deposit-substrate interaction for copper and iridium were confirmed by XPS. The formation of cobalt oxide – substrate interface was deduced from RHEED patterns. The results are compared to the layers prepared by Physical Vapor Deposition (PVD) [2].

The cobalt oxide epitaxial layers were further used as substrates for deposition of palladium particles of nanometer size. The palladium was deposited in several steps and the structure and palladium–cobalt oxide interaction were studied by RHEED and XPS, respectively. The results showed three-dimensional growth of palladium particles with (111) epitaxial plane. The resulting surface morphology of the palladium–cobalt oxide model system was confirmed by Atomic Force Microscopy (AFM). Our studies proved that these layers can be successfully used for model studies of physical and chemical properties of pure and palladium doped catalysts.

[1] V. Johanek, P. Svenda, K. Masek, Int. J. of Hydrogen Energy 46 (2021) 17197
[2] V. Uvarov, J. Krutel, K. Masek, J. Myslivecek, V. Johanek, App. Surf. Sci. 593 (2022) 153430

Vacuum Upgrades & Developments at ISIS – The UK Neutron and Muon Research Facility

Sunil Patel[1]
[1] *ISIS Facility, United Kingdom*

Large Vacuum Systems of Particle Accelerators, June 18, 2024, 10:30 - 12:30

ISIS Neutron and Muon Source is based at the STFC Rutherford Appleton Laboratory (RAL) in Oxfordshire and is a world-leading centre for research in the physical and life sciences. It is owned and operated by the Science and Technology Facilities Council, one of the councils that forms UK Research and Innovation (UKRI).

In December 2024 the ISIS facility will celebrate 40 years of operation. Over these years the vacuum systems used in the linac, synchrotron, target stations and also on the many experimental instruments, have been upgraded to improve reliability and to meet the challenges of working at the cutting edge of science and technology.

In this presentation I will discuss the work carried out to achieve these improvements in vacuum performance and some of the challenges faced meeting the technical specification of these projects.

I will also discuss the Endeavour programme, a £90 million investment to increase experimental capacity at ISIS that will see the construction of 4 new instruments and 5 upgrades on ISIS.

Finally I provide an update on ISIS 2 project – a proposed new facility to the RAL site.

Tetrafluoromethane influence on carbon-based nanocomposite nc-CrC/a-C thin films

Dr Wojciech Pawlak[1], Adam Roślak[1], Wioletta Strzałkowska[1], Józef Doering[1], Marcin Makówka[1], Anna Jędrzejczak[1], Łukasz Kołodziejczyk[1], Jecek Balcerzak[1], Łukasz Jóźwiak[1], Ireneusz Piwoński[2]

[1] Lodz University of Technology, Poland, [2] University of Lodz, Poland

Advanced Thin Film Characterisation, June 19, 2024, 16:00 - 17:30

Carbon-based nanocomposite coatings are known for very good tribological properties. However, fluorination in the presence of CF4 has rarely been attempted. The work included the preparation of an nc-CrC/a-C nanocomposite coating on a gradient CrCN sublayer and checking the effect of CF4 fluoridation in the last phase of deposition. The XPS method revealed that fluorine does not combine with carbon in the nanocomposite coating and is instead bound to chromium at the expense of chromium carbides.

Searching for the evidence of correlated two-electron tunneling in field emission resonance from light emission on Ag(100) surfaces

Dr. Wei-Bin Su[1], Dr. Shin-Ming Lu[1], Mr. Ho-Hsiang Chang[1], Dr. Wen-Yuan Chan[1], Prof. Chia Seng Chang[1]
[1] *Institute of Physics, Academia Sinica, Taiwan*

Electronic Structure of Materials, Surfaces and Interfaces, June 18, 2024, 10:30 - 12:30

Our previous studies have discovered that the linewidth of field emission resonance (FER) observed on the surfaces of MoS2 and Ag(100) using scanning tunneling microscopy can vary by up to one order of magnitude [Fig. 1(a)]. This phenomenon originates from a correlated two-electron tunneling through the exchange interaction [1,2]. Due to this mechanism, the quantized state in FER is occupied by two electrons of opposite spin, different from the conventional viewpoint that FER quantized state is occupied by only one electron since field emission is one-electron tunneling process. Because FER electrons are excited electrons, the relaxation of FER electrons emits light. In this study, we investigated whether light emission of FER provides evidence regarding paired electrons. We discovered on the Ag(100) surface that optical spectra revealed two types of peak signal that can be related to the paired electron, as shown in Figs. 1(b) and 1(c). The twin-peak feature (peaks a and b) in Fig. 1(b) indicates a spin-spin interaction between electrons in which a triplet state is formed. The 3-eV peak (peak c) in Fig. 1(c) indicates an Auger-type excitation in which, one electron is excited to a higher energy state by photons resulting from the radiative decay of surface plasmons induced by another electron. Therefore, the features of the twin peaks and the 3-eV peak are the evidence of correlated two-electron tunneling.

[1] W. B. Su et al., Nanoscale Adv., 2, 5848 (2020).
[2] W. B. Su et al., Phys. Rev. B 105, 195411 (2022).

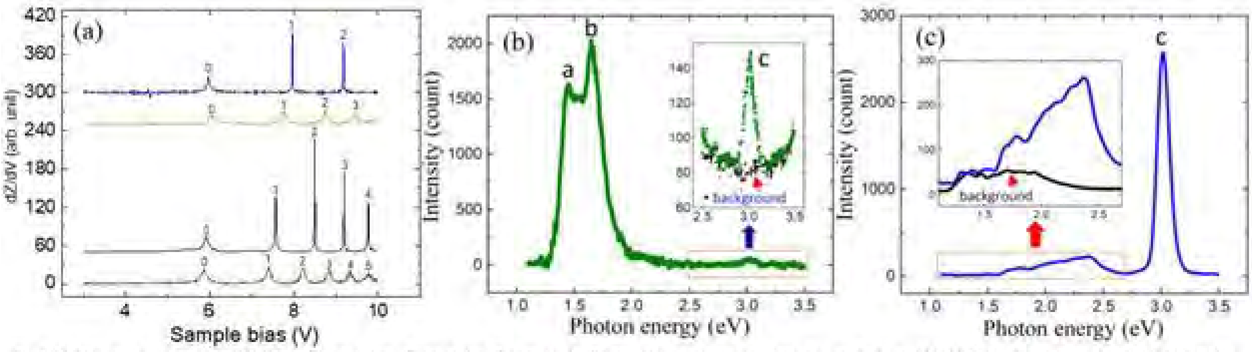

Fig. 1 (a) FER spectra showing a FER linewidth variation of one order of magnitude. (b) Optical spectrum showing twin peaks (a and b). (c) Optical spectrum showing 3-eV peak c.

Atomic Layer Deposition of HfS2 on Pristine and Functionalized Oxide Interfaces: Model Studies from Surface Science

Georg Fickenscher[1], Lukas Fromm[2], Julien Steffen[2], Andreas Görling[2], Jörg Libuda[1]
[1]Interface Reasearch and Catalysis, ECRC FAU Erlangen-Nürnberg, Germany, [2]FAU Erlangen-Nürnberg, Germany

Oxide Surfaces and Nanomaterials - Spectroscopy, Imaging and Physicochemical Processes, June 18, 2024, 10:30 - 12:30

Transition-metal dichalcogenides (TDMCs) like HfS2 have drawn lots of attention in the field of microelectronic materials. Innovative deposition methods like atomic layer deposition (ALD) open new possibilities for the processing of low-dimensional semiconductors based on TMDCs. ALD allows controlling layer thicknesses precisely and achieving excellent layer quality. However, to achieve continuous, defect-poor, and pinhole-free films, control over the nucleation process is essential.
In this study, we investigated the initial nucleation processes during ALD of HfS2 on Co3O4(111) surface under ultrahigh-vacuum conditions (UHV). The nucleation and growth steps were monitored by infrared reflection absorption spectroscopy (IRAS).[1] HfS2 was grown by sequential dosing of tetrakis(dimethylamido)hafnium (TDMAH) and D2S onto Co3O4(111) exposing well-defined OD groups and partially dissociated OD/D2O aggregates.
We found that the initial half cycle of the ALD process comprises several regimes. Initially, TDMAH loses all ligands by reacting with mobile OD/D2O species. With increasing TDMAH exposure, the stoichiometry of the deposit changes. We observed the formation of partially hydrolysed Hf(NMe2)n(O)x(OD)m species and the consumption of OD/D2O aggregates. Finally, the Hf(NMe2)n(O)x(OD)m species react with TDMAH until all OD groups are consumed.
To control the nucleation process, we have investigated ALD of HfS2 on both functionalized and non-functionalized self-assembled-monolayers (SAMs) on Co3O4(111).[2] We compared the growth on the hydrocarbon-terminated biphenyl-4-carboxylic-acid (BP4CA) SAM to the OH-terminated 4′-hydroxy-4-biphenylcarboxylic-acid (4HBP4CA) SAM. We observed that the deposition of HfS2 can be efficiently controlled by the surface termination. We observed no deposition on the BP4CA-SAM, while HfS2 grows on the OH-terminated 4HBP4CA-SAM. For the 4HBP4CA-SAM, the initial nucleation again consists of several regimes with the stoichiometry of the Hf(NMe2)nORm nuclei changing during the first half-cycle.

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Initial Stages of Water Absorption on CeO2 Surfaces at Very Low Temperatures for Understanding Anti-Icing Coatings

Anna Cecilie Aasland[1], Simon P. Cooil[2], Damir Mamedov[3], Håkon I. Røst[4], Johannes Bakkelund[1], Zheshen Li[5], Smagul Karazhanov[3], Justin W. Wells[1,2]

[1]Department of Physics, Norwegian University of Science and Technology (NTNU), Norway, [2]Centre for Materials Science and Nanotechnology, University of Oslo, Norway, [3]Department for Solar Energy Materials and Technologies, Institute for Energy Technology), Norway, [4]Department of Physics and Technology, University of Bergen, Norway, [5]Department of Physics and Astronomy - Centre for Storage Ring Facilities Aarhus University, Denmark

Water and Environmental Surfaces, June 19, 2024, 16:00 - 17:30

Anti-icing coatings preventing ice from forming on surfaces can reduce damage and dangerous situations in society [1]. Since different applications require different properties of the anti-icing coatings, it is important to find coatings suitable for their application, and techniques which can efficiently evaluate the relevant properties.

X-ray photoelectron spectroscopy (XPS) is routinely used to study the chemical composition of coatings. However, despite its ability to detect small amounts of H_2O, XPS is not commonly used to investigate the early stages of H_2O absorption or anti-icing behaviour on surfaces.

CeO_2 coatings are hydrophobic, robust, and transmit light [2], but their anti-icing properties and how their surface chemistry initially changes when they are cooled and exposed to H_2O have not been studied.

To investigate this, CeO_2 coatings were grown by sputter deposition and measured with XPS before and after cooling the coatings to ≈100K and exposing them to H_2O at an atmosphere of 1×10^{-8} mbar.

The XPS measurements in Fig. 1 show that little to no ice forms on the surface of CeO_2 after H_2O exposure. Contrarily, the sampleholder spectrum clearly indicates that there is ice on the Mo sampleholder on which the CeO_2 samples were mounted. This lack of ice on CeO_2, even when it is present on the surrounding areas, suggests that thin films of CeO_2 have great potential as future anti-icing coatings. Furthermore, the measurements demonstrate that XPS is a sensitive technique which can be used to simultaneously investigate the chemical composition and the anti-icing properties of surfaces.

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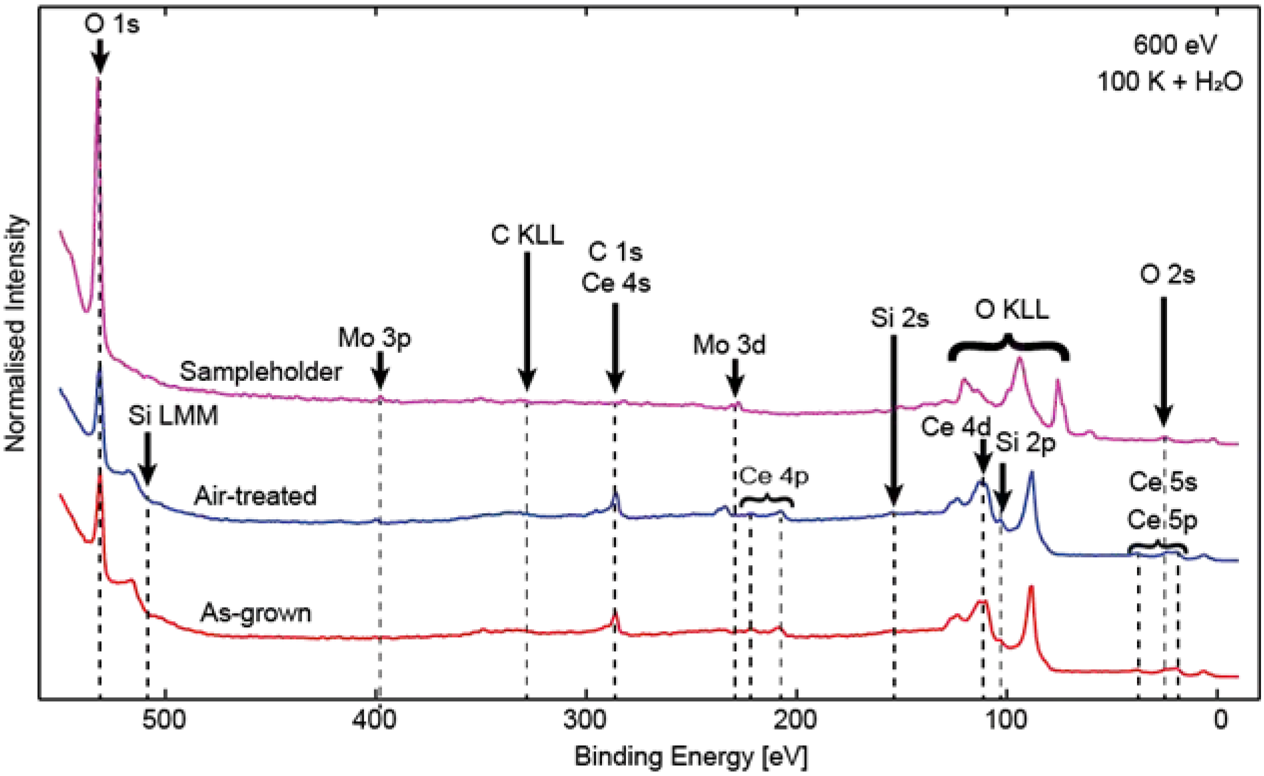
[2] D. Mamedov et. al, Materials Today Communications 35, 106323 (2023).

Figure 1: XPS scan of two CeO_2 samples (As-grown and Air-treated) and a Mo sampleholder measured with photoexcitation energy hv=600eV at T=100K after depositing H_2O.


O 1s
600 eV
100 K + H₂O
C KLL
C 1s
Ce 4s
O 2s
Mo 3p
Mo 3d
Si 2s
O KLL
Sampleholder
Si LMM
Ce 4d
Si 2p
Ce 4p
Air-treated
Ce 5s
Ce 5p
As-grown
Normalised Intensity
500
400
300
200
100
0
Binding Energy [eV]

Vacuum System for Measuring Diffusivity and Permeability: Case Studies on Zerodur Glass, Kapton®, and PET Plastic

Prof. Sefer Avdiaj[1], Ms Lyra Hoxha[2], Mr. Ibrahim Hameli[1]
[1]University of Prishtina. Department of Physics, Kosova, [2]University of Wurzburg, Germany

Special Vacuum Chambers and Components, June 17, 2024, 16:00 - 17:35

This paper introduces an innovative vacuum system designed for accurate measurements of diffusivity and permeability in various materials. We present the development and application of this system, alongside experimental data for zerodur glass, Kapton®, and Polyethylene terephthalate (PET) plastic.
Our vacuum system is carefully engineered to create ultra-high vacuum conditions, essential for accurate diffusivity and permeability measurements. It comprises state-of-the-art components carefully integrated to ensure minimal interference and maximal precision. The system's design emphasizes versatility, enabling the study of a wide range of materials with varying properties.
Utilizing this system, we conducted a series of experiments to investigate the diffusivity and permeability characteristics of zerodur glass, Kapton®, and PET plastic. Our methodology involved subjecting samples to controlled vacuum environments on one side and the other side is subject a controlled varying higher pressure while monitoring their response over time. Through careful data collection and analysis, we obtained comprehensive insights into the diffusion and permeation behaviors of these materials.
Our results reveal distinct diffusivity and permeability profiles for each material. Zerodur glass exhibits low diffusivity and impermeability, making it suitable for applications requiring exceptional barrier properties also for gases such Helium. In contrast, Kapton® and PET plastic demonstrate higher diffusivity and permeability, suggesting potential applications in situations where controlled gas transfer is desired.
This research contributes to the understanding of material behavior under vacuum conditions and showcases the capabilities of our innovative vacuum system.

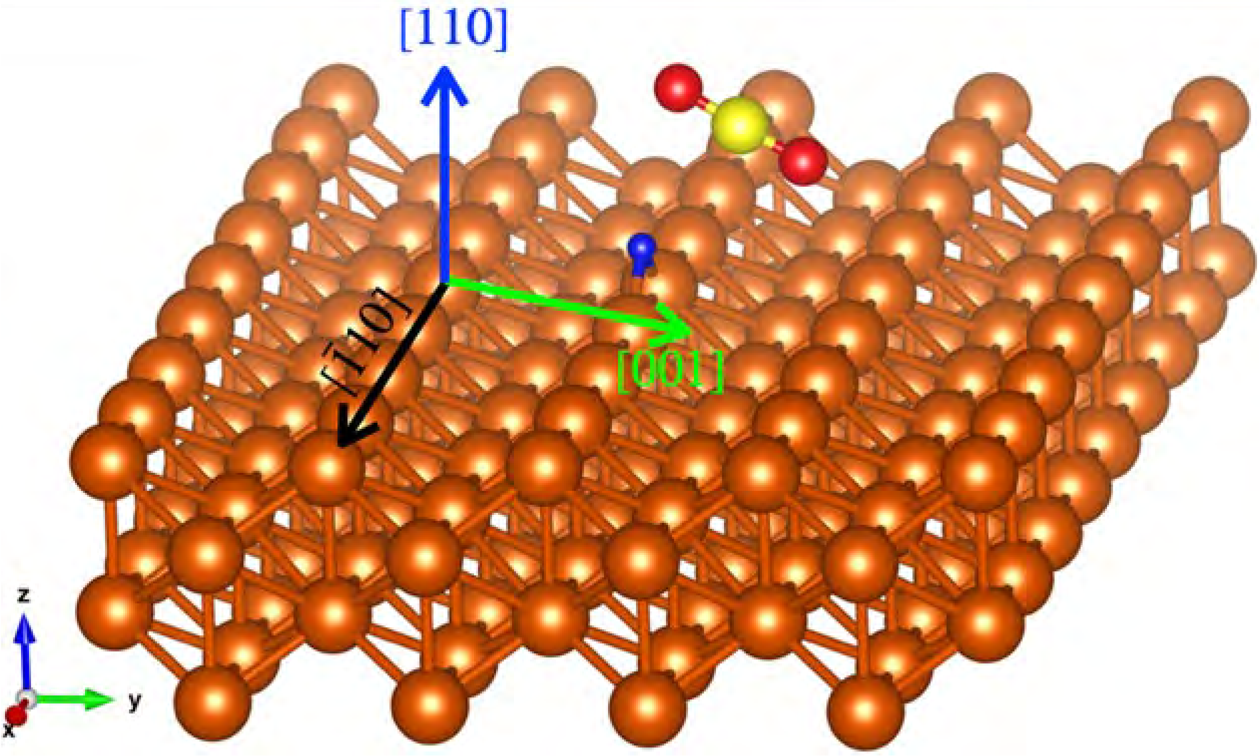
Direction Dependence of CO2 Incidence on Cu(110) Lattice Vector in the CO2 Hydrogenation Reaction

Fahdzi Muttaqien[1], Wa Ode Nur Fitriah Rajaelo[1], Fikri Akbar Mubarok[1], Atthar Luqman Ivansyah[1], Septia Eka Marsha Putra[3], Suprijadi Haryono[2], Yoshitada Morikawa[4]

[1]Faculty of Mathematics and Natural Sciences, Institut Teknologi Bandung, Indonesia, [2]Instrumentation and Computational Physics Research Group, Faculty of Mathematics and Natural Sciences, Institut Teknologi Bandung, Indonesia, [3]Engineering Physics, Institut Teknologi Sumatera, Indonesia, [4]Department of Precision Engineering, Graduate School of Engineering, Osaka University, Japan

Catalysis and Electrocatalysis including Single Atom and In Operando Studies 2, June 19, 2024, 16:00 - 17:30

The mechanistic insight of methanol synthesis on Copper (Cu) catalyst from CO/CO_2 hydrogenation has been studied extensively in more than decades. Due to the complexity of methanol synthesis path, one fine Cu surface structure, which is composed by step and kink sites or other defects, may not accommodate the catalytic enhancement of all the intermediate steps. Formate (HCOO) formation from CO_2 hydrogenation is rate determining step in the methanol synthesis, and one of the Eley-Rideal (ER) type reaction. The ER type reaction suggests that incoming CO_2 directly reacts with pre-adsorbed hydrogen without making any interaction with surfaces. In this research, we examine the effect of CO_2 incoming direction as a function of Cu(110) lattice vectors and the role of surface line-defects to the mechanism of HCOO formation. We obtain that the formation energies of HCOO formation depends on CO_2 incoming direction relative to the surface lattice vectors. Those energies are lower than that of reactions on Cu(111), indicating surface-dependence of HCOO formation on Cu catalysts. However, surface line-defects on Cu(110) produces similar formation energies as Cu(111). We believe our work may improve the understanding of the catalytic reaction of CO_2 hydrogenation into HCOO and helps develop molecular beam technique to enhance reaction rate of HCOO formation.



W–Zr thin-film metallic glasses: Thermal behavior and evolution of properties

Sarka Zuzjakova[1], Michaela Cervena[1], Stanislav Haviar[1], Jiri Houska[1], Petr Zeman[1]
[1]University of West Bohemia, Czech Republic

Functional Coatings 1, June 17, 2024, 14:00 - 15:30

Metastable solid materials such as amorphous or nanocrystalline alloys, supersaturated solid solutions, high-temperature or high-pressure phases persisting at normal conditions, have been of great interest due to a possibility to explore novel structures with unknown properties. These materials are kinetically determined and can be therefore synthesized only by non-equilibrium processes. Recently, we have shown that using magnetron sputter deposition, we were able to prepare W–Zr thin-film alloys with several metastable structures in respect to the equilibrium phase diagram [1]. The present study focuses on systematic investigation of the evolution of properties of W–Zr thin-film metallic glasses with three different Zr contents (32 at.%, 48 at.% and 61 at.%) after annealing in synthetic air. The films were annealed to temperatures in the range 300°C–600°C and after cooling down to room temperature the evolution of their structure, elemental composition, hardness, electrical resistivity and optical properties was studied. Attention was also paid to their oxidation behavior during dynamical heating to 600°C in synthetic air. The results obtained show a very interesting thermal behavior during annealing in air. No protective surface oxide layer grows on the surface of the films up to 550°C, but oxidation leads to the formation of very compact, homogeneously oxidized substoichiometric W–Zr–O films with an amorphous structure. The mass gain increases smoothly for all three films as oxygen penetrates the entire volume of the amorphous films. The lowest final mass gain and the latest onset of oxidation (≃350°C) is observed for the lowest Zr content (32 at.%) investigated. Controlled oxidation of these films to selected temperatures leads to a significant enhancement of mechanical properties and tuning of their optical and electrical properties. All evolution trends will be thoroughly presented.

References

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Phosphorus buffer layer for electronic decoupling of Zinc-Tetraphenylporphyrin from a metal substrate: a combined spectroscopy and microscopy study

Mattia Bassotti[1], Mr Carlo Calcatelli[1], Dr Luca Floreano[2], Dr Luca Schio[2], Dr Dimas G. De Oteyza[3], Mr Sergio Salaverria Bugallo[3], Dr Giacomo Giorgi[4], Dr Frederik Schiller[5], Dr Alberto Verdini[1,2]

[1]Dipartment of Physics and Geology, University of Perugia, Italy, [2]IOM-CNR, Laboratorio TASC, Italy, [3]Nanomaterials and Nanotechnology Research Center (CINN), CSIC-UNIOVI-PA, Spain, [4]Department of Civil & Environmental Engineering (DICA), Università di Perugia, Italy, [5] Centro de Física de Materiales CSIC/UPV-EHU-Materials Physics Center, Spain

Self-Assembly, Characterisation and Reactivity of 2D Structures of Molecules at Surfaces, June 21, 2024, 10:30 - 12:00

Porphyrins are organic molecules playing vital role in many biological fundament processes, including oxygen transport (hemoglobin) and photosynthesis (chlorophyll). Their versatility and remarkable electronic properties have recently boosted the scientific interest on this class of compounds, leading to diverse applications in fields such as sensors, catalysis and organic electronics [1]. However, porphyrins thin-film deposited on a interacting metal substrate can undergo alteration of the HOMO/LUMO features and molecule geometry [2], hindering their utilization in actual devices. In this work, we introduce a novel strategy to address this problem, employing a phosphorus (P) monolayer to inhibit electronic transfer between the Cu(110) substrate and a Zinc-Tetraphenylporphyrin (ZnTPP) monolayer (ML). Near Edge X-Ray Absorption Spectroscopy (NEXAFS) was exploited to compare the empty states of a ZnTPP ML deposited on P/Cu(110) and on bare Cu(110), showing that P interlayer preserves the LUMO features, which are quenched if ZnTPP is grown on the bare Cu(110) (see Fig.1a). Ultra-Violet Photoemission Spectroscopy (UPS) combined with Scanning Tunneling Spectroscopy (STS) confirms this, and further correlates the LUMO with the HOMO levels (see Fig.1b) for a better understanding of the decoupling effectiveness. Scanning Tunneling Microscopy (STM) was performed together with Density Functional Theory (DFT) calculations to delve into the details of the ZnTPP/P interaction mechanism, enabling us to correlate non-equivalent molecules with non-equivalent P atoms anchoring sites (see Fig. 1c).

References

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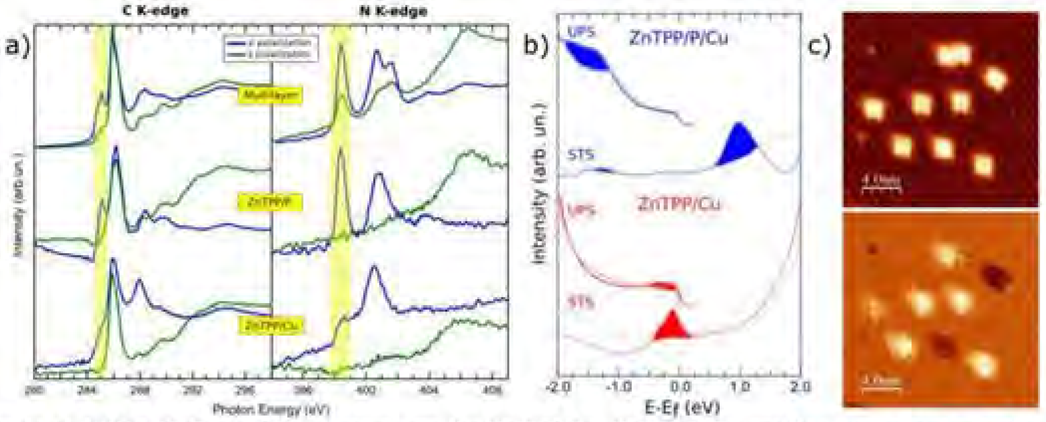

Figure 1: a) NEXAFS C and N K-edge spectra for ZnTPP/Cu, ZnTPP/P/Cu and Multilayer systems, the latter serving as reference for a low-interacting ZnTPP layer. In yellow is highlighted the LUMO level, which appears quenched without P interlayer, while preserved and similar to the multilayer case for the ZnTPP/P system; b) UPS and STS spectra taken for ZnTPP on bare copper (red) and on P/Cu (blue). The filled areas are used to spot features changes between the systems, in particular the unoccupied level at 1eV for ZnTPP/P/Cu that shifted to a HOMO level for ZnTPP/Cu system, in response to the metal electronic transfer. c) STM topography (top) and conducting map (bottom) reveal the non-equivalency of ZnTPP molecules on top of P.

Evolution of atomic-scale structure and vibrational properties of Graphdiyne nanoribbons: an insight into novel 2D carbon allotropes

Alice Cartoceti[1], Paolo D'Agosta[1], Francesco Tumino[2], Simona Achilli[3], Guido Fratesi[3], Nicola Manini[3], Giovanni Onida[3], Alessio Orbelli Biroli[4], Valeria Russo[1], Andrea Li Bassi[1], Carlo Spartaco Casari[1]
[1]Department of Energy, Politecnico di Milano, Italy, [2]Department of Chemistry, Queen's University, Canada, [3]Department of Physics 'Aldo Pontremoli', Università degli Studi di Milano, Italy, [4]Department of Chemistry, Università di Pavia, Italy

Carbon Materials 2, June 19, 2024, 10:30 - 12:35

Graphdyines (GDYs) are novel 2D carbon allotropes with mixed sp-sp2 hybridization, characterized by highly appealing and tunable optoelectronic properties [1-2]. On-surface synthesis (OSS) techniques not only allow the obtainment of extended 2D carbon networks with engineered structure on metallic substrates [3], but they also pave the way for in situ scanning-probe microscopy/spectroscopy (STM/STS) investigations at the molecular level, allowing to unveil GDYs structural and electronic properties [4-5]. Herein, we present a study on structural and vibrational properties of on-surface synthesized (OSS) 1,4-bi(bromoethynyl)benzene (1,4-bBEP) networks on different metallic surfaces, namely Au(100), Au(111) and Ag(111). The morphological and atomic-scale structure evolution was investigated through scanning tunneling microscopy (STM), while Raman spectroscopy unveiled their vibrational properties. Thanks to the combination of these two complementary techniques, it was possible to perform a punctual in situ monitoring of the networks' transition from metalorganic (MoF) to covalent organic (CoF), following a step-like annealing temperature increase. The as-deposited MoF network appears as densely packed and highly oriented 2D domains, i.e. nanoribbons, composed of self-assembled 1D metal-organic chains. On the other side, the annealed system shows a progressive disordering of the chains within the 2D domains following the thermally-activated removal of the metal adatoms forming the covalent network, as suggested by the evolution of distinctive Raman features, associated with sp and sp2 contributions. These findings contribute to understanding the growth mechanism and the structural and vibrational properties of 1,4-bBEB 2D networks on metal surfaces, enabling the design of novel functional carbon nanostructures.

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A non-obvious source of surface meandering

Marta Chabowska[1], Hristina Popova[2], Magdalena Załuska - Kotur[1]
[1]Institute of Physics Polish Academy Of Sciences, Poland, [2]Institute of Physical Chemistry Bulgarian Academy of Sciences, Bulgaria

Advances in Experimental and Theoretical Methods 3, June 17, 2024, 16:00 - 17:35

The surface morphology plays an important role to fabricate electronic and optoelectronic devices. The observed various surface patterns are consequence of the kinetic effects of epitaxial growth process on the surface including step edges. Particularly, Ehrlich-Schwoebel barrier (ESB), which is an additional diffusion barrier crossing down the step and attach to the lower step edge, is a decisive factor for the morphology. It is well known that the presence of ESB results in various interesting surface phenomena including step meandering.

Our approach to the phenomenon of surface meandering is based on looking at the surface from the point of view of the potential at the surface. We introduce the model which show how surface pattern depends on this potential. Results obtained on a basis of a new approach to previously introduced (2 + 1)D vicinal Cellular Automaton model [1-2] led us to a non obvious conclusion: the mere presence of the potential channel at the bottom of the step is sufficient to obtain meanders at the surface. We analyze how the meander wavelength depends on various parameters such as potential depth, diffusion rate, initial particles concentration. Next, we show how the additional presence of ESB changes the obtained structures.

Fig. 1. Meanders obtained for the initial particles concentration $c_0=0.003$, number of diffusional steps nDS=5, terrace length $l_0=5$, simulation time $t=10^6$ and potential channel with jump probability out of it given by P=exp(-2.5) a) without b) with ESB. System size 200 x 300.

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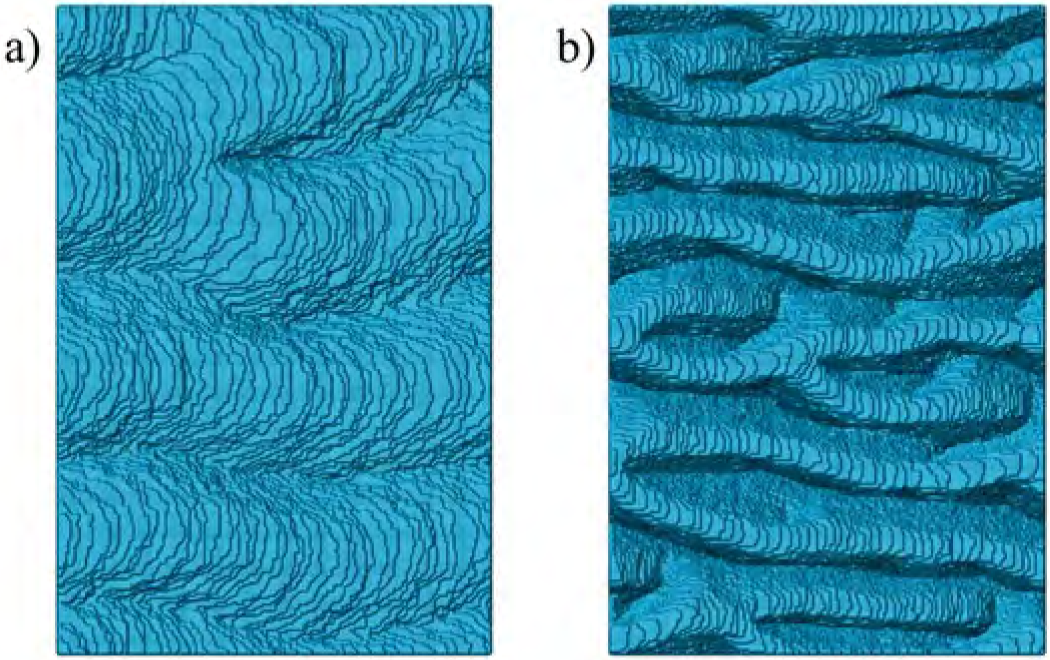
Acknowledgments: Research is financially supported by The Polish National Center for Research and Development (grant no. EIG CONCERT JAPAN/9/56/AtLv AlGaN / The authors thank prof. V. Tonchev for useful discussions and collaboration.


a)
b)

Ab initio Simulation of Molecular Crystal Regrowth from Solution

Mr Huanyu Zhou[1,2], Nicholas M. Harrison[1,2]
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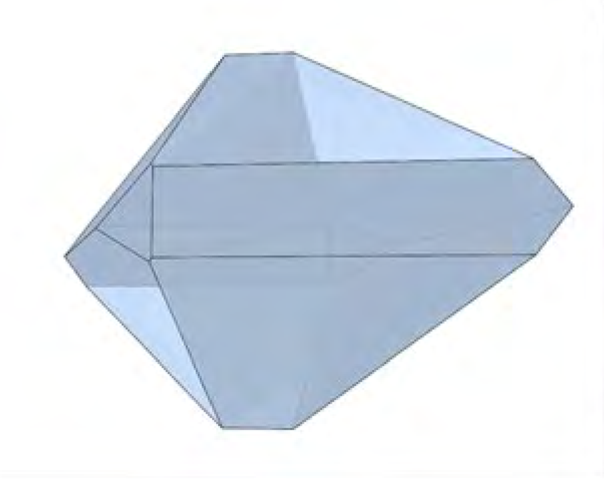
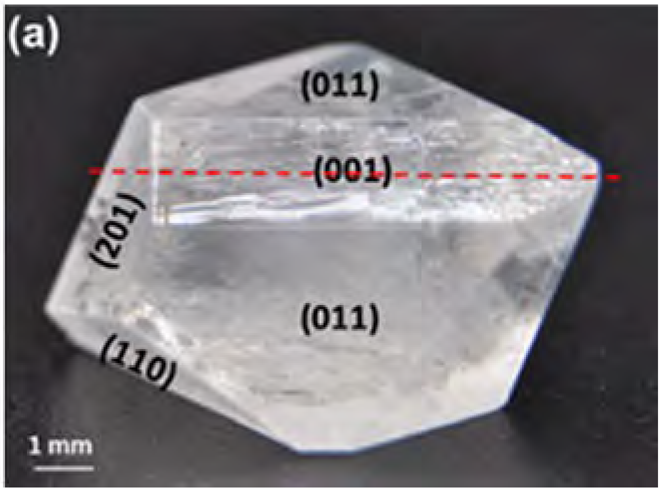
2D Materials and Van der Waals Heterostructures 2 and Ferroelectric Behaviour, June 20, 2024, 11:00 - 13:00

Morphology of molecular crystals significantly influences their processability and physical properties, which has stimulated broad interest of pharmaceutical industries and scientific research. To understand the mechanism underpinning the morphology of crystals regrown from solutions, the state-of-the-art simulation techniques play a unique role, as the delicate solid-solvent interface structure can be probed at atomic scale. Here, paracetamol, as an important medication for pain and fever, is studied using density functional theory with reference interaction site method (DFT-RISM). Various facets of paracetamol are modelled and interfaced with continuum solvents of ethanol to elucidate a recently reported unconventional crystal regrowth behaviour post breakage (Mater. Horiz., 2023, 10, 1425-1430). The predicted morphologies show good agreement with experimental data, illustrating that critical interfacial energetics are captured and reproduced reliably by DFT-RISM. Solvation effects influenced by physiochemical properties of both facets and solvents are analysed to reveal the origin of distinct regrowth behaviours across facets. As a kinetic process dominated by hydrogen bond, the polarity of paracetamol facets and solvents has been proved critical to solvent structure, charge transfer and electrostatic potential near surface, thus activating or passivating the regrowth of certain facets at the presence of solvent. The intriguing competition between thermodynamic and kinetic factors that dominate morphology of the regrown crystal is elucidated in this study, stressing the peculiar nature of the solid-solvent interfaces and the necessity of adopting multi-scale and hybrid simulation techniques such as DFT-RISM. This study is the first example of applying DFT-RISM to simulate the interface structures and properties during molecular crystal regrowth, which provides a prototype for future investigations on regrowth kinetics and morphology control strategies of other crystalline materials.





Aluminum fiber optical vacuum feedthroughs for harsh environments

Christoph Bartlitz[1], Florian Löwinger[1], Klaus Bergner[1], Heiko Wunderlich[1], Andreas Trützschler[1], Kristian Kirsch[1]
[1]Vacom GmbH, Germany

Special Vacuum Chambers and Components, June 17, 2024, 16:00 - 17:35

Fiber optical components are used in a wide variety of places, both in scientific experiments and in production processes in vacuum systems. In principle, these components enable interference-free transmission of the finest measurement signals over long distances, robust sensor technology and maximum transmission speed. Hermetic optical fiber feedthroughs based on stainless steel, ceramics and predominantly quartz glass have become established for coupling and decoupling light signals to vacuum- and process chambers.

In some applications, however, these fiber feedthroughs can reach the limits of their range of use and thus become a limiting factor for the overall system. This is especially relevant for processes in harsh environments, where high temperatures or ionizing radiation are present. Such conditions call for the use of new materials and concepts to mitigate the effects.

For these requirements, we designed and tested an optical fiber feedthrough whose metallic components are made entirely of aluminum. Because, aluminum alloys contain light elements, such as Al, Mg, Si, and thus offer a small cross section for radioactive activation. Whereas, neutron radiation tends to activate high-Z materials at stainless steel or titanium, thus rendering stainless steel or titanium vacuum vessels radioactive itself. Concerning high temperature applications, we report on customized high-temperature fiber optical feedthroughs including an adhesive-free hermetic sealing.

These technologies enable the application of optical fibers as in-vacuum diagnostic within these harsh high-temperature and radioactive environments. Thereby, the diagnostic is driven by fiber Bragg gratings (FBGs) in the optical fiber itself. The application of FBGs as an in-vacuum temperature sensor is demonstrated, where an optical fiber containing a bunch of several FBGs becomes a compact, stable, robust, and flexible network of local sensors at different positions in vacuum with several km signal path.

Enabling vacuum process monitoring with time-of-flight spectroscopy

Kristian Kirsch[1], Klaus Bergner[1], Sebastian Röhrig[1], Marco John[1], Andreas Trützschler[1]
[1]*Vacom GmbH, Germany*

MS-6: RGA User Meeting 3, June 19, 2024, 16:00 - 17:30

As the complexity of industrial vacuum processes increases, detailed knowledge of the vacuum itself becomes even more important. A crucial aspect to manage this challenge is fast in-situ monitoring and control of process parameters such as pressure and residual gas composition. Improving process control in this way minimizes production errors, avoids damage to process equipment and ensures longer operating times. The capabilities of hot cathodes and quadrupole mass spectrometers are limited for this complex task, as they can only measure either the total pressure or the gas composition. One answer to this challenge is our novel ion source NOVION®, which combines the well-known technology of time-of-flight spectroscopy with our patented ion trap to an industrially available gas analyzing application.

In this talk we present the fundamental physical principles of the novel ion source and explain the compact combination of time-of-flight spectroscopy with our own patented ion trap. On the one hand we demonstrate the capability of precise total pressure measurements over a wide pressure range. On the other hand, we show the available possibilities to use the novel ion source in partial pressure measurement mode, leak detection and detection of air leaks.

We discuss advantages and limits in different applications as well as best practice in the field and we show ways to push the principle to its limits at high pressures without compromising performance or lifetime of the filaments.

Influence of contamination on MoS2/Au interface

Mr Rafał Dunal[1], Mr Witold Kozłowski[1], Mr Iaroslav Lutsyk[1], Mr Michał Piskorski[1], Mr Paweł Krukowski[1], Mr Paweł Dąbrowski[1], Mr Maxime Le Ster[1], Mrs Aleksandra Nadolska[1], Mr Przemysław Przybysz[1], Mr Wojciech Ryś[1], Mr Klaudia Toczek[1], Mr Paweł Kowalczyk[1], Mr Maciej Rogala[1]

[1] *Faculty of Physics and Applied Informatics, University of Lodz, Poland*

From Nanostructured thin films to nanoparticles. Reactions at nanostructures, June 18, 2024, 16:00 - 17:30

One of the innovative approaches for data storage is the resistive switching technology in which logical states are represented by the conductivity states of the memory cell. It consists of two electrodes and a switchable material in between them. Polarisation of the electrodes with an external electric field leads to a transition from a high resistivity to a low resistivity state which represent logical states “0” and “1”. A very promising group of materials for this application are 2D materials due to their atomically thin structure and electronic properties covering a wide range of appliations from insulators to conductors or even superconductors. Thanks to their huge surface/volume ratio the interface/material condition has a significant impact on the flow of the current.

In our work, we investigated the impact of interface quality between MoS2 and gold electrode in nanoscale with the use of AFM. The whole process of samples preparation has been done in controlled conditions preceded by the gold substrate sputtering and annealing cycles to obtain a clean interface. Additionally, another set of samples was prepared with the standard tape and polymer transfer technique in the wet air to investigate the impact of contaminations agglomerated between the material and substrate. We show that for pure interface conditions the electronic structure of MoS2 is influenced by gold substrate. In turn, for samples made in the air we observe the influence of the contaminants on the band gap. By the use of nanoscale force spectroscopy and local conductivity measurements, we will characterize the interface properties and show the possibility of their modifications.

This work was supported by National Science Center, Poland, under the Grant 2020/38/E/ST3/00293

Deposition study of NbTiN superconducting thin films prepared by reactive DC and HiPIMS magnetron (co)sputtering.

Dr. Aleksandr Zubtsovskii[1], Prof. Dr. rer. nat. habil. Xin Jiang[1]
[1] *Institute of Materials Engineering, University of Siegen, Germany*

Functional Coatings 2 and Superconducting Thin Films, June 17, 2024, 16:00 - 17:35

Exploration and improvement of low-temperature superconducting (SC) thin films represent a frontier of technological advancement with profound implications for quantum technologies, including high-efficiency particle detectors, advanced quantum computing architectures, and the improvement of coplanar waveguide superconducting resonators. Implementation of modern deposition techniques, specifically High-Power Impulse Magnetron Sputtering (HiPIMS), enable the fabrication of superconducting thin films with tailored microstructural properties that directly influence their SC transition temperatures Tc, London penetration depth, and critical magnetic field Hc. For instance, materials with higher critical temperatures reduce the operational costs associated with cryogenic cooling, while those with superior magnetic field tolerance expand the feasibility of superconducting devices in high-field applications.

Particularly, NbTiN can be suggested as a promising candidate for thin film application in the development of superconducting RF cavities and waveguide resonators [1]. Due to its high critical temperature (Tc ≥ 15) and low normal state resistivity, NbTiN thin films may surpass (in the form of multilayer S(I)S structures) current efficacies of bulk Nb SRF cavities and niobium-based films [2].

In this work, we deposit NbTiN films on silicon and copper substrates by reactive DC and HiPIMS magnetron sputtering as well as hybrid DC/HiPIMS co-sputtering. In particular, we explore the influence of the deposition parameters, e.g. deposition pressure, cathode power and Ar to N_2 ratio, on the surface morphology, film microstructure and superconducting performance of the deposited material. Findings for an optimised parameter set of film deposition will be presented. The resulting optimised parameter set will, subsequently, be implemented into multilayer S(I)S structures to enhance their superconducting performance.

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Characterisation of a novel detector and analyser of low-energy electrons for surface analysis

Yousef Alharbi[1], Mr. Oskar Fossberg[1], Dr. Chris Walker[1], Dr. Gabriele Bertolini[1], Dr. Andrew Pratt[1], Prof. Steve Tear[1]
[1] *University of York, United Kingdom*

Advances in Experimental and Theoretical Methods 1, June 17, 2024, 11:00 - 12:35

The detection and analysis of low-energy electrons, such as secondary electrons, and Auger electrons plays a crucial role in the fields of surface science and materials characterisation. The quantification of these electrons requires knowledge of the inelastic mean free path (IMFP) which is a crucial physical parameter that describes the transport properties of electrons in solid samples. A novel approach to low-energy electron detection and analysis is using an instrument called a Bessel box energy analyser (BBA) [1]. Previously, a BBA was designed and developed to be compact and easily mounted, controlled, and relocated in a range of electron microscopes and UHV systems [2]. In standard SEMs, energy analysis of electrons emitted from a sample is not possible using standard Everhart Thornley detectors. In an SEM, the BBA provides a wide range of information using electron spectroscopy as we have shown [2].
In the current study, we outline the application of a BBA to the investigation of ejected electron emission spectra from a variety of different materials. We present ejected electron spectra obtained using this analyser for carbon (HOPG), silicon and other metallic elemental standards. Also, we identify using Elastic Peak Electron Spectroscopy (EPES), plasmon loss features for these materials covering a wide range of atomic numbers. The yield of ejected electrons for the HOPG sample and elemental standards was measured and the IMFP was investigated using EPES in a UHV environment. Additionally, we show detection of AES peak energies and shapes using the BBA allowing identification of sample chemical states [3].

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Low energy electron irradiation as mitigation strategy for two potential showstoppers in future gravitational wave detectors

Luisa Spallino[1], Marco Angelucci[1], Roberto Cimino[1]
[1]LNF-INFN, Italy

Large Vacuum Systems, June 17, 2024, 11:00 - 12:35

The mitigation of all potential noise sources detrimentally affecting gravitational wave (GW) detection is mandatory for present and future GW interferometers. Here we approach two apparently uncorrelated issues: the electrostatic charge forming on test masses at room and cryogenic temperature, and the build-up of a frost layer on cryogenically cooled mirrors.

Electrostatic charge has been shown to affect LIGO data taking. Its mitigation routinely requires mirror's long exposures (hours) to a relatively high pressure (tenth of mbar) of N_2 ions flux.

Cryogenic mirrors in future GW detectors are ideal to reduce thermal noise and to obtain the desired detection sensitivity at low frequency. However, operating at temperatures ~10 K presents several challenges, one being on the cryogenic vacuum system hosting the cold mirrors. Gases composing the residual vacuum will tend to cryosorb on the mirror surfaces forming a contaminant ice layer ("frost"). This can severely perturb mirror optical properties preventing detection with the design sensitivity.

Noticeably, the method used at LIGO to mitigate electrostatic charging cannot be applied on cryogenically cooled mirrors without forming on its surface an unacceptably thick condensed N_2 layer.

Low energy electrons (few hundreds eV) are known to be very efficient in inducing gas desorption. Also, by properly tuning the energy of the incident electrons, an electron beam can be used to neutralize both positive and negative charges on the mirror's dielectric surface. Electrons are also known to interact only with the very top layers (some nm) of any irradiated surface and seems ideal to neutralize charge and induce frost desorption without damaging the mirror surfaces' optical properties.

Here we present an experimental work demonstrating that low energy electrons may be indeed used as a mitigation method to cure surface charging and frost formation.

The NIST on a Chip Program, Quantum Based Sensors for the Pressure, Vacuum, and More!

Dr. Jay Hendricks[1], Ms. Barbara Goldstein
[1]Nist, United States of America

Vacuum Metrology, June 20, 2024, 11:00 - 13:00

This presentation covers vacuum metrology history of how we got to where we are today and gives a forward-looking vision for the future of measurement science and its important role in our daily lives. The talk will focus a bit on the use of quantum-based measurements and photonics has the potential revolutionize sensor technologies. The role of NIST as a National Metrology institute (NMI) is briefly described considering the world-wide redefinition of units that occurred on May 20th, 2019. The re-definition of units is now aligned with physical constants of nature and fundamental physics which opens new realization routes with quantum-based sensors and standards. The NIST on a Chip program (NOAC) is briefly introduced in this context.

The technical core of the lecture will be a deeper dive into research on measurement methods for pressure, the Fixed Length Optical Cavity (FLOC) and for vacuum the Cold Atom Vacuum Standard (CAVS). What is exciting about many of these new measurement approaches is that they are both primary (relying on fundamental physics), are quantum-based and use photons for the measurement readout which is key for taking advantage of the fast-growing field of photonics. The FLOC enables the elimination of mercury barometers worldwide and the CAVS is the first primary standard for making vacuum measurements below 1.3x10-5 Pa. A Sensitive Photonic Thermometer (SPOT) will be introduced, along with other sensing technologies that the NOAC program is currently investigating, such as flux, magnetic field, mass and torque.

Quantum-based metrology systems, however exciting, do raise new challenges and several important questions: What will be the role of metrology institutes in the is new ecosystem of metrology and measurement? What will be the NMI role for quality systems and measurement assurance for these new quantum-based systems? This talk will begin to explore these important philosophical questions.

Identification of Metal Centers in a Bimetallic Ni/Co-HITP Metal-Organic Framework

Dr Sisheng Shu[1], Mr Fubiao Gu[1], Sparsh Tyagi[1], Professor Martin Castell[1], Dr Christopher Patrick[1]
[1]*University Of Oxford, United Kingdom*

Spectroscopy and Microscopy of Nanostructures Modelling Nanostructure Properties, June 20, 2024, 11:00 - 13:00

The family of metal-organic frameworks (MOFs) with M3(HXTP)2 stoichiometry (M = transition metals; HXTP = 2,3,6,7,10,11-hexa-substituted triphenylenes) are made up of near planar-squarely coordinated metals and trinucleating bidentate planar ligands and form hexagonal honeycomb structures. These MOFs have high electrical conductivities, and hence potential application in chemiresistive sensing, electrocatalysis and novel microelectronic devices. M3(HXTP)2 MOFs are often referred to as 2D MOFs because of their planar structure, but the materials that are synthesized through wet chemical techniques usually consist of stacked van der Waals-bonded layers resulting in 3D materials. Vacuum growth techniques, as demonstrated here, enable on-surface synthesis of true 2D materials with monolayer thickness [2].

We demonstrate the creation of monolayer single metal (Ni, Co) and bimetallic NixCo3-x(HITP)2 metal-organic frameworks (MOFs) synthesized on Au(111) surfaces in ultra-high vacuum. The MOFs are characterized by scanning tunneling microscopy (STM), which reveals the growth processes and hexagonal structures. The pure Ni3(HITP)2 and the bimetallic NixCo3-x(HITP)2 frameworks have a similar isotropic island morphology, while the Co3(HITP)2 islands have a ribbon shape. Individual Ni and Co metal centers can be atomically identified by their different apparent height in the STM images of the bimetallic framework, as shown in the image to the left. Density functional theory (DFT) calculations indicate that the apparent height difference is caused by electronic effects rather than representing a true difference of topography. The STM images further reveal that in the mixed-metal MOF the Ni and Co centres are distributed randomly.

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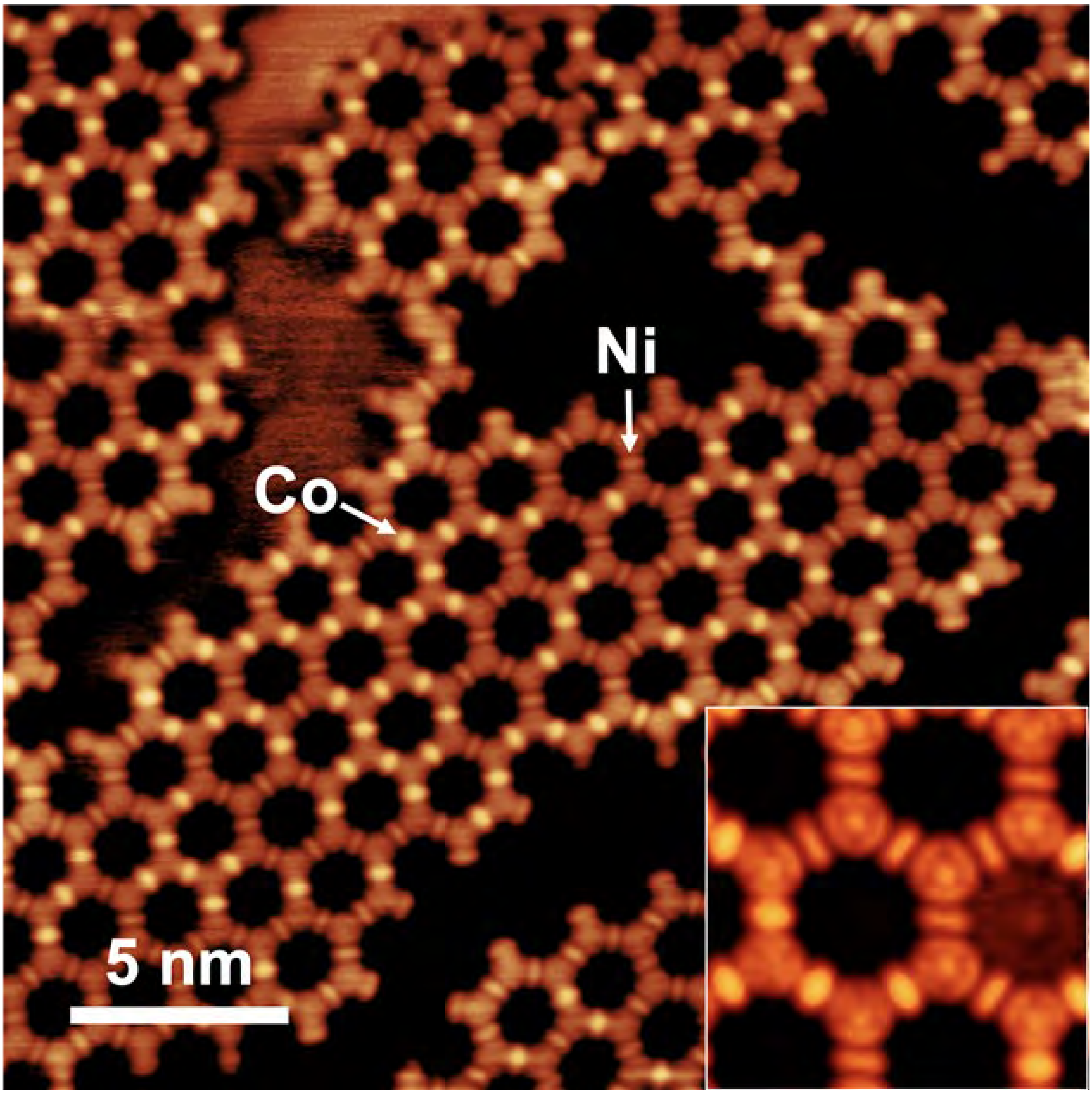
Ni
Co
5 nm

Fabrication of Thin-layer InSb-based Planar Devices

MSc Eng. Piotr Kałuziak, MSc Eng. Jan Raczyński[1], PhD Eng. Semir El-Ahmar[1], PhD Wojciech Koczorowski[1]
[1]Faculty of Materials Engineering and Technical Physics, Institute of Physics, University of Technology, Poland

2D Semiconductors, June 18, 2024, 14:00 - 15:30

For many decades, indium antimonide (InSb) has been a well-studied material that is highly valued for its low energy gap of approximately 0.18 eV at room temperature, as well as its exceptional electric charge carriers mobility value, which stands at 77000 cm2/(V·s) [1]. The development of device fabrication technologies opens new possibilities for InSb thin layers. The lithography process application followed by metals deposition under vacuum conditions to the graphene layer makes it possible to fabricate sophisticated planar architectures with unique useability[2]. A slight modification of such structuring procedure allows the transfer of the technology to layers of greater thickness, e.g. InSb.

High-quality InSb thin films are fabricated using the flash evaporation technique under HV conditions on a gallium arsenide (GaAs) substrate. Following the modified structurisation procedure the Hall and TLM structures were fabricated to determine the galvanometric properties of the InSb-based hybrid systems. In addition, the structure to test the efficacy of the strip magneto sensor (SMS) in the InSb was proposed [3]. As a result of the high charge carrier mobility of InSb, it is predicted to obtain a significant magnetoresistive effect in specific geometry configurations.

The research has received funding from the National Centre for Research and Development No. LIDER/8/0021/L-11/19/NCBR/2020 and partly from the Ministry of Education and Science (Poland) under Projects No. 0512/SBAD/2420 and 0512/SBAD/6217.

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Polarity compensated Perovskite surfaces as a support for single-atom catalysis

Mr Aji Alexander[1]

[1]Department of Surface and Plasma Science, Charles University, Czech Republic, [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, Poland, [3]IOM-CNR, Istituto Officina dei Materiali, AREA Science Park Basovizza, Italy

Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 3, June 20, 2024, 11:00 - 13:00

A. Alexander1, D. Wrana1,2, P. K. Samal1, J. Škvára1, L. Albons1, J. Redondo1, L. Fusek1, I. Píš3, V. Johánek1, J. Mysliveček1, M. Setvin 1

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Perovskite surfaces recently gain popularity in the catalysis community due to their promising chemical properties, ability to separate electron-hole pairs during light harvesting, and the presence of ferroelectricity in many perovskites [1]. While perovskites have a unique set of interesting bulk properties, their surfaces are much less understood; the main unanswered questions are their structural stability, chemical reactivity, and catalytic selectivity.

This presentation will cover the possibility of modifying the catalytic activity of doped KTaO3 (001) and $SrTiO$3(001) perovskite by extrinsic metals, mainly cobalt, as well as methods to compensate the polarity that appears on their pristine surface. I will use combined STM/AFM measurements in conjunction with XPS to demonstrate the thermal stability and the dispersion of guest atoms as single adatoms on the polarity-uncompensated, $KTaO$3(001) [2]and $SrTiO$3(001) surfaces. The temperature evolution of absorbed species, as well as the interaction of the cobalt with the surface under various reducing and oxidizing environments, will be highlighted. This explains how cobalt's metallic, oxide, and hydroxide phases vary depending on the environment.

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R&D of the EAST plug-in cryopump for long-pulse and high-performance plasma operation

Dr. Zhaoxi Chen[1], Mr. Chengpeng Zhang[1,2], Dr. Qingxi Yang[1], Dr. Guodong Wang[3], Prof. Yuntao Song[1]
[1]Institute of Plasma Physics, Hefei Institutes of Physical Science, Chinese Academy of Sciences, , China, [2]University of Science and Technology of China, China, [3]Hefei University of Technology, China

Vacuum pumps, June 21, 2024, 10:30 - 12:00

Particle exhaust plays an important role in the recycling control and performance improvement for the fusion plasma, and it's one of the key factors that restricting the steady-state operation of tokamak. Cryopump has high pumping speed for hydrogen isotopes and helium, and without moving components that can be affected by the strong background magnetic field, thus, it's widely used on most of the operating research tokamaks and it's regarded as the best particle exhaust solution for the future fusion power plants too. On EAST tokamak, two in-vessel cryocondensation pumps are currently used, by which the 120 million degrees Celsius plasma operation for 101 seconds and the 70 million degrees Celsius plasma operation for 1056 seconds were successfully achieved. However, the pumping performance degradation caused by heat flux deposition is a major challenge for EAST to realize long pulse and high heating power discharge. In response to this issue and considering the spatial constraints of EAST, two sets of plug-in cryopumps based on cryoadsorption are planned to be developed and installed. In order to validate the design and key manufacturing technologies of the EAST plug-in cryopumps, one full-size prototype was developed and tested. The prototype exhibits good pumping speed of approximately 9255 L/s for hydrogen, 7001 L/s for deuterium, and 5290 L/s for helium. And its pumping performance is relatively stable under the working pressure from 10-4 Pa to 10-1 Pa. This work provides theoretical and technical support for the efficient particle exhaust under EAST high heating power discharges, which can help EAST to realize the 10 MW 100s discharges. It also laid a technical foundation for the cryopump development for the Chinese Fusion Engineering Test Reactor (CFETR).

Impurities as a source of regular patterns on the surface

Magdalena Załuska-Kotur[1], Marta Chabowska[1]

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Advances in Experimental and Theoretical Methods 3, June 17, 2024, 16:00 - 17:35

Most of the processes that determine the shape, stability and content of dopants and impurities take place on the surface of the growing crystal. It is also a fascinating arena of far- from-equilibrium self-organizing processes, which result in the regular ordering of surfaces into bunches, meanders, nanowires or other patterns. A vicinal cellular automaton model (VCA) was proposed, which enabled the study of surface dynamics over a long period of time [1-3]. We have shown that the VCA model can be used as a very flexible tool for modeling surface phenomena. It allows us to investigate how the process of diffusion in different surface potential energy landscapes determines the way crystals grow and to separate the effect of diffusion from the effect of step permeability. We show that when the impurities contribute their own potential field, this leads to the formation of regular meandering, bunched step structures or nanowires, even if their positions are random. We show that it is possible to control the pattern formation process using the appropriate type and number of added atoms. The obtained patterns and surface dynamics are compared with experimental results.

*In collaboration with Hristina Popova (Sofia), Vesselin Tonchev (Sofia) and F.Krzyżewski (Warsaw)

Fig. Examples of surface pattern induced by the presence of 30 % impurities. a) surface potential b) meanders c) bunches d)nanowires

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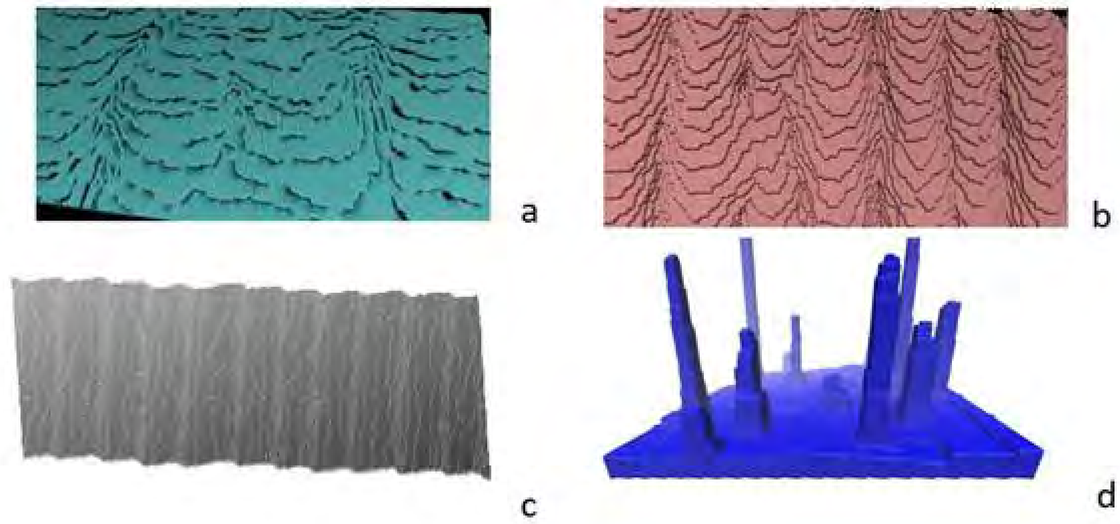

Photocathode Electron Source R&D at Daresbury Laboratory

Dr. Lee Jones[1,2], Mr. Hugh Churn[1,2], Dr. Tim Noakes[1,2]

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Electronic Structure of Materials, Surfaces and Interfaces, June 18, 2024, 10:30 - 12:30

Synchrotron Radiation Sources have been the workhorses powering scientific research and innovation for nearly 5 decades. The last decade has seen light source technology develop to the point where the incoherent radiation developed by storage ring sources is surpassed by the brilliance of coherent X-ray sources based on linear accelerators driving Free-Electron Lasers. These Fourth Generation Light Sources require high brightness electron beams. To achieve this, a photocathode electron source with a high quantum efficiency and low intrinsic emittance which is also robust with a long operational lifetime and low dark current is essential. Achieving all of these fundamental requirements is challenging, particularly as some of them are in competition. Consequently, the field of photocathode R&D remains an active and challenging aspect of particle accelerator research.

Effective photocathode research requires a unique range of equipment and capabilities. The experimental facilities to support photocathode R&D at the STFC Daresbury laboratory have evolved progressively and are recognised as world-class. We have expertise in III-V semiconductor photocathodes for high-current DC guns, metal photocathodes for ultrafast electron pules, and alkali metal semiconductor photocathodes for high beam current sources. These technologies underpin the operation of Infra-Red and X-ray Free-Electron Lasers, and also longitudinally-coherent electron sources for Ultra-Fast Electron Diffraction experiments.

Our photocathode research facilities include the unique TESS* system to characterise photocathode energy spread and spectral response. We present a summary of the photocathode R&D capabilities at the Daresbury Laboratory, and link this to the active CLARA** accelerator programme and future aspirations for a UK XFEL***.

* Transverse Energy Spread Spectrometer (TESS) - Rev. Sci. Instrum. 93, 113314 (2022)

** Compact Linear Accelerator for Research and Applications (CLARA) – PRSTAB 23, 044801 (2020)

*** UK XFEL Science Overview and Conceptual Design Options Analysis at https://xfel.ac.uk/wp-content/uploads/2023/02/XFEL_Science_Case-STKA00183.07-v3-interactive.pdf

Diamond-II Vacuum Instrumentation & Interlock Systems

Hugo Shiers[1]
[1]Diamond Light Source, United Kingdom

Large Vacuum Systems of Particle Accelerators, June 18, 2024, 10:30 - 12:30

Diamond Light Source is the UK’s national synchrotron. Currently underway is the Diamond-II upgrade programme, an in-place upgrade for the Diamond storage ring, which will reduce beam emittance, increase brightness, and enable three new beamlines.

Diamond utilises vacuum gauge and Ion pump interlocks with Omron PLCs for vacuum instrumentation protection and for accelerator (machine) protection. Diamond-II will have upgraded PLCs and use gauge and ion pump interlocks along with analogue signals from the gauges and ion pumps providing additional functionality which will be used for vacuum protection, machine projection, along with Gas Bremsstrahlung and water ingress interlocks.

This paper discusses the vacuum control system for Diamond-II along with the proposed vacuum equipment for Diamond-II. It will detail proposed vacuum intervention procedures and show how it is planned to keep sector vessel venting to a minimum during repairs with some novel equipment. In addition, the implementation method for the Gas Bremsstrahlung and water ingress interlocks will be discussed. Finally, it will be discussed how the vacuum instrumentation and controls from Diamond to Diamond-II will be migrated in a seamlessly manner.

Residual gas analysers (RGAs) on the Diamond Light source:

Hugo Shiers[1], Dr Neil Warner, Dr Chris Burrows
[1]*Diamond Light Source, United Kingdom*

MS-6: RGA User Meeting 1, June 19, 2024, 10:30 - 12:35

Diamond Light Source is the UK's national synchrotron. Currently underway is the Diamond-II upgrade programme, an in-place upgrade for the storage ring, which will reduce beam emittance, increase brightness, and enable three new beamlines.

Diamond utilises RGAs on the all the accelerators, frontends, and beamlines for gas species trending, leak checking and general troubleshooting. There are some 130 RGAs on the Storage Ring, Insertion Devices & Frontends alone, controlled and selectively archived through the DIAMOND EPICS control system. How these RGAs have been utilised, maintained, and serviced over the last 17 years will be discussed, along with results of various studies using the RGAs on the accelerators.

Drawing from the current experience of Diamond, we are looking at how we will install, integrate, and utilise the RGAs on Diamond-II, incorporating novel ways to install the RGA heads and considering the different ways we can utilise them within our control systems. The plans and ideas for the RGA systems on Diamond-II will be discussed with particular emphasis on the applications and maintenance of the systems.

The vacuum system of SIS100 at FAIR – First operating experience gained during the string test

Mr. Stefan Wilfert, Mr. Ivan Pongrac, Mr. Stefan Zeller

Large Vacuum Systems of Particle Accelerators, June 18, 2024, 10:30 - 12:30

The international accelerator project FAIR, with its construction commencing in 2017, recently entered a new phase of realization: the installation work of the accelerator components for the new superconducting heavy ion synchrotron SIS100 has begun in the 1.1 km long underground ring tunnel. Prior to this, a crucial milestone was reached in the design verification of the machine. At the series test facility of GSI, a short but fully operational arc segment of the future SIS100 ring was built up and successfully tested for the first time. The so-called string test is made up of three cryo-magnetic modules (two dipoles and one quadrupole) and a cryostat end cap, to which a short part of the later room temperature vacuum system of the SIS100 is connected. All these interconnected modules with their beam-guiding components form an approx. 15 m long, fully-functional model of the future UHV/XHV system for beam transport. While conventional pump technology is used in the approx. 1 m long bakeable room temperature part, the major part of the string beam vacuum system is operated at LHe temperatures in order to generate and maintain the low residual gas pressures required for machine operation. The purpose of the string test is, among other things, to verify the vacuum system design and to gain experience of its operating behavior. We report on its commissioning, first measurements, findings, and observations during operation and draw the first tentative conclusions.

Unravelling Fundamental Limits: Isotopic Labelling and Correlative NanoSIMS/XPS Analysis of Nickel Catalysts in Alkaline Electrolysers

Eleanor Ender[1], Dr Cindy Tseng[2], Yifeng Wang[2], Dr Reshma Rao[2], Dr Alex Walton[1], Dr Katie Moore[1]
[1]University Of Manchester, United Kingdom, [2]Imperial College London, United Kingdom

Advanced Thin Film Characterisation, June 19, 2024, 16:00 - 17:30

The current status of hydrogen production predominantly relies on fossil fuel sources. Due to the growing demand for sustainable and green energy, there is a significant focus on alternative methods of hydrogen production.

Alkaline electrolysis is one of the key methods for producing hydrogen using renewable energy sources. This process involves the electrolytic splitting of water molecules into hydrogen and oxygen using an electric current. The process can be powered by renewable sources, making it a cleaner and more sustainable method. However, scale-up is limited by a requirement of better understanding of the surface chemistry of the catalyst materials and reaction mechanisms.

Nickel has been a popular electrode material for water splitting since between the 1920s and 1970s due to its good alkali resistance, electrochemical activity, and not being too expensive. While nickel compounds have shown promising results, there are concerns of catalyst degradation and deactivation. Studies suggests that nickel electrode deactivation occurs in long-term experiments due to nickel hydride formation on the surface.

This work aims to understand the fundamental limits to the performance of alkaline electrolysers and nickel catalysts, investigating deactivation through isotopic labelling experiments and correlative Nanoscale secondary ion mass spectrometry (NanoSIMS) and X-ray photoelectron spectroscopy (XPS). The measured catalysts will undergo hydrogen evolution reaction (HER) in deuterated electrolyte at different timescales to determine time of deactivation. In order to investigate the mechanism of deactivation isotopic ratio depth profile analysis with NanoSIMS will be performed to determine distribution of deuterium within the sample. Additionally, XPS analysis will be employed to offer chemical insights into the nickel compounds formed after deactivation.

This research will compare the migration of deuterium content during HER operation and correlate it with the formation of different nickel species. This will uncover the species responsible for deactivation of alkaline electrolyser nickel catalysts.

Towards Robust Dichroism in Angle-Resolved Photoemission

Jakub Schusser[1,2], Hibiki Orio[1], Maximilian Ünzelmann[1], Johannes Heßdörfer[1], Muthu P.T. Masilamani[1], Florian Diekmann[3], Kai Rossnagel[3,4], Friedrich Reinert[1]
[1]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany, [2]New Technologies Research Centre, University of West Bohemia, Czech Republic, [3]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Germany, [4]Institute of Experimental and Applied Physics, Kiel University, Germany

Advances in Experimental and Theoretical Methods 1, June 17, 2024, 11:00 - 12:35

Dichroic techniques are highly relevant in the field of topological materials, layered systems, and spin-polarized electronic states [1-3]. Dichroism in angle-resolved photoemission is per se a matrix element effect, which depends on the initial and final states as well as on the perturbation by the light field. Although matrix element effects in ARPES such as dichroism are important for addressing properties of the initial state wave functions, the results can strongly depend on experimental geometry or final state effects. Combining experimental data on bulk WSe2 taken at soft x-ray photon energies with state-of-the-art photoemission calculations, we demonstrate that a dichroic observable called time-reversal dichroism remains unaffected against variation of photon energy, light polarization, and the angle of incidence [4]. The robustness of this matrix element effect indicates a considerable benefit over other dichroic techniques and encourages further experimental and theoretical investigations.

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[2] Beaulieu, S. et al., Physical Review Letters 125 (21), 216404
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[4] Schusser, J. et al., https://doi.org/10.21203/rs.3.rs-3758849/v1

Exploring the Interplay of Ti–Sn Co-Doping in Photoelectrochemical Water Splitting of Hematite Nanowires

Mr. Francisco Javier Fernández Alonso[1,2,3], Dr. Paula Quitério[4], Dr. Rui Vilarinho[4], Prof. João P. Araújo[4], Prof. Adélio Mendes[5], Prof. Miguel Manso-Silván[1,2,3], Prof. Vicente Torres-Costa[1,2], Dr. Arlete Apolinario[4], Dr. Célia Tavares de Sousa[1,2,3]

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Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 4, June 21, 2024, 10:30 - 12:00

Photoelectrochemical (PEC) water splitting has emerged as a promising avenue for sustainable energy production, offering a solution to the increasing demand for clean energy sources [1]. Hematite, recognized for its abundance, cost-effectiveness, non-toxicity, and stability, stands out as a potential semiconductor for efficient water splitting [2]. However, the inherent limitations of bare-hematite-based PEC cells, characterized by low photocurrent density, demand the exploration of innovative strategies to enhance their efficiency [3]. In this study, we investigate the synergistic effects of three key approaches: improving crystallinity through high-temperature annealing [3], enhancing specific surface area through nanostructuring, and heteroatomically doping the structure to enhance photoanode conductivity. Hematite nanowires were synthesized via a hydrothermal method, with Ti-doping introduced during synthesis and subsequent co-doping with Sn during an additional 800 °C annealing process, in which also the crystallinity was enhanced. Notably, the incorporation of Ti dopant resulted in a remarkable 30-fold increase in photocurrent density under simulated solar illumination, from 0.03 mW/cm² to 0.63 mW/cm², while co-doping with Ti and Sn further boosted the performance to 1.27 mW/cm². By elucidating the impacts of heteroatom doping on hematite properties and its interplay with high-temperature annealing processes, this research contributes to the development of efficient nanostructures tailored for sustainable energy conversion applications.

References:
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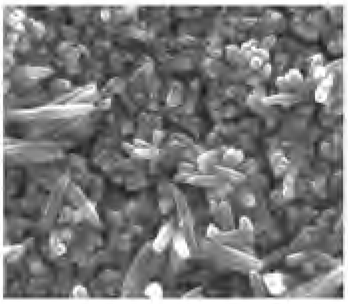
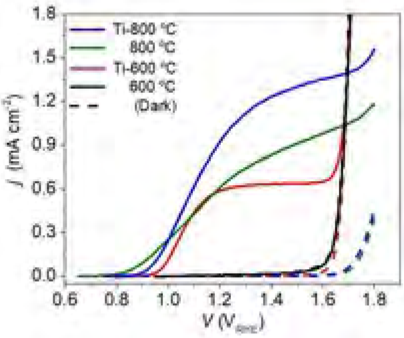
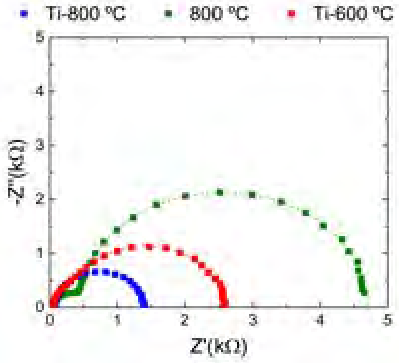
[2] J Zhao et al., Journal of Energy Chemistry 79, 601 (2023).
[3] P Quitério et al., Journal of Physical Chemistry C 124(24), 12897 (2020).







Boosting Visible Light Photocatalysis with Synergistic Plasmonic Effect and Electron Trapping on Au-loaded Se-doped Ta2O5 Heterostructures

Mr. Francisco Javier Fernández Alonso[1,2,3], Dr. Carlo Marini[6], Dr. Fernando Agulló-Rueda[4], Mr. Nelson Naveas[1,2,5], Dra. Célia Tavares de Sousa[1,2,3], Prof. Vicente Torres-Costa[1,2], Prof. Miguel Manso-Silván[1,2,3]

[1]Departamento de Física Aplicada, Universidad Autónoma de Madrid, Spain, [2]Instituto de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, Spain, [3]Centro de Microanálisis de Materiales, Universidad Autónoma de Madrid, Spain, [4]Instituto de Ciencia de Materiales de Madrid, Centro Superior de Investigaciones Científicas, Spain, [5]Departamento de Ingeniería Química y Procesos de Minerales, Universidad de Antofagasta, Chile, [6]CELLS–ALBA Synchrotron, Spain

Functional Coatings 1, June 17, 2024, 14:00 - 15:30

In recent years, there has been a significant increase in interest in processing materials exhibiting visible light photocatalytic activity. This growing attention arises from the pressing necessity to innovate new approaches for energy production, pollutant degradation, water splitting, purification, etc. [1,2]. In the present work, porous films of oxygen-deficient Se-doped Ta_2O_5 have been synthesized by the sol-gel method and characterized. Their photocatalytic activity in the degradation of ciprofloxacin has been studied both under solar and UV light and compared with that of compact thin films of Ta2O5. The UV photocatalytic efficiency of porous samples is a factor of 10 higher than that of compact samples, which is attributed to their much larger specific surface area. Also, it has been observed that photodegradation under solar illumination occurs exclusively for Se-containing samples. This phenomenon is attributed to the synergistic effects of Se-doping, which narrows the band gap, and the presence of Se4+ associated energy levels. These levels act as electronic traps, suppressing electron-hole recombination.

The effect of Au nanoparticle loading on the structure has also been studied. A synergistic effect has been observed between Se-doping and loading with Au nanoparticles. Our study points to a plausible reduction in radiative recombination at Se4+ mid-band levels of the electrons promoted to the conduction band because of the excitation of the Au nanoparticles by the local surface plasmon resonance.

References

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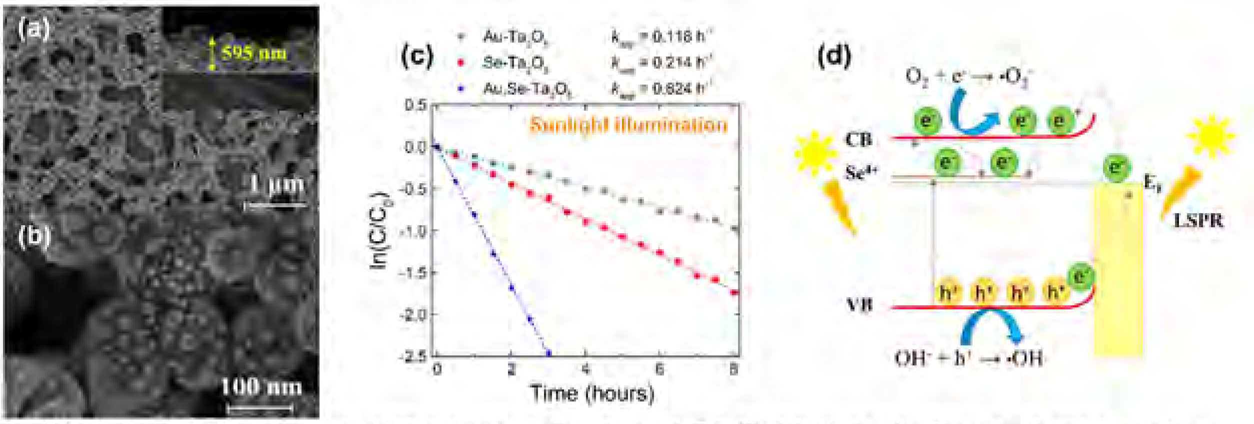

Figure 1. SEM images of the porous Se-doped Ta_2O_5 films (a) before and (b) after Au nanoparticle loading. (c) Temporal evolution of the concentration of ciprofloxacin under solar illumination. Note that $k_{app}(Au,Se\text{-}Ta_2O_5) > k_{app}(Se\text{-}Ta_2O_5) + k_{app}(Au\text{-}Ta_2O_5)$. (d) Proposed mechanism for enhanced visible-light photocatalytic activity.

Photoluminescence of Diamond-Like Carbon Quantum Cones with Dispersive Spectrum Distributed in Time: Nano Monochromator

Arturs Medvids[1], P Ščajevs[2]
[1]Riga Technical University, Latvia, [2]Vilnius University, Lithuania

Carbon Materials 2, June 19, 2024, 10:30 - 12:35

A quantum cone is a structure consisting of a large number of quantum dots with a gradually decreasing diameter from the base to the top of the cone. This distribution of quantum dots leads to a dispersive radiated spectrum. The red edge of the spectrum is determined by the band gap of the semiconductor, and the blue edge by the quantum confinement of excitons on top of the cones [1]. We observe the kinetics of photoluminescence, obeying the stretch exponential law, from quantum cones formed on the surface of DLC [2]. They are explained by an increase in the lifetime of excitons along the height of the cone and an increasing concentration of excitons at the base due to their drift in the quasi-build-in electric field of the quantum cone. Such time dependence of the photoluminescence spectrum gives the possibility of its discrimination on time. The possible visualization of the quantum cones tops of DLC using irradiation by a UV light source is shown in figures d, e, and f. A quantum cone is a nano source of light with a dispersive spectrum along the height of the cone-nano monochromator. These features will make it possible to build the smallest spectrometer to measure the absorption spectrum of individual nanoparticles or viruses.

Figure. AFM images of DLC samples: (a), (b), and (c) surfaces and the fluorescent microscope images (d), (e), (f) at UV excitation.

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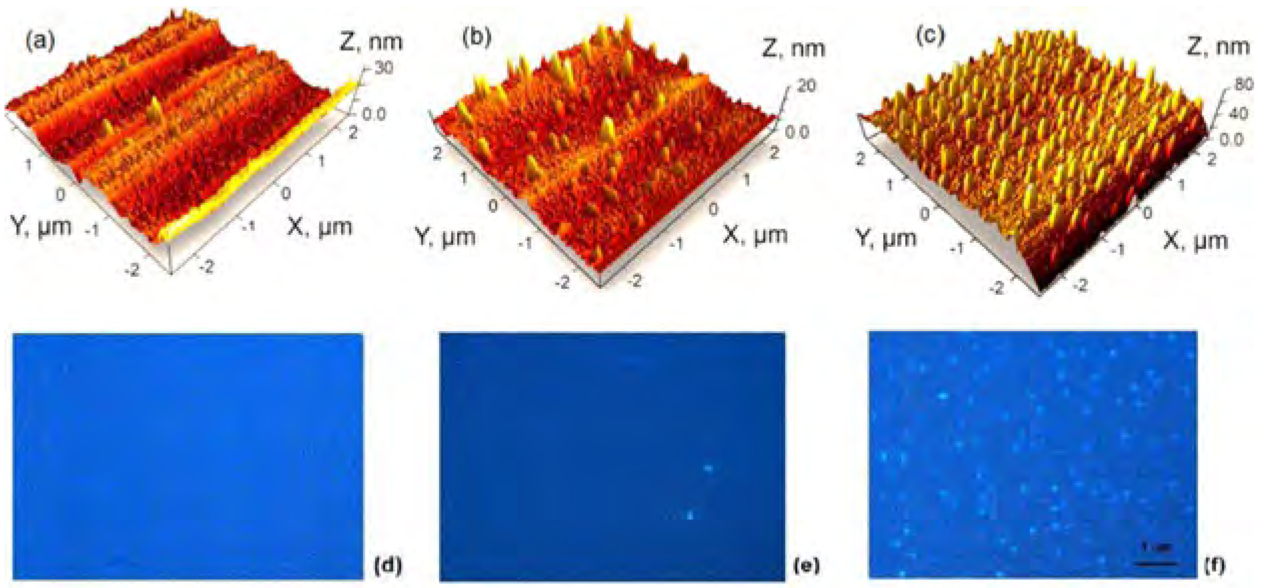
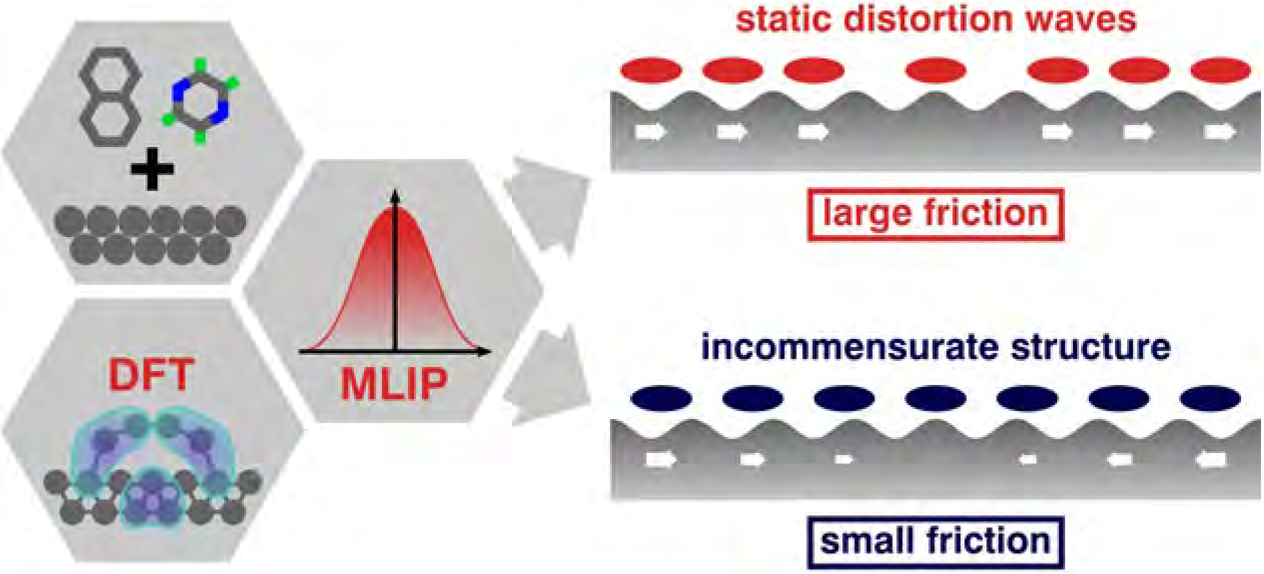


Optimization of incommensurate organic/inorganic interface structures to study superlubricity

Lukas Hoermann[1], Johannes J. Cartus, Oliver T. Hofmann
[1] *University Of Warwick, United Kingdom*

Biointerfaces/Biophysics/Biosensers, June 19, 2024, 10:30 - 12:35

Organic/inorganic interface systems are highly relevant due to their tunability and propensity to form incommensurate structures which potentially exhibit superlubricity between organic and inorganic surfaces. The study of interface properties necessitates precise modelling of interface geometries as well as the electronic structure using accurate first-principles electronic structure methods. However, the system size of incommensurate structures renders such calculations intractable. Hence, investigations into incommensurate interfaces have been constrained to very simple model systems or highly simplified methods. To overcome this constraint, we have devised a machine-learned interatomic potential (MLIP) using Gaussian process regression. This potential can accurately compute energies and forces for structures containing thousands to tens of thousands of atoms, offering a level of precision on par with traditional first-principles methods, all while significantly reducing computation costs. Through this method, we quantify the breakdown of the low-friction state in incommensurate structures due to the formation of static distortion waves. Moreover, we extract design principles for incommensurate interface systems that inhibit the formation of static distortion waves and facilitate low friction coefficients.



A structural study of CO ligation to Cu adsorbed on Fe3O4 (001)

Fulden Eratam[1]
[1]Diamond Light Source, United Kingdom

Catalysis and Electrocatalysis including Single Atom and In Operando Studies 1, June 19, 2024, 14:00 - 15:30

A structural study of CO ligation to Cu adsorbed on Fe3O4(001) – Fulden Eratam1, Benedikt Klein1,2, Lena Puntscher3, Matthew Stoodley1,2, Alexander Generalov4, Alexei Preobrajenski4, Tien-Lin Lee1, Gareth Parkinson3 and David Duncan1 – 1. Diamond Light Source, Didcot, UK – 2. University of Warwick, Coventry, UK– 3. TU Wien, Vienna, Austria– 4. MAX IV, Lund, Sweden.

Single atom catalysts (SACs), monodispersed metal adatoms on isolated centres of a support, can potentially increase catalytic efficiency, selectivity, and stability1. The coordination state of the supported metals is a key parameter in the selectivity of SACs2 and is typically identified using X-ray absorption near edge spectroscopy (XANES). Therefore, the coordination of Cu adatoms on magnetite (Fe3O4), a popular oxide support, has been studied using the near edge X-ray absorption fine structure (NEXAFS) / XANES measurements obtained from the Cu L-edge, before and after CO ligation. The Cu adatoms have been previously identified by normal incidence X-ray standing waves (NISW) to two-fold coordinate to surface O at the bulk-continuation cation sites3, whereas CO adsorption has been shown to pull these atoms out of the surface by 0.2 Å4. The current work highlights the effect of one such CO distortion on the XANES data and presents Cu L-edge XANES of Cu single metal adatoms adsorbed on Fe3O4(001) before and after CO coordination. In the absence of CO, it is found that Cu adatoms produce a XANE spectrum very similar to that of Cu2O. Meanwhile, CO coordination is found to produce a significant enhancement in the intensity of a pre-edge feature, observed at an energy range typical of CuO (Fig1).

Fig1: The effect of CO ligation on the Cu L-edge XANES of Cu/Fe3O4(001).

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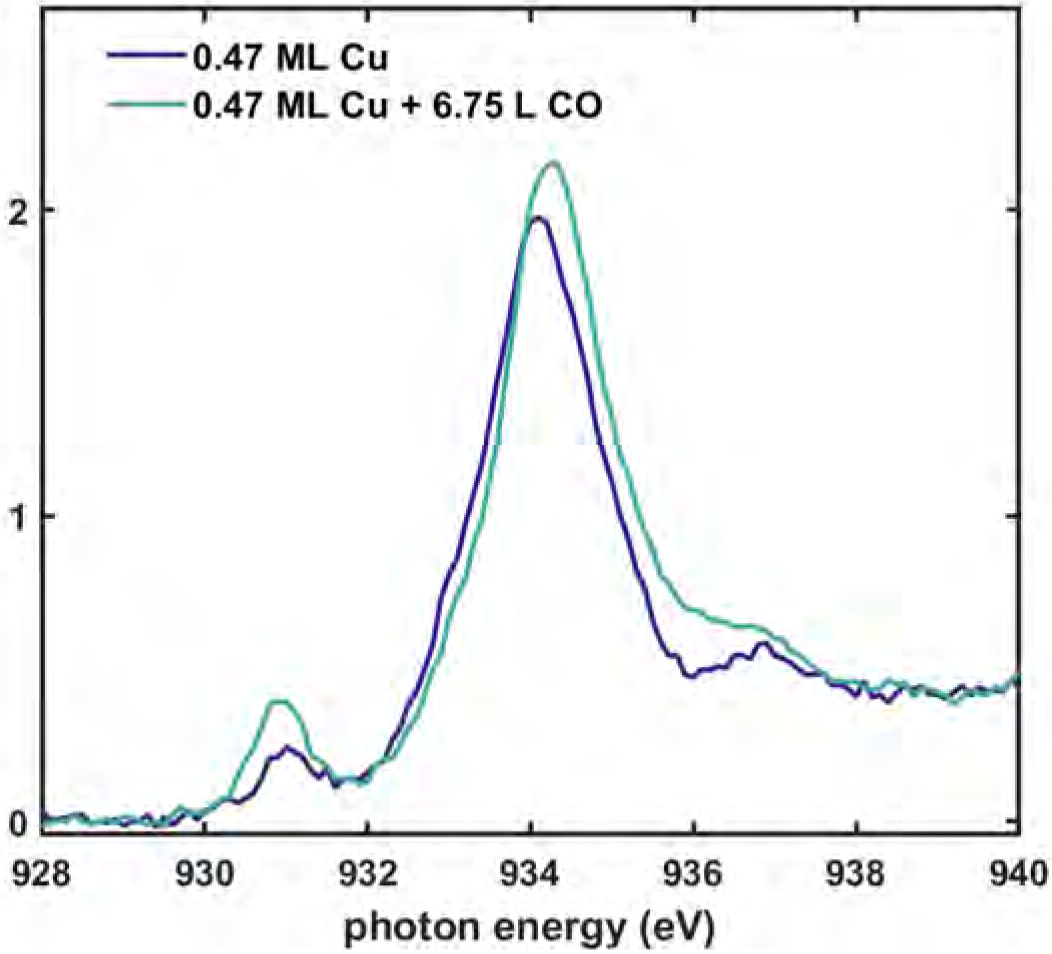
0.47 ML Cu
0.47 ML Cu + 6.75 L CO
0
1
2
928
930
932
934
936
938
940
photon energy (eV)

Imaging and spectroscopic study of topological defects in graphene grown by bottom up synthesis

Mr Matthew Stoodley[1,2], Dr Benedikt Klein[1,2,3], Mr Joel Deyerling[4], Dr Luke Rochford[1,2], Mr Dylan Morgan[1], Mr Michael Clarke[5], Dr David Hopkinson[2], Mr Sam Sullivan-Allsop[6], Dr Fulden Eratam[2], Dr Lars Sattler[7], Dr Sebastian Weber[7], Dr Gerhard Hilt[7], Dr Alexander Generalov[8], Dr Alexei Preobrajenski[8], Mr Leon Williams[2], Dr Tien-Lin Lee[2], Dr Alex Saywell[5], Dr Roman Gorbachev[6], Professor Sarah Haigh[6], Dr Christopher Allen[9], Professor Wilhelm Auwärter[4], Professor Reinhard Maurer[1], Dr David Duncan[2,5]

[1]University of Warwick, United Kingdom, [2]Diamond Light Source, United Kingdom, [3]Korea Basic Science Institute, South Korea, [4]Technical University of Munich, Munich, Germany, [5]University of Nottingham, United Kingdom, [6]University of Manchester, United Kingdom, [7]Carl von Ossietzky Universität, Germany, [8]Max IV Laboratory, Sweden, [9]University of Oxford, United Kingdom

MS-3: On-Surface Synthesis of 1D and 2D Functional Graphitic Materials, June 19, 2024, 10:30 - 12:35

Typically, the introduction of defects into graphene requires post-processing methods such as ion sputtering or plasma etching.[1,2] Here, we present a bottom-up synthesis method yielding graphene with incorporated topological defects on a copper substrate. In the chemical vapour deposition process we use an aromatic precursor that contains the same structural elements as the desired defect. During the growth of the graphene lattice, the topology of the precursor is partly retained and topological defects are formed in the carbonaceous network. We have utilised imaging techniques such as scanning tunnelling microscopy (STM) and non-contact atomic-force microscopy (nc-AFM) to characterise the electronic and physical structure (Figure 1), respectively. We have tested the durability of these graphitic films via etching of a copper foil substrate and transferring them to a transmission electron microscopy (TEM) grid for imaging. By utilising nc-AFM and TEM we have quantified the number of these topological defects which can be introduced by varying the copper substrate temperature during growth. Further, we have spectroscopically studied the defective graphene using the techniques of normal incidence X-ray standing waves (NIXSW), near edge X-ray absorption fine structure (NEXAFS) and X-ray photoelectron spectroscopy (XPS) to elucidate the structural and chemical changes induced by varying defect concentration. Structurally, our results indicate that the adsorption height varies inversely with the defect concentration. Good agreement was found between our simulated XPS and NEXAFS spectra with experiment using state-of-the-art density functional theory hybrid functionals.

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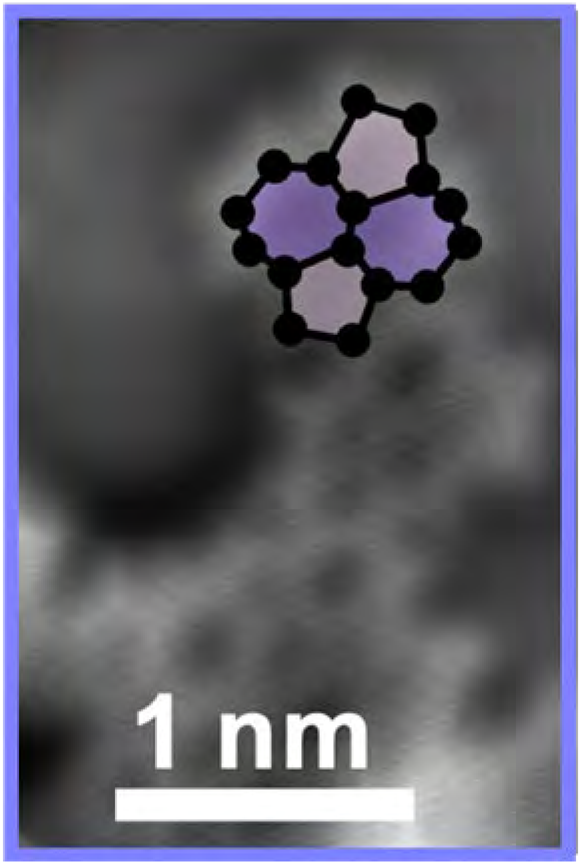
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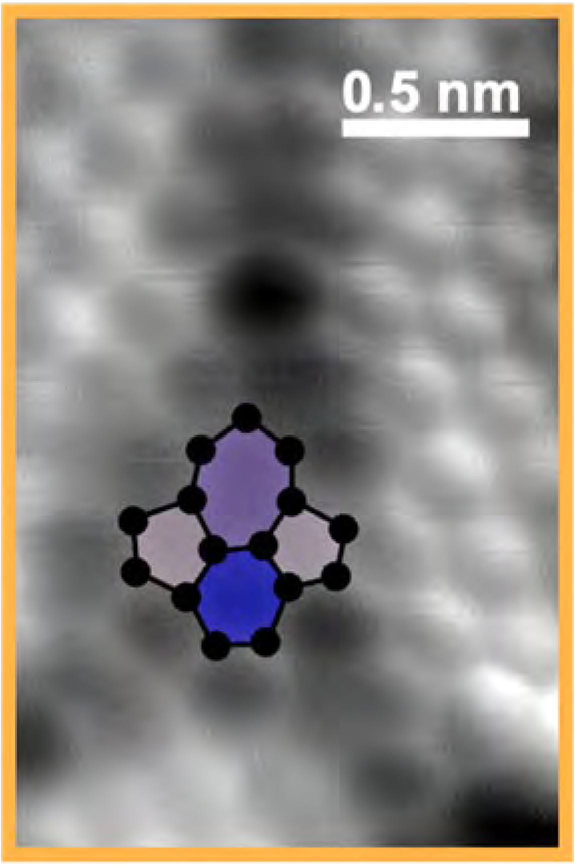
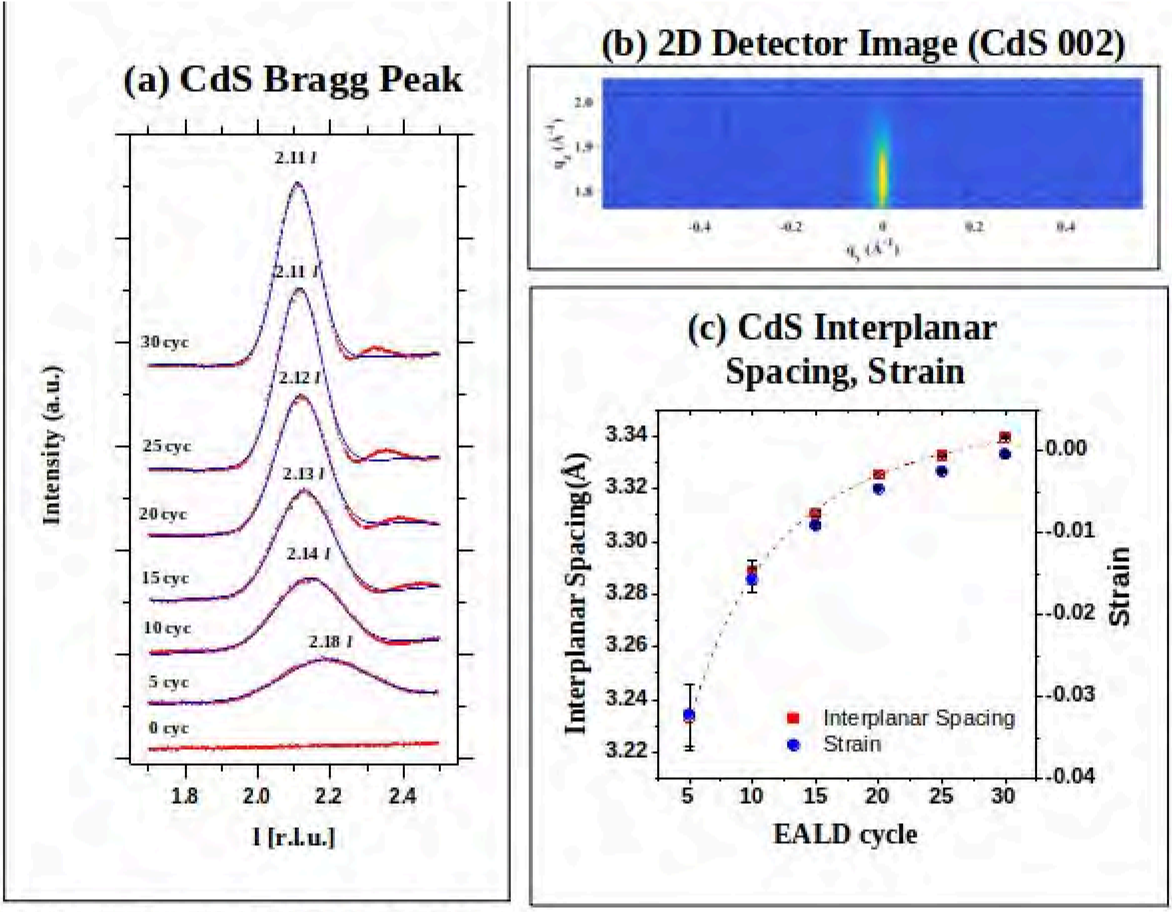

0.5 nm

An electrochemical approach to the growth of semiconductor thin films

Francesco Carla[1], Matthew Snelgrove[2], Adam Morris[3]
[1]Diamond Light Source, United Kingdom, [2]Bernal Institute, University of Limerick, Ireland, [3]University of Bath, United Kingdon

2D Semiconductors, June 18, 2024, 14:00 - 15:30

Electrochemical atomic layer deposition (E-ALD) is a method used for the growth of highly crystalline semiconductor thin films on conductive substrates. This technique exploits surface-limited electrochemical reactions, and is based on the alternate deposition of different elements in solution. The process can be performed using relatively simple and inexpensive setups and has been proved effective for the growth of epitaxial thin films on single crystal surfaces. The use of such substrates represent a barried for the possible application of the technique for microfabrication and possible industry integration. In order to overcome this limitation we have investigated the possibility of using polycrystalline surfaces as substrate for E-ALD reactions. In this contribution we'll present the results of a comparative study performed on the E-ALD of CdS on Au(111) and polycrystalline Au at the I07 beamline of the Diamond Light Source synchrotron. The growth process on both substrates has been characterized using Surface X-ray Diffraction and X-ray Reflectivity experiments that have been performed using a flow cell designed for in-situ electrochemistry. The results of the x-ray experiments and additional data obtained post-growth using laboratory techniques show that is effectively possible to use E-ALD for the preparation of high quality crystalline films.



CdS growth on Au(111) by E-ALD
(a) (002) Bragg peak evolution during growth
(b) CdS (002) Bragg peak showing high order and crystallinity (no evidence of powder rings observed)
(c) Relationship of the interplanar spacing and strain with E-ALD cycles.

N-heterocyclic carbenes – The design concept for densely packed and thermally ultra-stable aromatic self-assembled monolayers

Mateusz Wróbel[1], **Daria M. Cegiełka**[1,2], Andika Asyuda[3], Krzysztof Kozieł[4], Michael Zharnikov[3], Piotr Cyganik[1]

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Low-dimensional Thin Film Materials, June 17, 2024, 11:00 - 12:35

Self-assembled monolayers (SAMs) of N-heterocyclic carbenes (NHCs) on metal substrates are among the most commonly investigated systems in the context of molecular-scale engineering of surfaces and interfaces. Interest in NHC SAMs is mainly driven by their extreme chemical stability[1] and assumingly higher thermal stability[2] compared to archetypal thiolate SAMs. The majority of NHC SAMs' forming molecules are designed employing imidazolium in the role of anchoring group. The prevailing view in literature is that only by attaching the bulky side groups to nitrogen heteroatoms in imidazolium moiety, the standing up and stable NHC SAMs can be achieved.[3,4] However, such approach leads to monolayers with much lower packing density compared to thiolate SAMs. We demonstrate, combining several spectroscopic methods (X-ray photoelectron spectroscopy, near-edge X-ray absorption fine structure spectroscopy), and temperature-programmed secondary ion mass spectrometry analysis, that upright oriented, densely packed and ultrahigh thermally stable NHC SAMs can be formed by using NHCs molecules with small methyl side groups in combination with simple, solution-based preparation procedure.[5] While SAMs exhibiting such features are especially suitable for applications in organic electronics, where overheating problems and high-temperature fabrication procedures are common issues, the high density and upright orientation makes them a good platform for further functionalization.

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Underpotential deposition of nickel oxyhydroxide nanoislands for better understanding of the alkaline oxygen evolution reaction

Harry Taylor[1], Alex Walton[1]
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Catalysis and Electrocatalysis including Single Atom and In Operando Studies 2, June 19, 2024, 16:00 - 17:30

Hydrogen will play a key role in fighting climate change by providing a clean fuel source in hard-to-decarbonise industries and energy storage. Currently, 96% of hydrogen production is from fossil fuels. Green hydrogen is the production of hydrogen using electrolysis powered by renewable energy sources. The oxygen evolution reaction (OER) is often referred to as the bottleneck of electrolysis due to its kinetically sluggish 4 electron transfer processes. Better catalysts are required to increase green hydrogen production. Currently expensive, and often rare, catalyst materials, such as iridium and ruthenium are used. First row transition metal oxides have been shown as a potential, cheap and sustainable, alternative to these materials.

One of these alternatives for alkaline OER is nickel oxyhydroxide (NiOOH). The active phase of the bulk catalyst is a highly disordered layer of NiOOH, making it difficult to characterise on the atomic scale. We have created a model system of well-defined NiOOH nanoislands on atomically flat gold(111) surface to fully understand the relationship between structure and function of the catalysts. Underpotential deposition is the phenomenon of electrodepositing a monolayer of one metal onto another metal. In this case, we have used the technique to deposit a metal oxide onto another metal with submonolayer coverage (nanoislands). The structure of the nanoislands is characterised using a combination of high-resolution atomic force microscopy (HR-AFM) and angle resolved x-ray photoelectron spectroscopy (AR-XPS). Electrochemical measurements and operando XPS are used to determine the catalytic activity and stability of the systems.

Positive and Negative Impacts of Hydrogen Bonds on Photocatalytic Hydrogen Evolution

Zhongqiu Lin[1,2], Hikaru Saito[1], Hiromasa Sato[1], Toshiki Sugimoto[1,2]
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Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 4, June 21, 2024, 10:30 - 12:00

Understanding the behavior of water molecules at solid–liquid interfaces is crucial for various applications such as photocatalytic water splitting, a key technology for sustainable fuel production and chemical transformations. Despite extensive past studies, the impact of the microscopic structure of interfacial water molecules on photocatalytic reactivity has not been thoroughly examined, primarily due to the abundance of bulk water molecules that hinders the observation of interfacial water. In this work, we conducted experiments in a water vapor environment and controlled water adsorption layers, ranging from angstroms to nanometers, on various TiO_2 photocatalysts. With this approach, we directly demonstrated the crucial role of hydrogen bond (H-bond) networks in photocatalytic hydrogen evolution by combining real-time mass spectrometry and Fourier-transform infrared spectroscopy. We observed a monotonic increase in the H_2 formation rate with increasing relative humidity (RH) up to 70%, indicating that reactive water molecules were present not only in the first adsorbed layer but also in several overlying layers. In contrast, at RH above 70%, when more than three water layers covered the catalyst surface, the H_2 formation rate began to decrease dramatically because of the structural rearrangement and hardening of the interfacial H-bond network induced during further water adsorption. This unique many-body effect of interfacial water was consistently observed for various TiO_2 particles with different crystalline structures, including brookite, anatase, and a mixture of anatase and rutile. Our results demonstrated that depositing several water layers in a water vapor environment with RH ~70% is optimal for photocatalytic hydrogen evolution rather than liquid-phase reaction conditions in aqueous solutions. This work provides molecular-level insights for designing interfacial water conditions to enhance photocatalytic performance.

Flexible thin film surface acoustic wave technology for transdermal drug delivery

Jikai Zhang[1], Duygu Nahar1[1], Hui Ling Ong[1], Peter Arnold[1], Meng Zhang[1], Hamdi Torun[1], Mohammad Mohammad[1], Yong-Qing Fu[1]
[1]Northumbria university, United Kingdom

Biomaterials 2 and Bioengineering, June 18, 2024, 14:00 - 15:30

Transdermal drug delivery, as an alternative to oral and intravenous subcutaneous injection drug delivery, allows painless delivery of drugs or macromolecules through the skin into the body [1]. Unlike needle injection, transdermal drug delivery method offers minimally invasive delivery [2] in addition to avoidance of drug degradation in the stomach [3], and potentially controlled release of drugs [4]. Various technologies have been evaluated as means to enhance drug delivery through the relatively impervious epidermal layer of the skin, however precise delivery of large hydrophilic molecules is still a challenge even with microneedles or other energized (electrical, thermal or ultrasonic) patches, which are often difficult to integrate into small wearable devices. This study developed a flexible thin film surface acoustic wave (SAW) platform to facilitate transdermal delivery of macromolecules with fluorescein isothiocyanate up to 2000 kDa. ZnO thin films were deposited onto alumnium substrates and flexible thin film SAW devices were prepared. Two surrogates for human skin have been used to evaluate SAW energized devices, i.e., delivering dextran through agarose gel and also across stratum corneum of pig skin into the epidermis. Mechanical agitation, acoustothermal effect, and microscale acoustic cavitation induced by SAWs activated on the skin surface were identified as the main mechanisms for promoting drug transdermal transmission. Our studies showed that SAW based transdermal drug delivery is dependent on the combined effects of wave frequency and intensity, duration of applied acoustic waves, temperature, and drug molecules molecular weights.

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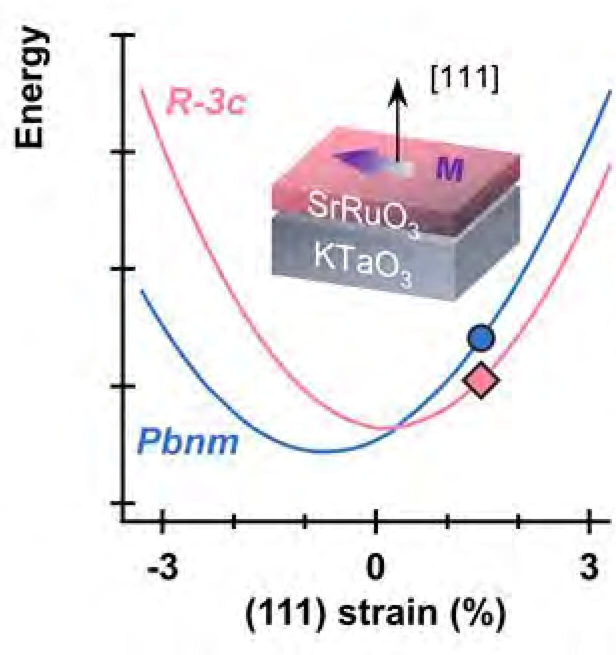
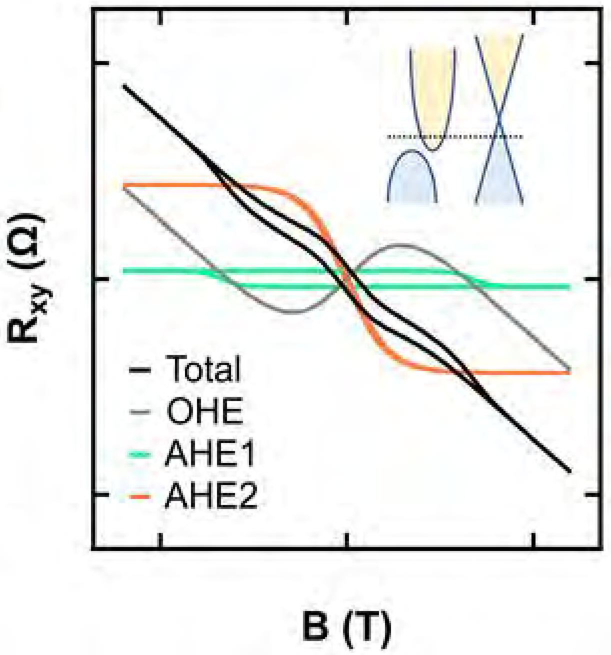
Magnetism and Berry phase manipulation in an emergent structure of perovskite ruthenate by (111) strain engineering

Prof. Xiaoran Liu[1], Zhaoqing Ding[1], Dr. Xuejiao Chen[2], Prof. Qinghua Zhang[1], Prof. Zhicheng Zhong[2], Prof. Jiandong Guo[1]
[1]Institute Of Physics, Chinese Academy Of Sciences, China, [2]Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, China

Functional Coatings 2 and Superconducting Thin Films, June 17, 2024, 16:00 - 17:35

The interplay among symmetry of lattices, electronic correlations, and Berry phase of the Bloch states in solids has led to fascinating quantum phases of matter. A prototypical system is the magnetic Weyl candidate $SrRuO_3$, where designing and creating electronic and topological properties on artificial lattice geometry is highly demanded yet remains elusive. Here, we establish an emergent trigonal structure of $SrRuO_3$ by means of heteroepitaxial strain engineering along the [111] crystallographic axis. Distinctive from bulk, the trigonal $SrRuO_3$ exhibits a peculiar XY-type ferromagnetic ground state, with the coexistence of high-mobility holes likely from linear Weyl bands and low-mobility electrons from normal quadratic bands as carriers. The presence of Weyl nodes is further corroborated by capturing intrinsic anomalous Hall effect, acting as momentum space sources of Berry curvatures. The experimental observations are consistent with our first-principles calculations, shedding light on the detailed band topology of trigonal $SrRuO_3$ with multiple pairs of Weyl nodes near the Fermi level. Our findings signify the essence of magnetism and Berry phase manipulation via lattice design and pave the way towards unveiling nontrivial correlated topological phenomena.





Exploration of Defect Superstructures in Graphene

Benedict Saunders[1], Dr Lukas Hoermann[1,2], Professor Reinhard Maurer[1,2]
[1]Department of Chemistry, University of Warwick, United Kingdom, [2]Department of Physics, University of Warwick, United Kingdom

MS-3: On-Surface Synthesis of 1D and 2D Functional Graphitic Materials, June 19, 2024, 10:30 - 12:35

Graphene has been meticulously studied due to its remarkable mechanical, electrical, and thermal properties. It is well documented that introduction of various dopants and defects in the lattice can be used to tune the material's properties for a specific application, such as in electronics, sensors, or catalysis. In order to design graphene with specific properties, one must achieve control over the composition and concentration of defects. This requires a fundamental understanding of the stability of defects and their interaction in a superstructure. We present a comprehensive surface structure determination approach using the SAMPLE structure search code, extended to enable the systematic generation of defective superstructures, using a combination of Density Functional Theory and machine learning. Henceforth, we show the capabilities of our approach for a proof-of-principle application on free-standing graphene with heteroatom, vacancy, and topological defects. Finally, we use the SAMPLE code to gain physical insight into the interactions between these defects, paving the way for effective and rational growth models of topologically designed defective graphene.

Investigating the Tribological Behavior of Bioinspired Surfaces in Agro-waste and Alumina Reinforced AA6063 Matrix Hybrid Composites.

Prof Peter Apata Olubambi[1,2], <u>Dr Festus Ben</u>[1,2,3]

[1] Centre for Nanomaterials and Advanced Materials, University of Johannesburg, South Africa, [2] Department of Metallurgy, University of Johannesburg, South Africa, [3] Centre for Advanced Material Research and Development, Federal Polytechnic Ede, Nigeria

Biointerfaces/Biophysics/Biosensers, June 19, 2024, 10:30 - 12:35

The tribological behaviour of three bioinspired agro-waste ashes, including bean pod ash, cassava peel ash, and coconut husk ash, integrated as reinforcements in alumina-reinforced AA6063 matrix hybrid composite was investigated. The hybrid composites were fabricated using the double stir-casting method to ensure uniform dispersion, of both the natural and synthetic reinforcements within the aluminum matrix. The objective was to engineer bioinspired materials that not only exhibit lightweight properties but also boast exceptional hardness and wear resistant characteristics. The specific wear rate exhibited notable variations with sliding velocity across the distinct agro-waste reinforcing materials. This observation is in stark contrast with the behaviour observed in the single reinforced alumina/AA6063 and the unreinforced matrix, underscoring the unique bioinspired tribological attributes of the agro-waste-based hybrid composites. Furthermore, the hardness values demonstrated a proportional increase corresponding to the weight percentage of agro-waste ash contents. Improvement in wear resistance was also observed. These nuanced bioinspired tribological behaviors presents opportunities for tailored load-bearing applications, derivable from the agro-waste-based hybrid composites. With their potential to offer lightweight yet robust components, these composites show promise across a spectrum of industrial domains, including automotive, automobile, and electronics. As such, this study not only advances our understanding of bioinspired tribological phenomena but also paves the way for the development of innovative materials with diverse applications and enhanced performance attributes.

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Interaction between pentacene molecules and monolayer transition metal dichalcogenides

Dr Juliana Morbec[1], Mr Edward Black[1]
[1]*Keele University, United Kingdom*

Catalysis and Electrocatalysis including Single Atom and In Operando Studies 2, June 19, 2024, 16:00 - 17:30

Combining two-dimensional (2D) materials with organic materials can be very attractive for applications that require flexibility and where size and weight are important parameters to be considered, such as in wearable, portable and mobile applications. Organic materials usually exhibit excellent optical absorption efficiency and photo- and temperature-induced conformational changes, while 2D materials often show relatively high carrier mobility, superior mechanical flexibility, and tunable electronic and optical properties. Combining both systems can stabilize the organic materials and lead to heterostructures with both high carrier mobility and high optical absorption efficiency, which is promising for solar energy conversion. In this work we investigate, by means of density-functional-theory calculations, heterostructures composed of organic molecules (for example, pentacene and azulene) and transition metal dichalcogenides (TMD) for application in photovoltaic devices. We examine the interaction between the molecules and monolayer TMDs as well as the band alignment of the heterostructures, considering effects of the molecular coverage, rotation and dielectric screening.

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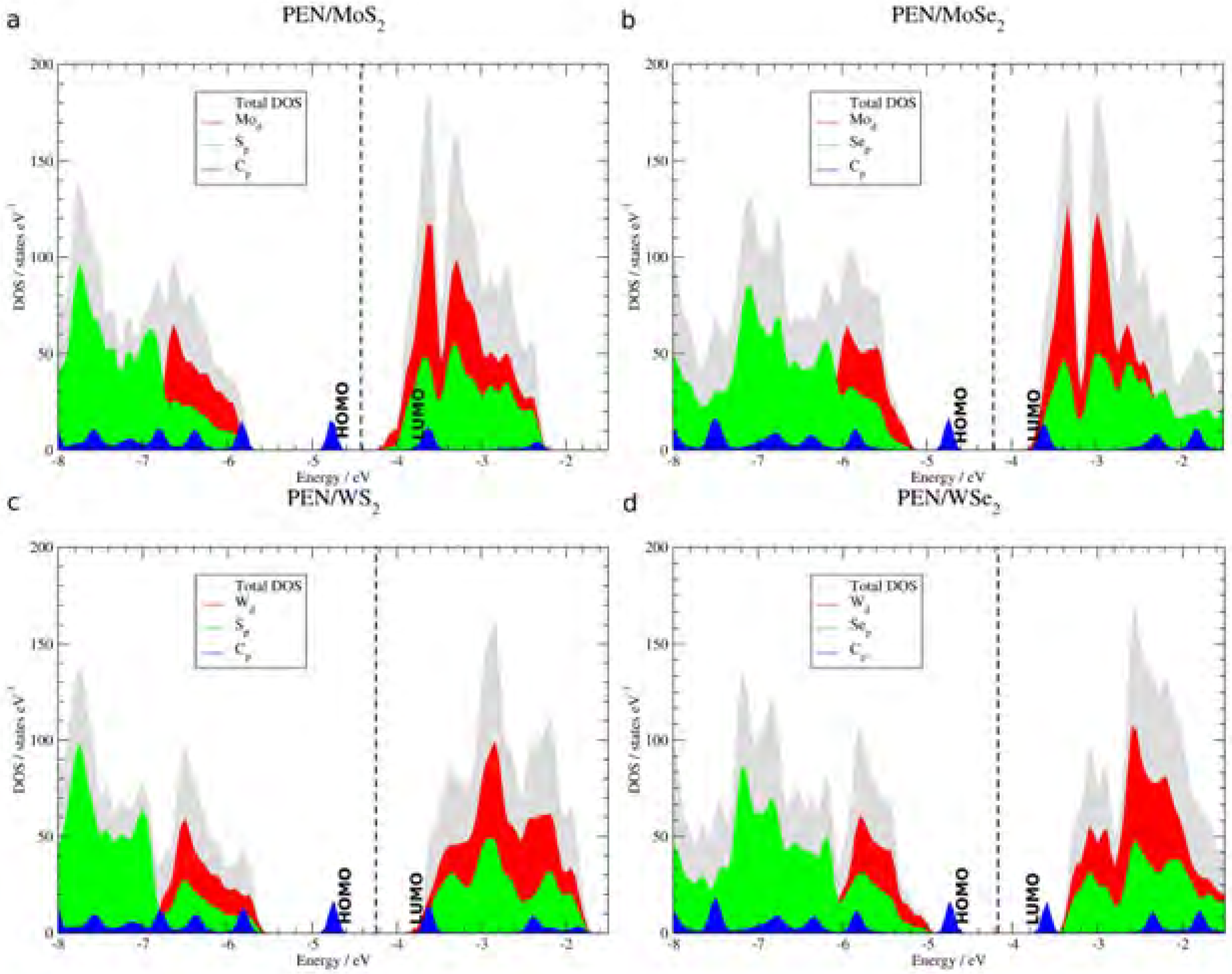

Lattice dynamics of low-dimensional systems investigated with surface spectroscopy

Jiandong Guo[1]
[1]Institute Of Physics, Chinese Academy Of Sciences, China

2D Materials and Van der Waals heterostructures 1, June 19, 2024, 14:00 - 15:30

To understand the mechanism of how the lattice determines the physical properties of condensed matters, it is important to investigate the lattice dynamics by analyzing the phonon energy and lifetime. High resolution electron energy loss spectroscopy (HREELS) is a powerful tool for the measurements of phonon dispersion of solids from their surfaces. We developed this technique by introducing the hemispherical electron analyzer and realized the energy/momentum two-dimensional detection of surface elementary excitations including phonon and plasmon. By using the new HREELS, the topological nodal rings of the monolayer graphene, both dispersive and nondispersive, are identified directly. The nonanalytical V-shaped phonon dispersion of the monolayer BN on Cu foils are observed, evidencing the distinct nature of the two-dimensional polar system. The microscopic mechanism of the superconductivity enhancement at FeSe/SrTiO3 interface is also clarified as the interfacial electron-phonon interaction measured by HREELS.

Reflection imaging with a helium zone plate microscope

Sabrina Daniela Eder[1], Ranveig Flatabø[1], Thomas Reisinger[1], Gianangelo Bracco[2], Peter Baltzer[3], Bjørn Samelin[1], Bodil Holst[1]

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MS-1: Recent Developments in Surface Microscopy, June 18, 2024, 10:30 - 12:30

Neutral helium atom microscopy is a novel microscopy technique which offers strictly surface-sensitive, non-destructive imaging. Several experiments have been published in recent years where images are obtained by scanning a helium beam spot across a surface and recording the variation in scattered intensity at a fixed total scattering angle θSD and fixed incident angle θi relative to the overall surface normal [1 - 6]. These experiments used a spot obtained by collimating the beam (referred to as helium pinhole microscopy). Alternatively, a beam spot can be created by focusing the beam with an atom optical element. However up till now imaging with a focused helium beam has only been demonstrated in transmission (using a zone plate) [7]. Here we present the first reflection images obtained with a focused helium beam (also using a zone plate). Images are obtained with a spot size (FWHM) down to 4.7 μm ± 0.5 μm, and we demonstrate focusing down to a spot size of about 1 μm. Furthermore, we present experiments measuring the scattering distribution from a focused helium beam spot. The experiments are done by varying the incoming beam angle θi while keeping the beam-detector angle θSD and the point where the beam spot hits the surface fixed - in essence, a microscopy scale realization of a standard helium atom scattering experiment.

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Molecular Ordering on Surfaces at the Limit of Vanishing Coupling Strengths: TMPH/Cu(111)

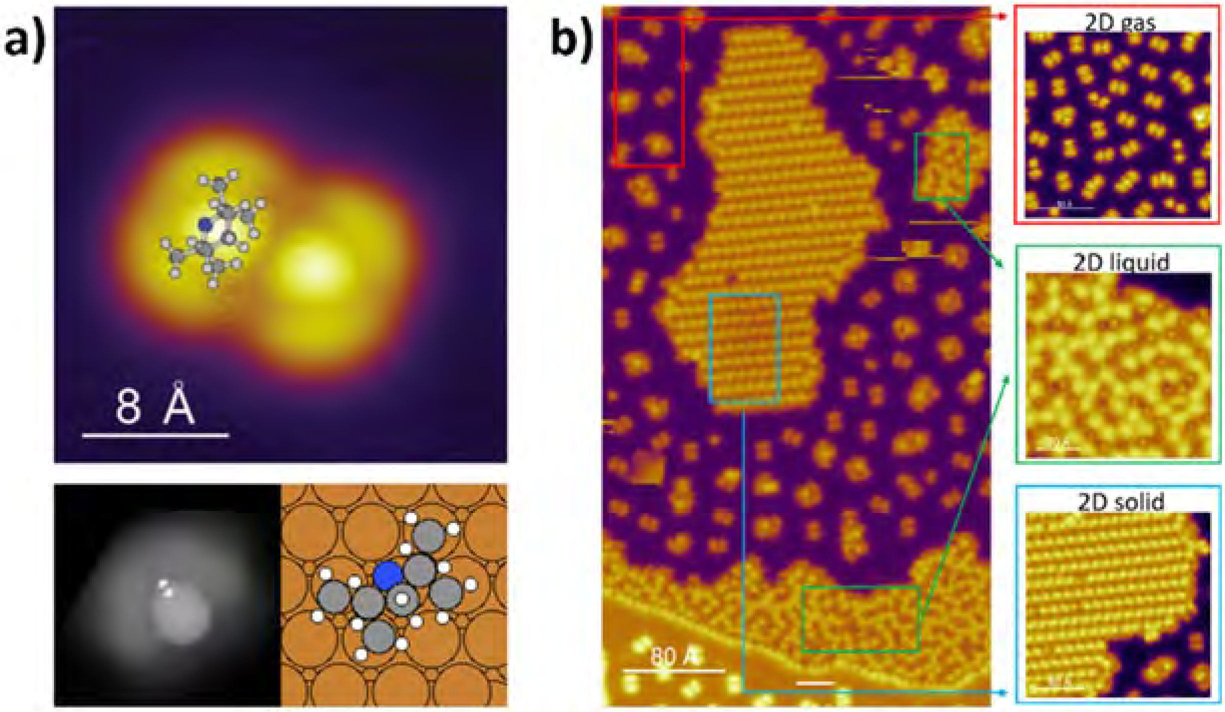
Miki Fukushima[1], Dr Renald Schaub[1]
[1] *School of Chemistry, University of St Andrews, United Kingdom*

Self-Assembly, Characterisation and Reactivity of 2D Structures of Molecules at Surfaces, June 21, 2024, 10:30 - 12:00

Several factors conspire to drive molecular ordering at surfaces, including intermolecular forces, the molecule-substrate interaction strength, temperature and kinetics, and molecular structure and symmetry. In the limit of very minute interaction strengths, ordering can be obtained by lowering the temperature. As it decreases towards absolute zero, thermal motion diminishes, allowing for enhanced control and stability of molecular assemblies on surfaces. This pursuit is grounded in the recognition of the pivotal role that molecular ordering plays in determining the physical, chemical, and electronic properties of surface-bound structures. A question of interest therefore becomes: When do interaction strengths become too weak to sustain molecular ordering at near-zero temperatures?

Herein, the adsorption of 2,2,6,6-Tetramethylpiperidine (TMP) on Cu(111) is investigated under ultra-high vacuum and low-temperature (~5K) conditions by Scanning Tunnelling Microscopy (UHV-LT-STM). The system represents an extremely weakly coupled system consisting of a two-fold symmetric non-planar molecule and a three-fold symmetric support.

At low coverages, we identify a 2D gas-like phase composed of monomers and dimers of TMP, each in a different adsorption configuration. From DFT calculations, we identify the adsorption geometry of TMP in its dimeric form. Most interestingly however, the monomer exhibits a three-fold symmetry incompatible with any static geometry of TMP. And yet, facile tip-assisted manipulations can induce the monomers to form dimers and vice-versa. We prove that the monomeric TMP exists in a highly activated rotational state, akin to a translation pinned around the N-C pivot point. With increasing TMP coverage, saturation and condensation are reached, with the emergence of small, disordered droplets. These can be grown by further inclusion into extended, but disordered liquid-like molecular islands. When the full monolayer coverage is nearly reached, crystalline structures are observed within disordered islands. Therefore, three TMP/Cu(111) phases (solid, liquid, gas) are seen to coexist at 5 Kelvin.



Updates on the factors determining the design of an XHV system for an Ion-trap Quantum Computer

Sam Lodge[1], Paul Smith[1], Andrew Chew[1], Nigel Burch[1], Peter Jones[1], Pete Lamb[1], Emiliano Lucchetta[1], Paul Milner[1], Derek Clement[2], Tanya Sinha[2], Amin Abolghasemi[3], Joe Randall[3], Luuk Earl[3], Frank Rathmann[1]

[1]Edwards Ltd, United Kingdom, [2]Gamma Vacuum, United States of America, [3]Universal Quantum, United Kingdom

Special Vacuum Chambers and Components, June 17, 2024, 16:00 - 17:35

An XHV system for an ion trap quantum computer has been developed where a target operating pressure of <10-12 mbar has been identified to maximise ion/qubit lifetime. Considerations made for the final design will be presented with respect to material choice and treatments, pump selection and the consequences of a low allowable bakeout temperature.

Contributions to the total residual gas load from leaks, permeation and outgassing will be reported as will other factors including conductance optimization and vibrations.

Molecular dynamics investigation of the role of lattice heating in laser-driven hydrogen evolution at copper surfaces

Alexander Spears[1], Wojciech Stark[1], Professor Reinhard Maurer[1]
[1] *University Of Warwick, United Kingdom*

Plasmonics and Excited States at Surfaces, June 19, 2024, 10:30 - 12:35

Light-induced ultrafast dynamics entail the energy transfer between light, electrons, and phonons at interfaces. Whether or not this energy transfer can be harnessed to selectively drive photocatalytic processes remains an open question. Molecular dynamics with electronic friction (MDEF) provide a fully anharmonic mixed quantum-classical description of electron-phonon coupling, whereby electronic friction is usually approximated with a homogeneous electron gas model. While this method has previously been used to model state-resolved scattering experiments or to determine vibrational lifetimes after femtosecond laser pulses, its validity has yet to be fully assessed.

We compare the dynamics of laser-driven hydrogen recombination across different copper surface facets using machine-learning interatomic potentials based on electronic structure theory to enable the efficient statistical sampling of chemical dynamics.

Using this approach, we compare results from thousands of simulations based on electronic friction using first-order response theory and the homogeneous electron gas model and analyse the ability of different approximations to accurately describe the non-adiabatic energy transfer between the surface and adsorbates.

These methods also allow us to investigate the influence of lattice heating after an ultrafast laser pulse.

Modification of the surface of a macroporous Ni electrocatalyst for hydrogen production using Ag and Pd nanostructures

Dr. María Sánchez-Loredo[1], Ramiro Medina-Orta[2], Emma Ortega[2], Valentín Pérez-Herranz[2]
[1]Universidad Autónoma de San Luis Potosí, Mexico, [2]Universitat Politècnica de València, Spain

Supported Nanostructures, June 17, 2024, 14:00 - 15:30

Metal nanoparticles have shown an efficient catalytic performance in the hydrogen production by alkaline water electrolysis, a promising method to produce hydrogen as a clean renewable energy carrier. However, the reduction of the energetic investment for large-scale production still requires special efforts, and can be achieved through the improvement of the intrinsic catalytic activity of the electrodes, or by enlarging the active surface area. In this work, the hydrogen production using multicomponent catalysts with low Ag, Pd and Ag/Pd loading, supported on macroporous nickel electrodes, is reported. The high activity and conductivity of silver nanoparticles was expected to complement the activity of the nickel electrodes on the Hydrogen Evolution Reaction (HER). Pd nanoparticles incorporation was carried out depositing a colloidal dispersion, followed by heat-treatment, with the aim to provide more active sites enhancing the HER activity. The study of the electrochemical activity in the HER was carried out using pseudo-steady-state polarization curves and electrochemical impedance spectroscopy at different temperatures, and the results were correlated with their nanostructured porous structures (some with morphologies characterized by corners and edges). The values of η100 (overpotential invested to produce a fixed amount of hydrogen) and jm (an indicative of the catalytic activity per unit mass of metal nanoparticles), obtained with the modified electrode with lower Pd loading, improve those obtained by other authors who applied bimetallic AgPd nanoparticles for the HER [1-3]. The incorporation of nanostructures (Pd over Ag) provided morphologies with more active sites, significantly improving the catalytic activity of the electrode and reducing the energy investment required to produce hydrogen.

Acknowledgments: CONACYT-COPOCYT/472041

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Growth dynamics and mechanical properties of TiAl(Si)N monolayers and multilayers deposited by HiPIMS on Si and WC-Co substrates

Thiago De Souza Lamim[1], Diego Martinez-Martinez[1], Jean-Baptiste Chemin[1], Yves Fleming[1], Adrian-Marie Philippe[1], Nathalie Valle[1], Marianne Penoy[2], Ralph Useldinger[2], Laurent Bourgeois[2], Patrick Choquet[1]
[1]Luxembourg Institute of Science and Technology (LIST), Luxembourg, [2]Ceratizit Luxembourg, Luxembourg

Low-dimensional Thin Film Materials, June 17, 2024, 11:00 - 12:35

TiAl(Si)N coatings are promising candidates for machining difficult-to-cut engineering materials due to their high hardness, wear resistance, and oxidation resistance. Their multilayer structures are expected to combine and enhance these properties [1]. This work investigates the growth of two TiAl(Si)N multilayer systems deposited by HiPIMS on Si and WC-Co substrates. The first consists of TiAlSiN layers with different Ti:Al ratios between each sublayer. TiAlN/TiAlSiN multilayers form the second system with the same Ti:Al ratio but different bilayer thicknesses. Microstructural characterisations were performed using FESEM. XRD in Grazing incidence and Bragg-Brentano configurations were employed to identify the phases and texture. Additionally, the structural aspect and growth dynamics of these films were studied by TEM, Electron Diffraction and XRD pole figures. Furthermore, the mechanical properties were analysed by nanoindentation.

The multilayers are formed by the same phases present in the constituting monolayers: hexagonal + cubic and cubic + cubic (Fig. 1). However, both cubic monolayers showed different textures, changing from (220) to (111) with the addition of Si in the films. Surprisingly, the texture of the cubic + cubic multilayers differed from both initial monolayers and was influenced by the substrate: (420) for Si substrate and no clear presence of peaks for WC-Co. The cubic + cubic multilayers showed a columnar growth structure, indicating a continuity of the crystalline phases throughout the sublayers. On the other hand, such continuity was interrupted for the hexagonal + cubic multilayer, where the columnar growth was no longer observed. The chemical contrast of annular dark field STEM and EDS mapping confirmed the multilayer structure for both systems. The hardness of the multilayers tends to be similar to the average values of their weakest sublayer when the thickness ratio is equal to 1.

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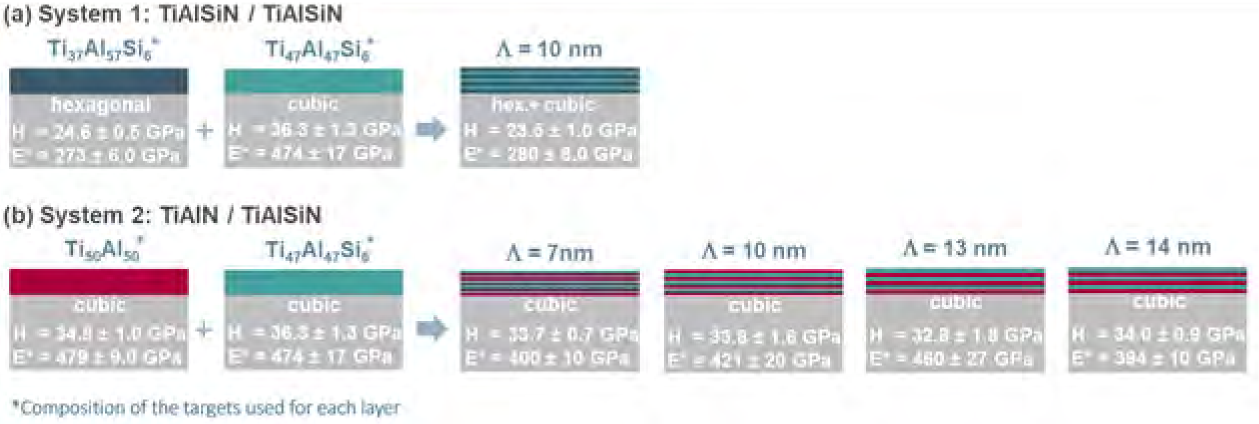

Monolayer exfoliated MoS2 studied with Atom micro diffraction

Dr. Sam Lambrick[1,2], Nick von Jeinsen[1], Ke Wang[1], Alek Radic[1], Yiru Zhao[3], Ismail Sami[3], Vivian Perez[1], Manish Chhowalla[3], Andrew Jardine[1]

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MS-1: Recent Developments in Surface Microscopy, June 18, 2024, 10:30 - 12:30

Atom micro diffraction employing neutral helium atoms has emerged as a pioneering technique for investigating atomic-scale surface structures[1]. Leveraging the unique properties of thermal energy neutral atoms, particularly their absolute surface sensitivity, atoms are an ideal probe for studying two-dimensional (2D) materials. Among these materials, transition metal dichalcogenides (TMDs), such as MoS2, have garnered significant interest in optoelectronics, especially when functionalized through vacancies and defects[2].

In this study, we applied atom micro diffraction utilizing our scanning helium microscope (SHeM) to investigate monolayer exfoliated MoS2. The spatial resolution afforded by SHeM allowed us to perform atom diffraction studies on a exfoliated monolayer of a TMD, a class of materials that have previously only been measured with atom scattering in a layered bulk structure. We perform analysis comparing the diffraction from monolayer and bulk MoS2, explore the temperature dependence of the diffraction, while also considering the influence of the substrate. Additionally, we explored the scattering behaviour from surface sulphur vacancies in the monolayer[3], which has proved difficult to do with established techniques.

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Quadrupole Residual Gas Analysis developments at TNO

René Koops[1], Timo Huijser[1], Arnold Storm[1], Léo Blanc[1], Gijs Snijders[1], Marina Gomes Rachid[1], Mark van de Kerkhof[2], Eva Mondt[2], Jan Hulva[2], Jeroen van den Brink[2]
[1]TNO, Netherlands, [2]ASML, Netherlands

MS-6: RGA User Meeting 1, June 19, 2024, 10:30 - 12:35

Extreme ultra-violet lithography (EUVL) is the current leading edge lithography methodology in Semicon industry. EUVL requires vacuum to ensure light transmission through the optics. This vacuum needs to contain very low partial pressures of contaminant species to ensure the lifetime of the optics inside the EUVL stepper. TNO has been heavily involved in EUVL technology from the early start, for a large part through research focused on optics lifetime and contamination control challenges.

From this point of view we have, amongst other topics, been involved in the definition of Ultra Clean Vacuum (UCV) and outgassing standards for EUVL technology. Most of our research and equipment relies heavily on residual gas analysis by use of RGA's (quadrupole Residual Gas Analyzers) which are becoming more and more popular in the (Semicon) industry.

RGA's are robust, relatively fast, require relatively small volume claims and are not relying on (strong) permanent magnetic fields. This makes RGA's a logical choice for industry, whereas for (fundamental) research other types of mass spectrometers can be of interest depending on their individual characteristics.

Despite these advantages for industry, the demands on performance keep being pushed close to and beyond hardware limits. Especially in the field of EUVL technology, the demands on dynamic range of measurement and lower detection limits for trace contaminants in a clean matrix gas are continuously being stretched.

In this presentation I would like to showcase an overview of what RGA related work we have done and plan to do in the future. This includes our efforts in lowering detection limits and increasing the dynamic range of measurements, development of brand-independent data handling SW, tuning and calibrating facilities and a variety of RGA-use within our labs and research.

Traceable partial pressure and leak rate measurements applying ISO/TS 20175

Matthias Bernien[1]
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MS-6: RGA User Meeting 1, June 19, 2024, 10:30 - 12:35

The calibration of quadrupole mass spectrometers (QMSs) is challenging due to the insufficient stability of their detection sensitivity. In order to perform traceable partial pressure and outgassing rate measurements reference pressures or gas flows must be provided in-situ for the relevant mass-to-charge ratios, respectively. ISO/TS 20175:2018 describes procedures that can be used to perform in-situ calibrations of QMSs.

The presentation will provide an overview on ISO/TS 20175:2018 covering the calibration of QMSs for continuous leak monitoring of vacuum systems, leak rate measurements with a tracer gas, residual gas analysis and outgassing rate measurements. The working principles of QMSs and the sources of instability are detailed to highlight the need for the procedures described in ISO/TS 20175:2018. When measuring low partial pressures of one gas in the presence of another gas with much higher partial pressure, so-called interference effects, i.e., a reduction in sensitivity to the former gas must be taken into account. For the calibration with respect to gas flows the effective pumping speed at the vacuum system must be considered in addition to the sensitivity of the QMS. In conclusion, the presentation aims to provide an understanding for the principles underlying the procedures described in ISO/TS 20175:2018 and how to achieve traceability when using QMSs.

Surface and bulk structure of spinel nanoparticles MFe2O4

Doctor Pilar Ferrer[1], Charlotte Hall[1,2], Dave C Grinter[1], Georg Held[1], Ricardo Grau-Crespo[2]
[1]Diamond Light Source, United Kingdom, [2]University of Reading, United Kingdom

Nanoparticles, June 18, 2024, 14:00 - 15:30

Ferrites are metal oxides with the spinel structure, AB2O4, where A represents divalent metal cation (e.g. Co2+, Cu2+, Zn2+) and B represents the trivalent cation, Fe3+. In a normal spinel the A and B cations occupy tetrahedral (Td) and octahedral (Oh) positions respectively. In order to understand the behaviour of nanoparticles of these metal ferrites for the photocatalytic water splitting reaction, we use a combination of computational simulations and experimental data to investigate the bulk and the surfaces properties of MFe2O4 (A =Co, Cu or Zn).
The A and B cations can redistribute across the Td and Oh sites and our results showed that the Td/Oh ratio of the Fe cation on the bulk was different from the surface. Calculations show that the electronic structure and band gap is affected by the cation distribution which in turn influences the catalytic properties. Bulk characterization was done by Anomalous X-Ray scattering, X-Ray Diffraction and XANES while the surface characterization was carried out by X-ray magnetic Circular Dichroism and Near Edge X-Ray Absorption Fine Structure (NEXAFS).

Dynamics of metal particles on rutile $TiO_2(110)$ under near-ambient pressures of O_2, H_2, and CO_2

Florian Kraushofer[1], Matthias Krinninger[1], Sebastian Kaiser[1], Johanna Reich[1], Friedrich Esch[1], Barbara A. J. Lechner[1]

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Catalysis and Electrocatalysis including Single Atom and In Operando Studies 2, June 19, 2024, 16:00 - 17:30

Catalysts on reducible oxide supports often change their activity significantly at elevated temperatures due to the strong metal-support interaction (SMSI), which induces the formation of an encapsulation layer around noble metal particles [1]. However, the impact of oxidizing and reducing treatments at elevated pressures on this encapsulation layer remains controversial, partly due to the ‘pressure gap’ between surface science studies and applied catalysis. Furthermore, the effects of encapsulation can be difficult to disentangle from those of sintering, which is also enhanced at elevated pressures.

In the present work, we employ near-ambient pressure scanning tunneling microscopy (NAP-STM) and X-ray photoelectron spectroscopy (NAP-XPS) to study the effect of reducing (H_2) and oxidizing (O_2, CO_2) atmospheres on Pt particles on rutile $TiO_2(110)$ at 600 K and pressures from ultra-high vacuum (UHV) up to 1 mbar. We find that controlling the sample stoichiometry is crucial, as even blank $TiO_2(110)$ surfaces exhibit very different reactivity to H_2 and CO_2, depending on the degree of bulk reduction, and the SMSI effect is suppressed on near-stoichiometric samples. On reduced samples, CO_2 acts as a weakly oxidizing gas, encapsulating particles in a non-classical SMSI mechanism similar to that observed in O_2 [2]. In contrast to the classical SMSI state, in which particles remain dynamic and somewhat accessible to adsorbates, they are permanently passivated when overgrown in oxidizing conditions. Small sub-nm clusters exhibit enhanced sintering in all three gas atmospheres before encapsulation occurs. Surprisingly, even large Pt nanoparticles dynamically restructure at 600 K in H_2, although the SMSI overlayer remains unchanged.

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Development of imaging-type spin-resolved photoemission microscopy apparatus

Koichiro Yaji[1], Shunsuke Tsuda[1]
[1]National Institute For Materials Science, Japan

Advances in Experimental and Theoretical Methods 2, June 17, 2024, 14:00 - 15:30

In developing novel materials and improving their performance, it is essential to clarify the electronic states near the Fermi level, which directly contribute to the physical properties. Recently, there has been a growing need to measure local electronic states down to sub-micrometers. Spin-resolved photoemission spectroscopy is a powerful technique that can investigate the spin-polarized electronic states in materials. However, the measurement efficiency of spin-resolved photoemission spectroscopy is extremely low compared to that of spin-integrated photoemission spectroscopy. Here, we show an imaging-type spin-resolved photoemission microscopy (iSPEM) equipped with a multi-channel spin detector developed at the National Institute for Materials Science (NIMS). A 10.9-eV laser is used as the excitation light. Compared to conventional machines using the single-channel spin detector, our iSPEM machine significantly improves the data acquisition efficiency in spin-resolved photoemission spectroscopy by four orders of magnitude. Spin-integrated (-resolved) photoemission imaging in real-space mode achieved a spatial resolution of 30 nm (420 nm). We demonstrate the spin polarization imaging of polycrystalline iron with the real space mode and spin-resolved Fermi-surface imaging of Bi(111) in the momentum space mode.

Velocity slip coefficient measurements at cryogenic temperatures using a Spinning Rotor Gauge

Mrs. Johanna Wydra[1], **Dr. Alexander Marsteller**[1], Mr. Vincent Skrobocz[1], Mr. Tim Poppe[1], Dr. Simon Niemes[1], Dr. Michael Sturm[1], Dr. Robin Größle[1]
[1] Karlsruhe Institute Of Technology, Germany

Vacuum Gas Dynamics, June 18, 2024, 16:00 - 17:30

The velocity slip coefficient is an important parameter for modelling of rarefied gas dynamics, describing the interaction between gas atoms or molecules and the surface.
When operated at pressures in the slip regime, a spinning rotor gauge (SRG) is sensitive to the viscosity, the velocity slip coefficient and the tangential momentum accomodation coefficient.
We have built and operated the Cryo-ViMA (cryogenic viscosity measurement apparatus) experiment, which uses an SRG in the slip regime aimed at measuring the viscosity of tritium over a temperature range from 80 K to room temperature.
The analysis required to extract the viscosity from our measured data also gives a value for the velocity slip coefficient, which can be related to the tangential momentum accomodation coefficient.
In this contribution we present the velocity slip coefficient in dependence of temperature as measured with our setup for helium and hydrogen isotopologues with the stainless steel rotor of our SRG.

Understanding the passivation layer formed by tolyltriazole on copper, bronze, and brass surfaces

Al Rossin[1], Dr Federico Grillo[1], Dr Stephen Francis[1], Dr David Miller[1,4], Dr Andrew Rossall[2], Prof Jakob van den Berg[2], Dr Gregory Hunt[3], Prof Christopher Baddeley[1]

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Metal Surfaces - Adsorption, Desorption and Reactions 1, June 17, 2024, 11:00 - 12:35

Tolyltriazole (TTAH) is used industrially as a corrosion inhibitor for copper alloys, particularly in organic media.[1-2] In this study, the morphology and chemistry of the layer formed by TTAH on copper and copper alloys under realistic conditions is investigated, with focus on the effects due to the presence of tin or zinc in the substrates. A combination of X-ray photoelectron spectroscopy (XPS), medium energy ion scattering (MEIS), and scanning transmission electron microscopy (STEM) has been used. It was found that an inhomogeneous metal-organic layer forms on the surface of copper specimens, likely in the form of copper nanoparticles surrounded by Cu-TTA complexes. This layer increases in thickness for at least 30 days. Chemically, the copper species in the layer are initially in the +2 oxidation state, but after longer exposure to TTAH, mostly Cu(I) is observed. In bronze samples, tin does not appear to segregate to the surface layer. In brass samples, zinc is depleted from the bulk and forms a thicker Zn-TTA layer.

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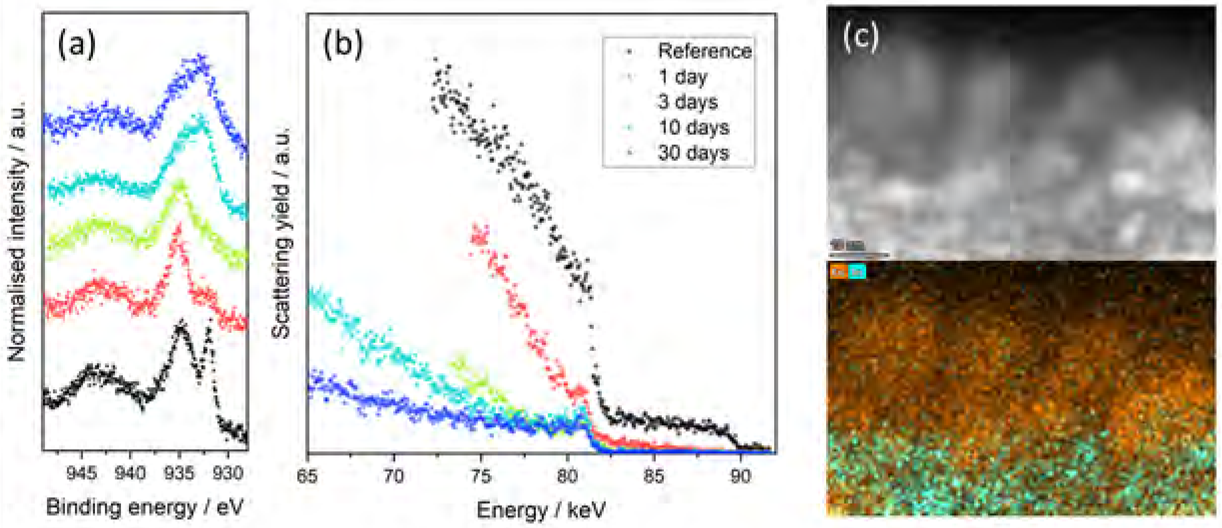

Figure 1: (a) Cu $2p_{3/2}$ XPS, (b) MEIS, and (c) cross-sectional STEM and EDS characterisation of phosphor bronze treated with TTAH at elevated temperature and pressure.

Probing molecular diffusion on 2D materials with neutral matter

Philipp Seiler[1], Viktoria Schwab[1], Noah J. Hourigan[1], Marco Sacchi[2], Anthony Payne[2], Anton Tamtögl[1]
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2D Materials and Van der Waals Heterostructures 2 and Ferroelectric Behaviour, June 20, 2024, 11:00 - 13:00

Lineshape broadening upon inelastic scattering from surfaces (Figure 1(a)) can be used to determine the characteristics of molecular diffusion on pico- to nanosecond timescales[1,2] with low-energy neutral beams being the gentlest probing technique[3]. Using this technique, we have studied the diffusion of both water and much more complex molecules on 2D materials.

Using neutron spectroscopy, we follow the nanoscopic motion of triphenylphosphine (P(C6H5)3 or PPh3) on graphite with a motion similar to that of a molecular motor. PPh3 “rolls” over the surface with an almost negligible activation energy for rotations and motion of the phenyl groups and a comparably small activation energy for translation. The unique behaviour of PPh3 is due to its three-point binding with the surface, increasing the adsorption energy while the effective diffusion barrier remains small [1] illustrating that the molecular degrees of freedom in larger molecules are intimately connected with the diffusivity[1,2].

We further illustrate that for H2O diffusion on epitaxial h-BN, the single-molecule perspective is highly complex. In contrast to motion over graphene[4], single H2O molecules can easily re-orientate, and their motion can no longer be treated as a series of jump-like motions by point-like particles occupying equivalent adsorption sites. We establish that, despite a water adsorption energy similar to graphene, an extremely low activation energy exists on h-BN, giving rise to motion with a strong normal component and a fast rearrangement of the water molecules' orientation during diffusion. We rationalise these findings in the context of the potential energy surface and molecular friction on h-BN/Ni(111). As illustrated in Figure 1(b), upon inclusion of the supporting metal substrate, H2O exhibits a much smaller friction on h-BN/Ni(111) compared to graphene/Ni(111), in stark contrast to the free-standing 2D materials[5].

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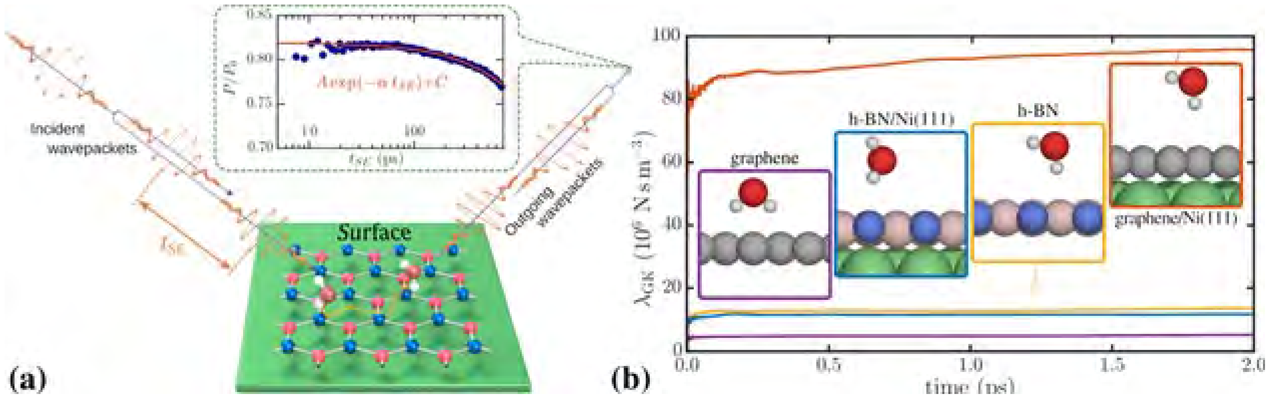

Advancements in ultra-high sensitivity mass spectrometers for atom scattering

Nick von Jeinsen[1,2], Dr Susanne Schulze[1], Mr Tom Spencer[1], Dr Andrew Jardine[1], Dr David Ward[1,2], Dr John Ellis[1]

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MS-6: RGA User Meeting 3, June 19, 2024, 16:00 - 17:30

As surface physics techniques like helium atom microscopy advance, the desire for ever-greater resolution creates a challenge. While a smaller probe size and improved angular resolution offer more detailed scattering information, they often come at the cost of a significantly weaker measurable signal [1]. Hence, the current work focuses on the improvement of the detection via the design and development of a next-generation mass spectrometer optimised for low mass detection, which is based on previous work by M. Bergin et al. [2].

The instrument has an extended ionization volume, where electrons emitted from a hot filament are confined using a solenoidal magnetic field to give a high ionization probability. Electron space charge is used to confine and extract the gas ions formed, which are then passed through a magnetic sector mass filter before reaching an ion counter. The design and constrained implementation of each improved iteration of the major components are described in turn with a number of industry first technological implementations, followed by a summary of the overall performance of the detector focussing on detection efficiency, time response, and background count rates.

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Ferroelectricity on as-cleaved perovskite surfaces

Dominik Wrana[1], Llorenç Albons[2], Marta Macyk[1], Andrzej Jasicki[1], Aji Alexander[2], Jesus Redondo[2], Igor Sokolovic[3], Pavel Kocan[2], Michele Reticcoli[4], Konrad Szajna[1], Martin Setvin[2], Franciszek Krok[1]
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2D Materials and Van der Waals Heterostructures 2 and Ferroelectric Behaviour, June 20, 2024, 11:00 - 13:00

Ferroelectric polarization of bulk crystals is a well-known effect contrary to the ferroelectricity manifestation on the very surface. Electric fields generated by ionic displacements are altered by surface reconstruction, buckling of atoms, and shifts in electronic states. In order to use the spontaneous polarization of ferroelectrics towards photo- and piezocatalysis one needs to develop a full model of the actual effect of polarization on surfaces.

Here we investigate one of the most important classes of stable catalytic materials, oxide perovskites, which are known to exhibit record-high efficiencies toward water spitting [1]. Careful analysis of ferroelectricity exhibited on surfaces of single crystals of as-cleaved ferroelectric $BaTiO_3(001)$, $KNbO_3(001)$, and quantum paraelectric $KTaO_3(001)$ reveals phenomena at both single-atomic and macroscales [2]. SEM data provides the spatial information of 90° ferroelectric domains, which typically have a width of 5-20 um and length of up to hundreds of um. By the employment of contact AFM it turns out to be possible to detect smaller 180° domains in the lateral/friction signal.

I would like to conclude my presentation by showing the capabilities of qPlus ncAFM to not only reveal the atomic arrangement of the (1x1) reconstruction of as-cleaved perovskite surfaces but also to demonstrate a reversible ferroelectric polarization of the material at the nanoscale, by application of different tip-sample bias voltages.

This research was supported by the National Science Centre, project SONATA 2022/47/D/ST5/02439.

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RFEAs for Plasma Assisted Thin Film Deposition Tools

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Plasma Science 2, June 19, 2024, 14:00 - 15:30

Plasma plays a crucial role in various thin film deposition techniques such as PECVD, ALD, Magnetron and HiPIMS etc. These methods offer precise control over film properties like thickness, composition, and structure. To optimize a plasma source for particular application, careful selection of process parameters such as gas pressure, RF source power, bias power, pulsing frequency, and duty cycles is essential. These parameters govern the ion energies and ion flux reaching over the substrate. Therefore, it becomes imperative to measure ion energy distribution functions and ion flux, providing valuable insights into the behavior of energetic ions on wafers. Such insights are crucial for controlling the deposition process and fine-tuning film properties.

Impedans offers a comprehensive range of retarding field energy analyzers (RFEAs) designed to address the need for wafer-level measurements within plasma environments [1]. Positioned at the substrate, these RFEAs offer insights into surface interactions within the plasma. The Semion RFEA measures the uniformity of positive and negative ion energies and flux hitting a surface, at multiple locations inside a plasma chamber using an array of integrated sensors. The Quantum is an advanced RFEA, that combines energy retarding grids with an integrated quartz crystal microbalance (QCM). Quantum provides measurements of the ion energy and flux as well as the ion-neutral ratio and deposition rates. The ion-neutral ratio serves as a critical parameter for optimizing film properties. This talk will showcase measurement challenges and innovative solutions offered by Impedans RFEAs in various thin film deposition tools.

References

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Particle deposition by droplet evaporation: the role of surface interactions

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Nanoparticles, June 18, 2024, 14:00 - 15:30

Achieving a homogeneous deposition of particles by evaporation is a key problem in many industrial applications, such as coatings [1]. The assembly of nanoparticles near the three-phase contact line, known as the “coffee ring” effect, is a well-known example of a complex phenomenon that stems from capillary flow and the pinning of the three-phase line [2]. The evaporation rate has also been shown to affect the structure of self-assembled nanoparticles [3]. Thus, understanding the interplay between solvent, colloids, surface, and process conditions is key to optimizing the homogeneity of surface distributions. In this work, we use coarse-grained computer simulations that allow for the systematic exploration of surface structure as a function of interparticle interactions. The evaporation process is modelled by defining a region far from the liquid-vapor interface where particles are deleted. By means of a geometric analysis (Voronoi tessellation) of the resulting structure, we correlate the homogeneity of the distribution with the controlling parameters of the simulation. This study sheds light on the optimization of deposition processes by spray and evaporation.

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On-surface synthesis of sulphur and oxygen-doped eleven-ring analogues of acenes

Irena Padniuk[1,2], Otilia Stoica[3,5], Mariusz Krawiec[4], Rémi Blieck[3,5], Rafał Zuzak[1], Antonio M. Echavarren[3,5], Szymon Godlewski[1]

[1]Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, Poland, [2]Jagiellonian University, Doctoral School of Exact and Natural Sciences, Poland, [3]Institute of Chemical Research of Catalonia (ICIQ), Barcelona Institute of Science and Technology, Spain, [4]Institute of Physics, Maria Curie-Sklodowska University, Poland, [5]Departament de Química Organica i Analítica, Universitat Rovira i Virgili, Spain

Supported Nanostructures, June 17, 2024, 14:00 - 15:30

Acenes are a class of molecules composed of linearly fused benzene rings. The wide range of their properties makes them promising candidates in many applications, particularly in (opto)electronics or spintronics [1-2]. Our recent investigations focused on tuning the features of acenes by incorporating non-benzenoid rings or heteroatoms into their structure [3]. Here, we present an on-surface synthesis of a set of eleven-ring analogues of acenes, built explicitly as a heptacene core with additional benzothiophene or benzofuran moieties, especially heptaceno[2,3-b:11,12-b′]bis[1]benzothiophene, heptaceno[2,3-b:11,12-b′]bis[1]benzofuran and heptaceno[2,1-b:11,10-b']bis[1]benzofuran [4]. We confirmed the presence of the synthesised target compounds on Au(111) using ultra-high resolution scanning tunnelling microscopy (UHR-STM). Notably, our findings revealed that, unlike the sulphur-doped molecules, the oxygen-doped products self-assemble on the Au(111) surface. Moreover, the electronic structure of the systems and their differences were deeply investigated by scanning tunnelling spectroscopy (STS) and were corroborated with the calculations based on density functional theory (DFT). Specifically, we focused on the influence of the benzothiophene and benzofuran units on the molecular properties. Distinctly, we found that the arrangement of benzofuran moieties relative to the heptacene core impacts the system's properties. Additionally, we compared the electronic structure of our compounds with those of corresponding isoelectronic structures and with members of the acene family. Based on this, we resolved the role of thiophene and furan rings and, finally, the meaning of heteroatom-doping in the properties of the synthesised systems.

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Neutral Atom Microscopy: Science and Applications

Prof Paul Dastoor[1]
[1]University Of Newcastle, Australia

MS-1: Recent Developments in Surface Microscopy, June 18, 2024, 10:30 - 12:30

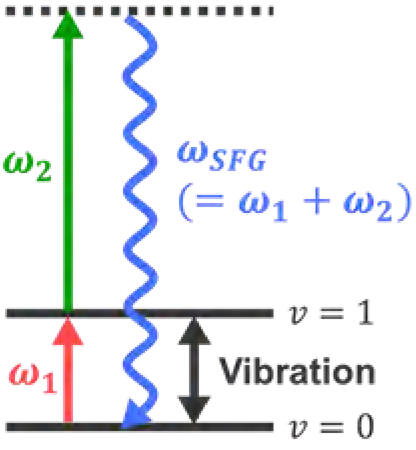
The development of microscopic imaging has been fundamental to scientific advancement since the 16th century. Indeed, as Freeman Dyson stated, “new directions in science are launched by new tools much more often than by new concepts”. A case in point is the design, development and demonstration of the new field of Neutral Atom Microscopy (NAM). Following its inception, over a decade ago, several scanning helium microscopes (SHeMs) have now been built around the world. By exploiting helium’s large scattering cross-section to atomic scale surface features, its neutral/inert nature and extremely low energy (~60 meV), these exciting new instruments are opening a new window on science, providing for the first time completely non-damaging imaging using beams of neutral helium atoms. This talk will discuss the role of microscopy in science and describe how the development of the SHeM revolutionises the imaging of materials and the potential impact of damage-free microscopy. The presentation will also highlight the importance of international collaboration in the development of this new technology.

Pioneering tip-enhanced near-field nonlinear nanospectroscopy of interfacial molecules beyond the diffraction limit

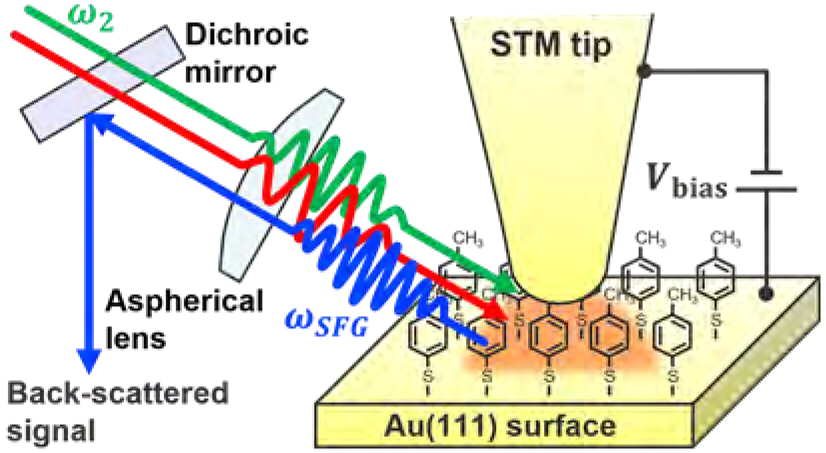
Dr. Shota Takahashi[1], Prof. Atsunori Sakurai[1,2,3], Mr. Tatsuto Mochizuki[1,2], Prof. Toshiki Sugimoto[1,2,3]
[1] Institute for molecular science, Okazaki, Japan, [2] Graduate institute for advanced studies, SOKENDAI, Japan, [3] Laser-Driven Electron-Acceleration Technology Group, RIKEN SPring-8 Center, Japan

Advances in Experimental and Theoretical Methods 3, June 17, 2024, 16:00 - 17:35

The surfaces and interfaces of materials are the regions where the spatial inversion symmetry of the bulk is broken, leading to unique molecular behaviors not observed in bulk materials. Vibrational sum frequency generation (SFG) is a second-order nonlinear spectroscopic technique widely used to investigate such surface-specific molecular behaviors. However, due to the diffraction limit of light, the spatial resolution of conventional SFG measurements has been limited to sub-micrometer scales. The information obtained from SFG signals has thus been restricted to the ensemble-averaged properties and structures of more than 10^8 molecules within an optical focusing spot. This has hindered site-specific understanding of molecular details in heterogeneous surfaces. In this study, we overcame this constraint by integrating SFG spectroscopy with a scanning tunneling microscope (STM) and developing a tip-enhanced near-field SFG system for molecular vibrational nanospectroscopy. By irradiating the nanogap between an Au tip and Au substrate in the STM with femtosecond excitation lasers, we induced plasmonic localization and enhancement of the incident electromagnetic fields, thereby amplifying SFG signals from a small number of molecules within the ultrasmall gap. Leveraging this new nanospectroscopic technique, we successfully verified molecular adsorption structures at the surface with a high spatial resolution of less than 20 nm, exceeding the optical diffraction limit and surpassing the resolution achievable with conventional far-field SFG spectroscopies. Moreover, we found that varying the STM voltage applied across the nanogap induces a signal enhancement exceeding 2000% in near-field SFG intensity within a voltage sweeping of just a few volts. The electrically tuned non-resonant background signals served as a sensitizer to further enhance molecular vibrational near-field SFG signals through heterodyne interference effect, improving the chemical sensitivity of the tip-enhanced SFG spectroscopy. Our results open new avenues for detailed exploration of correlated chemical and topographic information using the tip-enhanced SFG nanospectroscopy.



Energy diagram of SFG process



Tip-enhanced near-field SFG

Surface conductivity on metal monolayer films formed on Si(111) studied by low temperature scanning tunneling microscopy/potentiometry

Dr. Masahiro Haze, Masayuki Hamada[1], Junya Okazaki[1], Prof. Yukio Hasegawa[1]

[1] *University of Tokyo, Japan*

Electronic Structure of Materials, Surfaces and Interfaces, June 18, 2024, 10:30 - 12:30

The surface electrical conductivity is affected by the local defects, such as atomic vacancy, impurities and steps. In order to study these phenomena in nanometer scale, scanning tunneling potentiometry (STP) has been developed, which allows us to directly access the surface transport properties. This microscope, which is based on scanning tunneling microscopy (STM), enables us to make an image of topograph and electrochemical potential of a sample surface, simultaneously with atomic scale special resolution and uV level high potential sensitivity under the current flowing parallel to the sample surface. However, STP measurements have not been performed at low temperature and under magnetic fields, though many interesting phenomena, such as Hall effect, are expected.

Here, we have developed STP system which works at cryogenic temperature and under high magnetic fields. As a sample, we employed Pb atomic monolayer films formed on Si(111) substrates, which are ones of the well investigated metallic systems. We successfully measured surface potentials at nanometer scales, and we found that the conductivity is not affected by steps on striped incommensurate (SIC, the coverage is 4/3 monolayers) phase. In addition we found that there is a potential gradient perpendicular to the current direction under magnetic fields, suggesting that we can detect the Hall effect in nanometer scales.

Interfacial structure on the Pt(111) electrode modeled under ultrahigh vacuum conditions

Prof Masashi Nakamura[1], Keita Okuda[1], Nagahiro Hoshi[1]
[1] *Chiba University, Japan*

Metal and Oxide Single Crystal Surfaces - Growth, Preparation, and Characterisation, June 18, 2024, 16:00 - 17:30

The adsorbed hydroxide (OHad) layer is formed on platinum electrodes at positive potentials, which affects many important electrochemical reactions, such as alcohol oxidation reactions and the oxygen reduction reaction. The stability of the OHad layer on the Pt electrodes is strongly governed by the hydrophilicity of the cation interacting with OHad in the electrical double layer (EDL). Therefore, elucidating the detailed hydration structure and role of cations in the EDL is a key research goal. In this study, the structures of H_2O, OHad, and Li were investigated using infrared spectroscopy. By optimizing the coverage of OHad (θOH) and Li (θLi), the bending mode of PtOH (δPtOH) band on the Pt(111) surface under ultra-high vacuum (UHV) conditions matches with that on the Pt(111) electrode at 0.8–0.9 V vs RHE in LiOH solution[1,2], indicating that a quasi-EDL composed of OHad species interacting with hydrated Li+ on Pt(111) was successfully modeled under UHV conditions. According to the interfacial structure modeled under UHV conditions, θOH = 0.3, and Li interacts directly with OHad at a stoichiometric ratio (θOH/θLi) of two. Modeling of the EDL, including the outer Helmholtz plane, is beneficial for identifying the microscopic details of the EDL under electrochemical conditions.

References

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[2] K. Okuda, M. Alaydrus, N. Hoshi, I. Hamada, M. Nakamura, J. Phys. Chem. C, 126, 4726 (2022).

3D (metal) vs. 2D (oxide) nanoparticles on MgO smoke

Slavica Stankic[1], Jacek Goniakowski[1], Cédric Baumier[2], Franck Fortuna[3]
[1]Sorbonne Université, CNRS UMR 7588, Institut des NanoSciences de Paris (INSP), France, [2]Laboratoire de Physique des deux Infinis Irène Joliot-Curie (IJCLAB/SCALP), France, [3]Institut des Sciences Moléculaires d'Orsay (ISMO), France

Nanoparticles, June 18, 2024, 14:00 - 15:30

Metallic or oxide nanoparticles embedded in an oxide substrate or supported on its surface are used in a large number of applications. Controlling their morphology and atomic structure opens a way to adjust their properties (catalytic reactivity/ selectivity, magnetization etc.). We have previously shown that MgO smoke serves as an excellent support for the growth of silver nanoparticles which systematically adopt the shape of a truncated octahedron [Nanoscale, 5 (2013), 2448.]. Stepped MgO surfaces or contact lines between stacked crystallites were shown to completely dominate the nucleation behavior of silver providing conditions for its growth close to the equilibrium. (100)Ag//(100)MgO epitaxy was evidenced and the Ag(110) facet identified for the first time in case of supported silver particles.
In this study we report on the site-specific growth of In2O3 on MgO smoke. We combined TEM experiments and atomistic simulations to analyze the In2O3 adsorption/ adhesion on MgO surfaces of different orientations. Indium oxide shows a strong tendency to selectively wet MgO surfaces in form of uniformly organized 2D layers. On small MgO cubes, In2O3 was observed only in corners whereas the edges of larger cubes provide enough space to additionally accommodate uniformly and almost equidistantly distributed In-oxide layers (Figure (a)). On the contrary, no indium was observed on (100) MgO surface. STEM and corresponding EDX mapping (Figures (b), (c) and (d)) confirm that the layers of higher z-contrast are indium rich while the HRTEM and SAED reveal that MgO smoke supported In2O3 adopts the corundum crystal structure. These findings are supported by DFT calculations which show that indium adatoms and/or impurities tend to form a strongly interacting layer on some low-index MgO facets only. On these facets, due to the strong interfacial interaction, the optimal structure of ultra-thin In2O3 films obtained from global optimization differs from the bulk-like bixbyite one.

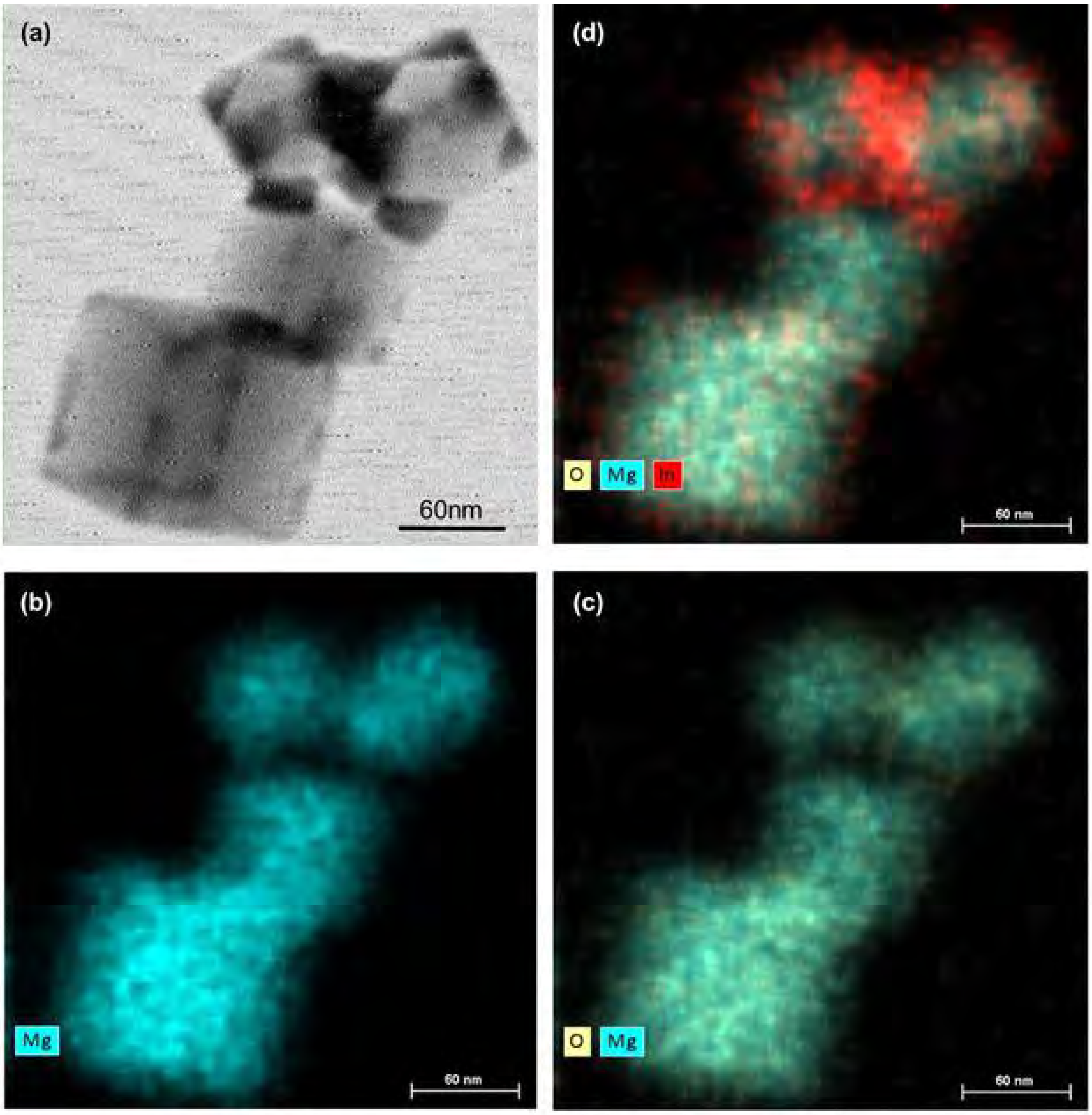

Figure: (a) STEM image and corresponding EDX mapping for Mg (b), MgO (c) and MgOIn (d), showing that the layers of higher z-contrast are indium rich. The image in (a) also shows the indium distribution over MgO cubes as a function of their size.

Simulating plasma-surface interactions with ion and molecular beams experiments: interest for nuclear fusion

Florin Ghiorghiu[1], Axel Dunand[1], Mykola Ialovega[1], Matthieu Latournerie[1], Aleksandr Afonin[1], Marco Minissale[1], Thierry Angot[1], Etienne Hodille[2], **Régis Bisson**[1]
[1]Aix-Marseille Univ, CNRS, PIIM, France, [2]CEA, IRFM, France

Plasma Science, June 18, 2024, 16:00 - 17:30

Harnessing nuclear fusion's power is the goal of ITER, an experimental reactor involving 35 nations and under construction in France. In ITER, a magnetically confined plasma of hydrogen isotopes (deuterium (D) and tritium (T)) is heated to millions of Kelvin, and power exhaust is realized on reactor walls made of tungsten (W). A detailed understanding of W interactions with D and T is needed because T is scarce and radioactive.
Without entering in the details of power exhaust, it is important to realize that the reactor walls are constituted of technical W, i.e. natural impurities such as oxygen (O) and carbon (C) atoms present in the W native oxide may play a role with respect to D and T interactions.
In this presentation we will present laboratory studies where deuterium ions and molecular beams are used to disentangle the complexity of plasma-wall interactions and surface science methods are employed to measure reaction kinetics and inform on microscopic mechanisms. In contrast to usual assumptions [1], the W native oxide appears to be resistant to D ions sputtering and lead to significant trapping of D in the bulk of W, a potential nuclear safety issue [2]. To better understand this behavior, D ions implantation in W with its native oxide is compared with D ions implantation in clean W(110), in O or C sub-monolayers on W(110), and in 30 nm thick crystalline WO_3. These impurity layers of different thickness behave quite differently. The competition between surface trapping and bulk trapping is evidenced by comparing D ions implantation and D_2 molecules exposure. Theoretical modeling using macroscopic rate equations initialized by DFT calculations that help to rationalize these different behaviors will be presented [3,4].

[1] https://doi.org/10.1103/PhysRevLett.111.225001 (2013)
[2] https://doi.org/10.1088/1741-4326/ac583a (2022)
[3] https://doi.org/10.1088/1741-4326/aa6d24 (2017)
[4] https://doi.org/10.1088/1741-4326/ad2a29 (2024)

Ultrathin oxide/graphene heterostructures

Professor Andrea Picone[1]
[1]Politecnico Di Milano, Italy

Advanced Thin Film Fabrication, June 19, 2024, 10:30 - 12:35

Graphene interfaced with oxide ultrathin films is a particularly appealing system for the development of new devices, since the dielectric layer can be used to modulate the physical properties of the carbon monolayer. Furthermore, graphene can be used as a template to synthesize novel two-dimensional oxide materials.[1] Despite such an extreme technological and scientific interest, only few successful examples of sharp graphene/oxide interfaces have been reported so far, since the growth of atomically flat ultrathin oxide films on the honeycomb monolayer is hampered by the extremely low surface free energy of graphene, which promotes the nucleation of three-dimensional clusters. Here, by using standard surface science techniques, I will analyze the structural, chemical and electronic properties of transition metals oxide (CrxOy and FexOy) and rare earths oxide (ErxOy)ultrathin films grown on the graphene/Ni(111) substrate.[2,3] The experimental results reveal a rich variety of graphene heterostructures, depending on the element used and the synthesis procedure.

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From Cr carbide to Cr oxide through a graphene layer
Appl. Surf. Sci., 599 (2022), Article 153926

From Vibrationally resolved to time-resolved spectroscopy with scanning tunnelling microscopy

Vibhuti Rai[1,2], Nico Balzer[3], Gabriel Derenbach[2], Christof Holzer[4], Marcel Mayor[5], Wulf Wulfhekel[2,6], Lukas Gerhard[2], Michal Valášek[3]

[1]Department of Physics, Freie Universität, Germany, [2]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology (KIT), Germany, [3]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Germany, [4]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology (KIT), Germany, [5]Department of Chemistry, University of Basel, Switzerland, [6]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), , Germany

Plasmonics and Excited States at Surfaces, June 19, 2024, 10:30 - 12:35

Scanning tunneling microscopy (STM) provides sub nanometer spatial resolution, allowing studies of phenomena down to single molecules and atoms. Recently, STM has been used to understand the mechanism of light emission on a single molecular level. For a molecule to emit light into the far field, it needs to be electrically decoupled in the STM geometry, typically achieved by the use of an insulating layer between the molecule and the metallic substrate. Here, we show another approach to efficient electrical decoupling through a chemical route. This is achieved by anchoring individual chromophores via extended tripodal scaffolds. In this study, we demonstrate that NDI chromophores coupled to a gold substrate via a tripodal scaffold and via a vacuum barrier to the tip of an STM enable spectrally and spatially resolved electroluminescence. We show that specific vibrons of the chromophore, which are mechanically decoupled from the substrate, give rise to hot-luminescence (HL) bands, whereas vibrons coupled to the substrate do not show HL [1-2]. Furthermore, we present a method to study the dynamics of low-energy excitations such as vibrons, excitons, spins, etc., by combining THz pump-probe scheme into STM junctions [3]. This enables STM to achieve picosecond temporal resolution.

[1] Rai, et al. Nat Commun 14, 8253 (2023)
[2] Rai, et al., Phys. Rev. Lett. 130, 036201 (2023)
[3] Cocker, et al. Nature Photonics 7, 620–625 (2013)

HREELS investigation of phonon and plasmon dispersion across the TiSe2 CDW phase transition

Prof. Valentina De Renzi[1], Andrea Tonelli, Roberto Biagi, Enrico Da Como
[1]*Università di Modena e Reggio Emilia and Istituto CNR-NANO, Italy*

Plasmonics and Excited States at Surfaces, June 19, 2024, 10:30 - 12:35

The existence of excitonic insulators was predicted by W. Kohn and co-workers in their seminal paper in the late sixties [1]. Since then, several systems have been considered as candidates for this exotic phase, among which TiSe2 has been extensively addressed. The origin of the low-temperature charge density wave (CDW) phase in TiSe2 has been long debated. While the softening of acoustic phonon mode is a general feature of CDW transitions, the softening of the low-temperature plasmon mode is considered as a fingerprint of exciton condensation. Recently, two papers based on High-Resolution Energy-Loss Spectroscopy (HREELS) have addressed this issue, finding conflicting results; whilst Kogar and co-workers [2] claimed evidence of the softening of the low-T plasmon at the critical momentum q_c=0.5 r.l.u., Lin et al. [3] stated that Landau damping is the responsible for the plasmon loss disappearing already at very low q.

In this work, we further investigate this issue, carefully comparing HREELS spectra at selected q, taken below and above the transition temperature Tc. We measure the dispersion of both acoustic and optical phonon modes along the ΓM direction (Fig.1a), showing the softening of the lowest-lying acoustic phonon below Tc (Fig.1b). The low-T plasmon feature - at variance with Lin results - is still visible up to q=0.12 r.l.u. At higher q, the higher-energy phonon modes overlap with the plasmon, making it difficult to disentangle the latter from the formers. Nevertheless, a careful analysis of our data speaks against plasmon softening. Though our results do not completely clarify the origin of the TiSe2 CDW-transition, by providing important pieces of information, they contribute to understanding this unresolved puzzle.

[1] D. Jerome et al., Phys Rev. 158, 452 (1967)
[2] A. Kogar et al., Science 358, 1314 (2017)
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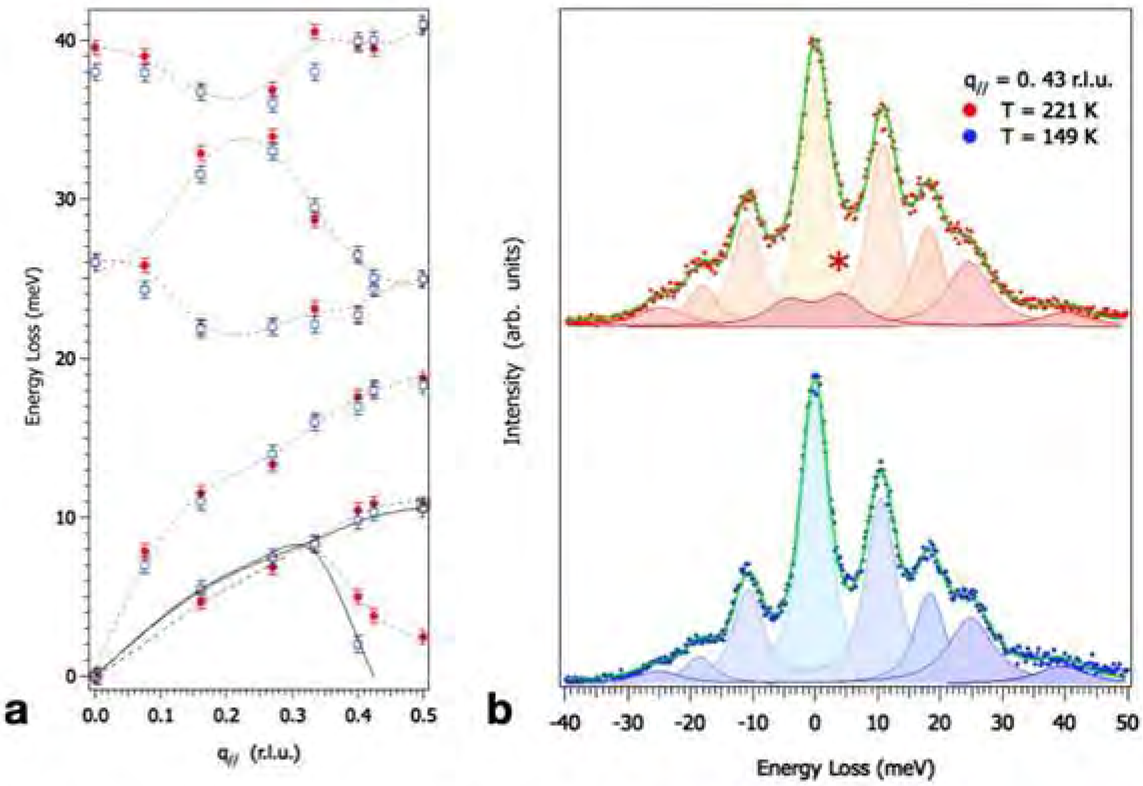
a
Energy Loss (meV)
0
10
20
30
40
0.0
0.1
0.2
0.3
0.4
0.5
q// (r.l.u.)
b
q// = 0. 43 r.l.u.
● T = 221 K
● T = 149 K
*
Intensity (arb. units)
-40
-30
-20
-10
0
10
20
30
40
50
Energy Loss (meV)

Insight into the diffusion of electrically active and inactive impurities using Secondary Ion Mass Spectrometry

Adrianna Rejmer[1,2], Iwona Pasternak[2,3], Walery Kołkowski[3], Andrzej Materna[1,4], Emil Tymicki[1,4], Ayse Ozcan-Atar[5], Emanuele Pelucchi[5], Włodzimierz Strupiński[2,3], Paweł Michałowski[1]
[1]Łukasiewicz Research Network Institute of Microelectronics and Photonics, Poland, [2]Faculty of Physics, Warsaw University of Technology, Poland, [3]VIGO SYSTEM, Poland, [4]ENSEMBLE3 Sp. z o.o, Poland, [5]Tyndall National Institute, Ireland

Electronic Materials, Energy Reduction and Carbon Reduction 2, June 21, 2024, 10:30 - 12:00

The precise determination of the spatial distribution of dopants in a structure and the prediction of its temperature behavior is crucial for the practical applications of semiconductors. Standard dynamic Secondary Ion Mass Spectrometry (SIMS) provides depth profiles of impurity atoms without distinguishing between electrically active and inactive parts. Whereas Electrochemical Capacitance Voltage (ECV) technique yields depth profiles of all carriers present in the structure. The observation of significant discrepancies between the profiles measured by these two techniques sparks discussion on the varying diffusion of electrically active and inactive impurities.

In our experiment, a highly Si-doped GaAs layer of 500 nm thickness, embedded between undoped GaAs layers (GaAs/GaAs:Si/GaAs), was investigated. Samples were subjected to thermal treatment at various temperatures ranging between (800-1000)°C for 30 minutes and tested using standard and Ultra Low Impact Energy (ULIE) SIMS [1], along with ECV technique.

The depth profiles obtained using ULIE-SIMS allow for the investigation of the behavior of the Si in GaAs in various roles [2]: Si on Ga sites acting as n-type dopant, Si on As sites doping for p-type, and silicon existing in the form of Si pairs. This approach enables insight into the diffusion of individual contributions from substitutional Si to total Si concentration and analysis of self-compensating effects present in highly doped GaAs:Si samples. The proposed complementary use of SIMS and ECV techniques shows great promise to be a highly beneficial tool in the optimization of growth processes, determining the cause of electrical inactivity, and controlling the dopant activation process.

Figure 1. The comparison of the net electrically active Si concentration (ULIE-SIMS) and carrier concentration (ECV) depth profiles.

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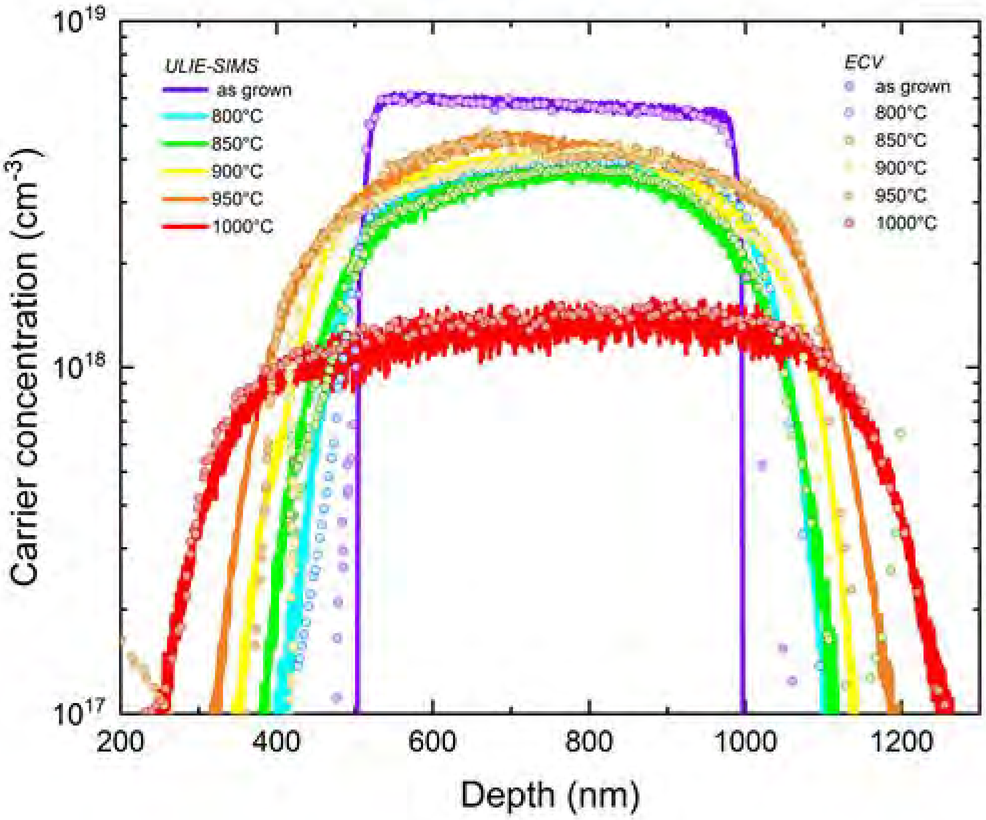
ULIE-SIMS
as grown
800°C
850°C
900°C
950°C
1000°C
ECV
as grown
800°C
850°C
900°C
950°C
1000°C
Carrier concentration (cm-3)
10^{19}
10^{18}
10^{17}
200
400
600
800
1000
1200
Depth (nm)

How substrate roughness affects dewetting: an analysis based on the thin film equation

Luca Repetto[1], Giuseppe Firpo
[1]Department of Physics - Università di Genova, Italy

Functional Coatings 1, June 17, 2024, 14:00 - 15:30

Providing strategies for regulating the stability of thin films in contact with solid substrates has a relevant impact in various fields. It can offer solutions to coating failures [1] as well as provide new strategies for the fabrication of functional nanostructures [2]. The role played in these processes by the substrate has been pointed out by several authors [3-5]. Here we consider how roughness amplitude and morphology influence the dewetting of films by reporting the analysis of simulated dewetting morphologies obtained by solving a modified thin film equation that keeps into account the effect of substrate topography.

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Adding a Dimension to Atom-by-Atom Assembly

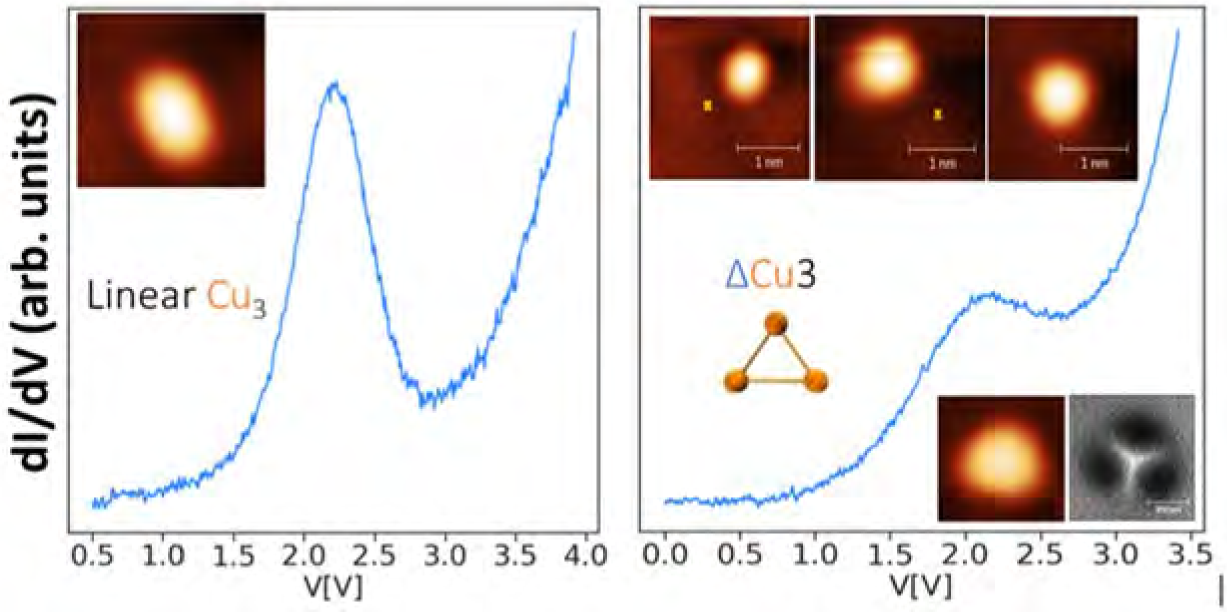
Filipe Junqueira[1], Connor Fields[1], Dr. Brian Kiraly[1], Shabnam Naseri[3], Andreas Larsson[3], Prof. Lev Kantorovich[2], Philip Moriarty[1]
[1]School of Physics and Astronomy, University Of Nottingham, United Kingdom, [2]Dept. of Physics, King's College London, United Kingdom, [3]Department of Engineering Sciences and Mathematics, Lulea University, Sweden

From Nanostructured thin films to nanoparticles. Reactions at nanostructures, June 18, 2024, 16:00 - 17:30

In the years since Crommie et al's landmark and revolutionary "quantum corral" paper appeared [Science 262 218 (1993)], a remarkably diverse and increasingly sophisticated array of artificial atomic lattices and nanostructures have been assembled by lateral manipulation of atoms using the tip of a scanning probe microscope – an essentially 2D process. Examples of atom-by-atom (or molecule-by-molecule) assembly that move beyond sliding, pushing, and/or pulling adsorbates across a surface to translate and attach atoms/molecules via vertical manipulation are much rarer, not least because this generally requires significantly better control of the chemistry of the tip apex.

Here we use vertical manipulation (in qPlus AFM mode) to form a simple atomic cluster – a triangular Cu3 trimer – that cannot be assembled via lateral atom manipulation, highlighting the key importance of exploiting the complete 3D potential energy landscape associated with scanning-probe-driven mechanochemical reactions. We interpret our experimental scanning tunnelling microscopy/spectroscopy (STM/S) and qPlus AFM data using an extensive set of nudged elastic band (NEB) calculations that give key insights into the surprising "self-healing" nature of the tip apex geometry observed experimentally: despite repeated deposition of atoms from the tip, the same imaging resolution (and spectroscopic signiature) is often retained for many manipulation cycles.

Fig. 1(a): Differential conductance (dI/dV) spectrum of a linear Cu3 trimer formed via lateral manipulation of Cu atoms using the strategy first described by Fölsch et al. [PRL 92 056803 (2004)]; (b) Upper inset: Triangular Cu3 trimer assembled using deposition of Cu atoms from the tip in qPlus AFM mode. This cluster cannot be assembled via lateral manipulation. Each "X" marks the position at which the tip was moved towards the Cu(111) sample surface to deposit an atom. Lower inset: STM image and qPlus AFM image of the triangular Cu3 trimer acquired with a CO-functionalised tip.



Directing Jahn-Teller Dynamics via Submolecular Resolution Tunneling Spectroscopy

Yitao Wang[1], Ilya Popov[2], Ali Sufyan[4], Sajjad Muhammad[3], Andreas Larsson[4], Nicola Manini[5], Brian Kiraly[1], Elena Besley[2], Philip Moriarty[1]

[1]School of Physics and Astronomy, University Of Nottingham, United Kingdom, [2]School of Chemistry, University of Nottingham, United Kingdom, [3]CBI Green Chemicals and Energy Centre, University of Nottingham Ningbo Campus, China, [4]Department of Engineering Sciences and Mathematics, Lulea University, Sweden, [5]Dept. of Physics, Università degli Studi di Milano, Italy

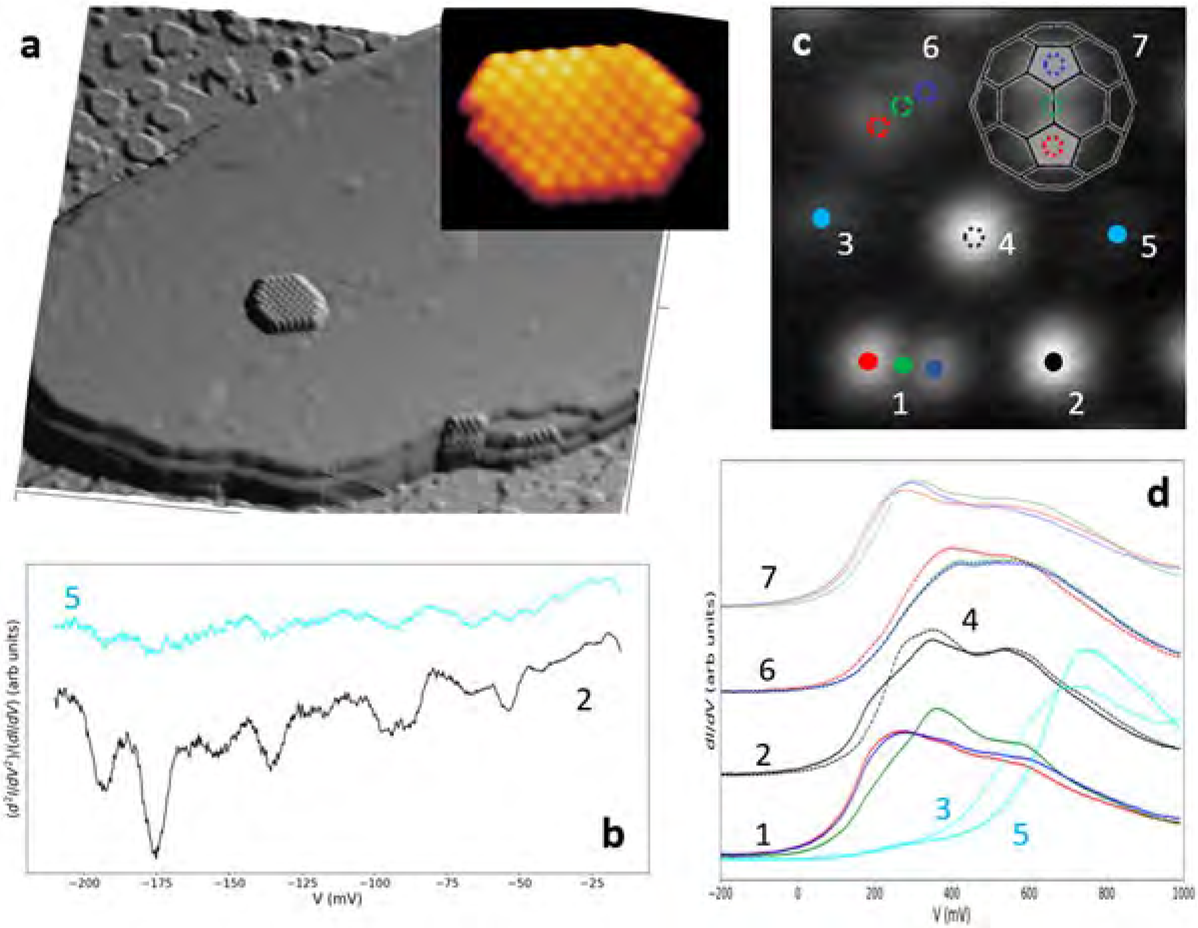
Spectroscopy and Microscopy of Nanostructures Modelling Nanostructure Properties, June 20, 2024, 11:00 - 13:00

"Any non-linear molecule with a spatially degenerate electronic ground state will undergo a geometrical distortion that removes that degeneracy.." [HA Jahn and E Teller, Proc. Roy. Soc. A 161 220 (1937)]. The static Jahn-Teller effect, and its dynamic counterpart, are compelling examples of the core role that symmetry -- and, by extension, group theory -- plays in the electronic properties of matter at the molecular, mesoscopic, and macroscopic levels.

Here, we probe the dynamic Jahn-Teller (dJT) effect in a molecular system that is rich in JT physics/chemistry due to its exceptionally high symmetry: the fullerenes. We build on a previous observation of the spectroscopic signature of the dJT effect in C60 [T. Frederiksen, et al. Phys. Rev. B 78, 233401 (2008)] to probe the variation of Jahn-Teller coupling between electronic and vibrational degrees of freedom within single molecules. Electron injection into nodes vs antinodes of the molecular orbital density significantly modifies the dJT-derived spectroscopic lineshapes (Fig. 1).

As first highlighted by Franke et al. [J. Phys. Chem. Lett. 1 500 (2010)], inelastic tunnelling spectroscopy of C60 adsorbed on Pb(111) surfaces yields all of the Jahn-Teller active modes of the molecule, in stark contrast to the strong suppression -- or complete absence -- of IETS signal on other metal surfaces. Motivated by Franke et al.'s findings, our IETS and dI/dV measurements were carried out on (111)-oriented Pb islands grown on Cu(111). We have carried out a comprehensive series of DFT calculations to elucidate the role of Pb(111) in enabling high resolution IETS measurements of vibrational/vibronic structure.

Fig. 1(a) STM images of a Kr@C60 island on Pb/Cu(111); (b) IETS spectra of molecules 2 and 5 shown in (c), a constant height image (V=-50 mV) of a molecular island, and (d) variation in dI/dV signatures for each of the molecules shown in (c).


a
b
5
2
(d²I/dV²)/(dI/dV) (arb units)
−200
−175
−150
−125
−100
−75
−50
−25
V (mV)
c
1
2
3
4
5
6
7
d
7
6
4
2
3
5
1
dI/dV (arb units)
-200
0
200
400
600
800
1000
V (mV)

DFT-Based Simulation of Helium Interaction Potentials with MoS2 Surfaces for Scanning Helium Microscopy Applications

Min Lin[1]
[1] University of Cambridge, United Kingdom

MS-1: Recent Developments in Surface Microscopy, June 18, 2024, 10:30 - 12:30

Scanning Helium Microscopy (SHeM) has emerged as a powerful surface microscopy technique that leverages neutral helium atoms as probe particles. This method is capable of generating detailed helium atom diffraction patterns on a microscopic scale, providing invaluable insights into surface structures and phenomena. Despite its proven efficacy, limited work has been undertaken to model the interactions between helium atoms and sample surfaces within the SHeM framework [1].

In this study, we employed Density Functional Theory (DFT) to simulate the interaction potentials between helium atoms and MoS2 surfaces, a material of significant interest due to its unique properties and applications. Our approach involves the calculation of helium-MoS2 interaction potentials using DFT, followed by incorporating these potentials into Multiscat [2], a program designed for conducting close coupling calculations. This innovative methodology allows us to predict diffraction patterns observed in SHeM, particularly the differentiation between two distinct phases: MoS2-1T and MoS2-2H by examining the variations in diffraction peaks along their principal axes.

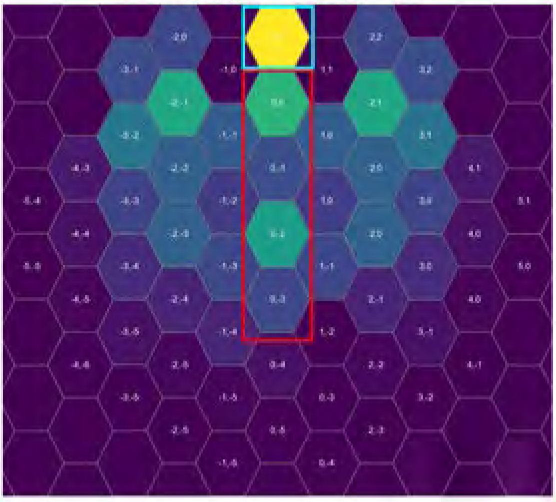
Furthermore, we extend our simulation efforts to the LiF(001) surface, where our results align with previously measured outcomes [1], thereby validating our simulation approach. Our findings not only enhance the understanding of helium-surface interactions in the context of SHeM but also demonstrate the potential of DFT-based simulations in advancing the capabilities of SHeM, offering a more nuanced and accurate depiction of surface structures and interactions.

[1] 2D Helium Atom Diffraction from a Microscopic Spot
Nick A. von Jeinsen, Sam M. Lambrick, Matthew Bergin, Aleksandar Radić, Boyao Liu, Dan Seremet, Andrew P. Jardine, and David J. Ward
Phys. Rev. Lett. 131, 236202 – Published 6 December 2023

[2] Manolopoulos, D. and Wyatt, R. (1988) Quantum scattering via the log derivative version of the Kohn variational principle. Chemical Physics Letters, 152(1), 23–32.


MoS2_1T

Incident Angle = 45°, Phi = 60.0°


MoS2_2H

Incident Angle = 45°, Phi = 60.0°

CrN/NbN and TiN/NbN nanoscale multilayer coatings deposited by high power impulse magnetron sputtering for biomedical applications

Dr Arunprabhu Arunachalam Sugumaran[1]
[1]Sheffield Hallam University, United Kingdom

Biomaterials 1, June 18, 2024, 10:30 - 12:30

CoCrMo alloys have been widely used for biomedical applications such as knee and hip replacement joints due to their excellent biocompatibility, mechanical and corrosion properties. However, the major drawback of using these alloys is the release of toxic, carcinogenic Cr and Co elements due to tribocorrosion. It has been reported that the performance of these implants can be enhanced by depositing suitable monolithic or multilayer coatings. The aim of this work was to investigate the mechanical, tribological and corrosion behaviour of CrN/NbN and TiN/NbN nanoscale multilayer coatings deposited on CoCrMo alloy. Combined high power impulse magnetron sputtering (HIPIMS)/direct current magnetron sputtering (DCMS) technology was used for the deposition to take advantage of highly ionised metal rich HIPIMS plasma without compromising the deposition rate. An industrial size Hauzer HTC 1000-4 system enabled with HIPIMS technology was used for the deposition of the coatings. X-ray diffraction analysis revealed a preferred crystallographic orientation of (200) for TiN/NbN and (111) for CrN/NbN. Microstructural analysis using scanning electron microscopy showed that these coatings are extremely dense without any intercolumar voids. CrN/NbN multilayer coating showed better adhesion, nanohardness, tribological properties, corrosion resistance and fatigue resistance as compared to the TiN/NbN multilayer coating. Ellipsometry measurements showed a strong plasmonic behaviour for TiN/NbN multilayer coating with a clear metallic behaviour at high wavelengths and low losses. The photocatalytic potential of both coatings is compared.

Optimisation of graphene oxide synthesis and accurate determination of the carbon/oxygen ratio

Jack Bradley[1], Prof. Steve Tear[1], Dr Andrew Pratt[1]
[1] *School of Physics, Engineering & Technology - University Of York, United Kingdom*

Carbon Materials 2, June 19, 2024, 10:30 - 12:35

Graphene oxide (GO) membranes, formed from compacted flakes of graphene oxide, have a wide range of applications including for healthcare technologies, nanofluidics and nanofiltration [1-3]. Critical to the material's performance and behaviour in these applications is the relative amount of carbon and oxygen present throughout the membrane with just small changes in this ratio significantly altering its properties. Hence, in order to understand the C/O ratio of GO, as well as control it for a particular application, a reliable method for accurately quantifying the amount of each element is required. The work presented here will discuss a methodology to evaluate the C/O ratio of GO produced via four different variations of the established Hummers' method [4]. Whilst the Hummers' method is the accepted method of GO synthesis, a host of variations exist. Here, the effects of pre- and post-treatment during GO synthesis will be analysed. Results from characterisation using X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FT-IR), and Raman spectroscopy, amongst other techniques, will be presented and discussed. From these results, the effects of gas expansion and hydrogen peroxide in the GO synthesis will be explored with a view to establishing an optimised procedure. Focusing on XPS, the use of carbon and oxygen Auger peaks to help quantify the C/O ratio will be assessed for native and thermally-reduced GO membranes.

[1] P. D. Bentley et al., AIP Adv. 11, 025314 (2021)
[2] K. G. Zhou et al. Nature 559, 236 (2018)
[3] Q. Yang et al., Nature Mater. 16, 1198 (2017)
[4] W. S. Hummers et al., J. Am. Chem. Soc. 80: 1339 (1958)

Using DFT-predicted O 1s spectra to investigate the chemistry of phenylphosphonic acid on rutile TiO2(110)

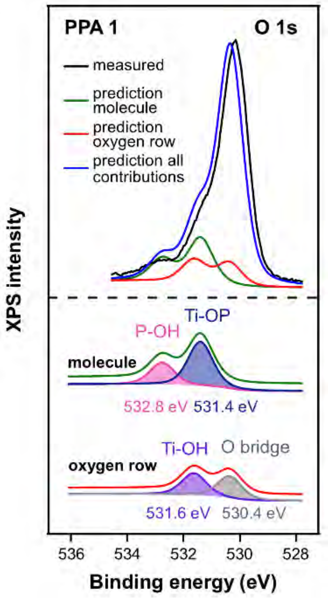
Ole Lytken[1], Alexander Wolframa[1], Maximilian Muth[1], Julia Köbl[1], Andreas Mölkner[1], Sascha Mehl[3], Nataliya Tsud[2], Hans-Peter Steinrück[1], Bernd Meyer[1]
[1]University of Erlangen-Nuremberg, Germany, [2]Charles University, Czech Republic, [3]Elettra, Italy

Oxide Surfaces and Nanomaterials - Spectroscopy, Imaging and Physicochemical Processes, June 18, 2024, 10:30 - 12:30

We have combined synchrotron XPS and NEXAFS measurements with DFT calculations to study the chemistry of phenylphosphonic acid on rutile TiO2(110). Upon adsorption at room temperature, we observe a complex O 1s spectrum, a single P 2p multiplet and the disappearance of small polarons in the Ti 2p and valence-band regions. Upon heating to 450 - 500 K, the O 1s spectrum changes, an additional P 2p species appears, the polaron signals reappear even stronger and NEXAFS indicates a more flat-lying molecule.

Using DFT calculations, we have determined the most-stable adsorption configurations on the surface. For these configurations we have calculated the O 1s binding energies of all oxygen atoms, including the adsorbed molecule and the first three trilayers of the TiO2(110) substrate, which for a (2×4) unit cell with four adsorbed molecules contains 96 oxygen atoms. In addition, we have used the orientations of the phenyl rings from the DFT structures to calculate the expected polar and azimuthal angular dependencies in carbon K-edge NEXAFS and compared those with our experimental observations.

Below 450 K, we find a singly-deprotonated bidentate species to be in perfect agreement with the experimental observations. Above 500 K, the desorption of water creates oxygen vacancies, and we find a mixed bidentate and rotated-tridentate adsorption structure to be the best match for the experimental observations.



Simulation of Pressure Distribution and Efficiency of Ion Passage in Vacuum Chambers of the U400R Cyclotron Complex

Alexander Tikhomirov[1], George Gulbekyan[1], Boris Gikal[1], Igor Kalagin[1], Nikolay Kazarinov[1], Vasiliy Semin[1], Kirill Gikal[1], Oleg Chernyshev[1]

[1]Joint Institute For Nuclear Research, Flerov Laboratory Of Nuclear Reaction, Russian Federation

Special Surfaces and Outgassing, June 17, 2024, 14:00 - 15:30

The results of numerical simulation of vacuum conditions for the design of vacuum systems of the upgraded cyclotron complex U400R are presented. The developed method for estimating ion losses is based both on numerical modeling of the pressure distribution in vacuum chambers of practically any arbitrary geometry, and on calculating cross sections for recharging ions with residual gases. This method was implemented using computer programs GENAP and VACLOS, which provide a good agreement to experiments during a long-term experience of acceleration of heavy ions in cyclotron complexes of FLNR. These computer programs were used to design vacuum systems of accelerator complexes, such as the DC-72 cyclotron in Slovakia, the CYTREC cyclotron complex in Dubna, the DC-60 cyclotron complex at the Astana University in the Republic of Kazakhstan, the DC-110 cyclotron complex at the Dubna Center of Nano & Nuclear Technologies and the DC-280 heavy ion cyclotron complex at the FLNR, JINR.

Adsorption, growth and decay dynamics of silver on Si(001)

Kai Huang[1]
[1]*Guangdong Technion-israel Institute Of Technology, China*

Plasmonics and Excited States at Surfaces, June 19, 2024, 10:30 - 12:35

The growth of metal films on semiconductors is of interest in the fabrication of miniaturized semiconductor devices. Amongst the numerous systems in this field, the growth of Ag-films on Si(001) has been heavily examined, since it serves as a prototype model for an abrupt metal/semiconductor interface.

Here, we present studies on the adsorption, growth and decay dynamics of silver on Si(001).First, we examined the atomistic structure of the silver films formed on Si(001) at room temperature. It had been long assumed that silver dimers, Ag4, served as the fundamental unit of the film. By using Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT) simulations, we show that it is a tetramer structure, Ag4, that accounts for the (2x1) and (2x2) periodicities of the silver film. Second, we examined the growth dynamics of silver film on Si(001). By varying the substrate temperature between 100 K and 230 K, STM and DFT identified three growth stages en route to forming an extended silver film, each exhibiting distinct dynamics. Our results demonstrate the complexity in epitaxial film growth, as resulted from the hot-atom motion upon the monomer adsorption of deposits, and the migration of adsorbed aggregates of a variety of sizes. Third, we present findings that relate to the thermal stability of silver film on Si(001), i.e. the decay dynamics. Extended in-situ monitors of the film evolution between 245 K and 276 K, unambiguously demonstrate the decay of the silver film, from which the relevant energetics are determined. Complementary measurements, using annealing/quenching method, gave evidences that the decayed Ag forms as clusters migrating over both naked and silver-covered silicon surfaces. Additionally, the decay of silver film was found to be enhanced in the vicinity of three-dimensional silver islands.

The Impact of Substrate on Hafnium Oxide ALD from its Amido Precursor - An APXPS Study.

Dr Rosemary Jones[1], Dr Giulio D'Acutno[1], Dr Payam Shayesteh[1], Dr Indiana Pinsard[1,5], Dr Roman Tsyshevsky[3], Dr Jean-Jacques Gallet[4], Dr Fabrice Bournel[4], Dr Florence Lim[4], Miss Foqia Rehman[1], Dr Lucía Pérez Ramírez[4], Dr François Rochet[4], Dr Esko Kokkonen[6], Dr Ashley Head[7], Prof Maija Kuklja[3], Prof. Rainer Timm[1,5], Prof Joachim Schnadt[1,5,6]

[1]Lund University, Sweden, [2]Stanford University, United States of America, [3]University of Maryland, United States of America, [4]Sorbonne Université, France, [5]NanoLund, Sweden, [6]Max IV, Sweden, [7]Brookhaven National Laboratory, United States of America

Advanced Thin Film Characterisation, June 19, 2024, 16:00 - 17:30

The introduction of atomic layer deposition, ALD, to the microelectronics industry has introduced a large number of new possible materials, able to be deposited in layers with atomic thickness control. One such material is the high-κ oxide HfO2; thermally stable and ultrathin HfO2 films deposited by ALD are a significant contender to replace SiO2 as the gate oxide in capacitor applications. In such a device the typical support remains Si, and thus the HfO2 gate oxide/Si interface is an integral part of the device. In addition, the combination of TiO2 and HfO2 have shown to exhibit impressive gate oxide characteristics. The quality of these interfaces can dramatically affect the performance of the device. We present a mechanistic study of the first deposition cycle of HfO2 on Si(111) and TiO2 surfaces using tetrakis(dimethylamido) hafnium (TDMA-Hf) and water as precursors using operando ambient pressure XPS (APXPS)[1-3]. This methodology allows to observe the chemical reactions in a time-resolved manner, giving both mechanistic and kinetic details during the reaction. We present three operando ALD studies of these interfaces demonstrating the importance of subtrate and it's preparation in the initial reaction with TDMAHF. Thermal SiO2 compared to partially oxidised Si(111) [1,2] showed vastly different reaction mechanisms and kinetics, significantly slower for thermal SiO2 were observed, as well as unwanted side reactions occurring leading to C and N species remaining at the interface. In the case of TiO2[3] we are able show how the temperature and pressure impacts on reaction mechanisms, as well as demonstrating the role of bulk oxygen in forming HfOx species in the first half cycle.

[1] R. Jones et al. J. Vac. Sci. Technol. A 42, 022404 (2024)
[2] G. D'Acunto et al. Chem. Mater. 2023, 35, 2, 529–538
[3] G. D'Acunto et al. J. Phys. Chem. C 2022, 126, 29, 12210–12221

Measurement and modelling of low-pressure inductively coupled plasmas in nitrogen/oxygen mixtures

Lars Schücke[1,2], Angie Natalia Torres Segura[2], Ihor Korolov[2], Peter Awakowicz[2], **Andrew Gibson**[1,3]
[1]Research Group for Biomedical Plasma Technology, Faculty of Electrical Engineering and Information Technology, Ruhr University Bochum, Germany, [2]Faculty of Electrical Engineering and Information Technology, Ruhr University Bochum, Germany, [3]York Plasma Institute, School of Physics, Engineering and Technology, University of York, United Kingdom

Plasma Science, June 18, 2024, 16:00 - 17:30

Low pressure inductively coupled plasma (ICP) sources are widely used for surface processing applications, particularly in the semiconductor industry. They are also of interest for other applications such as surface sterilisation. In both, fluxes of reactive species and high-energy photons to surfaces are important determiners of process outcomes. Because of this, understanding and control of these fluxes is important for knowledge-based process control, and ultimately the development of better-performing micro- and nano-scale devices.

This work focuses on the formation of nitric oxide (NO) and ultraviolet (UV) photon emission from the NO(A) state in the 200 – 300 nm range. NO and UV emission formation are studied in a double-coil inductively coupled plasma source operated in N_2/O_2 mixtures, at pressures between 10 and 40 Pa. Absolute densities of ground state NO are measured using laser induced fluorescence (LIF). Absolutely calibrated optical emission spectroscopy (OES) is used to measure absolute UV photon emission, and to infer the neutral gas temperature through analysis of the N_2(C-B) emission band. Electron densities and temperatures are measured using a Multipole Resonance Probe (MRP). A simple plasma chemistry model is developed to relate absolute photon emission to the other measured parameters to better explain the experimental observations. It is found that the NO density and UV emission show a complex dynamic across the E-H mode transition of the ICP source, which can be related to changes in the electron density and gas temperature. The chemistry model reveals that UV emission is dependent on the densities of both electrons and excited N_2 molecules. Implications for these results for surface processing in both the biomedical and semiconductor industries will be discussed.

This work was funded by the German Research Foundation (DFG) project number 424927143. Thanks also to the team at House of Plasma GmbH for support with the MRP.

Soft-Landing meets Mass-Spectrometry - gentle UHV deposition for large, reactive or fragile molecules to create functional nano-architectures

Andreas Walz[1,2], Annette Huettig[1,2], Michael Walz[1,2], Hartmut Schlichting[1,2], Johannes V. Barth[1]
[1]Technical University of Munich, Germany, [2]pureions GmbH, Germany

Supported Nanostructures, June 17, 2024, 14:00 - 15:30

Cutting-edge research in the field of nanoelectronics, solar technology, catalysis and nano-scale bio-applications requires an unbiased understanding of the structure-related properties of their building blocks. Technically, many restrictions do exist: Thermal evaporation in vacuum (MBE, OMBE) is limited to volatile substances. Solution-based techniques often lack purity and quality. However, soft-landed building blocks sorted by mass, charge or structure recognition methods play a fundamental and increasing role in such studies. The pool of possible molecules and ionization techniques is exhaustive: The ions are generated from various substances spanning the whole chemical spectrum including single metal atoms or clusters up to larger nanoparticles on one hand, and from small organic molecules up to several kilo- and megadalton proteins or DNA. Numerous methods such as electrospray, MALDI, laser ablation, magnetron sputtering, plasma techniques and more are established. These diverse sources exhibit a wide range of ionization levels - from singly charged up to several thousand-fold charged. Furthermore, most ion sources operate at elevated pressures and typically require collimation of the generated ions to a narrow beam and its transfer to higher vacuum for m/z filtering.

In-line with this, we present the development and performance of an ion beam deposition device currently supplied by an ESI-source. Successfully processed examples originating from various chemical groups are presented, comprising GNR, foldamer, porphine derivatives and nucleic acids. The main body contains RF-driven ion guides with high transmission (>80% efficiency) and low residual gas loads. A digital square-wave quadrupole mass filter provides adjustable amplitude and frequency resulting in a virtually unlimited m/z-range and resolving power, e.g., of >650 m/Δm FHWM at 20 % transmission. The footprint of an entire UHV deposition system is almost benchtop in size, about 50 x 100 cm. Due to its modular nature, all components may easily be integrated/connected to other systems/components.

Barriers for molecular dissociation: Can correlated electronic structure methods help?

Dr. Katharina Doblhoff-Dier[1], Benjamin Oudot[1], Dr. Andy Powell[1], Dr. Nick Gerrits[1], Dr. Theophile Tchakoua[1,4], Prof. Geert-Jan Kroes[1], Dr. Jörg Meyer[1], Dr. Heriberto F. Busnengo[2,3], Dr. Mark F. Somers[1]
[1]Leiden University, Netherlands, [2]Instituto de Física Rosario (IFIR), CONICET-UNR, Argentina, [3]Universidad Nacional de Rosario, Argentina, [4]Utrecht University, Netherlands

Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 3, June 20, 2024, 11:00 - 13:00

Barriers for molecular dissociation are notoriously difficult to compute accurately when using “standard” electronic structure methods, such as density functional theory based on the generalized gradient approximation[1]. This impedes accurate predictions for reaction probabilities.

In this talk, I will discuss what we can learn from barrier heights computed based on the random phase approximation and quantum Monte Carlo calculations[2]. The discussion will be based on two complementary test systems, namely H2 dissociating on Al(110) and on Cu(111). These systems allow us to scrutinize some shortcomings of density functional theory based on the generalized gradient approximation in predicting dissociative chemisorption as well as the potential benefits of quantum Monte Carlo approaches and calculations based on the random phase approximation.[2]

Furthermore, I will demonstrate how “anchoring” of density functional theory results to results from correlated electronic structure methods can allow for accurate predictions of the reaction probability without requiring infeasible computational resources.[3] For our test case, H2 dissociating on Al(110), a single quantum Monte Carlo-based “anchoring” point proved sufficient to allow for a near-chemically accurate, first-principles prediction of the probability for dissociative chemisorption at various molecular beam energies.

[1] N. Gerrits, E.W.F. Smeets, S. Vuckovic, A.D. Powell, K. Doblhoff-Dier and G.-J. Kroes (2000)
Density functional theory for molecule–metal surface reactions: when does the generalized gradient approximation get it right, and what to do if it does not
J. Phys. Chem. Lett. 11(24): 10552–10560.
[2] B. Oudot and K. Doblhoff-Dier: in preparation
[3] A.D. Powell, N. Gerrits, T. Tchakoua, M.F. Somers, H.F. Busnengo, J. Meyer, G.-J. Kroes, K. Doblhoff-Dier (2024)
Best-of-both-Worlds Predictive Approach to Dissociative Chemisorption on Metals,
J. Phys. Chem. Lett.: 15,307–315

Optimising NEG Coating for PETRA IV: Resistivity and Sticking Probability Measurements

Dr Ruta Sirvinskaite[1], Dr Lutz Lilje[1], Ralph Boespflug[1], Dr Sergey Antipov[1], Marco Schroeder[1], Anna Winiarska[1], Nils Plambeck[1]

[1]DESY, Germany

Non-evaporable getter coatings, June 18, 2024, 14:00 - 15:30

Non-Evaporable Getter (NEG) development at DESY has been ongoing to accommodate PETRA IV machine requirements. While most of the PETRA IV beam vacuum chambers will be manufactured from oxygen-free silver-bearing (OFS) copper and coated with NEG, getter film performance on these substrates has not been tested as extensively as on the stainless-steel. In order to investigate pumping and impedance properties of the columnar and dense NEG films, TiZrV and Zr layers of varying thicknesses (1 and 5 µm) were sputtered on eight Cu-OFS tubes. The 1 µm films were activated at temperatures ranging from 140 to 250 °C to determine the sticking probabilities for H2 and CO as well as CO pumping capacity. By measuring the attenuation of the RF signal along the four tubes coated with 5 µm NEG layer, resistivity of both NEG materials was evaluated. The results were then compared to previously reported findings for columnar and dense NEG films.

Seeing hard and soft materials with atoms

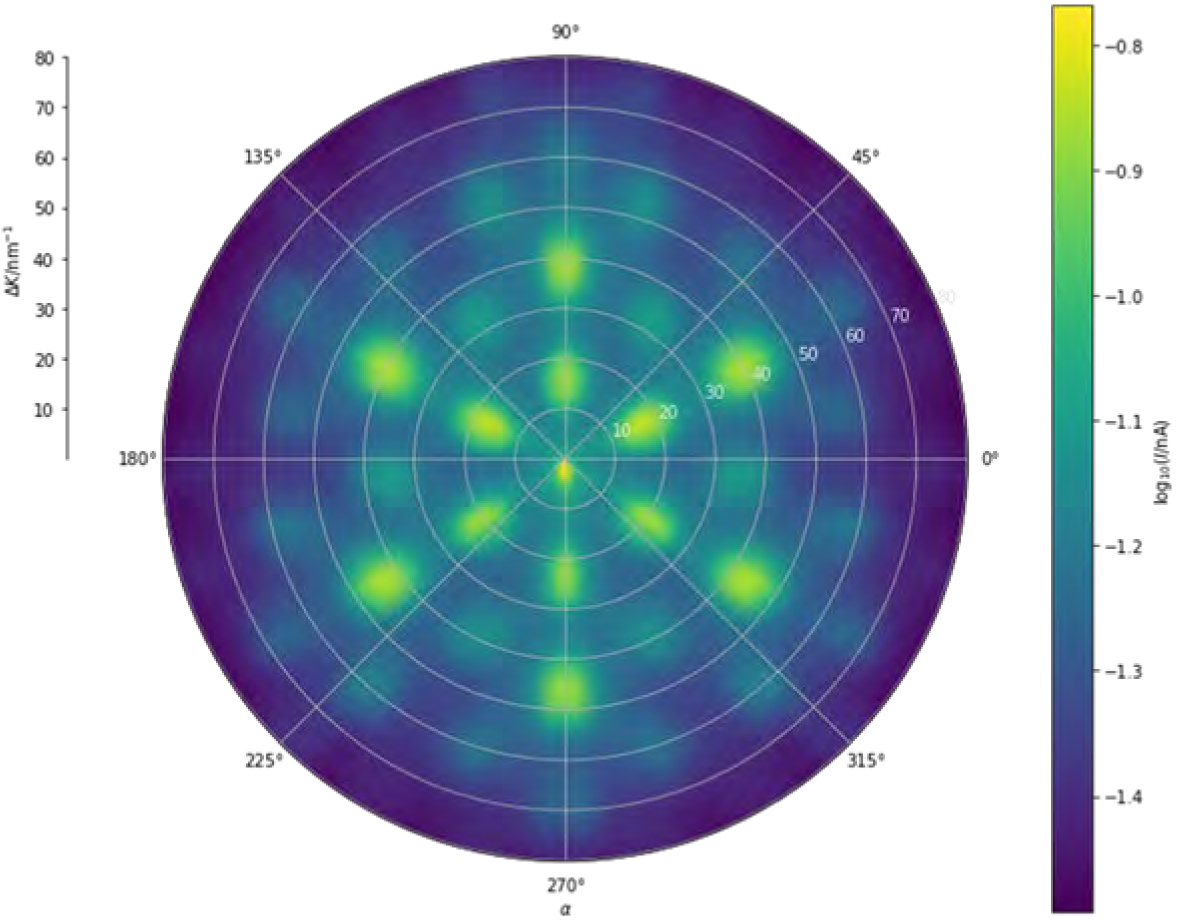
Dr David Ward[1], Prof Andrew Jardine[1], Dr Sam Lambrick[1]
[1]University Of Cambridge, United Kingdom

2D Materials and Van der Waals Heterostructures 2 and Ferroelectric Behaviour, June 20, 2024, 11:00 - 13:00

Recent advances in atom beam microscopy are presented with a focus on a new platform developed in Cambridge, now under commercial development at Ionoptika Ltd. The new platform has enabled significant improvements in capability which are demonstrated using several applied samples, including bacteria and bacteria biofilms which now accessible due to improvements in resolution measured with no surface treatment. And 2D materials where diffraction from the surface is used to enhance contrast and demonstrate a particularly interesting contrast mechanism.

Beams of noble gasses, have been used for surface science for many years due to their surface sensitivity while causing no damage, but application to real space imaging through spatial resolving power is more recent. The capabilities have enabled significant growth in the application of the technique, including chemical and diffraction enhanced contrast, depth profiling and real time 3D surface reconstruction. SHeM has been shown to reveal topographical structure completely non-invasively i.e. with no addition of a surface coating or contrast agents, which has significant applications in studying delicate samples.

In the current work there is a focus on two applied sample groups, 2D materials, particularly MOS2 where we demonstrate a capability to selectively image surface regions and reveal local structure. We also discuss some recent studies of soft samples where we address topics such as the role of an extra cellular matrix in determining bacterial biofilm formation. SHeM provides the unique ability to image the important interactions between surface topography and bacterial biofilm formation and growth without damaging or influencing the delicate biology of these systems.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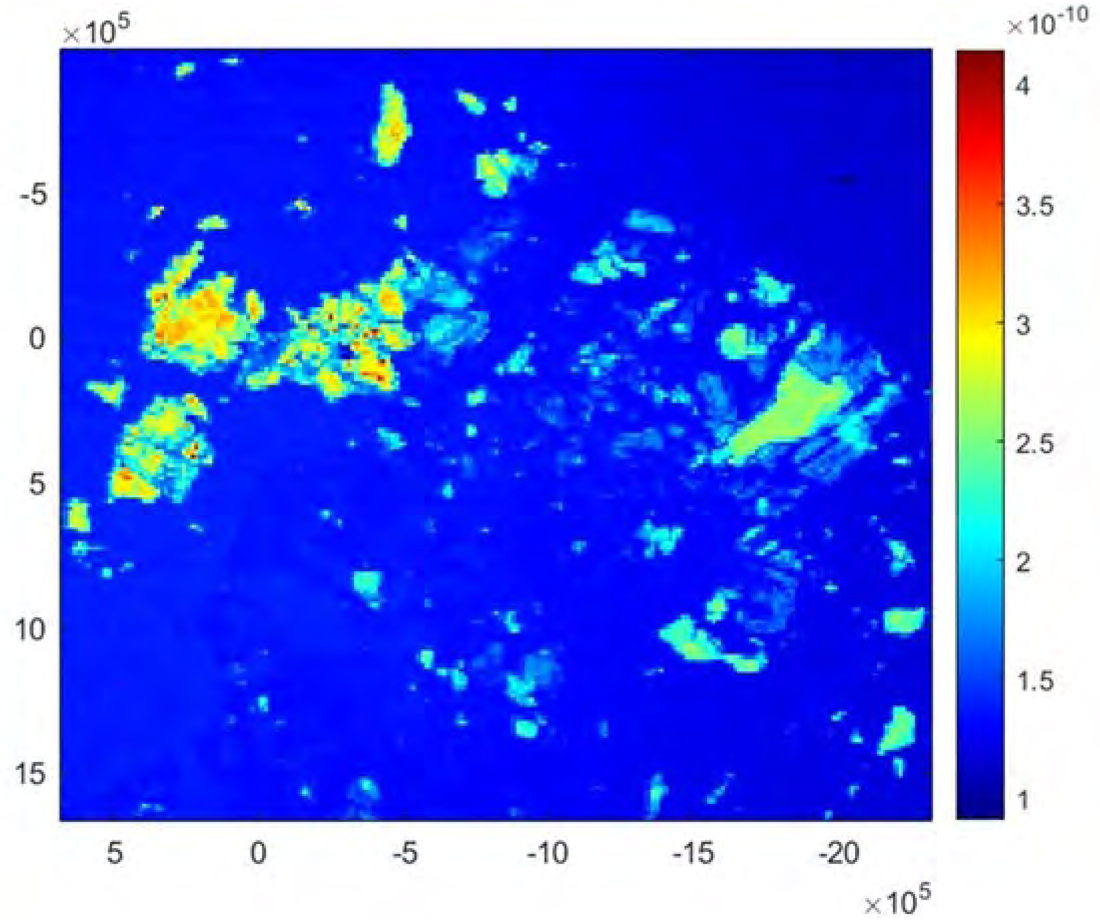
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Double envelope vacuum insulation panel to contribute the long-term thermal insulation performance

Takao Katsura[1]

[1]Hokkaido University, Japan

MS-4: Vacuum Insulation Energy Technologies for Energy Savings, June 20, 2024, 11:00 - 13:00

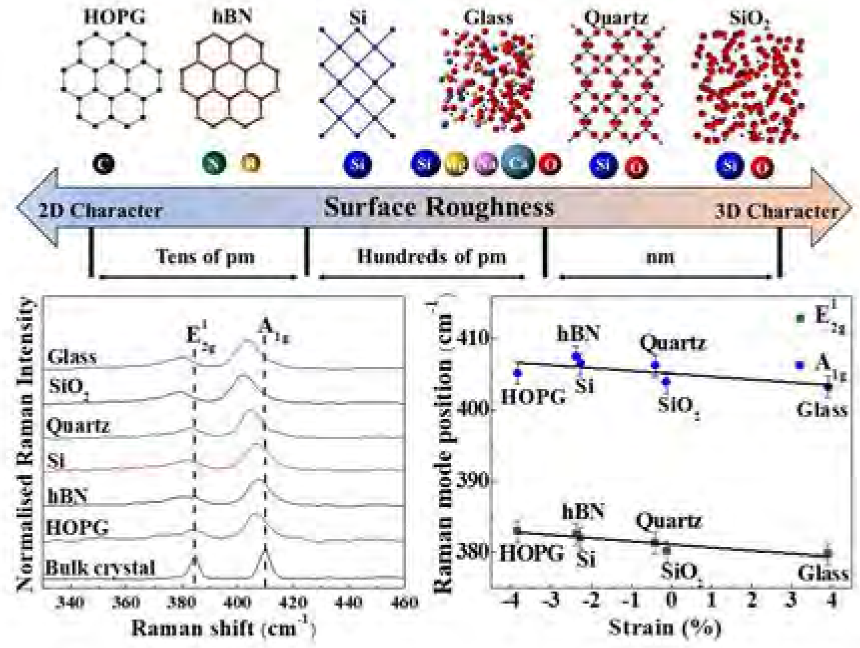
In order to realize vacuum insulation panels applicable to building insulation, it is necessary to overcome the challenge of maintaining the low pressure at which the high insulation performance can be achieved for several decades. We applied the double envelopes to VIPs and investigated longer service life of VIPs. The double envelope VIP is fabricated by fabricating a normal VIP, then wrapping the VIP with core materials, and then inserting it into the envelope for vacuum sealing. By applying the double envelopes, the pressure difference and the permeation of gas in inner VIP can be drastically reduced, resulting in a longer VIP lifetime. The effect of VIP longevity was clarified by simulation to predict the pressure increase inside the VIP and by accelerated tests to measure thermal conductivity once a month by placing the vacuum insulation material in a chamber at 80°C.

Substrate-induced strain in molybdenum disulfide thin films grown by aerosol-assisted chemical vapour deposition

Dr Nilanthy Balakrishnan[1], Lewis Adams[1], Dr Peter Matthews[1], Dr Juliana Morbec[1]
[1]School of Chemical and Physical Sciences, Keele University, United Kingdom

Low-dimensional Thin Film Materials, June 17, 2024, 11:00 - 12:35

Transition metal dichalcogenides have been extensively studied in recent years because of their fascinating optical, electrical, and catalytic properties. However, low-cost, scalable production remains a challenge. Aerosol-assisted chemical vapour deposition (AACVD) provides a new method for scalable thin film growth. In this study, we demonstrate the growth of molybdenum disulfide (MoS2) thin films using AACVD method. This method proves its suitability for low-temperature growth of MoS2 thin films on various substrates, including glass, silicon dioxide, quartz, silicon, hexagonal boron nitride, and highly ordered pyrolytic graphite. The as-grown MoS2 shows evidence of substrate-induced strain, see Figure 1. The type of strain and the morphology of the as-grown MoS2 highly depend on the growth substrate's surface roughness, crystallinity, and chemical reactivity. Moreover, the as-grown MoS2 shows the presence of both direct and indirect band gaps, suitable for exploitation in future electronics and optoelectronics.



THE RELEVANCE OF CATALYTIC SILICATE AND CARBON DUST SURFACE REACTIONS IN THE INNER SOLAR NEBULA

Youssef Guermassi[1], Petra Rudolf[1], Fayçal Raouafi[2]
[1]Surface Physics, The Netherlands, [2]Solid state Physics, Tunisia

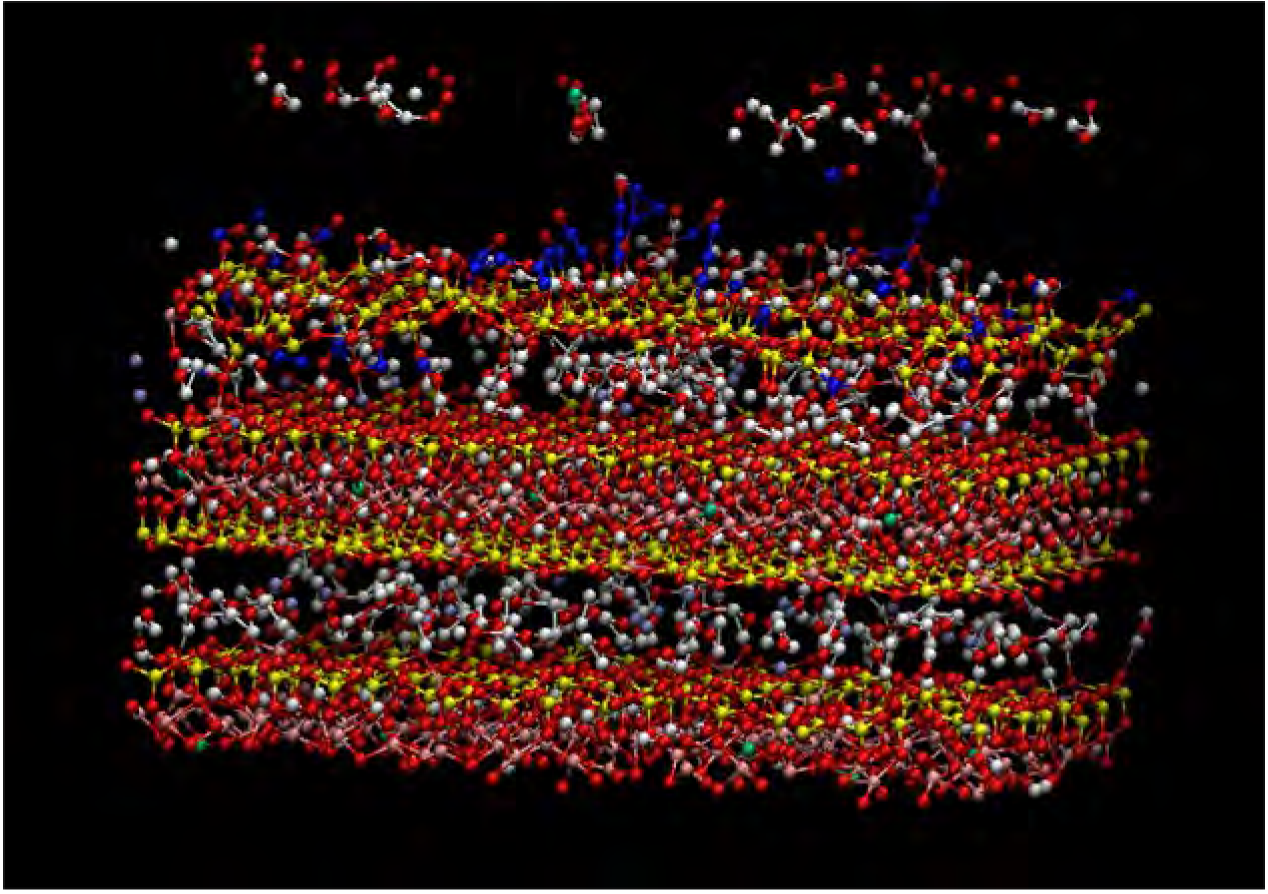
Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 4, June 21, 2024, 10:30 - 12:00

We live in a dusty Universe! Dust is not only found in our solar system among the planets, but it is present in a wide variety of objects throughout the Universe, mainly in those regions between stars called interstellar clouds. The interstellar medium particles -generally composed of an intimate mixture of silicate and carbon grains- and the interstellar gas are perpetually interacting. Our study aims to understand the dynamics of this interaction between the matter in the gas phase and the nanoparticles in new physical conditions and see how this

influences the chemical complexity of space, particularly in the formation of planets. A coherent and interdisciplinary approach is required to quantify the active and catalytic role of dust in space [1]. First of all, we will produce in the laboratory dust particles analogous to the silicate dust observed in the interstellar medium. Then, we will perform experiments to study the reactions on the surface of the dust grains under

astrophysical conditions and characterize the obtained products using the technique: of X-ray photoelectron Spectroscopy (XPS). Finally, we will exploit the results of our study to define relevant astrophysical environments using a molecular dynamic simulation and develop additional modules for these simulations that describe the new dust functionality.

[1] Alexey Potapov and Martin McCoustra. Physics and chemistry on the surface of cosmic dust grains: A laboratory view. International Reviews in Physical Chemistry, 40(2):299–364, 2021.



Vacuum Insulated Energy Saving Materials for Net Zero Energy Buildings

Saim Memon[1,2,3]

[1]Sanyou London Pvt Ltd, United Kingdom, [2]Birmingham City University, United Kingdom, [3]Jiangsu Sanyou Dior Energy-saving New Materials Co. Ltd, China

MS-4: Vacuum Insulation Energy Technologies for Energy Savings, June 20, 2024, 11:00 - 13:00

Vacuum insulated energy materials for energy savings such as vacuum insulated wallpaper (VIW), vacuum insulation panel (VIP and decorative integrated VIP are pivotal industrial R&D developments that help in achieving net-zero energy buildings due to their superior thermal efficiency and space-saving attributes. These vacuum insulated materials significantly reduce heat transfer, thereby lowering the energy needed for heating and cooling, aligning with sustainability goals by reducing buildings' carbon footprints. VIW and VIP are particularly effective in extreme climates, offering superior insulation with minimal thickness compared to traditional materials like XPS, EPS, mineral wool, or polyurethane. This results in less space required and lower overall energy consumption. In both cold-arid regions where heating is essential, and hot-arid areas where cooling demands are high, VIPs effectively prevent unwanted heat transfer, enhancing interior comfort while reducing energy use and associated carbon emissions. Overall, the application of VIPs in buildings not only supports stringent building regulations but also contributes to a sustainable, energy-efficient future. This keynote speech focus on addressing global challenges to pave the way for a sustainable, net-zero energy future using vacuum insulation energy technologies.

Reducing Iridium loading within acidic oxygen evolution catalysts for Green Hydrogen Production.

Dr. Norton West[1], Dr. Cindy Tseng[2], Dr. Alice Meng[3], Dr. Reshma Rao[2], Prof. Ifan Stephens[2], Dr. Katie Moore[1], Dr. Alex Walton[1]

[1]Photon Science Institute, University Of Manchester, United Kingdom, [2]Department of Materials, Imperial College London, United Kingdom, [3]Department of Chemical Engineering, Imperial College London, United Kingdom

Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 3, June 20, 2024, 11:00 - 13:00

Proton exchange membrane water electrolysers is one of two leading industrial methods that can enable green hydrogen production at scale, but the scarcity of iridium requires a reduction in the amount used within the anode of these devices. To achieve a reduction in iridium loading, the mechanisms of active catalytic sites must be understood so they can be produced reliably[1].

This work aims to understand the fundamental limits to the performance of acidic electrolysers and iridium oxide catalysts using correlative operando X-ray photoelectron spectroscopy (XPS) and Nanoscale secondary ion mass spectrometry (NanoSIMS)[2]. The measured catalysts have variable amounts of iridium loading with mixed metal oxides. To investigate acidic OER catalysts with reduced Iridium loading, operando XPS was performed with a custom designed cell to allow continuous OER catalyst operation during XPS measurements. This has been correlated with electrochemical activity of these catalysts measured in a three-electrode setup and depth profiling through the mixed metal oxide film with NanoSIMS to investigate changes in chemistry after cycling.

This work will compare the iridium species as a function of electrochemical potential. This will uncover the active species for mixed iridium oxides and direct design of iridium efficient electrocatalysts.

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Reactive remote plasma sputtering of TiOx thin films and controlled growth

Dr Hayley Brown[1], **Dr James Dutson**[1], Joshua Ellingford[1,4], Dr Steve Wakeham[1], Joe Lawton[2,1], Dr Mark Baker[2], Dr Vlad Stolojan[3], Prof Michael Thwaites[1], Dr Sarah Thornley[1]

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Advanced Thin Film Fabrication, June 19, 2024, 10:30 - 12:35

Rutile TiO2 thin films have been extensively studied in the last decades for several applications such as photocatalyst and self-cleaning applications. Typically, crystalline rutile TiO2 requires substrate heating or post anneal. This recent work demonstrates that pure rutile TiO2 thin films can be deposited using remote plasma sputtering without substrate heating.

In remote plasma sputtering a high density plasma is generated remotely from the target material and allows for independent control over the plasma density and ion energy. Previous research has shown that remote plasma sputtering is capable of depositing dense crystalline thin films at room temperature. In addition, remote plasma sputtering can offer a more stable reactive process due to the uniform erosion of the target material and elimination of the racetrack profile as seen in magnetron sputtering.

In this work the RF remote plasma power was kept constant (2.0 kW) and the properties of the films were studied as a function of deposition rate and substrate bias voltage. The film structural, optical, and surface properties were investigated by GI-XRD, SEM, transmission, and sessile drop measurements. All films deposited under zero bias conditions exhibited amorphous structures in GI-XRD and SEM images. Sufficient application of substrate bias was seen to promote columnar growth in cross-sectional SEM images with no detection of the anatase phase. Further increase of the substrate bias voltage caused a change in the texture of the rutile films from a low-energy [110] preferred orientation to a high-energy [101] and [002] preferred orientation. Contact angles of water with deposited films were found to increase with increasing substrate bias voltage and decreasing deposition rate. Film stress was also found to be influenced mainly by the substrate bias voltage. This work concluded that substrate bias and deposition rate where the key variables in obtaining room temperature rutile TiO2.

Electronic probing and manipulation of nanophotonic phenomena

Jaime Abad-Arredondo[1], Francisco José García-Vidal, Antonio. I. Fernández-Domínguez
[1]Universidad Autónoma De Madrid, Spain

MS-2: Light-matter Interaction at Atomic Scales, June 17, 2024, 16:00 - 17:35

Electrons have been invaluable in the development of tools to study nanoscale phenomena. In this talk we explore novel avenues to explore light-matter coupling at the nanoscale by leveraging electrons, made accessible through recent technical advancements. On the one hand, advances in nanofabrication allow the manufacturing of electrically driven nanogap antennas. By placing an excitonic material on top of the gap, hybrid light-matter states are formed. We demonstrate how the electrically controlled tunneling-electron-current can be used as a source to drive the polaritonic modes. This has direct applications to the development of on-chip nanophotonic quantum devices. On the other hand, recent advances in controlling the quantum properties of collimated free-electron beams have positioned them as promising probes for investigating quantum matter at the nanoscale. We provide a model Hamiltonian that captures the interplay between electronic transitions and optical modes. Our Hamiltonian is constructed using macroscopic Quantum Electrodynamics (QED) principles and is parameterized using the electromagnetic Dyadic Green's function. We apply this model to study state preparation on an isolated quantum-emitter (QE), and to perform polariton sensing with modulated free electrons in a hybrid QE-optical cavity setup.

Probing the solid/liquid interface in X-Ray Phtotoelectron Spectroscopy: A droplet-based approach

Dr Alex Walton[1]

[1]University Of Manchester, United Kingdom

Advances in Experimental and Theoretical Methods 1, June 17, 2024, 11:00 - 12:35

The ability to study the solid/liquid interface in situ is essential to gain fundamental understanding of electrochemical processes. A poor understanding of surface chemical processes at electrodes is a key bottleneck in the development of many energy technologies -e.g. alternative battery technologies or water splitting catalysts. X-Ray Photoelectron Spectroscopy (XPS) is one of the most powerful probes of surface chemistry available but addressing the electrode/electrolyte interface with XPS is a major technical challenge as it is buried by the electrode on one side and the electrolyte on the other - making detection of photoelectrons from this interface very difficult. There has been intense efforts to overcome these challenges by either establishing (electron-transparent) ultrathin wetting layers on sample surfaces (known as the “dip and pull” method) or by making ultrathin graphene electrodes through which the interface can be addressed.

I will present an alternative approach to establishing an ultrathin wetting layer on the sample surface, through which we can directly probe the electrode/electrolyte interface in-situ. We do this by introducing a droplet of electrolyte onto the sample, offset from the analysis area by a few millimetres. This “offset droplet” approach has the advantages of being applicable to virtually any sample, the capability to alter the solution composition dynamically and a short diffusion length from analysis area to the “bulk” droplet. I will outline the capabilities and the challenges of this technique and present some results applying it to the study of model electrocatalysts.

Performance modelling of a multistage roots vacuum pump

Mr Michael Galtry[1]
[1]Atlas Copco Vacuum Technique, United Kingdom

Vacuum pumps, June 21, 2024, 10:30 - 12:00

A tool for design and performance modelling of a multistage roots vacuum pump has been developed. This tool models individual stage performance, interstage leakage, purges and pump power requirement for cases involving single and multiple gas species, adjusting clearances within the pump according to rotor and stator temperatures for the given conditions. In this talk we look at the modelling techniques used in developing the model.

Reactive sputtering of undoped ZnO films with ultrafast photoluminescence

Dr. Jiri Olejnicek[1], Marilou Cadatal-Raduban[2], Aneta Písaříková[1], Michal Kohout[1], Lenka Volfová[1], Rainer Hippler[1], Nobuhiko Sarukura[3], Shingo Ono[4], Kohei Yamanoi[3], Zdeněk Hubička[1]

[1]Institute of Physics of the Czech Academy of Sciences, Czech Republic, [2]School of Natural Sciences, Massey University, New Zealand, [3]Institute of Laser Engineering, Osaka University, Japan, [4]Nagoya Institute of Technology, Japan

Advanced Thin Film Fabrication, June 19, 2024, 10:30 - 12:35

Ultrafast luminescence is crucial for applications requiring timing precision below 100 ps. This work introduces a few micron-thick undoped ZnO layers on low-cost soda lime glass substrates, fabricated using three different deposition methods. Depending on the used technology and experimental conditions, we managed to prepare ZnO films showing intensive UV luminescence with an ultra-fast 9 ps decay time. For preparation of these layers we used: (i) pulsed DC hollow cathode discharge with a zinc nozzle, (ii) DC magnetron sputtering from a ZnO target, and (iii) medium frequency (MF) magnetron sputtering from a zinc target in combination with electron-cyclotron wave resonance (ECWR) plasma. Methods (i) and (iii) utilized reactive sputtering from metallic targets (or hollow cathode) in an Ar/O2 mixture, while method (ii) utilized a ceramic ZnO target sputtered in pure Ar. We investigated the influence of deposition technique, substrate temperature, and post-deposition annealing. Plasma parameters were determined via optical emission spectroscopy and modified RF probe technique. Subsequently, crystallographic, optical, and photoluminescence properties were analyzed. X-ray diffraction confirmed the crystalline nature of all ZnO layers, predominantly exhibiting a wurtzite structure with preferred (002) orientation. However, variations in defect density, evident in Raman spectra and defect-related luminescence peaks, were observed depending on deposition conditions. Layers prepared by MF+ECWR revealed superior UV luminescence intensity, surpassing the other techniques by a factor of 10, and featured ultrafast decay times ranging from 25 to 9 ps.

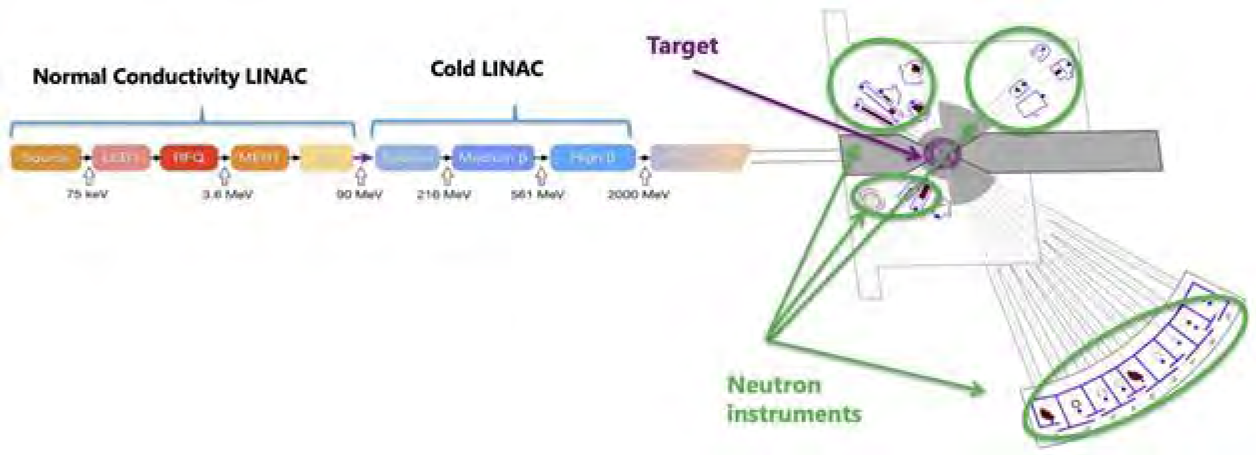
ESS vacuum system commissioning

Dr. Marcelo Juni Ferreira[1], Mr Adrien Besson[1], Dr. Laurence Page[1], Mr. Artur Gevorgyan[1], Mr. Hilko Spoelstra[1]
[1]European Spallation Source ERIC, Sweden

Special Surfaces and Outgassing, June 17, 2024, 14:00 - 15:30

The European Spallation Source (ESS) is a multidisciplinary research infrastructure and neutron source facility, based on a 2 GeV-5 MW proton linear accelerator (LINAC). ESS aims to be the brightest neutron facility, enabling novel science in fields such as biology research, environmental technologies, and fundamental physics. The facility includes superconductive radio-frequency cavities (SRF) to accelerate a proton beam and produce neutrons through the spallation process on a helium-cooled tungsten wheel, with the capacity to host 42 neutron instruments. The ESS Vacuum Group holds overall responsibility for all technical vacuum systems used in the Accelerator, Target, and Neutron Scattering Instruments (NSS).

An overview of the ESS Vacuum System's final installation steps will be provided, focusing on the neutron source, which includes the proton accelerator and target monolith. Details about the vacuum hardware and the Vacuum Control system will be presented as is for the first phase of commissioning. On the Neutron Instrument side, the concept of a higher energy neutron instrument, NNBAR, which follows the model of usual collider experiments, will also be introduced.



Iron-Induced Surface Transformations of Ceria: Insights from FeOx/CeO2(111) and Au/FeOx/CeO2 Systems

Shiva Oveysipoor[1], Lesia Piliai[1], Pablo Castro Latorre[2], František Pchalek[1], Martin Ormoš[1], Dr. Yuliia Kosto[1,3], Dr. Ivan Khalakhan[1], Dr. Tomáš Skála[1], Dr. Pere Alemany[2], Dr. Michael Vorochta[1], Dr. Konstantin M. Neyman[2], Dr. Albert Bruix[2], Dr. Peter Matvija[1], Prof. Iva Matolínová[1]
[1]Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University, Czech Republic, [2]Department de Ciència de Materials i Química Física and Institut de Química Teòrica i Computacional , Universitat de Barcelona, Spain, [3]Brandenburg University of Technology Cottbus-Senftenberg, Applied Physics and Semiconductor Spectroscopy, Germany

Catalysis and Electrocatalysis including Single Atom and In Operando Studies 1, June 19, 2024, 14:00 - 15:30

The catalytic efficiency of ceria (CeO2) in oxidation and combustion reactions can be increased significantly through modification by inexpensive reducible metals, such as iron. To understand the role of iron-ceria interaction behind the enhanced efficiency, we prepared well-defined model FeOx/CeO2(111) surfaces, and probed their structure and interfacial electronic properties via photoelectron spectroscopy (PES), scanning tunneling microscopy (STM), and low-energy electron diffraction (LEED) along with density functional theory (DFT) simulations.

Our results show that Ce ions are reduced to Ce3+ upon Fe deposition under ultrahigh vacuum (UHV), while Fe is oxidized and incorporated into uniformly distributed FeOx nanoclusters. At higher temperatures, partially oxidized Fe atoms form 3D amorphous particles and a corrugated 2D FeOx layer. Upon further annealing in O2, Fe oxidizes to Fe3+, 3D particles become crystalline and the ordering of the 2D FeOx layer improves. DFT simulations indicate that the 2D FeOx layer owes its stability to the structural corrugations and the transfer of charge from FeOx to CeO2. This novel 2D FeOx/CeO2(111) surface might play a key role in understanding the enhanced catalytic performance of ceria. Additionally, the 2D corrugated layer could act as a template for the growth of other metals with high catalytic activity, such as Au.

In this work, we prepared a model Au/FeOx/CeO2 surface containing the 2D FeOx layer to study the behavior of this system under CO oxidation conditions, in 1 mbar of the mixture of CO and O2, by STM and near-ambient pressure (NAP)-XPS. We discovered that the FeOx layer hinders the agglomeration of Au into large clusters, which may be directly linked to the improved catalytic activity and better long-term stability of Au catalysts supported by Fe-modified ceria.

Acknowledgment: The work was financially supported by the Czech Science Foundation, Project No. 20-13573S.

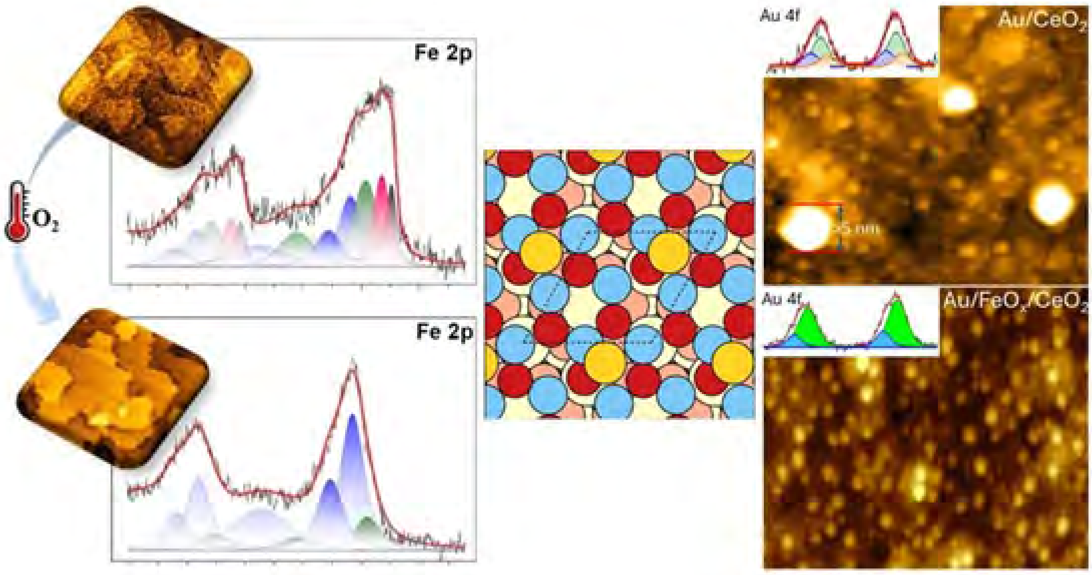


Figure 1. Spectroscopic and microscopic analysis of model $FeO_x/CeO_2(111)$ and $Au/FeO_x/CeO_2(111)$ systems

Electronic structure of fullerene derivative thin films with gold doping

Taiga Hirota[1], Dong Han[1], Tomoki Misaka[1], Hiroshi Ohoyama[1], Takashi Yamada, Takuya Matsumoto[1]
[1] *Graduate School of Science, Japan*

Carbon Materials 1, June 18, 2024, 16:00 - 17:30

Recently, it has been reported that a small amount of metal doping into carbon-based materials induced various physical properties. Our research group reported that the deposition of a small amount of gold on a thin film of [6,6]-phenyl-C61-butyric acid methyl (PCBM) significantly increases conductance. This increased conductance is due to the formation of a new molecular orbital in the band gap by the hybridization between the HOMO of the PCBM and the 6s orbital of gold atoms[1]. However, the relationship between the conductivity and the gold cluster size generated on the PCBM film was still unclear. In this study, we investigate the size of the gold cluster on PCBM film at a small amount of deposition.

The PCBM films were formed by spin-coating of PCBM chloroform solution on ITO glass substrates, and gold atoms were evaporated onto the PCBM films by thermal deposition method. X-ray photoelectron spectroscopy (XPS, Al Kα , hν=1486.6 eV) measurements were performed to evaluate the core level of Au 5d in vacuum (<10-9 Torr) at room temperature.

Fig. 1(a) shows XPS spectra of the Au 5d core level as a function of the amount of Au deposition. Fig. 1 (b) shows the split of Au 5d band as a function of the deposition amount of Au. According to the paper[2], the split of the Au 5d band depends on the cluster size of Au. The gold cluster size was estimated in the same manner as the paper[2]. Although the gold cluster was generated even at the 0.1 ML deposition, the cluster could not show conductivity considering the size and the coverage. Thus, we show the experimental evidence that the Au-PCBM orbital generation originates the conductance eliminating the possibility of Au cluster conduction.

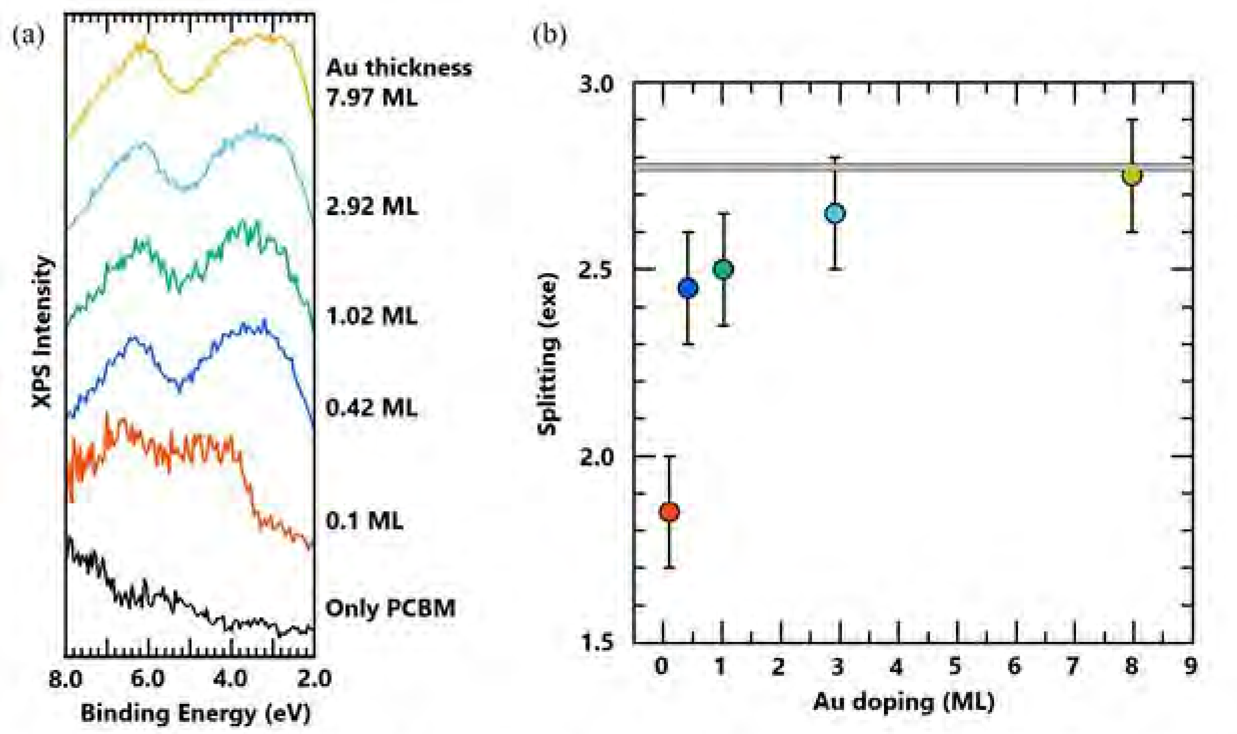


Fig. 1 (a) XPS spectra of Au 5d band depending on the amount of Au deposited on the PCBM film.
(b) Dependence of spectrum split width on gold deposition amount

Investigating the electrooxidation of Au in basic and acidic media

Jesús Redondo[1], Pankaj Kumar[1], Sabine Auras[2], Břetislav Šmid[1], Sophie Ju[1], Josef Mysliveček[1], Sara Barja[3]
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Catalysis and Electrocatalysis Including Single Atom and In Operando Studies 4, June 21, 2024, 10:30 - 12:00

The rate-limiting factor of the water-splitting reaction is the slow kinetics of the oxygen evolution reaction (OER) at the anode of a chemical cell[1]. The fundamental investigations of the anode material properties, its evolution during a (photo, electro) chemical reaction, and its interaction with the electrolyte are essential for systematically optimising the WS reaction. Gold is a non-critical, non-toxic material with low-supply risk. It has been shown that the performance of Au anodes for OER depends on the surface oxidation under certain potentials, and its interaction with the electrolyte cations. The formation and nature of Au oxides, and the influence of the electrolyte in the process, is still a challenging topic. The combination of ultra-high vacuum (UHV) techniques, attached to electrochemical (EC) set-ups (EC-UHV) allows for the fundamental investigations of anode/cathode materials[2].

Here, we explore the electrooxidation of Au(111) below and at the OER potential range in basic (KOH and NaOH) and acidic (H_2SO_4, $HClO_4$) solutions. We utilized a custom-made electrochemical set-up which allows transfer from/to UHV and electrochemical testing without exposing the samples to ambient conditions. The Au surface is electrochemically modified by immersion/emersion under potentiostatic control, cyclic voltammetry (CV) and chronoamperometry (CA) routines. We show how the applied potential and the cations/anions in the electrolyte influence the formation of Au oxides.

References

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Acknowledgments

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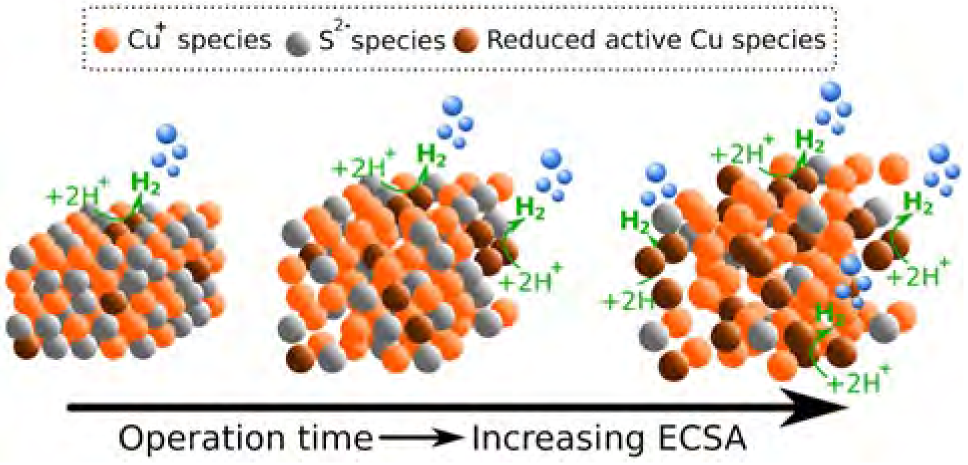
Surfase reconstrucion of Cu2-xS electrocatalyst under bias

Roser Fernandez-Climent[1], Jesús Redondo[1], Sixto Gimenez[2], Camilo Mesa[3], Jordi Arbiol[3], Maria Chiara Spadaro[3], Sara Barja[4], Frederik Schiller[4]
[1] Charles University, Czechia, [2] INAM-Universitat Jaume I, Spain, [3] Institut Català de Nanociència i Nanotecnologia, (ICN2), Spain, [4] Centro de Física de Materiales-CSIC, Spain

Catalysis and Electrocatalysis including Single Atom and In Operando Studies 1, June 19, 2024, 14:00 - 15:30

Copper sulfide electrocatalysts are promising Earth abundant and cost-effective materials able to drive different electrochemical conversions at mild pH conditions.

Herein it is explored the operando evolution of the Cu2-xS electrocatalyst to drive the hydrogen evolution reaction (HER). The electrochemical evaluation of the Cu2-xS electrocatalysts, exhibits hydrogen evolution rates that increase during ~1 month of continuous operation. Throughout operation time, Cu2-xS electrodes reach a state-of-the-art current of 400 mA cm-2 at -1 V vs RHE at mild conditions (pH 8.6), with practically 100% Faradaic efficiency for H2 evolution. The current density increased with the electrochemically active surface area of the electrodes. Consistently, improved electrode performance correlated with decreased Tafel slopes. Moreover, a comprehensive structural and chemical characterization of the electrodes before, during and after the HER was carried out, which was crucial for the proper interpretation of the results. Particularly, the analysis of Cu2-xS electrodes by operando spectroelectrochemistry (SEC), X-ray diffraction (XRD), and X-ray photoemission spectroscopy (XPS) simultaneously to the electrochemical tests revealed that the catalytic activity is mainly driven by catalytic centers located at Cu species. These results contribute to increase our fundamental understanding of heterogenous electrocatalyst transformation and consequent structure-activity relationship.



Time-Resolved Charge Observation of Photovoltaic Organic Thin Films by Tip-Synchronized Electrostatic Force Microscopy

Kentaro Kajimoto[1], Kento Araki[1], **Takuya Matsumoto**[1]
[1] Osaka University, Japan

Electronic Materials, Energy Reduction and Carbon Reduction 2, June 21, 2024, 10:30 - 12:00

The micro- or nanoscale generation, migration, and recombination of local charges (collectively referred to as charge dynamics) play essential roles in many natural and artificial systems or phenomena, including the brain, light harvesting, photosynthesis, catalysis, photovoltaic devices, and field-effect transistors. Charge tracking is intrinsically important for understanding the fundamental characteristics of these systems as well as the fabrication of functional materials and devices.

Tip-synchronized tr-EFM provides time-resolved charge detection at the tip position closest to the sample surface in the pump–probe framework, improving the sensitivity and spatial resolution in compared with standard EFM methods.

Recently, we were able to obtain a video showing photoexcited carrier migration on an organic photovoltaic device with a time resolution of 0.3 μs and sensitivity of 0.3 Hz [1]. The tip synchronization can be extended to dual-bias pump–probe measurements using constant-amplitude feedback control, frequency-shift electrostatic force detection, and lock-in detection of the probe pulse train modulation [2]. This method permitted highly sensitive detection of the electrostatic force under a constant tip–sample distance, thereby enabling time-resolved observation of the charge dynamics for the conductive polymer SPAN, which is a relatively poor conductor. Comparison of SPAN thin films with different doping levels revealed the individual differences in carrier density and mobility. The obtained results demonstrate that time-resolved EFM is a powerful tool for elucidating the charge dynamics of hopping conductors such as thermoelectric materials containing metallic grains.

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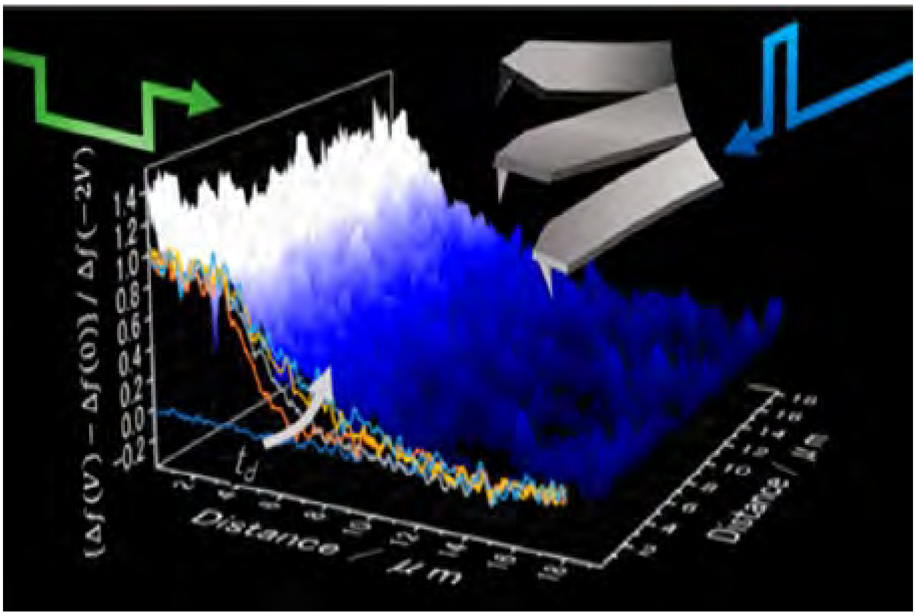
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Light-matter interaction of field emission resonances in a scanning tunneling microscope

Alberto Martin-jimenez[1], David Mateos[1,2], **Miguel Varea**[1], Rodolfo Miranda[1,2], Roberto Otero[1,2]
[1]Imdea Nanociencia, Spain, [2]Dept. de Física de la Materia Condensada, Universidad Autónoma de Madrid (UAM), Spain

MS-2: Light-matter Interaction at Atomic Scales, June 17, 2024, 16:00 - 17:35

The combination of scanning tunneling microscopy (STM) with laser light (pulsed or continuous) offers the unique possibility to investigate and control light-matter interaction at the atomic scale, which is critical for the development of novel technologies from diverse branches, such as quantum computing, optoelectronics, sensing, or catalysis, to mention a few. In our work, we investigate the effect of continuous wave (CW) laser illumination on the field emission resonances (FER) formed between a gold tip and an Ag(111) sample by measuring the derivative of the tunneling current as a function of the bias voltage. It was previously reported that the effect of CW illumination was that the lowest energy FER downshifts by the photon energy, being the hallmark of plasmon-assisted resonant tunneling [1]. We have extended these investigations and made a thorough experimental characterization of the effects induced by the laser power, tunneling current, and polarization of the excitation laser on the FERs. Interestingly, several peaks in the FER spectra appear/disappear upon laser illumination when varying polarization, laser power, or tunneling current, whose positions and intensities follow a non-trivial dependence. Our observations cannot be described only assuming plasmon-assisted resonant tunneling, indicating that the strong field confinement of the laser fields due to the tip-sample nanocavity may be responsible for the observed effects.

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Attempts to control the orientation of PdO on Pd(100)

Isac Bramer[1], Hanna Sjö[1], **Johan Gustafson**[1]
[1] *Lund University, Sweden*

Metal and Oxide Single Crystal Surfaces - Growth, Preparation, and Characterisation, June 18, 2024, 16:00 - 17:30

Pd is well known for its high activity for catalytic oxidation reactions. Several studies have shown that both metallic and oxidized Pd surfaces may be active, depending on the oxide surface orientation. While PdO(101) exposes coordinatively unsaturated Pd atoms, acting as active sites, PdO(100) does not and shows low activity. Hence, it is of great interest to be able to control the oxide growth to favour the active surface.

Previous studies have shown that the initial oxidation of Pd(100) results in a single-layer PdO(101) surface oxide, followed by multilayer PdO with similar orientation. When the oxide becomes thick enough, however, it becomes polycrystalline in conjunction with a drop in catalytic activity, probably related to the exposure of PdO(100)[1]. The actual growth of (100) oriented PdO has been found to be very difficult. Mehar et al., however, recently found that the sample temperature is key to controlling the orientation. Using atomic oxygen, it was found that below 600 K, the oxide grows exclusively as PdO(101), while above 600 K the result is a mixture of PdO(101) and PdO(100)[2].

We will here present a study where these findings were tested. Pd(100) was systematically oxidized at different temperatures and the oxide orientation checked with grazing incident X-ray diffraction. At high temperatures, we indeed found the growth of PdO(100), to an even larger extent than expected. At lower temperatures, where we expected exclusively PdO(101), we were very surprized to find PdO(501) instead. We will discuss possible reasons and implications of these results.

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Robust SrTiO3 Passivation of Silicon Photocathode by Reduced Graphene Oxide for Solar Water Splitting

Matjaž Spreitzer[1], Hsin-Chia Ho[1], Janez Kovač[1], Miha Čekada[1], Milutin Smiljanić[2], Nejc Hodnik[2]
[1]Jožef Stefan Institute, Slovenia, [2]National Institute of Chemistry, Slovenia

Functional Coatings 1, June 17, 2024, 14:00 - 15:30

Development of a robust photocathode using low-cost and high-performing materials, e.g., p-Si, to produce clean fuel hydrogen has remained challenging since the semiconductor substrate is easily susceptible to (photo)corrosion under photoelectrochemical (PEC) operational conditions. In the present work, we utilized pulsed laser deposition (PLD) to prepare a high-quality SrTiO3 (STO) layer to passivate the p-Si substrate using a buffer layer of reduced graphene oxide (rGO). Specifically, a very thin (3.9 nm ~10 unit cells) STO layer epitaxially overgrown on rGO-buffered Si showed the highest onset potential (0.326 V vs RHE) in comparison to the counterparts with thicker and/or nonepitaxial STO. The photovoltage, flat-band potential, and electrochemical impedance spectroscopy measurements revealed that the epitaxial photocathode was more beneficial for charge separation, charge transfer, and targeted redox reaction than the nonepitaxial one. The STO/rGO/Si with a smooth and highly epitaxial STO layer outperforming the directly contacted STO/Si with a textured and polycrystalline STO layer showed the importance of having a well-defined passivation layer. In addition, the numerous pinholes formed in the directly contacted STO/Si led to the rapid degradation of the photocathode during the PEC measurements. This study provided a facile approach for preparing a robust protection layer over a photoelectrode substrate in realizing an efficient and, at the same time, durable PEC device.

Tunable Electron-Phonon Coupling in Hexagonal Boron Nitride

Dr. Håkon Røst[1], Mr. Alv Johan Skarpeid[2], Dr. Simon Phillip Cooil[2], Ms. Anna Cecilie Åsland[3], Dr. Alexander Generalov[4], Dr. Alexei Preobrajenski[4], Dr. Craig Polley[4], Dr. Thiagarajan Balasubramanian[4], Dr. Bodil Holst[1], **Dr. Justin William Wells**[2]
[1]University of Bergen, Norway, [2]University of Oslo, Norway, [3]Norwegian University of Science and Technology, Norway, [4]MAX IV Laboratory, Sweden

Thin Film and Particle Deposition, 2D, June 18, 2024, 14:00 - 15:30

Over the last decade, the inert layered compound hexagonal boron nitride (hBN) has received significant attention for its compatibility with most low-dimensional van der Waals (vdW) materials [1,2]. It resembles graphene in lateral size, crystalline structure, and Debye frequency. Still, due to its dis-similar sub-lattices, it hosts a wide energy band gap separating the valence and conduction bands [3]. Recently, hBN was predicted to host strong electron-phonon coupling (EPC) in its electronic π- and σ-bands [4], reminiscent of the interactions that have been reported (and debated) from the σ-bands of graphene [5]. Since then, we have verified this EPC from energy renormalizations – or "kinks" – in the hBN π-band [6].

This presentation will discuss the observable EPC in mono- and multilayer hBN. Based on our most recent findings, we will showcase how the EPC changes with the substrate interaction; the number of stacked hBN layers; and the intercalation of interfacial adatoms (see Figure 1). We will also discuss the generality of EPC at large binding energies and its potential occurrence in other materials with finite electronic band gaps.

Figure 1: The measured band structure of epitaxially grown hBN when intercalated by increasing amounts of alkali ad-atoms. No obvious EPC "kink" was distinguished from the hBN as grown. All four panels have been overlaid by a nearest-neighbor tight-binding calculation (dashed line) placed at the initial band position (π1).

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[2] J. I.-J. Wang et al., Nano Lett. 15, pp. 1898-1903 (2015).
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[4] E. Thingstad et al., Phys. Rev. B 101, p. 214513 (2020).
[5] F. Mazzola et al., Phys. Rev. B 95, p. 075430 (2017).
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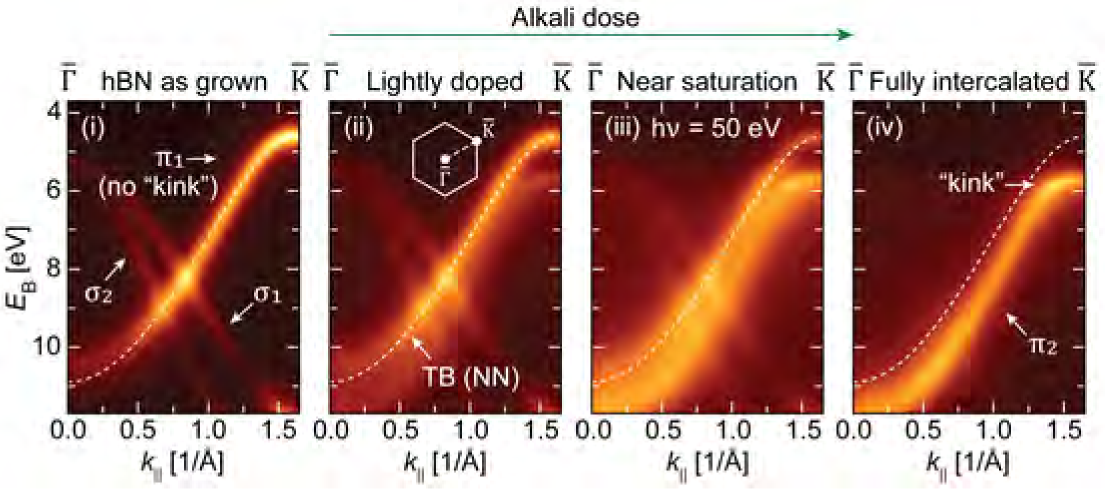

An XPS Study of the Ionic Liquid [C1C1Im][Tf2N] Adsorbed on Mn3O4(001) Thin Films

Dr. Jade Barreto[1], Timo Talwar[1], Dr. Florian Maier[1], Prof. Dr. Hans-Peter Steinrück[1]
[1] Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Oxide Surfaces and Nanomaterials - Spectroscopy, Imaging and Physicochemical Processes, June 18, 2024, 10:30 - 12:30

In the Solid Catalyst with Ionic Liquid Layer (SCILL) concept, a thin layer of ionic liquid (IL) modifies the catalytic surface in terms of enhanced selectivity and reactivity [1]. Since ILs are salts with low melting points typically below 100 °C and extremely low vapor pressure, they can be investigated in situ in ultra-high vacuum, as done over the last years studying the interfaces of thin IL films on metals by Angle-resolved X-Ray Photoelectron Spectroscopy (ARXPS) [2]. The reducible oxide Mn3O4 is an interesting support as it shows potential to be a catalyst in hydrocarbon oxidative reactions [3]. Here, we present the first study of an IL ([C1C1Im][Tf2N]) on the Mn3O4(001) surface by ARXPS. For that, we grow the oxide thin film (1 ~ 2 nm) onto the Au(111) surface, and then we adsorb the IL on this surface. The ARXPS results reveal intact adsorption at temperatures below 200 K as on observed many metals [2]. The temperature-programmed XPS shows multilayer desorption starting at room temperature. The remaining wetting layer is surprisingly stable up to around 350 K, while the same IL starts decomposing on Pt even below room temperature [4].

References:

[1] Kernchen, U., et al. Chemical Engineering & Technology: Industrial Chemistry-Plant Equipment-Process Engineering-Biotechnology, 30(8), 2007, 985-994.
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[3] Stobbe, E., et al. Catalysis Today, 1999, 47(1-4), 161-167.
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A new lead-free low-temperature hermetic edge seal for the fabrication of vacuum glazing

Prabhu Selvaraj[1], P C Eames[1]
[1]Loughborough University, United Kingdom

MS-4: Vacuum Insulation Energy Technologies for Energy Savings, June 20, 2024, 11:00 - 13:00

High performance low-cost vacuum glazing is a key development in realising more energy-efficient buildings. Vacuum glazing consists of two parallel glass sheets separated by a narrow, 0.15-0.3 mm wide vacuum gap. The glass sheets are separated and supported by an array of small pillars, required to maintain the vacuum gap against atmospheric pressure incident on the external surfaces of the two glass sheets. The vacuum gap with a pressure of less than 0.1Pa, sealed by a contiguous edge seal, minimizes heat transfer by conduction and convection across the glazing. Low-E coatings on the glass surfaces reduce IR heat transfer through the gap. Improved hermetic edge-sealing materials are required to address the challenges of cost, use of hazardous substances and issues of complexity of manufacturing of vacuum glazing. This work reports the use of a new lead-free alloy made of Sn-Zn-Al+Ti+Si+Cu+Er+Ce in the ratio 96:3:1 by weight % (Cerasolzer- GS-217), with a melting point of 217°C, to form a hermetic vacuum glazing edge seal. The design, construction, and performance of vacuum glazing prototypes of three different dimensions are reported. Sample A- 150mm x 150mm achieved a vacuum pressure of 0.02Pa, Sample B- 300mm x 300mm achieved a vacuum pressure of 0.03Pa, and Sample C- 500mm x 500mm achieved a vacuum pressure of 0.02Pa. The developed vacuum glazing edge seal uses J-B Weld epoxy-steel resin as a secondary seal to improve glazing robustness. A guarded hot box calorimeter was used to experimentally determine the thermal performance of the vacuum glazing. The experimentally determined overall heat transfer coefficient and temperature profiles along the central line of the vacuum glazing are in good agreement with predictions made using 3-D models.

The Vacuum System Design of FEBE on CLARA at STFC Daresbury Laboratory

Keith Middleman[1]
[1]STFC Daresbury Laboratory, United Kingdom

Vacuum Gas Dynamics, June 18, 2024, 16:00 - 17:30

The Front End Beam Exploitation (FEBE) beamline on CLARA will provide users with an exciting opportunity to perform a variety of experiments using the full 250 MeV electron beam that CLARA will deliver. Following user consultation, STFC Daresbury Laboratory have developed the multi-use beamline design to allow beam experiments combining electron beams, lasers and gas jet target experiments. The design incorporates the flexibility to re-configure experiments easily and incorporates a number of diagnostics pre and post the interaction point in the FEBE experimental hutch.

This paper describes the detailed design of the vacuum systems for FEBE on CLARA. It details the results of Monte-Carlo modelling that have been used to verify the vacuum system design on the whole as well as detailing some of the issues associated with the FEBE beamline and how we intend to overcome these. One of the major issues the design team had to accommodate was how the vacuum system can cope with the high gas load (plasma-wakefield) experiments where users intend to inject H2 or He to pressures in the 10-1 - 10-2 mbar range and what differential pumping arrangements have been put in place to protect the rest of the accelerator.

This paper will also show what designs have been adopted, how the design intends to protect the CLARA accelerator and what safety considerations have been included.

RGA vs Leak Detector – When to use an RGA?

Mr Cliff Harris[1]
[1]*Inficon, United Kingdom*

MS-6: RGA User Meeting 1, June 19, 2024, 10:30 - 12:35

Both an RGA and a helium leak detector use Mass Spectrometer sensors to detect leaks, but which is better?
Both have their place as a leak testing tool and both can detect leaks, so,
When should I use an RGA, what are the advantages?; isn't a helium leak detector much better for leak testing?

Electrical properties of Ti, Zr and V-based binary and ternary getter alloy thin films

Sylvain Lemettre[1], **Clément Bessouet**[1], Charlotte Kutyla[1], Laetitia Leroy[1], Alain Bosseboeuf[1], Thierry Sauvage[2], Olivier Wendling[2], Aurélien Bellamy[2], Stéphanie Escoubas[3], Christophe Guichet[3], Olivier Thomas[3], Johan Moulin[1]
[1]C2N, France, [2]CEMHTI, France, [3]IM2NP, France

Non-evaporable getter coatings, June 18, 2024, 14:00 - 15:30

In the perspective of designing future particle accelerators which could be UHV systems of very long size and/or with very small beam pipe dimensions, research focused on decreasing the surface resistance of NEG coating to reduce the impact of such coating on the beam dynamics [1]. Specifically, the objective is to reduce the surface resistance of the TiZrV NEG film without degrading its low activation temperature. To do so, attempts are made to decrease the film thickness [2], or to dope it with a conductive element such as Cu [3] or Ag [4]. But few and confusing information is available in the literature about the resistivity of NEG coatings [5]. In this work we investigated the electrical properties of thin Ti, Zr, V, ZrTi, ZrV, TiV and TiZrV getter coatings, and their dependence with chemical composition and microstructure.

150-250 nm thick films were co-evaporated under UHV on silicon wafers. Films resistivity and TCR were measured with a vacuum set-up equipped with a 4-probes head and heater. The microstructure of the films was determined by XRD and SEM. The atomic composition of the films in metallic, oxygen, carbon, nitrogen and hydrogen elements was measured by combining RBS, NRA and ERDA.

As expected, results show that the resistivity of a getter film is highly dependent of its chemical composition and microstructure (Figure 1). The most resistive coatings are the ones having the highest density of grain boundaries and the best getter properties, and vice versa. These results show that it is possible to control the NEG film resistivity by tuning the composition and deposition conditions.

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[4] Ge, J. Instrum. 18, (2023)
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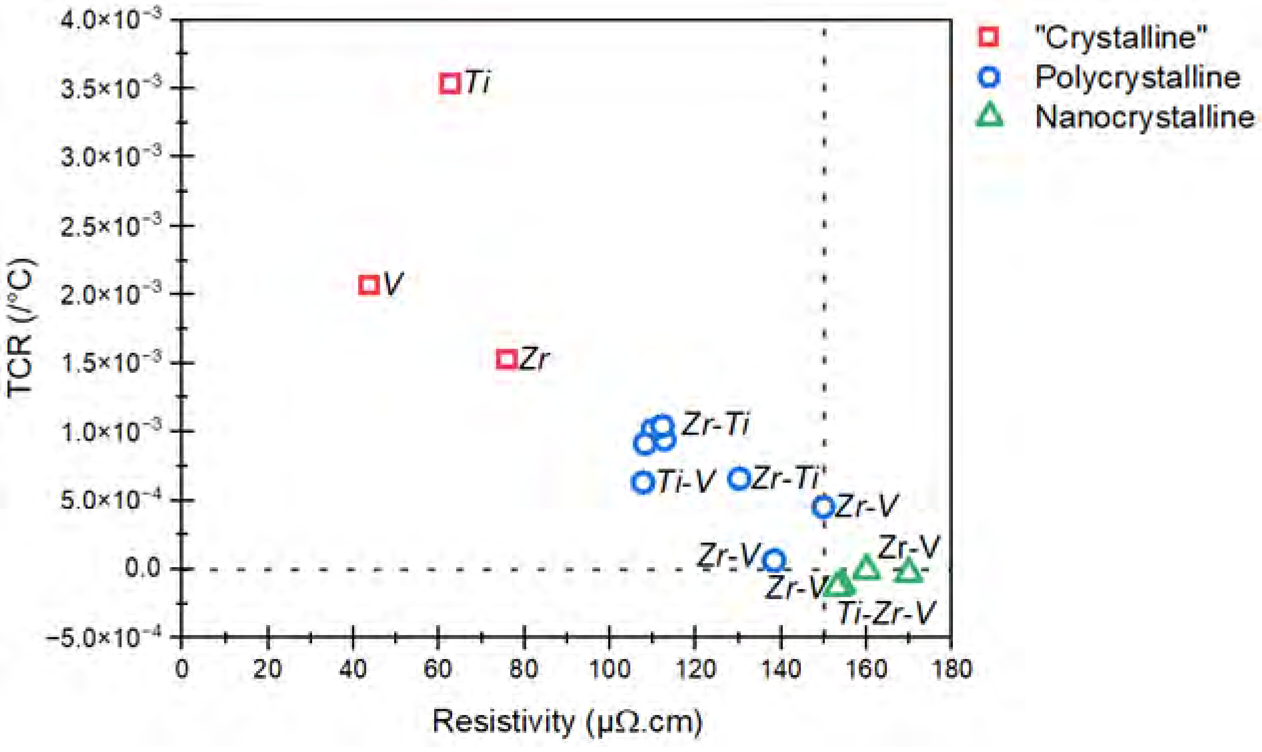

Excitation, suppression and generation of spokes in direct current magnetron sputtering discharges

Martin Rudolph[1], Wahyu Diyatmika[1], Oliver Rattunde[2], Edmund Schuengel[2], Dmitry Kalanov[1], Jörg Patscheider[2], André Anders[1,3]
[1]Leibniz Institute of Surface Engineering (IOM), Germany, [2]Evatec AG, Germany, [3]Leipzig University, Germany

Plasma Science, June 18, 2024, 16:00 - 17:30

A magnetron sputtering discharge is a source of metal atoms and ions that is used for the fabrication of thin films. The discharge belongs to the class of E x B discharges in which electrons perform a closed drift. Its projection onto the cathode is called racetrack. At typical operating conditions spokes can be observed that propagate along the racetrack. They are zones of high electron energy and consequently high metal and gas atom ionization. Their excitation results from a positive feedback mechanism initiated by a positive space charge fluctuation, which energizes drifting electrons. Electron impact ionization of atoms at this location produces additional electron-ion pairs which are rapidly separated by the electron drift. As a result, the positive space charge amplifies into a spoke instability. In this contribution we show how to manipulate the electron drift current by introducing steps in the magnetic field strength along the racetrack. We use a 300 mm diameter aluminum cathode, that we image using gated cameras during operation. At a strong-to-weak magnetic field step, we observe the excitation of intense spokes. We explain this observation by an accelerating electron drift at this location. The positive space charge created in that way acts as a seed that rapidly develops into an intense spoke. At the weak-to-strong magnetic field step, we observe a broad emission peak just after the transition, caused by the deceleration of electrons. Latter effect is known from rectangular magnetrons as a ‘cross-corner effect’. The observed effect is similar to a cross-corner effect known from rectangular magnetrons and we confirm here that this effect is primarily due to the change in the magnetic field strength and not caused by the geometry of the racetrack. The results may open up the possibility for ‘racetrack engineering’ in the future to fine adjust deposition processes for tailored thin films.

Scanning probe microscopy as a tool for nano-optical measurements

Pablo Merino[2], Martin Švec[1]
[1] Institute Of Physics, Czech Academy Of Sciences, Czech Republic, [2] Icmm, Spain

MS-2: Light-matter Interaction at Atomic Scales, June 17, 2024, 16:00 - 17:35

Exploration of essential photophysics at the level of individual molecules and atoms requires highly specialized optical spectroscopies. One of the working approaches is the use plasmonic nanostructures - in order to overcome the fundamental resolution limits achievable with visible and infrared light. Recent developments emerging in the field of Scanning Probe Microscopy (SPM) bring the unique opportunity to pursue intriguing, often hard-to-access interactions between light and matter with plasmonic tips at submolecular scale. The modes of operation can be switched between the electroluminescence, photoluminescence and tip-enhanced Raman spectroscopies, and applied to probe the eigenmodes, charges, vibronics and temporal evolution of the transient states in molecular emitters at nanoscopic scales.

[1] Nano Lett. 19, 8605-861 (2019)
[2] ACS Nano 15, 7694–7699 (2021)
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[4] Nature Comm. 13, 6008 (2022)
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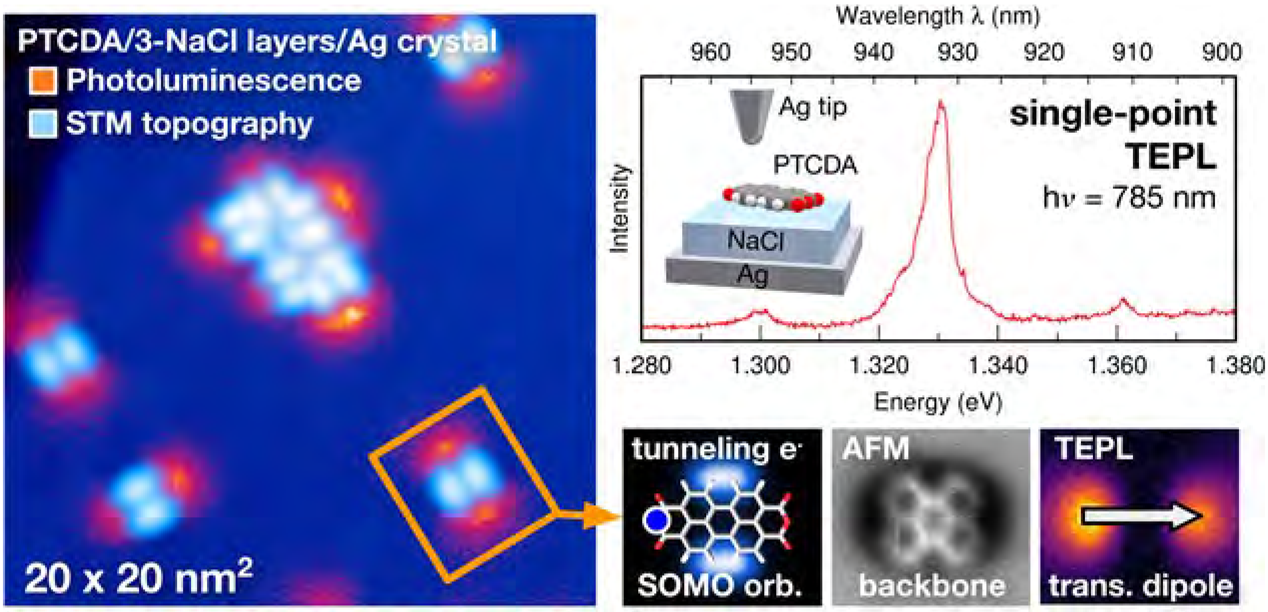


Computational prediction of interfaces between transition metal surfaces and two-dimensional MoS2

Dr Viktor Zolyomi[1], **Lara Kabalan**[1]
[1] STFC Hartree Centre, United Kingdom

2D Materials and Van der Waals heterostructures 1, June 19, 2024, 14:00 - 15:30

Transition metal dichalcogenides, such as MoS2, are layered van der Waals crystals naturally suited for exfoliation into thin films and two-dimensional crystals. They're used in a range of applications from sensing to optoelectronics. An ongoing challenge related to the application of these materials in nanoscale electronics, as well as corrosion protection of metal surfaces, is the lack of understanding of their electrochemistry on metal surfaces. In this work we investigate the binding energy and density of states of monolayer MoS2 on a series of transition metal surfaces (Ag, Au, Cu, Pd, Pt, Ti) in order to understand the strength of the interaction between the MoS2 and the underlying substrate. A correlation is demonstrated between the binding energy and the mean distance of the MoS2 from the substrate. Particularly strong interaction is identified in the case of the Ti surface, suggesting that MoS2 can be used as an effective ultrathin coating layer on Ti surfaces.

Timing the Escape of a Caged Electron

Connor Fields[1], Filipe Junqueira[1], Dr. Aleksandra Foerster[2], Dr. Sadegh Ghaderzadeh[2], Dr. Yitao Wang[1], Dr. Tyler James[1], Sofia Alonso Perez[1], Ilya Popov[2], Dr. David A Duncan[4], David McCue[4], Tien-Lin Lee[4], Sally Bloodworth[3], Gabriela Hoffman[3], Mark Walkey[3], Prof Richard J. Whitby[3], Malcolm J Levitt[3], Dr Brian Kiraly[1], Dr. James N O'Shea[1], Prof. Elena Besley[2], Philip Moriarty[1]

[1]School of Physics and Astronomy, University Of Nottingham, United Kingdom, [2]School of Chemistry, University of Nottingham, United Kingdom, [3]School of Chemistry, University of Southampton, United Kingdom, [4]Diamond Light Source, United Kingdom

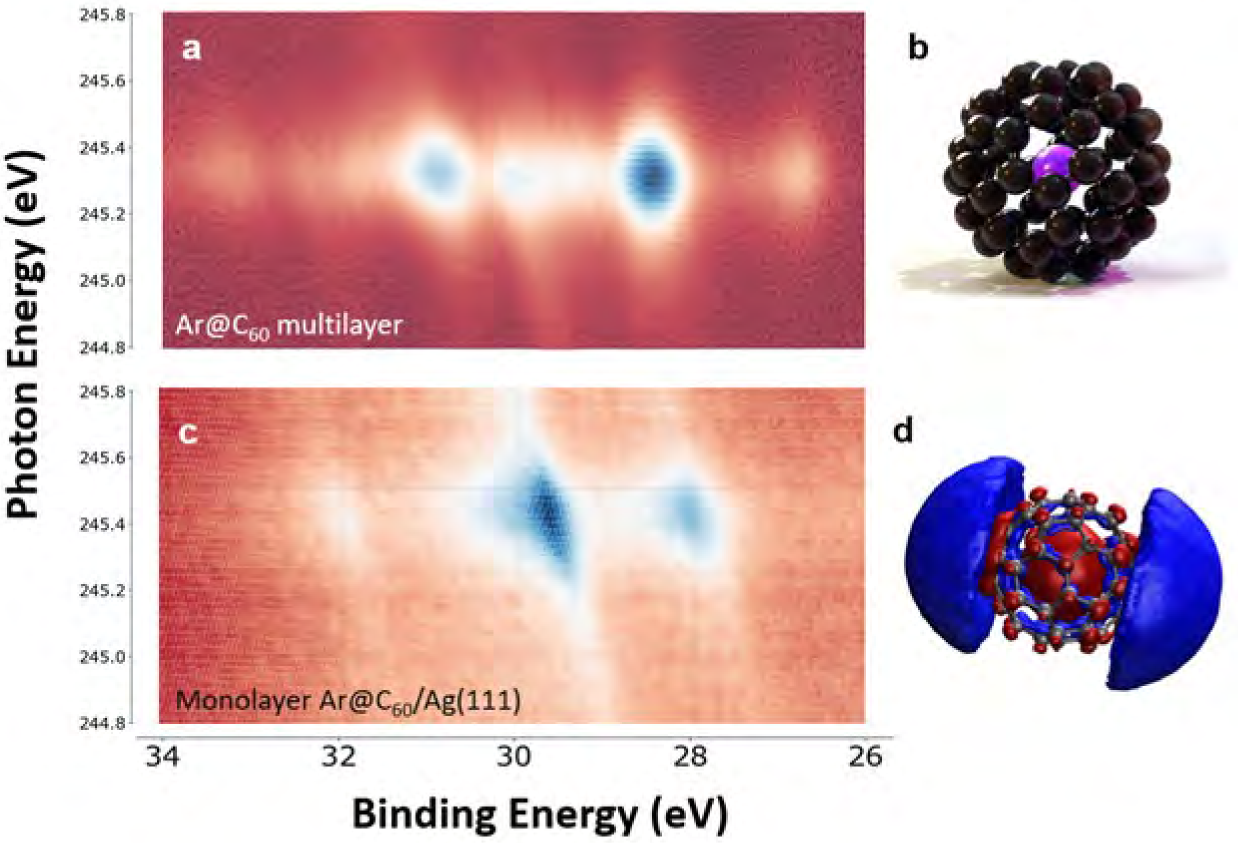
Carbon Materials 2, June 19, 2024, 10:30 - 12:35

Charge transfer in molecular and nanostructured systems is fundamentally dependent on the overlap of the orbitals comprising the transport pathway. In the limit of negligible mixing, electron transfer is severely restricted. This has key implications for molecular, nanoscale, and quantum technology architectures, for which delocalization (and decoherence) rates are essential figures of merit.

Here, we apply the core hole clock technique -- a synchrotron-based, energy-domain variant of ultrafast spectroscopy (Fig. 1(a),(c)) -- to measure the delocalization time of a photoexcited electron isolated inside a molecular cage, namely the Ar 2p5 4s state of Ar@C60 (Fig. 1(b)). De-excitation spectra have been acquired in the resonant Raman mode, where the photon energy bandwidth is significantly smaller -- in this case, ~ an order of magnitude smaller -- than the natural lifetime of the core-excited state. Moreover, for the case of an Ar@C60 monolayer on Ag(111), we have combined the resonant Auger measurements with X-ray standing wave analysis of the position of the Ar atom inside the fullerene cage, enabling the first direct correlation of adsorbate geometry with electron delocalization rate.

Despite the lack of C60-Ar hybridisation in the ground electronic configuration, coupling of the excited Ar state with the diffuse superatom orbitals of the fullerene is so strong that ~ 50% of the Ar 4s density is found outside the buckyball (Fig. 1(d)). This provides a novel, unexpected, and facile escape route for the incarcerated electron.

Figure caption: Fig. 1. (a) Resonant Auger map for a bulk film of Ar@C60 showing the presence of both traditional and spectator Auger decay; (b) artist's impression of the Ar@C60 molecule; (c) Auger map for an Ar@C60 monolayer on Ag(111) -- the spectator deexcitation channel is now entirely absent; (d) time-dependent density functional theory calculation of core-excited Ar 4s state (i.e. in presence of core-hole.)


a
Ar@C60 multilayer
b
c
Monolayer Ar@C60/Ag(111)
d
Photon Energy (eV)
245.8
245.6
245.4
245.2
245.0
244.8
34
32
30
28
26
Binding Energy (eV)

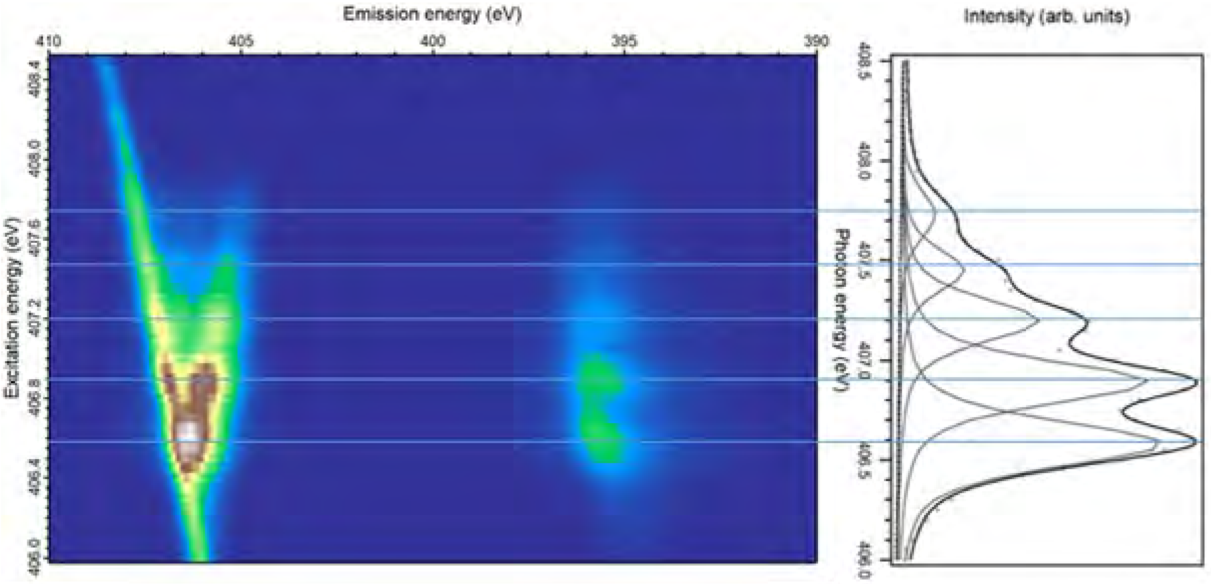
Vibronic coupling in N2@C60: A gas phase-solid state hybrid

Connor Fields[1], Yitao Wang[1], Filipe Junqueira[1], Aleksandra Foerster[2], Gabriela Hoffman[3], Mark C Walkey[3], Elizabeth S Marsden[3], Richard J Whitby[3], Malcolm J Levitt[3], David A Duncan[4], David McCue[4], Tien-Lin Lee[4], Victor Poree[5], Alessandro Nicolaou[5], Brian Kiraly[1], Elena Besley[2], James N O'Shea[1], Philip Moriarty[1]
[1]School of Physics and Astronomy, University of Nottingham, United Kingdom, [2]School of Chemistry, University of Nottingham, United Kingdom, [3]School of Chemistry, University of Southampton, , United Kingdom, [4]Diamond Light Source, , United Kingdom, [5]Synchrotron SOLEIL, France

Functional Coatings 2 and Superconducting Thin Films, June 17, 2024, 16:00 - 17:35

Endohedral fullerenes, in which an atom or molecule is incarcerated within a buckyball, represent a fascinating and exotic state of matter: the properties of the encapsulated species often retain gas phase character despite their embedding in a solid state matrix. This novel supramolecular system is particularly fascinating in the context of vibronic interactions, i.e. the coupling of electronic and vibrational wavefunctions.

We have used N K edge X-ray absorption and resonant photoemission/resonant Auger spectroscopy at Beamline I09 of the Diamond Light Source, combined with resonant inelastic X-ray scattering (RIXS) at the SEXTANTS beamline at SOLEIL, to probe the vibrational structure and vibronic coupling of the nitrogen molecule in N2@C60 (recently synthesised for the first time by molecular surgery in Whitby's group (University of Southampton)). Remarkably, the N K edge X-ray absorption spectrum (Fig. 1) for a bulk film of the endofullerene is not only as highly resolved as the gas phase spectrum, but there is a clear shift in the spacing of higher vibrational levels as compared to their gas phase counterparts, due to the greater degree of anharmonicity of the N-N potential within the fullerene. Dissipation of vibrational energy on the time-scale of the N 1s core-hole lifetime causes the resonant photoemission participator peak to disperse with constant kinetic energy, rather than constant binding energy. We shall discuss the implications of our results for the influence of vibronic coupling on electron transfer rates in endofullerenes.



Unlocking the Mysteries of Process Gases: Insights from Mass Spectrometry"

Mr Florian Heck, Mr Laurent Ducimetiere
[1]Pfeiffer Vacuum Sas, France, [2]Pfeiffer Vacuum GmbH, Germany

MS-6: RGA User Meeting 2, June 19, 2024, 14:00 - 15:30

Gas composition analysis plays a pivotal role across diverse fields of research and industries, facilitating a deeper understanding of processes, ensuring quality control, and optimizing efficiency. In this context, mass spectrometry emerges as a versatile and indispensable tool.

This presentation aims to explore the application of mass spectrometry in the following key areas:

- Providing a comprehensive understanding of process technology by elucidating the composition of process gases
- Ensuring continuous process reliability and security through real-time monitoring and data analysis
- Optimizing resource utilization and time efficiency by identifying opportunities for process optimization based on gas composition data

Attendees can expect to gain valuable insights into the methodologies and techniques employed for deciphering unknown gas mixtures through residual gas analysis, thereby highlighting the critical role of mass spectrometry in enhancing operational performance and driving innovation across various applications.

Poster Presentations

Pillow seal vacuum joints for the target area of the Super-FRS at FAIR

Dr. Neeraj Kurichiyanil[1], Mr. Christos Karagiannis[1], Dr. Helmut Weick[1], Mr. Karl Heinz Behr[1]
[1]GSI Helmholtz Centre for Heavy Ion Research, Germany

Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Superconducting Fragment Separator (Super-FRS) at the upcoming Facility for Antiproton and Ion Research (FAIR) is a large acceptance magnetic separator for production of rare isotopes and other secondary beams. The target area of Super-FRS, where the fragments are produced, is a sealed-off area due to high radiation background at the levels in which typical non-metallic vacuum components and joints would immediately fail and the level of activation will not permit any hands-on work on any vacuum seals. Nonetheless, as the about 30 meter long section is build from individual chambers, a replacement possibility in case of failure must be included. Moreover, the intense beam must not hit a chamber wall directly, and the secondary beams from the target require a large acceptance and different shapes of large apertures of the vacuum connections.

Pillow seal vacuum joints, featuring a double vacuum-groove design with separated pressure lines for the bellows and the sealing surfaces, in circular as well as in race-track shapes are developed and tested for the application in this area. Preliminary tests indicate a Helium leak-tighness better than 5e-8 mbar.l/s at inflation pressures up to 2 bar, satisfying the vacuum requirements of Super-FRS Target area. The design of these pillow seals including their insertion mechanism for remote handling is presented along with the vacuum test results on dedicated test bench.

Special and standard vacuum solutions at the Super-FRS at FAIR

Dr. Neeraj Kurichiyanil[1], Mr. Alexander Bergmann[1], Dr. Andreas Kraemer[1], Dr. Sivaji Purushothaman[1], Dr. Martin Winkler[1], Robin Juergen Similon[1]

[1]GSI Helmholtz Centre for Heavy Ion Research, Germany

Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

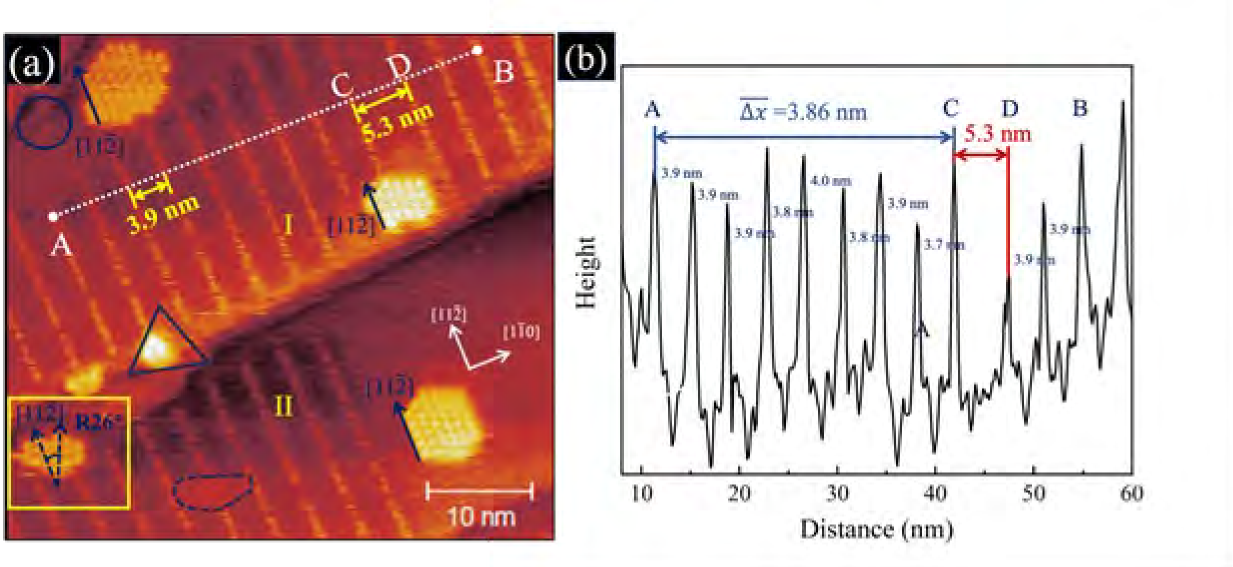
The Facility for Antiproton and Ion Research (FAIR), currently under construction in Darmstadt, will operate a large-acceptance Superconducting Fragment Separator (Super-FRS) for in-flight production and separation of exotic beams. This large aperture (DN400) un-bakeable single-pass machine presents unique challenges in its vacuum system design. In particular, beam-vacuum and insulation-vacuum components in high radiation areas should be radiation hard as well as foresee remote-handling, self-sealing vacuum joints and inserts must guarantee acceptable leak rates and out gassing, certain magnet vacuum chambers must be able to withstand beam losses, and the vacuum installations in the experimental areas along the beamline must take into account on-demand modifications tailored to the experiments. An overview of Super-FRS beam- and insulation-vacuum layout and design challenges along with details of conventional and special vacuum solutions applied for the Early Science stage of Super-FRS, is presented.

Cooperative Self-assembly of C60 and Decanethiol on Au(111)

Ying Gao[1], Dr. Quanmin Guo
[1]Univesity of Birmingham, United Kingdom

Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Self-assembled monolayers from organic molecules have been researched for many years motivated by their diverse potential uses, such as in organic molecular devices, solar cells, and sensors. What's more, organic molecular self-assembly can be used to create molecular templates for nanomaterial fabrication. Designing and controlling the supramolecular self-assembly architectures of materials at a few nanometers scale face many challenges. Thiol molecules can form several structural phases on the Au(111) surface. So far work has been performed with the δ phase of decanethiol (DT). Here, I report my work conducted with the lower coverage β phase of DT. The results show that with the low coverage of DT molecules, most C60 molecules formed closed-packed islands on the surface. Only a few areas with the disordered phase which we suspect is the cooperation result of DT molecules and C60 self-assembled themselves to stabilise at the surface via Var der Waals.

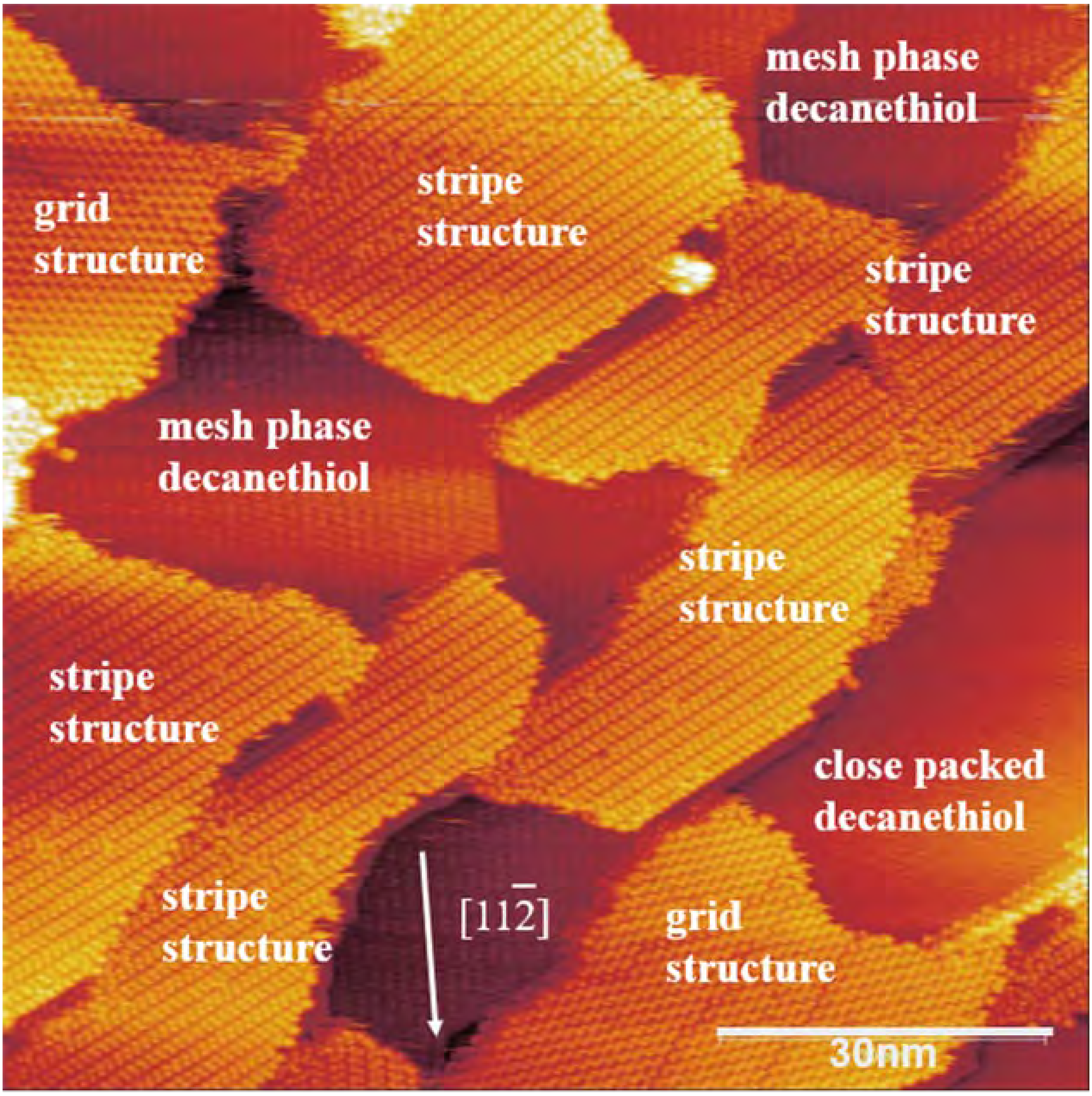


C70 Fullerene Self-Assembled Frameworks on Decanethiol/Au(111) Surface

Bosheng Li[1], Dr. Quanmin Guo[1]
[1] *School of Physics and Astronomy, University of Birmingham, Birmingham*

Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

In recent studies, complex supramolecular frameworks of C60 fullerene and octanethiol have been observed. Here we extend our study by replacing C60 with C70 fullerene. Firstly, a monolayer of decanethiol molecules were grown on Au(111) surface. A gentle thermal annealing of the monolayer in ultra high vacuum created the delta phase decanethiol. C70 molecules were then deposited onto the decanethiol/Au(111) at room temperature (295K). Low temperature scanning tunnelling microscope (LT-STM) was used to image the sample. Imaging was conducted at room temperature (295K) and LN2 temperature (77K). We found two types of C70/DT frameworks: i) the stripe structure and ii) the grid structure. The characteristics of these structures are mainly introduced.



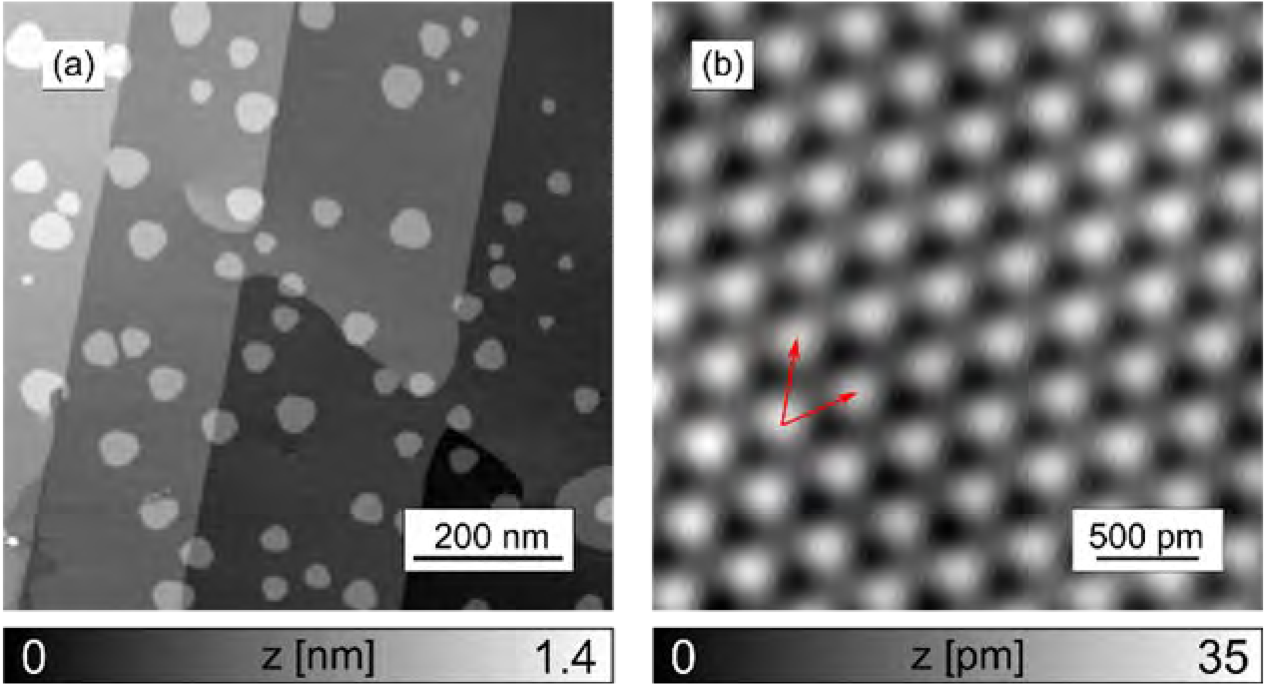
Mapping Electrostatic Potential on monolayer MnI2 islands

Daniel Rothhardt[1,2,3], Christopher Penschke[4], Peter Saalfrank[4], Regina Hoffmann-Vogel[3], Hans Hug[1,2], Amina Kimouche[3]

[1]Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, [2]Department of Physics, University of Basel, Switzerland, [3]Institute of Physics and Astronomy, University of Potsdam, Germany, [4]Institute of Chemestry, University of Potsdam, Germany

Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

There has been a growing interest in exploring two-dimensional (2D) materials beyond graphene. The introduction of a variety of atomically thin van der Waals crystals has inspired efforts to not only explore the electronic order but also to investigate the growth mechanism in these crystals. Here, we study the epitaxial growth of manganese iodide (MnI_2) on a Ag(111) single crystal. Two dimensional MnI_2 islands tend to grow on a specific buffer layer giving rise to the formation of twin domains rotated by 60°. We employ frequency-modulated (FM) scanning force microscopy in the non-contact mode, combined with FM-Kelvin probe microscopy (KPFM) and scanning tunnelling microscopy to investigate the electronic and topographic fingerprints of MnI_2 on Ag(111). The surface morphology undergoes a significant change under different evaporation conditions, which lead to an island shape transition and a more homogeneous growth mode. Occasionally, various phases have been formed giving rise to a reach variety of electronic structures as revealed by KPFM.



Status Vacuum System Design of IFMIF DONES

César Caballero Pérez[1], Marcelo Juni Ferreira[2], Volker Hauer[3], Anderson Sabogal[1], Daniel Sánchez-Herranz[1], Claudio Torregrosa[1]
[1]IFMIF/DONES, Spain, [2]ESS, Sweden, [3]KIT, Germany

Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

The International Fusion Materials Irradiation Facility-DEMO Oriented Neutron Source (IFMIF-DONES) will be an installation able to qualify materials to be used in future fusion power reactors. A linear accelerator will deliver high intensity deuterons to a liquid Li loop, which will create a flow of neutrons producing equivalent material damage to the expected in a fusion reactor. The Vacuum system must be capable of maintaining high vacuum conditions during operation with a high reliability. For this reason, a careful study of the vacuum has been assessed and implemented in the different sections of the accelerator; vacuum simulations are being performed to have a first estimation of the expected pressure profile; documentation to provide a good standardization of the subsystem is being produced; and the valuable knowledge from the prototype installation, IFMIF/Engineering Design and Engineering Validation Activities (EVEDA), is being taking into consideration in the engineering design activities. Additionally, two vacuum-related prototypes are being manufactured; the Multipurpose Vacuum Accident Scenarios (MUVACAS) prototype will provide the capability to perform experimental studies of air inrush in the last section of the accelerator; and the Quick Disconnecting System (QDS) prototype is developed to study the feasibility of remote handling of interfaces located between accelerator beam line and target chamber. The purpose is to show the design status of the accelerator vacuum subsystem along with the future challenges to tackle in the coming years.

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Size-controlled Cobalt Clusters trapped by a C60 template

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

In this study, the scanning tunnelling microscopy (STM) was used to investigate the capability of C60 templates in controlling the distribution and localization of single cobalt atoms or cobalt clusters at the nanoscale. The C60 template is in the form of a closed-packed monolayer and/or multilayer supported by a graphite substrate. The cobalt atoms from the evaporator seem to follow mostly a land-and-stick route with very limited lateral diffusion. Co atoms or small Co clusters are found to occupy the interstitial site within the C60 layers. Therefore, the C60 layers provide some guiding effect on the location of trapped atoms/clusters. The limited volume associated with the interstitial site prevents the formation of large clusters. The charge-transfer between cobalt and C60 molecules was then revealed by the dim and bright features in the STM images. The effectiveness of C60 template in directing the formation of size-controlled cobalt clusters was thus demonstrated at the atomic level. The cobalt-doped C60 networks were stable even after annealing the sample at a temperature much higher than that required for C60 desorption.

Size-controlled Cobalt Clusters trapped by a C_{60} template

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Introduction

Closed-packed C_{60} layers deposited on graphite (HOPG) are used as templates to trap cobalt atoms at room temperature in UHV. Thermally evaporated Co atoms are found to occupy the interstitials of the C_{60} layer. The smallest distance between the nearest neighbor Co atoms/clusters is around 1.75 nm. This growth method is potentially useful for making two-dimensional arrays of magnetic dots. It is not clear whether trapped Co exists as individual atoms in the form of small metal clusters.

Methodology

The HOPG substrate was cleaved in the air and degassed at 650 K in the UHV chamber for 1 hour. The vacuum condition was better than 10^{-9} mbar during STM scanning. The C_{60} molecules were deposited onto the HOPG surface and self-assembled into close-packed islands. The cobalt evaporation source was heated up to 1300 degrees and degassed thoroughly before deposition. The C_{60} molecules were deposited on the HOPG at the rate of 0.1ML/min. The STM imaging process was conducted at room temperature.

Results

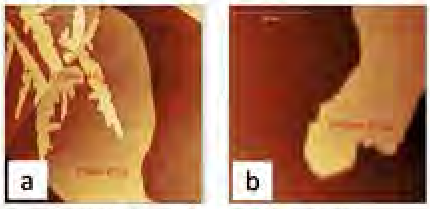

Figure 1. Large-scale (a) and local-scale (b) STM images of C_{60} layers on graphite.

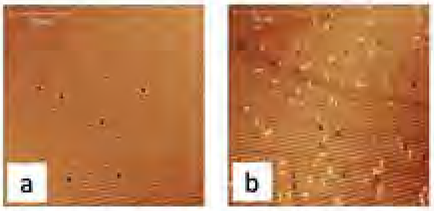

Figure 2. The first layer of the C_{60} template before (a) and after (b) the deposition of 0.025ML cobalt atoms (two images are from different areas)

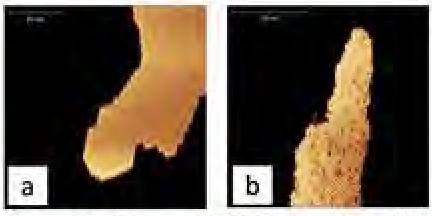

Figure 3. The second layer of the C_{60} template before (a) and after (b) the deposition of 0.025ML cobalt atoms (two images are from different areas)

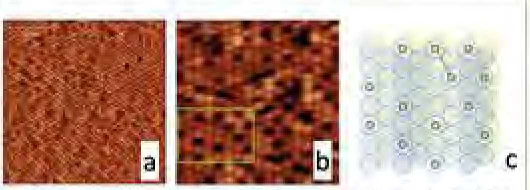

Figure 4. (a) STM images of the second layer C_{60} molecules following the deposition of 0.2 ML Co; (b) The second layer C_{60} molecules following the deposition of 0.2 ML Co and then were annealed at 650 K for 1 hour; (c) the schematic diagram corresponding to the rectangular area in (b). (The yellow circle represents a C_{60} molecule of the 1st layer; the blue circle represents a C_{60} molecule of the 2nd layer; the black circle indicate a possible location of Co between the 1st and 2nd layer of C_{60} corresponding to the dim C_{60} in (b); the red line marks the shortest distance of 1.73 nm between dim C_{60} molecules.)

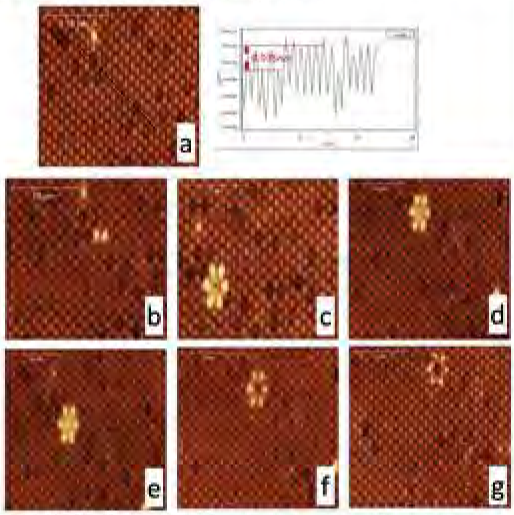

Figure 5. (a)-(c) STM images show the formation of a six-membered flower structure within the second layer of C_{60} during the continuous scanning process. I=600pA, U_{bias}=1.8V. The height profile measured along the black line in (a) shows a 0.035nm difference in the height of "dim" C_{60} compared with the normal one. (d)-(g) STM images of C_{60} molecules within the second layer under different bias voltages. (d) U_{bias}=2.1V, I=500pA (e) U_{bias}=1.9V, I=500pA (f) U_{bias}=1.7V, I=500pA (g) U_{bias}=1.5V, I=500pA. The bias-dependent behaviour suggests that the bright-dim contrast has an electronic origin. It is likely due to charge transfer between C_{60} and Co atoms.

Summary

The monolayer or bilayer C_{60} template was solely constructed by thermal-evaporating C_{60} molecules onto the graphite substrate with around 1.5 ML coverage. It has been studied that the interstitial sites within the layered C_{60} template give gold atoms chances to penetrate down to the bottom of the C_{60} monolayer and facilitate the formation of size- and shape-selected two-dimensional gold clusters on graphite.[1] In this research, a modified C_{60} network was synthesized after depositing cobalt atoms on the C_{60} layers, and the interaction between the cobalt atom and the C_{60} molecule was observed by the scanning tunneling microscope (STM). It appears that Co takes almost a land-and-stick route at RT. After annealing, the cobalt-C60 complex exhibited a self-regulated pattern in the STM images. The next step is to determine the structure of the trapped Co and find the number of Co atoms beneath each "dim" C60.

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Far- to middle-infrared absorption spectra of multi-layer graphene: DFT study

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Far- to middle-infrared (FIR/MIR) absorbances of multi-layer graphenes are theoretically investigated based on the density functional theory. We constructed two types of double-layer graphenes (DLGs) with (1x1) periodicity: AA and AB stackings, three types of triple-layer graphenes (TLGs) with (1x1) periodicity: AAA, ABA, and ABC stackings, and three types of twisted double layer graphenes, which are models of random stacking graphenes (RSGs).

We found that the absorbance spectra as a function of photon frequency, A(ω), are strongly dependent on the stacking structures and number of graphene layers (GLs) and are well understood based on the band structures and the selection rule for optical transition. AA-type multi-layer graphenes like AA-DLG and AAA-TLG have displaced Dirac cones (DDCs) whose Dirac points are shifted from the fermi level. A(ω)s are multi-step functions characterized with A(ω) of single-layer graphene (SLG) (~0.023). It does not exceed the product of A(ω) of SLG and the number of GLs. RSGs have almost degenerated Dirac-cone (DC) like bands. A(ω)s are almost twice of A(ω) of SLG, suggesting that large number of GLs are needed for large absorbance. For other systems like AB-DLG, ABA- and ABC-TLGs, electronic bands are parabolic near the K point and linear far from the K point. A(ω) has peaks at the energy corresponding to the vertices of parabolic band and are close to multiples of A(ω) of SLG in a linear-band region. Some of the peaks are more than ten times the A(ω) of SLG in spite of small number of GLs, indicating that they would be good FIR/MIR absorbance materials for some ω regions.

This work was supported by Innovative Science and Technology Initiative for Security Grant Number JPJ004596, ATLA, Japan. The calculations were performed by using the Numerical Materials Simulator of NIMS and the Earth Simulator (ES) of JAMSTEC.

Resistive switching behaviors through structural change of CoOx and CuxO films deposited by magnetron sputtering

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

We have studied the resistive switching behaviors of CoOx and CuxO films with structural changes by a post-thermal annealing process. These films deposited by RF magnetron sputtering were changed their structural phases by selection of ambient gases during post-thermal annealing at 300~700 °C. The resistive random-access memory (ReRAM) structures of Ti/Au/CoOx/p+-Si were fabricated with CoO or Co_3O_4 films by thermal annealing at 700 °C under N_2 and O_2 atmosphere, respectively. The ReRAM characteristics of the CoO device appeared much better than that of the Co_3O_4 device, also showing good uniformity from a cumulative probability distribution, long non-volatile retention of 10^4 s, good endurance of ~100 cycles, and excellent current ratio of 10^4. And the ReRAM properties appeared also in CuO-based devices, while Cu_2O ReRAM devices were not shown. Especially, CuO ReRAM device annealed at 500 °C showed the best properties with a resistive window of 8×10^2, good switching endurance of ~100 cycles, data retention for 10^4 s, and stable uniformity in the cumulative probability distribution. These results demonstrate the method to provide stable and good resistive switching properties of CoO and CuO films, which can be easily obtained through thermal annealing below 700 °C of CoOx and CuxO films.

Methodology for procedures for the detection of naturally occurring asbestos in soil sediments

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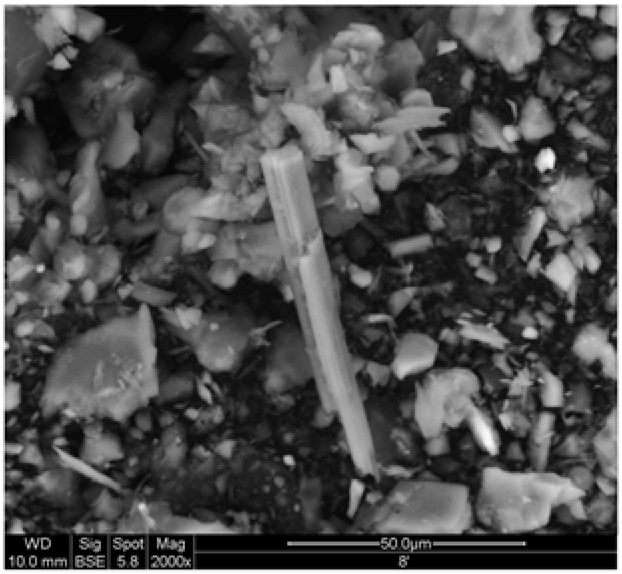
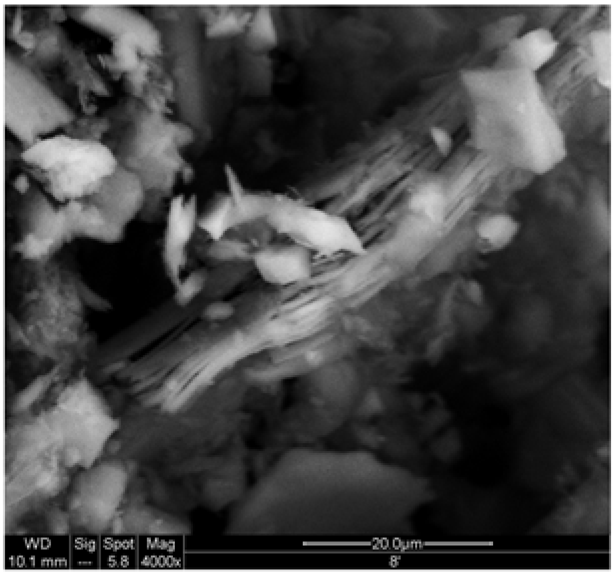
Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Asbestos is a group of natural silicates with an extremely long fibrous structure that is virtually infinitely cleavable. This material has exceptional properties and has been used for decades mainly in the construction industry. Its use dates back to BC. However, according to the International Health Organization (WHO), all types of fibrous asbestos are currently registered as proven human carcinogens. This is because it is a carcinogenic substance with mutagenic effects that poses a risk to the human body. There is a growing need for in-depth experimental research activities aimed specifically at monitoring and investigating the specific properties of naturally occurring asbestos and understanding the origin and biological effects of asbestos on the environment and subsequently on humans.

Global organizations are still trying to find and propose an overall policy to address the issue of exposure to industrial or natural fibrous dusts in the environment, which would include the following procedures: how to measure (concentration of fibres, their specific types), where to measure (to identify the locations of the most exposed areas), what measures to implement to reduce the concentration, and what legislation is needed to reduce the concentration of asbestos fibres and other fibrous structures in the environment.

The aim of the thesis is to summarise the current knowledge concerning the large-scale problem of asbestos occurrence in general and in the Pilsen region in the Czech Republic, to determine the appropriate methodology for detecting the presence of naturally occurring asbestos in soil sediments in a given locality based on experimental analyses motivated by analyses in other countries and to determine precisely the different types of asbestos from a series of samples.





On detailed characterization of annealed PECVD silicon oxynitride thin films: growth of nanocrystals

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Silicon oxynitride thin films have been studied and used in microelectronics and optoelectronics due to the possibility of controlling their optical, electrical and microstructural properties by changing the chemical composition and post-deposition annealing treatments. In this paper, the effect of high temperature annealing on microstructural and mechanical changes and crystallization process has been investigated for the annealed hydrogenated amorphous silicon oxynitride thin films. These a-SiOxNy:H films with excellent surface morphology were deposited on different substrates by a PECVD technique at low substrate temperature using a low-pressure N2O-SiH4-Ar gas mixture. It was observed that the films grown at R=N2O/SiH4=1 turned out to be silicon oxynitride Si-O-N films. Subsequently, all the as-deposited films were annealed at different temperatures up to 1100 °C in air ambition and subjected to physicochemical characterization. The influence of the post-deposition high temperature annealing treatment on the compositional (EDX, AES), morphological (SEM, profiler) and microstructural (TEM, XRD, Raman microscopy) properties, chemical bond configuration (FT-IR spectroscopy) and mechanical (nanoindentation) properties of these films were investigated and the experimental results are presented and discussed. High deposition rate (~60 nm/min), good hardness (around 13 GPa), low residual compressive stress (down to 0.3 GPa) of as-deposited amorphous films were obtained. Above 1000°C, transmission electron microscopy analysis showed that silicon nanocrystals (Si NCs) with an average radius between 3 and 9 nm were present in the annealed films. Annealed samples at these temperatures showed the c-Si diffraction peaks, which became narrower with increasing temperature. From the width of the Si (111) peaks, the average size of the Si-ncs and their dependence on temperature were determined and compared with those obtained from TEM measurements. XRD, Raman and transmission electron microscopy confirmed the phase separation and the formation of Si NCs in the films, and these experimental results are presented and discussed.

Spin effect in surface reactions by atomic hydrogen on Ni(111)

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Internal degrees of freedom in molecules such as vibration and rotation, play an important role in chemical reactions at surfaces. Atomic hydrogen (H) consists of an electron and a proton, each having spin 1/2. As the simplest molecule, the adsorption of H on surfaces is regarded as a proto-type reaction in surface chemistry, which has been extensively studied on various surfaces to date [1]. However, the role of the spin degree of freedom of H still remains unclear. Using a spin polarized atomic hydrogen beam [2], the spin effect in H adsorption and abstraction reactions on Ni(111) is studied. The results indicate that, the H reactivity is higher when its spin is oriented parallel to the surface spin direction of the Ni(111) compared with its spin direction is perpendicular to the surface.

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Formation of Fe nanoparticles on SrTiO3 (001)

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

The perovskite ceramic strontium titanate ($SrTiO_3$ or STO) presents remarkable properties that make it very promising for catalytic, photocatalytic, electronic, magnetic, spintronic, and biomedical applications. Stoichiometric $SrTiO_3$ is a transparent insulator with a 3.2 eV band gap, but doping $SrTiO_3$ with Nb can result in n-type semiconductor, or in a high-mobility metal, or even in a superconductor. The bulk $SrTiO_3$ crystal consists of alternating TiO_2 and SrO layers along the (001) direction, and an ideal (001) surface can be terminated by either of these two layers [1]. The deposition of Fe on $SrTiO_3$ (001) can provide Fe nanoparticles with various applications in the healthcare sector, such as nanoparticles serving as contrast agents in magnetic resonance imaging or in targeted magnetic therapy for cancer treatment. However, to further investigate these applications, it is necessary to perform adequate characterization of the properties and structures of the nanoparticles and substrates involved. Additionally, $SrTiO_3$ has also been investigated in several biomedical applications, with a good example being its use as a biomaterial in orthopedic and dental implants, due to its biocompatible properties. Therefore, combining the surface of $SrTiO_3$ with iron deposition allows for the exploration of a range of potential applications in healthcare. X-ray photoelectron diffraction (XPD) and low energy electron diffraction (LEED) have been successfully used for determination of different $SrTiO_3$ (001) surface structures [1]. This work deals with the investigation of the formation and structural characterization of Fe nanoparticles deposited on a Nb-doped $SrTiO_3$ (001) surface. The comparison between experimental and theoretical XPD involving multiple scattering calculations indicates the possibility of both TiO_2 and SrO terminations.

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Atomic interaction of titanium and titanium compounds surfaces with liquid sodium

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

The compatibility (wettability) of component materials with liquid sodium is one of the most important characteristics for efficient and safe utilization of liquid sodium in plants such as sodium-cooled fast reactor (SFR). In this study, atomic interactions at the interface between substrate materials (Titanium, Titanium oxide, or Titanium fluoride) and liquid sodium was investigated using the DV-Xα cluster method, one of the molecular orbital methods. And the difference in wettability was discussed from the calculation results. Although stainless steel is mainly used for the SFR, in this study, titanium materials are selected on substrate materials as fundamental research.

Interface models between substrate materials and sodium were constructed as shown in Fig. 1(a). Bond order obtained from calculation is an indicator for strength of covalent bond at the interface.

It has been found in previous our studies that the bond order ratio to the ratio of bond order between substrate material atoms and sodium atoms and between the substrate material atoms is correlated with contact angle which is indicator of wettability. [1] The larger the bond order ratio, the better the wettability. Figure 1 (b) shows the bond order ratio of each interface model. The bond order ratio for TiF_2 is the biggest among them, and decreases in the order of TiO_2 and titanium metal. It is 2.4 times larger than that of metallic titanium. From that reason, it can be speculated that TiF_2 has better sodium wettability than metallic titanium.

It is identified from this study that the atomic interaction at the interface with sodium changes significantly depending on the substrate material. It is also found that the wettability of the substrate material and liquid sodium can be inferred in viewpoint of the atomic interaction at the interface.

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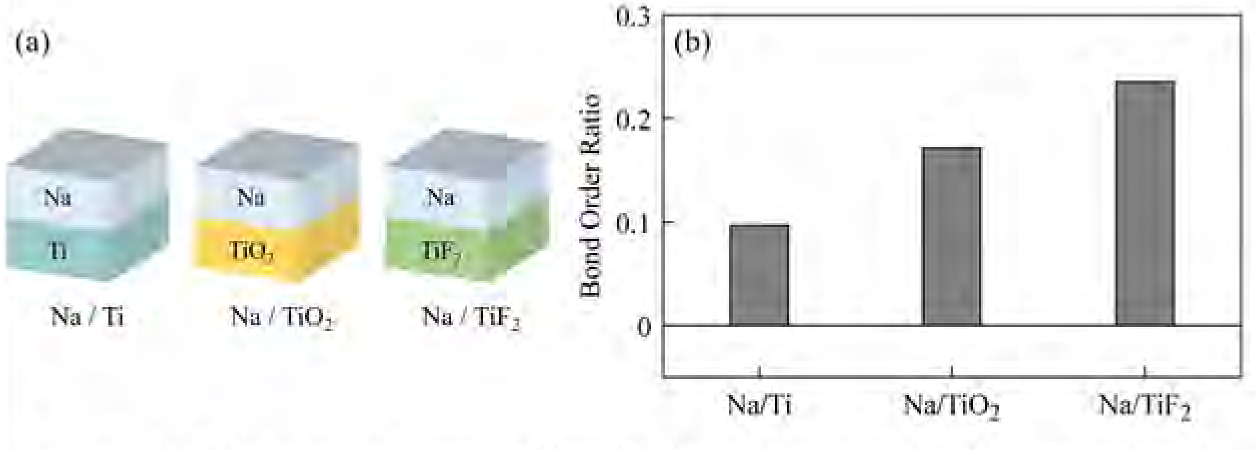

Figure 1. (a): The schematic diagram of interface in each cluster model, (b): Bond order ratio of each sodium / material interface.

Report on New Findings in Low-Energy Positron Diffraction (LEPD) Experiments for Surface Structure Analysis

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Low-energy electron diffraction (LEED) is one of the diffraction techniques traditionally used for the analysis of crystalline surface structures. However, LEED analyses are often plagued by discrepancies between experimental and calculated I-V curves, which can compromise reliability. These challenges are mainly due to highly anisotropic scattering factors and significant multiple-scattering, which current multiple-scattering (dynamical) LEED theories struggle to address fully.

As a complementary method, low-energy positron diffraction (LEPD), the positron counterpart of LEED, has been theoretically predicted to have significant advantages [1]. These include a simple and smooth scattering factor, less multiple-scattering and a shorter inelastic mean-free-path, which promises improved surface sensitivity and more accurate structure determination. We show that experimentally obtained LEPD I-V curves exhibit clearer and more defined Bragg peaks compared to LEED, resulting from significantly less multiple scattering and simple scattering factor. This result is consistent with theoretical predictions [1] and demonstrates the ability of LEPD to overcome the ambiguities of LEED analysis.

A LEPD system was developed several years ago at the Slow Positron Facility (SPF), KEK, which uses an intense slow-positron beam generated by a linear electron accelerator (LINAC). The experimental station has recently been significantly improved which enabled efficient data acquisition for more than 100 energies in just 2 hours on clean Cu(001) samples, enabling the practical use of LEPD for surface structure analysis. In addition, the sample is transported between the SPF and the Photon Factory (PF) at KEK while maintaining a clean surface in an ultra-high vacuum transport vessel, allowing both LEPD and angle-resolved photoemission spectroscopy (ARPES) experiments to be performed on the same sample. A comprehensive analysis of both the surface structure and the electronic band structure is planned.

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(Photo-)conversion of greenhouse gases on TiO2-based catalysts

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

(Photo-)conversion of greenhouse gases on TiO_2-based catalysts

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CH_4, CO_2 and N_2O are amongst the most prominent greenhouse gases accelerating the climate crisis, one of the major threads of the 21st century.[1] Therefore, capture and utilization of such gases, e.g. by (photo-)conversion to more valuable compounds is desirable.

The well-known photocatalytic properties of the widely available TiO_2 polymorphs anatase and rutile, combined with the high reactivity of defects such as Ti^3+ towards oxygen-containing molecules renders TiO_2 as an ideal model system to investigate cost-effective conversion of these greenhouse gases.[2,3] Also TiO_2 is known to form efficient hybrid catalysts with metal particles or metal-chalcogenide-clusters like nanostructured copper particles, $(WO_3)_3$ clusters or 2D TMDCs nanoparticles, e.g. MoS_2 to name only few examples.[4-6]

In this work we present model studies of the (photo-)conversion of small molecules such as CO_2 and N_2O on a TiO_2 Rutile (110) system with and without different types of co-catalysts present. To gain a comprehensive understanding, herein spectroscopic techniques (such as X-ray photoelectron spectroscopy (XPS) and FT Infrared Reflection Absorption Spectroscopy (FT-IRRAS)) will be combined with temperature- programmed desorption (TPD) experiments to probe the population of different reaction pathways and adsorption sites.

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Remote regulation on the hydration sites of adenine molecules via derivatization

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Hydration, as a ubiquitous and vital phenomenon in nature, has attracted great attention in the field of surface science concerning the fundamental interactions between water and organic molecules. However, the role of functional group derivatization is still elusive in terms of its potential impact on hydration. By the combination of high-resolution scanning tunneling microscopy (STM) imaging and density functional theory (DFT) calculations, the hydration of 9mA molecules was realized on Au(111) in real space, forming 9mA-H2O-9mA structures. In comparison with the hydration of adenine molecules, the methyl derivatization is experimentally found to remotely regulate the hydration sites, from the imidazole ring to the pyrimidine ring, and is further theoretically revealed to allow intramolecular electron redistribution and thus steer the priority of the hydration sites. These results provide sub-molecular understandings of the relationship between derivatization and hydration, which would shed light on the regulation of hydration processes in chemically and biologically related systems.

An Atomic Level Investigation of Na on SrTiO3(001)

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Surface structure studies of SrTiO3 crystals have yielded atomic-level structural and chemical knowledge of several of its reconstructions[1]. Detailed knowledge of SrTiO3 surface reconstructions forms a solid foundation for fundamental investigations of the evolution of a typical perovskite oxide surface as it interacts with alkali metals, an interaction with clear technological relevance to e.g. solid-state batteries[2].

We report STM and DFT data of Na deposited onto SrTiO3(001)-c(4x2). STM data reveals that Na adsorption favours step-edge formation, as the SrTiO3(001) surface grows sub-5 nm holes, one unit cell in depth, and typically separated by less than 10 nm (see Figure 1). Holes grow and their edges straighten with increasing annealing temperature. Step-edge-hole formation is accompanied by regions of √5x√5-R26.6 reconstruction, which has been reported for pure SrTiO3 in reductive environments[3]. DFT results indicate that Na adsorbed onto SrTiO3(001)-c(4x2) preferentially bonds the outer-most O of the Ti-O octahedra that make up Ti-rich SrTiO3 reconstructions. The most favoured sites are those where Na may bond disconnected Ti-O octahedra, seemingly to access as-uncorrelated-as-possible Ti(4p) states that can be reduced, as greater adsorption energies correlate with a greater the share of Ti(4p) in the DOS and with greater Ti(4p)-O(2p) band centre alignment.

Combined, STM features and DFT adsorption calculations make plausible the hypothesis that Na decorates SrTiO3(001)-c(4x2) step-edges, which reduces the surrounding surface to produce √5x√5-R26.6.

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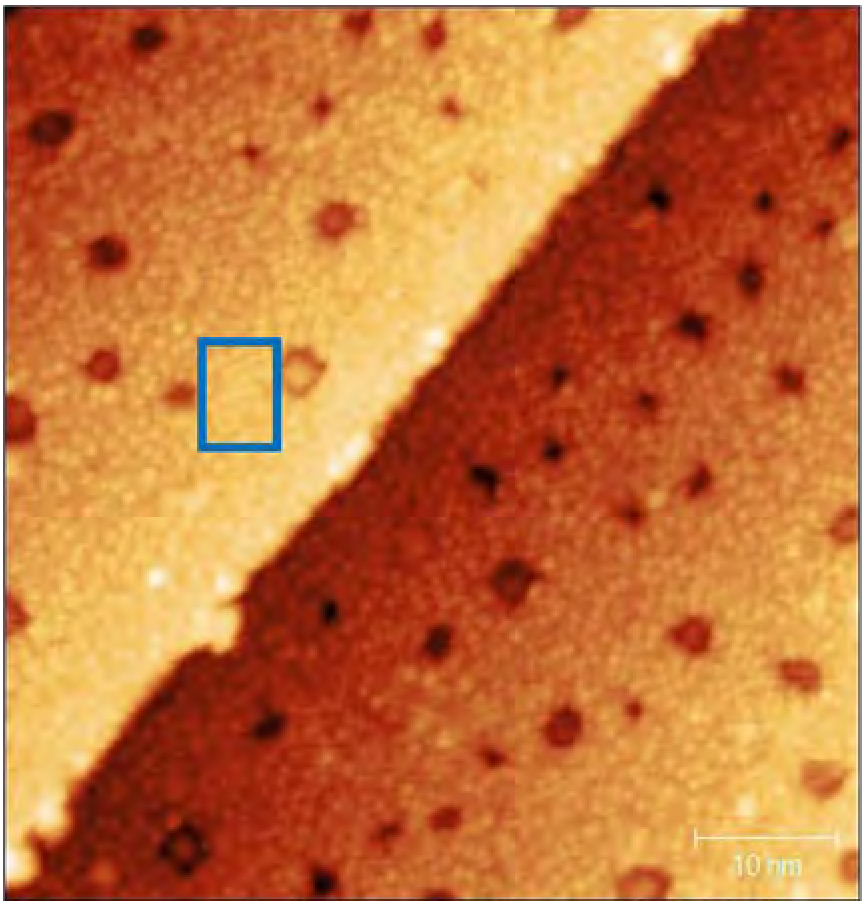

Figure 1: STM image of holes and √5x√5-R26.6^o on SrTiO3(001). The blue box indicates a √5x√5-R26.6^o region. Image size: 60x60 nm^2, annealing T = 500^{o}C, Na amount: 0.3 ML, current: 1.4 nA, bias: 0.8 V.

1

Study of the adsorption of double thiahelicene on metal surfaces by means of nc-AFM

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Helicene molecules are very attractive compounds due to their inherent chiroptical properties. Those characteristics made them suitable candidates in the building of optoelectronic devices such as 3D displays and circular polarized lasers [1]. Specifically, in the surface science field, research about helicene adsorption on surfaces has pursued to investigate the chirality phenomenon in 2D. In general, scanning probe microscopes have been employed for the surface morphology characterization of the samples. In particular, the Scanning Tunneling Microscope (STM) at low temperature regime has been widely used for the chirality recognition. By far, the studies of single helicenes on metal surfaces constitute the most predominant in the literature. However, the research about more complex molecular structures, self-assembly formation and influence of heteroatoms inclusion continue being interesting topics to address [2].

Here, we report the adsorption of a racemic mixture of double thiahelicene on metal surfaces by means of a room temperature custom-made nc-AFM setup. Our aim is to analyze the influence of thiophene functional groups and the surface reactivity in the adsorption pattern. For comparison, Cu(111) and Ag(111) monocrystals have been selected. In particular for the copper substrate, molecular wires formation oriented along one of the close packed surface directions were observed. The molecular wires can reach the 500 nm length and their structure are strongly impacted by the high mobility of the molecules. A set of flat oriented adjacent molecules, separated by 1.9 nm, form the internal structure of the wires. In contrast, on the silver surface only small and quite mobile molecular islands were observed. KPFM measurements illustrate a low contact surface potential difference on top of the molecules, indicating the perturbation of surface electron density upon adsorption of the molecules.

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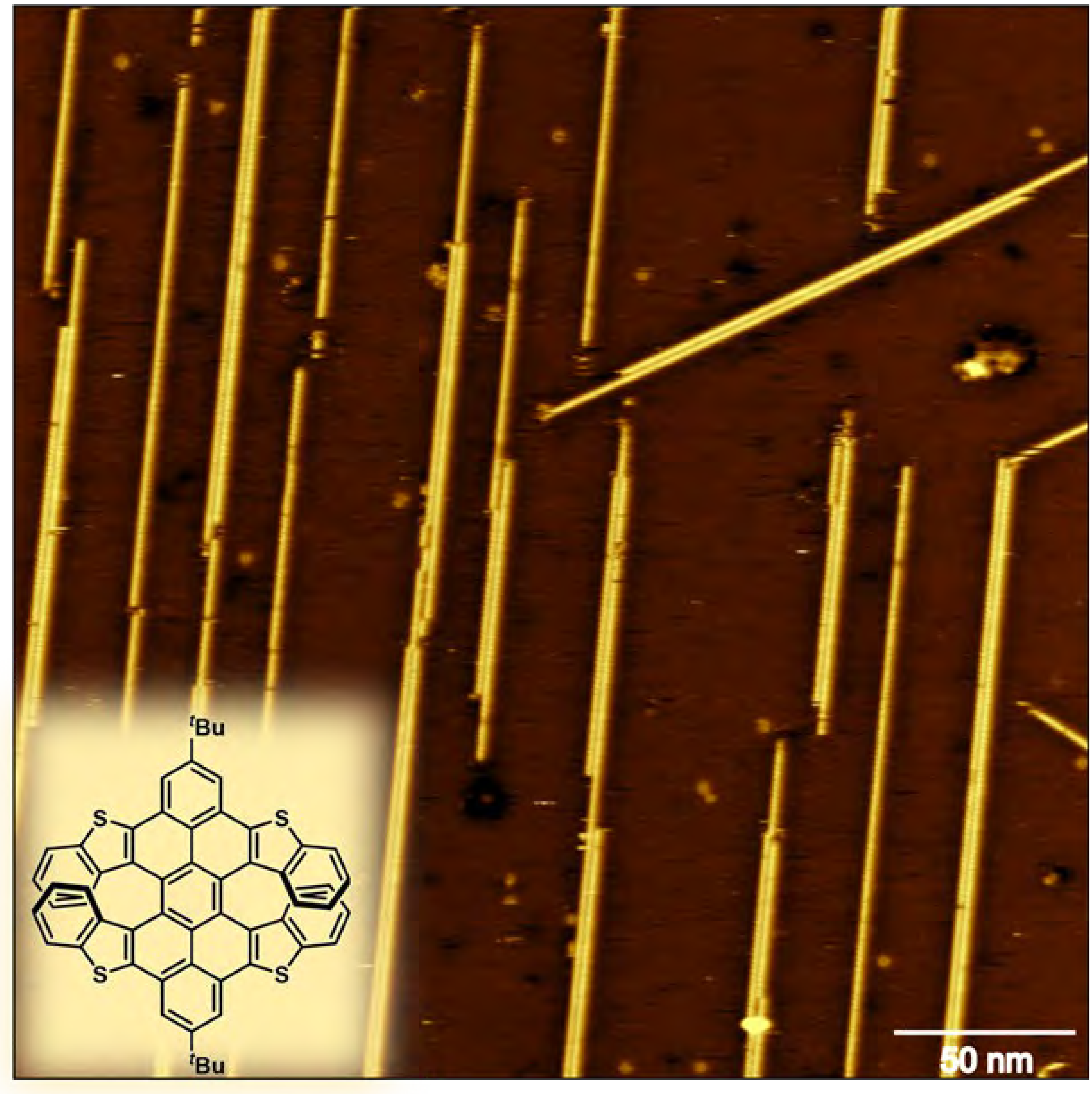
^{t}Bu
S
S
S
S
^{t}Bu
50 nm

Molecular adsorption on support-decoupled 2D Metal-Organic Frameworks: an STM study

Dominik Hruza[1], Zdeněk Jakub[1], Jakub Planer[1], Azin Shahsavar[1], Jan Čechal[1]
[1]CEITEC Brno University of Technology, Czech Republic

Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Metal-Organic Frameworks (MOFs) feature high density of identical metal sites, which makes them highly appealing for applications in single-atom catalysis. Here, we present an STM study of molecular adsorption on an Fe-TCNQ 2D MOF supported on graphene/Ir(111). The inert graphene effectively decouples the active Fe-N4 sites from the underlying metal, but it also induces small physical corrugation of the 2D MOF due to the underlying graphene/Ir moiré. We show that this dramatically affects the adsorption properties of the Fe-N4 sites atop. Specifically, the thermal stability of molecules bound to Fe-N4 sites above different regions of the graphene/Ir moiré varies by ~100 °C. We conclude that studying single-atom sites atop slightly corrugated, yet inert supports provides a unique opportunity to experimentally model the effects of small structural distortions on single-atom reactivity.

Structural transition of VSe2 on Au(111) induced by high sensitivity to CO gas

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Carbon monoxide (CO) is one of the well-studied reactants in many chemical catalytic reactions, and it is important to deeply understand the adsorption behavior as well as chemical reactivity of CO on a solid surface with regards to adsorption/desorption kinetics. Therefore, it is of great interest to study the process of CO adsorption and further catalytic reaction on one of the transition metal dichalcogenides, namely Vanadium diselenide (VSe2) because of its excellent catalytic activities. Herein, based on in-situ scanning tunneling microscopy (STM) study and density functional theory (DFT) calculations, we systematically investigated the absorption effect under different CO pressures. At relatively low pressure of CO (about 1x10-8 mbar), a few CO molecules adsorb on VSe2 and lead to the desorption of the top-Se atoms resulting in point defects. With the rise of pressure, the amount of absorbed CO increases, and the underlying V atoms also desorb due to the interaction of CO, finally leading to the structural transition of the whole VSe2. One thing to note is that, during the experiment CO atmosphere was injected as a continuous flow and some STM images were taken at the same time expressing the dynamic behavior of CO adsorption on VSe2, which has scarcely been in other static systems like UHV-STM.

Preparation of nickel oxide by pulsed laser deposition and its utilisation as hole transport layers for solar cells

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Nickel oxide has emerged as a promising material for hole transport layer (HTL) applications in silicon and perovskite solar cells [1, 2]. It possesses all the preferred properties, including suitable band alignment, a wide band gap, high hole conductivity, high visible light transmittance, and good stability. Although typical solution-processed NiOx layers are easier to process and are more cost-effective, pulsed laser deposition has undeniable advantages in producing high-quality layers with the exact desired stoichiometry. The present study demonstrates the tunability of the band gap by modifying the PLD parameters such as temperature, oxygen pressure and laser frequency. We were able to tune the band gap in the range of 3,6 to 4,1 eV while maintaining 1 % absorptance for 10 nm thick layers at 3,5 eV for all samples processed with a temperature higher than room temperature. By utilising a novel method that combines photothermal deflection spectroscopy with ellipsometry, it is now possible to observe the optical properties of layers ranging from 1 eV to 6 eV.

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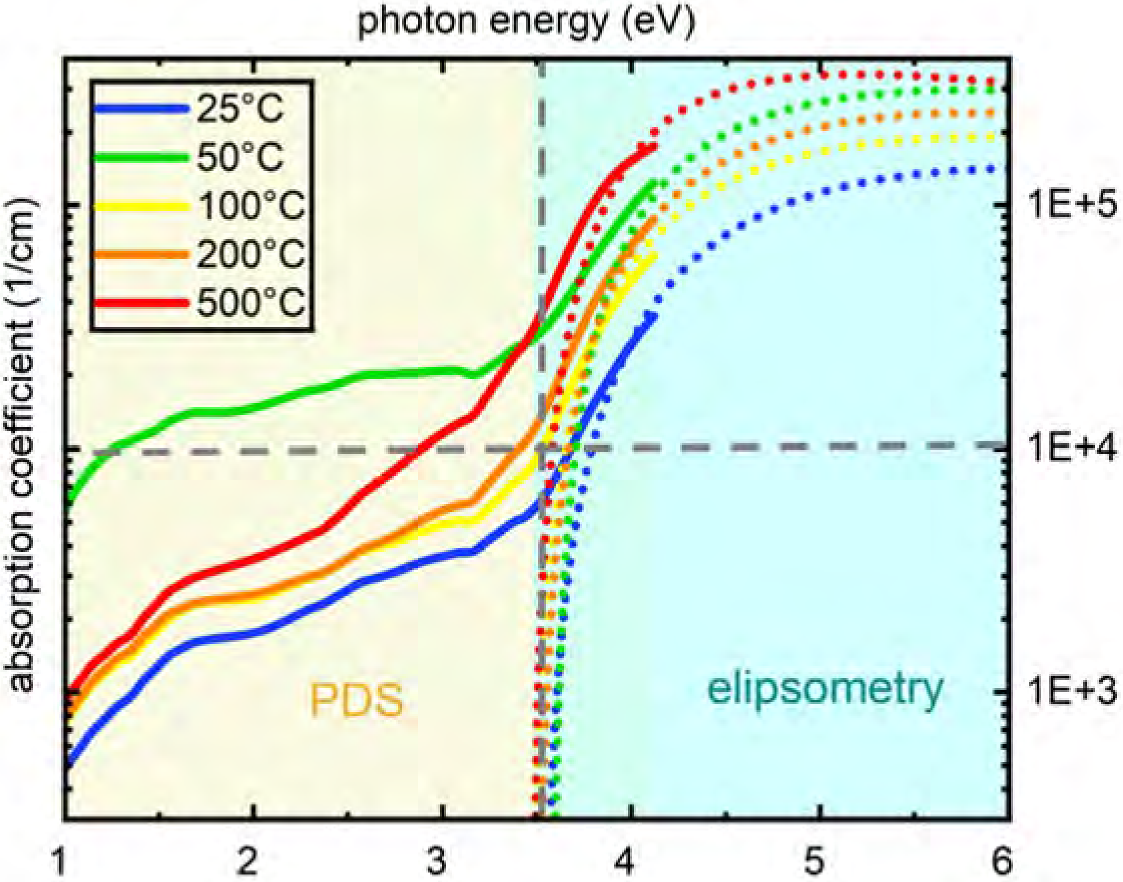
photon energy (eV)
absorption coefficient (1/cm)
25°C
50°C
100°C
200°C
500°C
PDS
elipsometry
1E+5
1E+4
1E+3
1
2
3
4
5
6

Investigation of the co-adsorption of N-heterocyclic carbenes (NHCs) and ethyl pyruvate on Pt surfaces

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Ethyl pyruvate is a well-researched prochiral molecule used in enantioselective heterogeneous catalysis[1] [2] [3]. The cinchonidine-modified Pt/Al2O3 catalysed hydrogenation of ethyl pyruvate hydrogenation reaction can achieve enantiomeric excess values of approximately 98% with a significant rate enhancement compared with the reaction over unmodified Pt[1].

N-heterocyclic carbenes (NHCs) are widely employed in homogeneous catalysis and organocatalysis[4] [5] [6]. Here we investigate whether NHCs have potential to be used as modifiers in enantioselective hydrogenation catalysis over Pt/Al2O3. A functionalised NHC (Figure 1a) is used to modify a Pt catalyst for the hydrogenation of ethyl pyruvate. Catalytic reactor data (Figure 1b) show that increasing the NHC concentration inhibits the reaction rate for ethyl lactate formation. To investigate how the NHC modifier influences the catalytic chemistry, Reflection Absorption Infrared Spectroscopy (RAIRS) and X-ray Photoelectron Spectroscopy (XPS) were used to probe the adsorption of ethyl pyruvate on NHC-modified Pt surfaces. The adsorption geometry adopted by the catalytic reagent as a function of NHC concentration provides insight into the catalytic behaviour.

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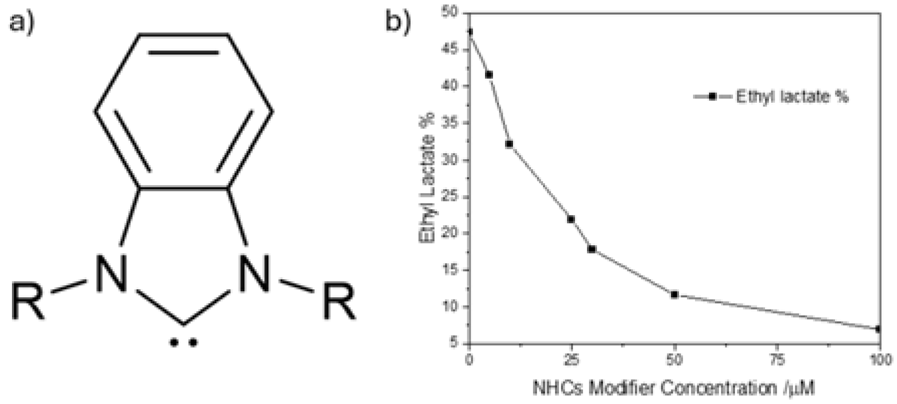

Figure 1. a) molecular structure of a generic benzimidazole NHC; b) effect of NHC concentration in isopropanol solution on the percentage formation of ethyl lactate (monitored by GC) after a reaction time of 5 hours using a 5% Pt/Al_2O_3 catalyst and a H_2 pressure of 5 bar.

Designing stable and reliable vanadium oxide thin films

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Energy-efficient devices have been significantly researched to minimize power consumption without compromising their functionality. A commonality between these devices is often the usage of a functional layer that responds to a specific externally applied stimulus. In this context, thermochromic materials (e.g., VO_2) which change their electronic and optical properties in response to the external temperature could find their applications in smart windows, passive smart-radiator devices, uncooled micro-bolometers, and other switching devices. In this study, a single-step process route for the fabrication of VO_2 thin films, which can be easily integrated into the production of energy-efficient devices, has been presented. The process employs a vanadium pentoxide (V_2O_5) sputtering target in an RF magnetron sputtering system for the deposition of vanadium oxide layer on both amorphous and crystalline substrates without requiring any post-treatment. The substrate temperature (Ts) and oxygen-flow-ratio (R_(O_2)) have been found to critically affect the stoichiometry of the deposited film. The resputtering phenomenon found to be dominant at elevated temperature, is pivotal in the formation of an oxygen-deficient phase, V_2O_3, at higher temperatures (Ts ≥ 873 K) from the oxygen-rich phases, V_2O_5 and V_6O_{13}, at lower temperatures (823 ≤Ts ≤ 873 K). Moreover, the structural phase transition (SPT) temperature of these vanadium dioxide films is 339 K, which agrees with the reported value of 340 K for a pure VO_2. Further, even with the microstructural variations, the observed phase transition in all the films is reversible and stable over multiple thermal cycles. In addition to temperature, applying another stimulus, electrical current through the film, also causes the semiconductor-to-metal transition (SMT), and the correlation between both stimuli has been established. Based on the obtained stoichiometries, a process model depicting the development of various VOx phases, which could act as a guide to fabricating the desired VOx compound, has been established.

Unravelling Surface Dynamics: Modelling Diffusion at Low Temperatures with Quantum Trajectories

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

The Helium Spin-Echo technique [1] has emerged as a powerful tool for measuring diffusion on a wide range of surfaces. Measurements of these surfaces provide us with a unique insight into the influence of quantum mechanics on the dynamics of adsorbates over picosecond timescales.
We outline recent work making use of quantum trajectories to predict the behaviour of systems such as Hydrogen on Ruthenium [2] and Hydrogen on Nickel [3]. As part of this work, we have developed a first-principles model of the adsorbate-surface interactions, which has shown to correctly predict the rate of diffusion both above and below the 'deep-incoherent' transition temperature. By identifying the essential components required to characterize diffusion at low temperatures, this model has helped us to simplify the description of the system, making use of the rotating wave approximation to reduce the full non-Markovian dynamics to an equivalent Markovian master equation. In doing so, we were able to greatly reduce the cost associated with simulating the dynamics of Hydrogen, whilst maintaining an accurate reproduction of the thermodynamics of the system.

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Hydrophilization of polyethylene terephthalate surface by deep-ultraviolet LED irradiations

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Many polymer materials are widely used for electronic devices. A polyethylene terephthalate (PET) is used in the electronics field, such as film capacitors and flexible substrates. However, when PET is used as a material for electronic devices, it is necessary to form a conductive thin film on the PET surface by coating or electroless plating, so adhesion with other materials is one of the problems.

In this paper, we describe about surface modification of PET using deep-ultraviolet (DUV) light. We determined using a DUV LED, which is one of the promising light sources. In the experiment, three deep-ultraviolet LEDs with emission wavelengths of 265 nm, 280 nm, and 310 nm, respectively, were irradiated to PET surfaces up to an integrated energy of 1000 J/cm² in air. A hydrophilicity, which is an index of adhesion, was evaluated by measuring the contact angle of the PET surface. The change of contact angles depend on the wavelength and the integrated energy of the LED. The contact angle of the non-irradiated PET surface was about 75°. In the case of 265 nm LED, the contact angle decreased sharply with the start of irradiation, reaching 5° or less at around the integrated energy dose of 350 J/cm², and then remaining almost constant. With the 280 nm LED, the contact angle decreased to around 5°at an integrated energy of 750 J/cm² and then became constant. On the other hand, the change of contact angle was not observed by 310 nm LED irradiations. These results suggest that it is possible to hydrophilize the PET surface by using DUV LED light, but it is dependent on the irradiation wavelength. Surface analysis by X-ray photoelectron spectroscopy (XPS) revealed that hydrophilic groups were formed on the PET surface by wavelength-dependent photochemical reactions induced by deep-ultraviolet light irradiations.

High-speed spectroscopic imaging ellipsometer based on monolithic polarizing interferometer: Inspection of the 2D van der waals materials

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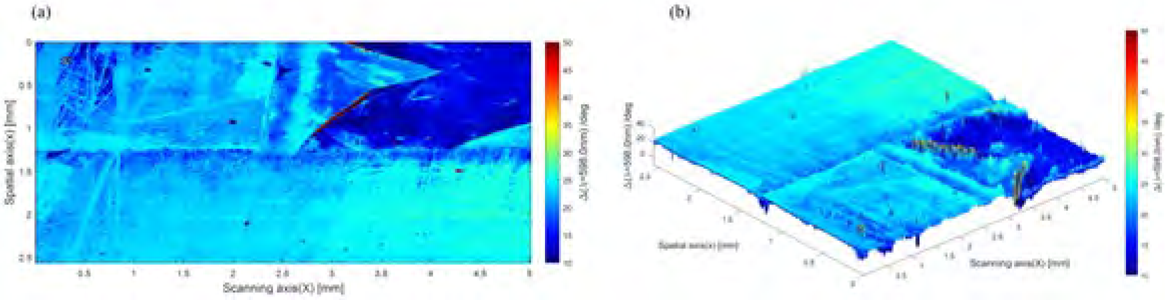
Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Spectroscopic ellipsometry (SE) stands as a widely used non-destructive optical technique utilized for examining thin film properties and periodic nanopattern geometry. As the feature size of integrated circuits is gradually decreased, the demand for high-speed SE solutions has escalated, ensuring efficient fabrication processes and optimal performance. Recently, we have proposed a new concept of dynamic imaging spectroscopic ellipsometer (DSIE) employing a monolithic polarizing interferometer and showed that we can provide a spatial resolution of around 50 by 50 microns. Our study explores methods to further refine the spatial resolution of the dynamic spectroscopic imaging ellipsometer by integrating a high magnification telecentric lens system for inspecting 2D materials. Traditional imaging ellipsoemeters, relying on null-type or rotating optical elements schemes, necessitate extended acquisition times, along with additional spectral scanning mechanisms for spectroscopic applications. However, the proposed microscopic imaging SE system can extract spatio-spectral ellipsometric phase map of 2D materials achieving spatial resolutions of a few microns within tens of msec. The proposed microscopic spectroscopic imaging ellipsometer demonstrated its remarkable potential of a microscopic high-speed SE inspection solution offering a high lateral resolution of a few microns. The proposed system can significantly enhance the visualization quality in 2D material inspection. We anticipate that its dynamic measurement capability with its highly localized spatial resolving power can create various impactful applications in 2D materials fabrication as well as semiconductor manufacturing fields.

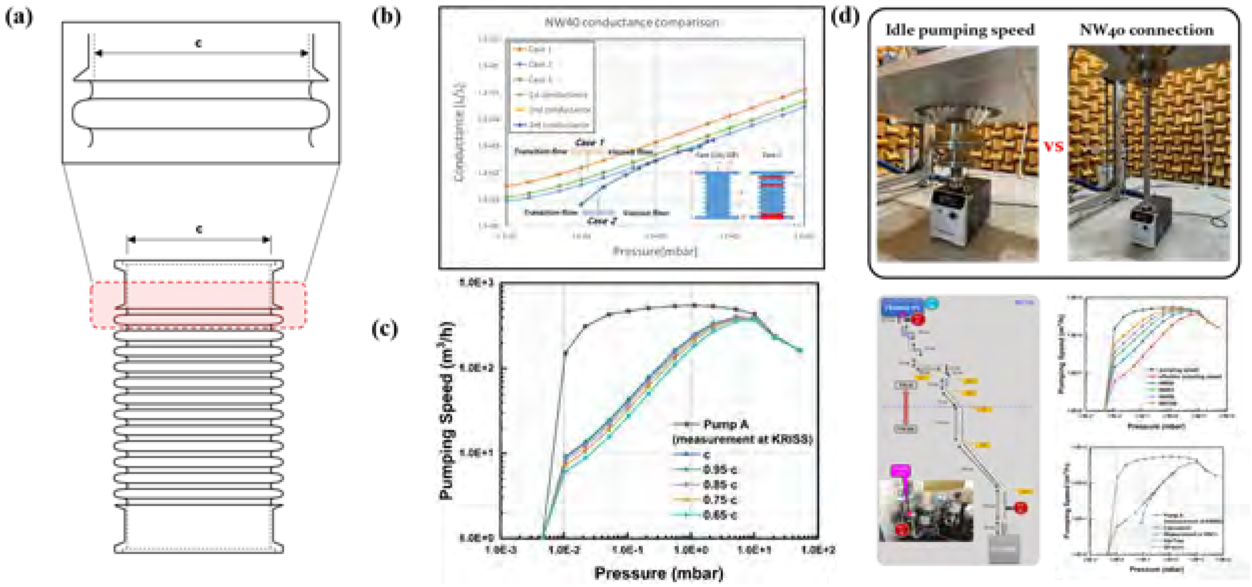


Impact of Conduit Geometry on the Pumping Speed Characteristics of Dry Vacuum Pumps

Jun-Ik Park[1], Jun Oh Kim[1], Sunmin Song[2], Chegal Won[1], Sang-Woo Kang[1]
[1]Strategic Technology Research Institute, Korea Research Institute of Standards and Science, South Korea, [2]Technical Team, K-KTech, South Korea

Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Dry Vacuum Pumps have been attracting much attention in high-tech vacuum industry because of many advantages such as simple pumping mechanisms, and free oil contamination. In Particular, manufacturing of a vacuum system requires a lot of cost and time, and pumps, essential for vacuum environment, are installed separately from the place where the actual process is performed using a conduit owing to space limitation, noise and vibration problem. Therefore, the design of the conduit between the pump and the process equipment is very important for the practical implementation of vacuum systems. In this study, the characteristics of a bellows type conduit commonly used in the vacuum industry and the pumping speed of a dry pump were measured and calculated through a theoretical calculation method of conduit conductance and an actual experiment. In addition, comparative verification was conducted through simulation using a commercial vacuum design program, VacTran. The calculated and measured pumping speed were quantitatively compared and analyzed in order to confirm the actual pump performance. These results provide a new route towards prediction of pump performance according to conduit geometry.



Technical details of the STFC nitrogen purge system required for PIP II HB650 Cryomodule String Assembly.

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

UKRI / STFC are committed to providing three of the four PIP II HB650 cryomodules required at Fermilab as part of the upgrade work required for the Deep Underground Neutrino Experiment. STFC Daresbury Laboratory is building new cleanroom facilities as part of the infrastructure requirements for the build of the cryomodules. This poster details a new nitrogen purge system, which allows a constant nitrogen purge to be applied to the internal vacuum faces of accelerating cavities as they are installed within the cavity string of the cryomodule. The purge system allows for fine control of a stable flow of nitrogen gas through the growing cavity string as the build progresses. The system can realise when the build is complete and therefore the vacuum vessel is sealed and can then stop the purge at an assigned pressure.

Analysis of Additive Manufactured Samples with Deposited Niobium Thin Films for Use on Particle Accelerators

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Due to the push for sustainable accelerators in recent years, new research is being conducted to combat the carbon and economic footprints that accelerators have, one of these ways is through thin films. This technology potentially has the effect of not only saving money through material sourcing but also saving energy by being able to run cryogenic facilities at 4.5K rather than 2K. According to sources (Pira, et al., 2023) this can result savings in cryogenic power of up to 3 orders of magnitude.

This paper represents the results from Niobium thin films being deposited onto copper and bronze additively manufactured substrates. Samples have been printed using Laser Powder Bed Fusion (LPBF). Some samples have been mechanically finished, others are as received. Samples are coated in a thin film of niobium and then analysed to determine the possibility and potential of using LPBF for particle science in the future.

0D quantum dots @ 2D nanosheet muti-dimensional nanostructure tin sulfide as black phosphorus analogue for high performance solar-driven photocatalyst

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Violet phosphorus (VP), also known as Hittorf's phosphorus, is promised a next-generation two-dimensional (2D) material with black phosphorus (BP). It is an intermediate in the process of synthesizing blacks starting with red phosphorus (RP), and has a unique activity. Since BP has proved problematic in the photocatalyst field, due to rapid recombination of electrons and holes. To overcome this, the tin sulfide (SnS) with the same structure of BP analogue was used to control the bands, implying that this method could be responsible for the increased efficiency. Specifically, SnS can absorb a wide range of visible light because its electron affinity is sufficiently low to generate hydrogen from water and its ionization potential is small. We successfully synthesized 0D/2D SnS multi-structures using the hydrothermal method and demonstrated that when the bandgap of SnS is wider than that of bulk materials and is tuned, this material can be used for more efficient photocatalytic applications. It demonstrated improved efficiency in the chromium hexavalent reduction and organic dye reduction photocatalyst, as well as in the hydrogen evolution photocatalyst.

Unveiling substrate role in 2D MoS2 growth: Pulsed Laser Deposition on non-metallic substrates for high-end applications

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Molybdenum disulphide (MoS2) is a 2D semiconducting material with peculiar electronic and optical properties [1]. The tunability of its bandgap, also subjected to an indirect-to-direct transition passing from bulk to monolayer, suggests it as a highly promising candidate in optoelectronics and low-power applications [2-5]. MoS2 is typically synthesized via chemical vapor deposition (CVD) or molecular beam epitaxy (MBE) [6]. However, pulsed laser deposition (PLD) has recently demonstrated to be a cleaner, and more reproducible approach to fabricate extended few/monolayer MoS2 films on various substrates [7]. The realization of MoS2-based integrated devices requires its direct growth/transferability on non-metallic surfaces. With this purpose, here we report on morphological and vibrational properties of 2D MoS2 systems grown via PLD onto non-metallic, SiO2/Si, glass, and metal, Au(111) substrates. The role of both substrates' type and deposition/annealing temperatures in affecting MoS2 properties are investigated, demonstrating also the obtainment of monolayer MoS2 on Au(111). Scanning electron microscopy (SEM), atomic force microscopy (AFM) and scanning tunnelling microscopy (STM) images allow to acquire information about films morphology, while their vibrational features and degree of crystallinity are explored via Raman spectroscopy. A custom wet-etching transfer procedure allowed relocate PLD-grown MoS2 films from Au(111) surfaces to SiO2/Si substrates. We finally report preliminary attempts to fabricate scaled Field Effect Transistors (FETs) based on PLD-grown and transferred few-layers MoS2 as channel material.

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Development of SLA 3D printed volumes for leak testing of LHC Hi-Lumi cryomodules at STFC

Mr Oliver Poynton[1,2], Dr Stuart Wilde[1,2], Mr Niklas Templeton[2], Mr Edward Jordan[2], Mr James Bourne[2]
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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

The Large Hadron Collider (LHC) is the world's largest and highest-energy particle accelerator and will remain so for at least the next two decades. To extend its discovery potential the LHC will need a major upgrade in the 2020s to increase its luminosity and thus event delivery rate by a factor of five beyond its nominal design value. The integrated luminosity goal will be a ten-fold increase of the nominal design. ASTeC (Accelerator Science & Technology Centre), Technology Department (TD) and the Cockcroft Institute (University of Lancaster), all based in Daresbury Lab (DL), have been tasked to play a key role in developing the superconducting Crab Cavity technologies for implementation on HL-LHC. Two crab cavity designs are being used; Double Quarter Wave (DQW) enabling vertical crab-crossing at the ATLAS detector interaction point and RF dipole (RFD) enabling horizontal crab-crossing at the CMS interaction point.
The project successfully completed manufacture of the first prototype cryomodule in 2023, to be tested in the SPS at CERN. The assembly process was extremely complex, and the team faced challenges in sequentially, and reliably, leak testing the assembly welds throughout the multi-year build process. For welds which could not be evacuated in the typical evacuation method, the team at DL used additive manufacturing technology to rapidly develop clamshells and differential pressure volumes for leak testing. 3D printed volumes were developed with sufficient density that baseline leak rates of <1e-12 mbar l/s could be achieved. This was rolled out as a full package of cost-effective leak test tooling for the cryomodule build. An overview of development, working practices & plans to further investigate additive manufacturing's future applications in vacuum systems is provided.

Oxidized zirconium alloys - evaluation of the tetragonal phase

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Zirconium alloys, thanks to their exceptional corrosion resistance and minimized neutron capture, are replacing the stainless steel used previously. As a material used in the nuclear power industry, they must undergo safety analyses. Zirconium alloys are used as a first barrier against the leakage of fission products into the reactor coolant and are highly stressed by the surrounding corrosive environment. Zirconium oxide forms on the surface of zirconium alloys exposed to this corrosive environment. The properties of this oxide depend on the original composition of the unoxidised alloy and are a function of the state of the corrosive environment (steam or water), the time and temperature of corrosion exposure. Zirconium oxide has a greater volume than the unoxidised zirconium material, resulting in high stresses at the oxide-metal interface. One possibility of relaxing this stress is the formation of a tetragonal phase of zirconium oxide, which has a smaller volume than the next emerging phase of zirconium oxide, i.e. monoclinic.

The aim of this work was to observe the evolution of zirconium oxide as a function of exposure time. In particular, to follow in detail the evolution of the key tetragonal phase of zirconium oxide, which, although stable at 1100 °C, is likely to be facilitated by the high compressive stress at the oxide-non-oxidized alloy interface. Its detection and study is possible by Raman spectrometry or X-ray diffraction.

Lifetime Studies of Caesium Telluride Photocathodes Grown at Daresbury Laboratory

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Fourth generation light sources require high brightness electron beams. To achieve this a cathode with a high quantum efficiency and low intrinsic emittance is required while also being robust with a long lifetime and low dark current. Alkali metal photocathodes have the potential to fulfill these requirements and, as such, are an important area of research for the accelerator physics community.

STFC Daresbury Laboratory's Photocathode R&D team operate multiple vacuum systems. The Alkali Photocathode Preparation Facility (APPF) at is capable of growing caesium telluride photocathodes using both sequential and co-deposition techniques. The Multiprobe machine can measure quantum efficiency (QE) and perform multiple surface analysis techniques including XPS, UPS and STM while the Transverse Energy Spread Spectrometer (TESS) can measure the photocathode's transverse energy distribution curve (TEDC) and subsequently extract its mean transverse energy (MTE).

We present our recent work studying the impact of residual vacuum gases on the photoemission properties of a caesium telluride photocathode, highlighting the decreased QE and increased MTE as a result of oxygen exposure. We also discuss other recent work by the photocathode team including lifetime studies of metal photocathodes, the impact of ultra-thin film MgO coatings and the effects of caesium implantation on copper.

Radiation Damage in Crystallography - A Tale of 2 Excitation Regimes

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Radiation Damage in crystallography is riddled with anecdotal evidence and heuristic interpretation of effects [1]. However, there are 50 years' worth of carefully measured empirical data mapping the field and steering strategies to 'avoid damage'. I will show a unifying theory that proposes a phenomenological model supported by an analog system simulation that explains 'damage' as the convolution of numerical artifacts coupled with the time evolution of the excitation deriving from x-rays traversing matter and releasing a parasitic e-beam shower. While appreciating that crystallography does work in general, the basic byproduct of this rationale is that there is no way to 'avoid damage' but one must rather embrace the effect and harness its power to surface electronic properties of materials and ultimately create better bulk models.

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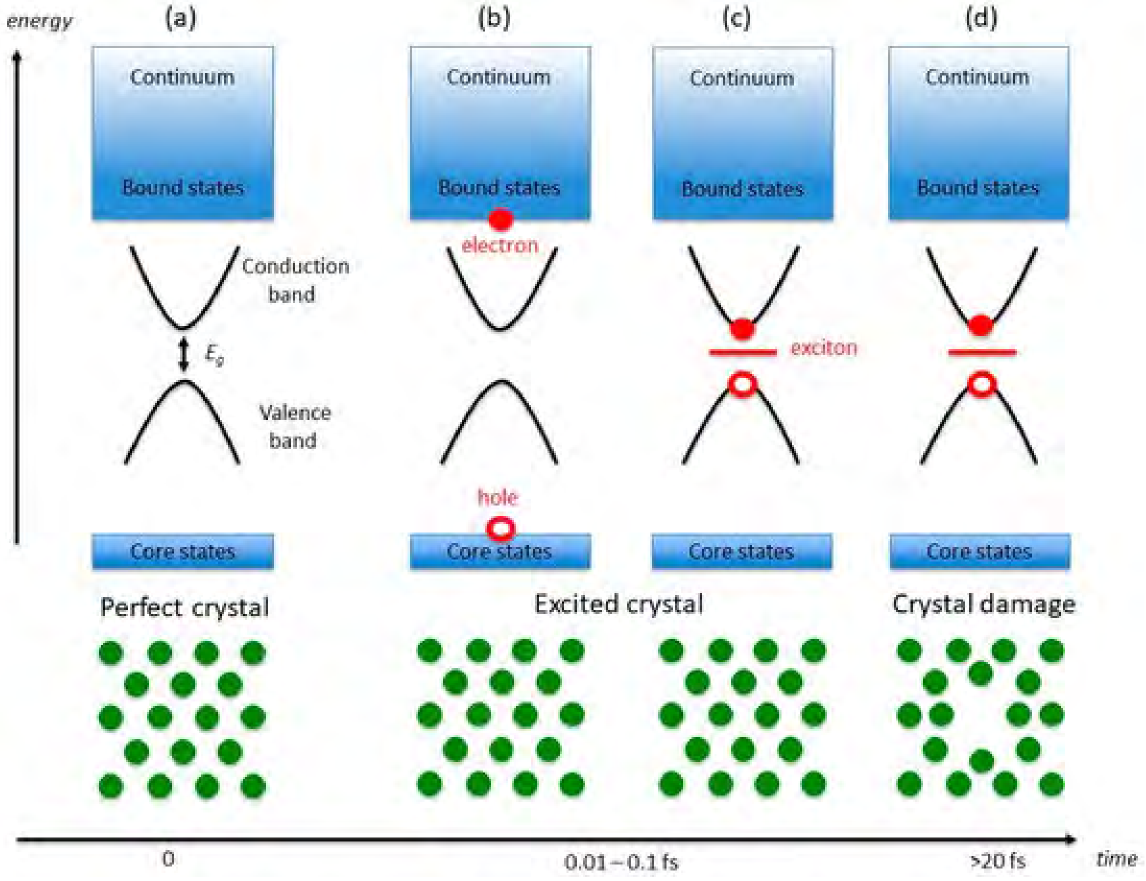

Formation of Two-Dimensional Ni-HITP Metal-Organic Framework on Au(111)

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Two-dimensional Metal-Organic Frameworks (2D-MOFs) are networks composed of metallic nodes connected by conjugated organic linkers [1]. For example, Ni centres react with hexaamino-triphenylene (HATP) molecules to form two-dimensional Ni3(HITP)2 MOF [2]. 2D MOFs have attracted significant attention because of their sufficiently high electrical conductivity for use in chemiresistive sensing and as electrocatalysts [3].

Theoretical predictions suggest that 2D-MOFs composed of transition metal centres (such as Ni) and triphenylene derivative linkers (like HATP) are topological insulators and exhibit the quantum anomalous Hall effect [4,5]. However, observing these non-trivial topological properties remains challenging. This happens because conventional wet chemical synthesis of these 2D MOFs yields multi-layered structures due to inter-layer interactions, whereas theoretical predictions are based on single-layer 2D-MOFs. To bridge this gap, synthesis of single-layer 2D MOFs is desirable.

We report the synthesis of single layer Ni3(HITP)2 MOF in ultrahigh vacuum (UHV) by separately evaporating HATP molecules and Ni onto Au(111) surface. Annealing these samples at temperatures up to 250 °C provides sufficient thermal energy for diffusion and for chemical reactions to take place. Using scanning tunnelling microscopy (STM) we are able to follow the evolution of the growth for the Ni3(HITP)2 MOF, enhancing our understanding about MOF formation. Our STM image interpretations are supported through density functional theory (DFT) calculations.

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Characterization of the biomedical surface by the XPS and HPXPS

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Nature has developed strategies to produce complex materials. Biomaterials is an important and inspiring field and needs special attention from scientists and engineers to create new reasonable biostructures. X-ray photoelectron spectroscopy (XPS) is valuable for the characterization of biomaterials [1], biointerfaces [2,3], and polymer surfaces [4,5] with detailed chemical and elemental information of the surface composition. We would like to promote the latest equipment, technology solutions, and innovations in the photoelectron spectroscopies field. Here it will be presented an innovative and compact spectrometer for routine X-ray photoemission spectroscopy and ambient pressure photoemission spectroscopy for the study of important phenomena in the current research. The design, construction, and technical parameters of a new X-ray source for imaging of biomedical surfaces with two types of analyser will be presented. We will report the technical solution of the new X-ray source and research results of XPS measurements conducted on the surface chemistry and electronic structures can be investigated, and the elemental composition is obtained in the imaging mode, with a micrometer resolution. Moreover, it will be demonstrated the investigation in ambient pressure conditions.

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Vacuum performance analysis using new cleaning solutions (on an UHV outgassing rig)

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Vacuum performance analysis using new cleaning solutions (on an UHV outgassing rig)
Rebekah Luff, Keith Middleman, Oleg Malyshev, Liam Smith

To achieve UHV conditions required for particle accelerators, the use of clean vacuum chambers and components are imperative. After previous studies [1], the current solution used at Daresbury Laboratory for cleaning particle accelerator components is HFE-72DE - this is a hydrofluroether with a dichloroethylene additive. However, under new PFAS regulations [2], HFE-72DE is being discontinued due to association with environmental pollutants and negative effects on human health.
The most cost-effective resolution is to use an alternative solution with analogous cleaning performance. Therefore, this work investigates the effectiveness of cleaning common particle accelerator materials with various solutions, and the results are to be compared to those achieved using HFE-72DE. This work is done using an UHV outgassing rig system.
Samples are deliberately contaminated, and their vacuum performance tested before and after cleaning. The cleanliness of samples is determined via the outgassing rate achieved. Previous work [1] shows 'clean' stainless steel to achieve an outgassing rate of 2x10-11mbarls-1cm-2 after bakeout to 250°C. Contaminated surfaces increased the outgassing rate, which prevents reaching desired UHV pressures for particle accelerators.
Electron bombardment [3] is also to be utilised to improve cleanliness by encouraging electron stimulated desorption (ESD). The cleanliness achieved is further determined by mass spectroscopy using a residual gas analyser and by ESD yield, which is compared to literature values for baked stainless steel - 10-2 to 10-3 molecules per photon [4].

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Merging reactive molecular beams and XPS to simulate high-pressure surface reactions

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Relevant catalytic reactions are studied by exposing the surface of interest to high-pressure gas environments. These include the reduction of greenhouse gases, such as CO_2 and CH_4 on metal surfaces. The ultimate reason for the high pressure needed in such reactions is the reduced number of molecules within the random gas that possess enough energy to overcome the activation barrier of the elementary chemisorption/dissociation step. However, the high pressure represents a challenge to carry out research in realistic operando conditions since the most powerful surface-sensitive techniques, such as X-ray photoemission spectroscopy (XPS) have the optimum performance in ultra-high vacuum (UHV) conditions. An alternative to investigate high activation barrier reactions with XPS in UHV consists of using a molecular beam (MB), which is a collimated stream of gas formed by the supersonic expansion from a high-pressure gas source. The resulting beam of molecules has a well-defined translational energy that can be tuned readily, as well as a narrow energy spread (10%). These properties translate into a scenario in which using a standard MB tuned to match the activation energy of, e.g., 0.6 eV (CO_2 on Cu), would be sufficient to achieve reaction rates that would otherwise require pressures over 20 bar.

We have implemented a UHV system that enables the simultaneous use of MB and XPS so that in gas/surface reactions the gas phase is tuned and monitored through time-of-flight techniques with molecular beams (TOF-MB), while the evolution of the surface chemical species is studied with XPS. Our comparative analysis of the Cu(111) oxidation by exposing it to a random O_2 gas, and to an energy-tunable O_2 beam demonstrates the validity and potential of the MB/XPS approach to assess gas/surface reactions with high activation barriers. First results from a similar analysis of Ru(0001) oxidation will also be presented.

Laser generated 2D MoOx functional surface nanostructures

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Transition metal oxides (TMOs) feature outstanding electro-optical properties relevant to novel applications such as photocatalysts for organic dye degradation, hydrogen generation, electrode materials for lithium-ion batteries, electrochemical sensors, biological applications, etc. Among them, molybdenum oxides (MoOx) show different oxidation states of the metal cation that allow the tuning of the stoichiometry from MoO3-x semiconducting phases towards metallic MoO_2. These phases have different optical properties, which are of interest for designing integrable photonic switches and optical sensing devices. To achieve this, it is necessary to develop successful deposition and processing technologies that enable the development of 2D MoOx functional elements.

A common approach to generating different MoOx phases in thin films consists of annealing the samples in ovens, a time-consuming process that does not allow a selective transformation of the MoOx. In this context, CW or pulsed laser irradiation arises as a potential solution to anneal MoOx thin films in a controlled and fast manner, creating surface nanostructures in localized areas.

In this work, we explore selective annealing by irradiation with an infrared (IR) pulsed laser source of amorphous sub-oxidized Mo oxide (MoO3-x) thin films grown by pulsed laser deposition on fused silica substrates. The results show the successful formation of polycrystalline spatially localized well-defined areas of Mo-oxide crystalline phases upon IR laser irradiation by properly selecting the irradiation time, repetition rate, and laser intensity. The localized static irradiation with high repetition rates of the MoOx thin film induced the transformation to α-MoO_3, whereas the irradiation by dynamically scanning the surface with the beam was able to create tracks made either of α-MoO_3 or spatially resolved MoO_2 and Mo_4O_{11} regions depending on the irradiation intensity and scan-speed. From these results, a mechanism for the formation of the observed Mo-oxide crystalline phases is proposed along with potential future research possibilities.

Effect of Li intercalation on the electronic properties of a SiC bilayer

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Two-dimensional (2D) materials have gathered interest from the scientific community since the emergence of graphene, due to their unique properties such as high surface to volume ratio, which hold importance for applications in sensors and energy storage. 2D materials possess the potential to enhance the capacity and power density of lithium-ion batteries (Li) to meet current energy demands [1]. The study of the interaction of Li with different types of 2D materials is crucial to improving the efficiency of new generations of rechargeable batteries. This work investigates the effect of interlayer Li on the geometry and electronic properties of a SiC bilayer. Previous results indicate that the most favorable adsorption site for Li is on Si atoms [2]. Concentrations from one to six Li atoms per unit cell were considered. The calculations are based on Density Functional Theory (DFT). Formation and binding energies were calculated, and phonon calculations were employed to verify the absence of negative frequencies, confirming the stability of the 2D material. It is observed that Li atoms transfer charge to both layers, reducing the band gap, consequently facilitating the movement of electric charge. This behavior is reflected in the electronic bands and density of states. To delve into the interactions, Crystal Orbital Hamilton Population (COHP) and isosurfaces of charge density difference were also analysed. The numerical results obtained could drive the development of practical applications for improved charge storage and longer duration as anodic material.

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MnxNbyOz nanostructures and ultrathin films on Au(111)

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Metal-supported two-dimensional (2D) metal oxides are a scientifically interesting and technologically important class of materials. The reduced dimensionality combined with oxide-support interactions leads to novel oxide phases, many of which have no equivalent in the bulk. Compared with binary systems, 2D ternary oxides have compositional flexibility that can add new degrees of freedom resulting in complex crystal structures. These have the potential for novel applications due to their unique electronic and optical properties.[1]

Previous studies have reported on 2D NbOx and MnOx phases on Au(111) substrates. Scanning tunnelling microscopy (STM) images show an epitaxial (2 x 2) honeycomb Nb_2O_3 monolayer on the Au(111) surface.[2] A complicated manganese oxide phase with a few monolayers thickness, called the MnOx fishbone phase, is observed via STM to grow epitaxially on the Au(111) substrate.[3]

Here we report successful on-surface synthesis of MnxNbyOz phases on the Au(111) surface. The growth evolution and structure of nanostructures and thin films are investigated by STM. The ternary oxides are grown by either co-deposition and oxidation of Mn and Nb, or using a binary NbOx / MnOx phase as a template. By adjusting the reacting conditions of the deposits, formation of distinctly different phases with various Mn / Nb ratios can be achieved. Our results show successful on-surface synthesis of 2D ternary oxides from binary oxides, which have also been realised on other systems.[4] The diversity of Au(111) supported MnxNbyOz nanostructures and films demonstrates the potential to tune surface functionality by adjusting the oxide stoichiometry.

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Effect of Ozonized Water Treatment on Aluminum 6063

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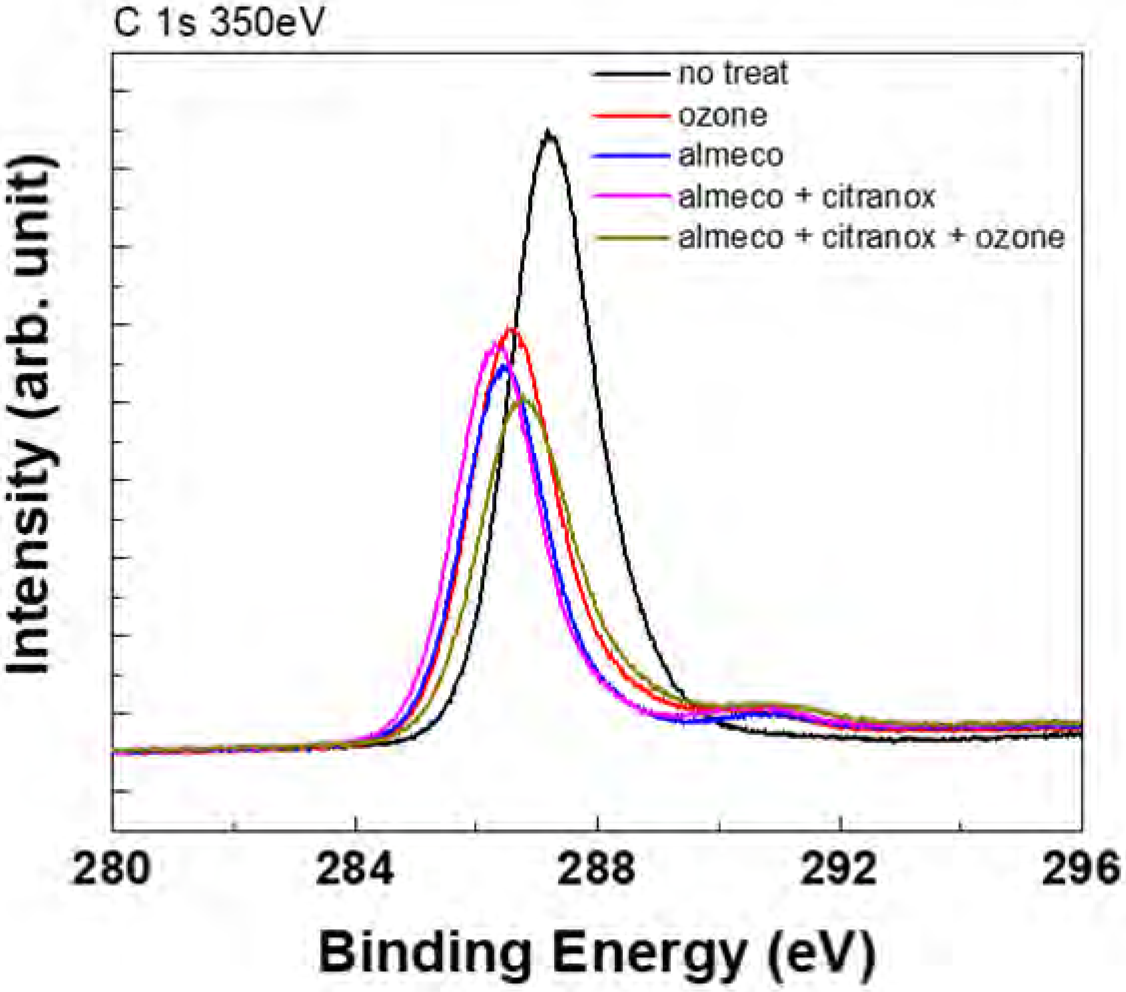
Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

This experiment aimed to determine the suitability of ozonized water cleaning technology for effectively removing initial organic impurities in aluminum 6063 vacuum chambers.

To achieve this, we conducted a comparative analysis using the conventional wet chemical cleaning method previously used at PAL (Pohang Accelerator Laboratory), ozonized water cleaning technology, and finally, a combination of both methods, followed by NEXAFS and XPS.

The experiment results confirmed that ozonized water cleaning technology effectively removes sp2 , sp3 carbon, and hydroxyl groups, as observed through by NEXAFS. Moreover, it was observed from the XPS C 1s peak analysis that the combined treatment of chemical reagents and ozonized water exhibited the most superior cleaning ability.

Furthermore, through the XPS Al 2p peak, it was confirmed that ozone treatment thickened the oxide layer compared to conventional methods, while also increasing the chemical composition of $Al2O3$ and reducing the proportion of amorphous oxide ($AlOx$). These results will undergo further comparative analysis through additional experiments to determine their correlation with the outgassing rate and Photon Stimulated Desorption (PSD) values of the aluminum vacuum chamber. We anticipate that this will provide guidance on the technological direction for next-generation aluminum surface treatments aimed at improving vacuum performance.


C 1s 350eV
no treat
ozone
almeco
almeco + citranox
almeco + citranox + ozone
Intensity (arb. unit)
280
284
288
292
296
Binding Energy (eV)

Temperature-Dependent Electronic Ground-State Charge Transfer in van der Waals Heterostructures

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The electronic ground state of single components of van der Waals heterostructures is reached through electronic charge rearrangement resulting from charge transfer (CT) processes. In this work, the impact of two factors on the CT amount is shown for a hybrid transition-metal dichalcogenide (TMDC)/molecule interface constituted of a molecular p-type dopant adsorbed on monolayer MoS2 on a graphite substrate. Results show that, next to the well established influence of the density of state distribution, a marked temperature dependence governs the CT amount and consequently the electronic level alignment. A noticeable reversible three-fold enhancement of the CT amount is shown when going from 7K to room temperature.

Bandstructure calculations including intracomponent electron-phonon coupling and intercomponent electronic coupling at different temperatures proved these two mechanisms to be the reason of the observed phenomenon.

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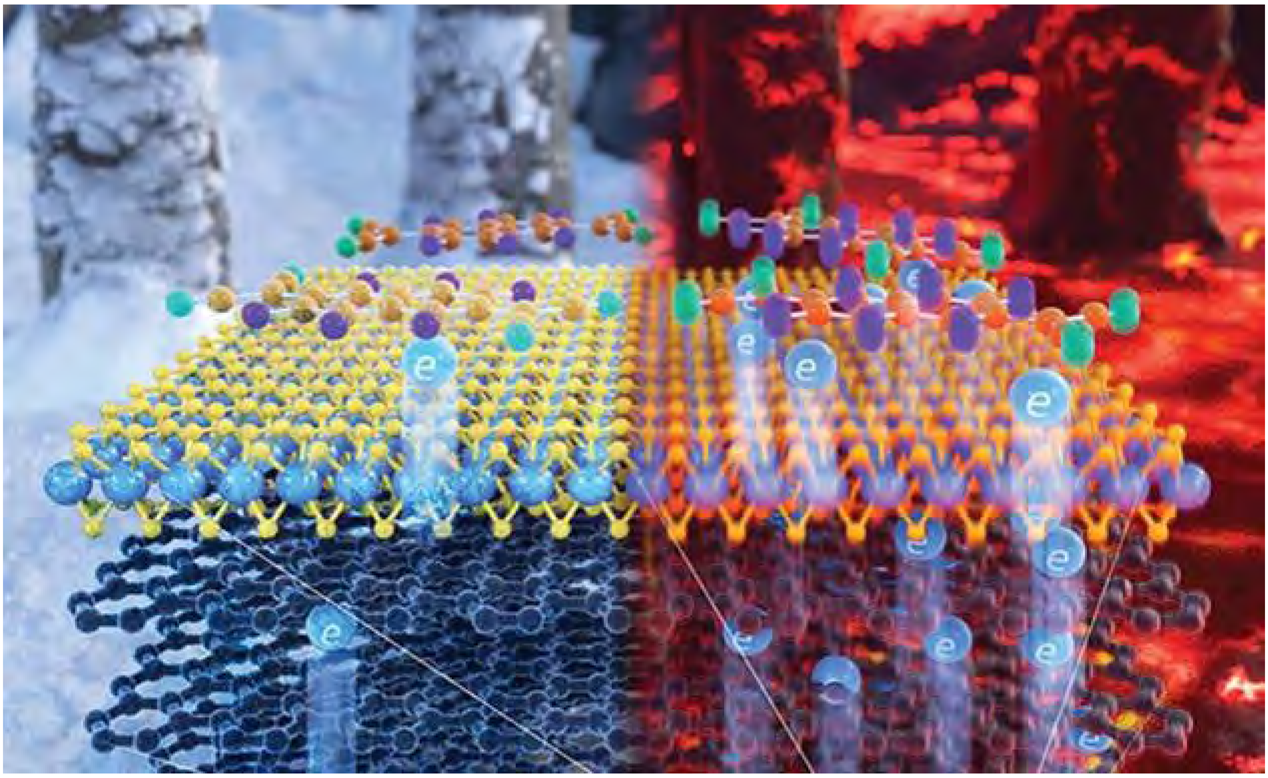

Adsorption and detection of NH3 on metal functionalized SnC nanosheet: A DFT study

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Ammonia (NH3) is a naturally occurring chemical in humans, animals, and plants. It is a colorless toxic gas with a very penetrating and characteristic odor. Despite its high toxicity, NH3 is almost unavoidable in some aspects of human activity because it is a common raw material used in chemical industries, fertilizers, and food processing. Ammonia sensors have many applications, including environmental monitoring, agriculture, medical diagnosis, and industrial waste management. Additionally, NH3 sensors have been used to diagnose hepatitis and some stomach and kidney diseases [1]. The functionalization of 2D nanomaterials has been reported to enhance their ability to interact with various molecules [2, 3]. In this work, we studied the effects of functionalization with different metal atoms (alkali, alkaline earth, and transition metals) on the adsorption and detection of NH3 in tin carbide monolayers (2D-SnC) using first-principles calculations based on DFT scheme. The electronic properties, adsorption energies, charge transfers, and recovery times were studied to analyze the feasibility of using this nanomaterial for the detection and adsorption of NH3. The results show strong adsorption of metal atoms on the monolayer. However, the interaction between NH3 and 2D-SnC was significantly enhanced because of the functionalization of the monolayer with metal atoms. The electronic properties and charge transfer changes suggest that the functionalized monolayer can detect and trap NH3 molecules.

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Improvement Mechanical Properties of Nb on Cu Structure for RF Cavity by Laser Radiation: Formation of Soft Cu Buffer layer

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Increasing the crystalline size of the Nb layer and Cu substrate in Nb on Cu structure after irradiation by Nd:YAG laser using XRD, SEM, and EDS measurements is observed, as shown in the figure. This effect leads to an increase in Nb hardness [1] and a decrease in Cu hardness according to the Hall-Pech effect [2]. Calculation of temperature distribution in Cu depending on the laser pulse duration shows that at nanosecond pulse duration, 1 µm layer at the Nb/Cu interface is formed, but at 10 ms pulse duration, 1 mm thick Cu substrate entirely becomes soft. In the first case, the thin, soft Cu layer plays the role of the buffer layer at the thermal shock (the decrease from room temperature to helium temperature in the accelerator of charged particles). Still, in the second case, the structure becomes unstable.

Fig. Dependence of Hardness and Crystallite size of Cu substrate on the Nd:YAG laser radiation intensity.

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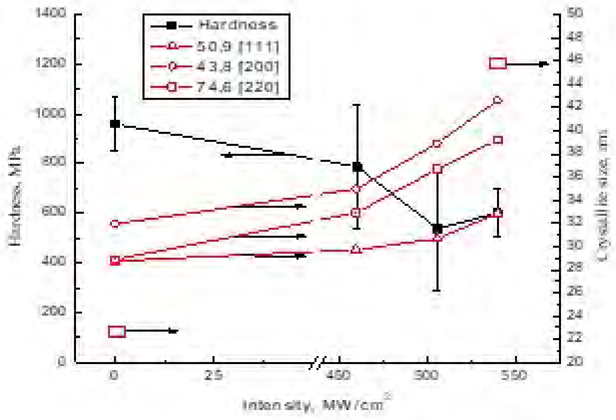

Effect of surface roughness and molecular templates on thin film thermoelectric performance

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

The observation of room temperature quantum interference (QI) effects in single molecules has opened up new possibilities for molecular electronics and thermoelectric materials. Molecular junctions are generally modelled and simulated using idealised contacts between the molecule and electrodes, something which does not translate easily to experiment when dealing with molecular films. Despite this, several recent reports now demonstrate that single-molecule QI effects can be translated into self-assembled monolayers (SAMs) [1, 2], which retain excellent thermoelectric properties, even with the absence of long-range order within the layers. The common wisdom is that to improve on this, the surface quality must be improved such that molecular ordering and the consistency of surface-molecule contacts are improved. Here we explore two methods for improving ordering and performance of organic thermoelectric layers. The effect of surface roughness is explored using a variety of gold substrates, including template-stripped gold, epitaxial Au(111) on mica, and 'rough' gold on quartz. We apply a range of preparation methods including ultra-high vacuum sputter-annealing, flame annealing, plasma, and solvent cleaning methods and monitor the improvement in surface structure with X-ray photoelectron spectroscopy (XPS) and high resolution atomic force microscopy (AFM). Following this we explore the potential for metal centred porphyrin based molecules as a template layer for second layer molecular growth, similar to previous reports which found multi component architectures resulting in a 50%-100% improvement in Seebeck coefficient [3].

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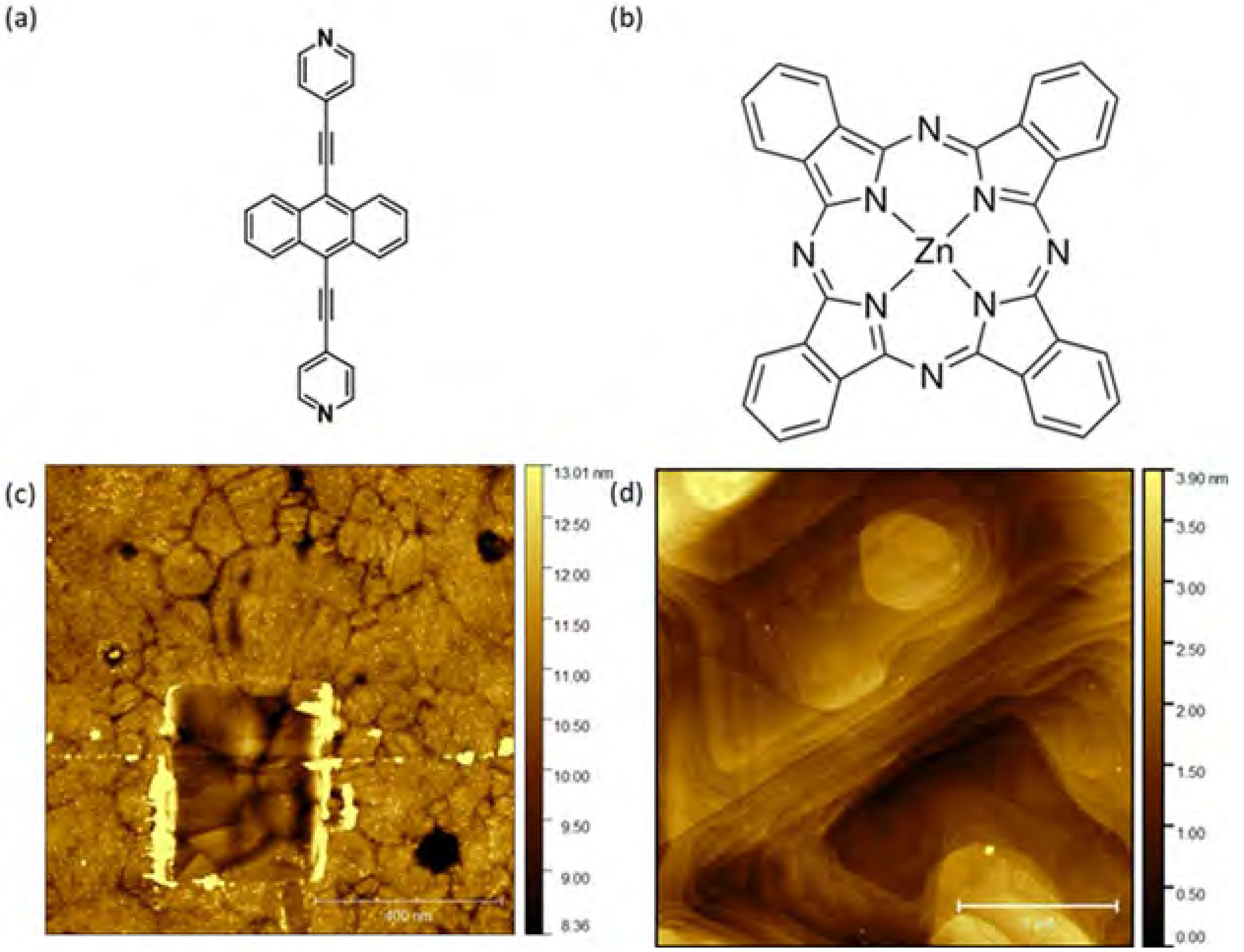
(a)
N
N
(b)
N
N
N
Zn
N
N
N
N
N
N
(c)
13.01 nm
12.50
12.00
11.50
11.00
10.50
10.00
9.50
9.00
8.36
400 nm
(d)
3.90 nm
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
1 µm

On-surface growth of 1D molecular wires characterised in ambient conditions

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Over the past few decades the size of electronics has been rapidly decreasing leading to major advancements in molecular electronics, in which the ultimate goal is to create single molecule electronic components [1]. One dimensional structures such as graphene nanoribbons (GNRs) [2] have become especially promising, partly due to their exceptional conductance and potential for high on-off ratios when integrated into electronic components [3,4]. The challenge remains that even small defects in the edges of these molecular wires can cause scattering and localisation of electrons, making bottom-up fabrication via on-surface synthesis an ideal method for defect free GNR growth [5].
Here, we use the precursor monomer 10,10'-dibromo-9,9'-bianthryl (DBBA) to fabricate GNRs on atomically flat Au(111) surfaces. DBBA is deposited under ultrahigh vacuum (UHV) conditions and subsequently annealed to thermally induce polymerisation and cyclodehydrogenation, forming molecular wires with a width of 7 carbon atoms. GNR growth is characterised in situ using temperature-programmed X-ray photoelectron spectroscopy (TP-XPS) and studied in ambient conditions using molecular-resolution atomic force microscopy (AFM) (see Figure 1 for a) images and b) description of the growth process). Following this, we discuss how to apply ambient high-resolution AFM to study on-surface growth on insulating surfaces, where polymerisation is catalysed by extrinsic metal cluster catalysts.

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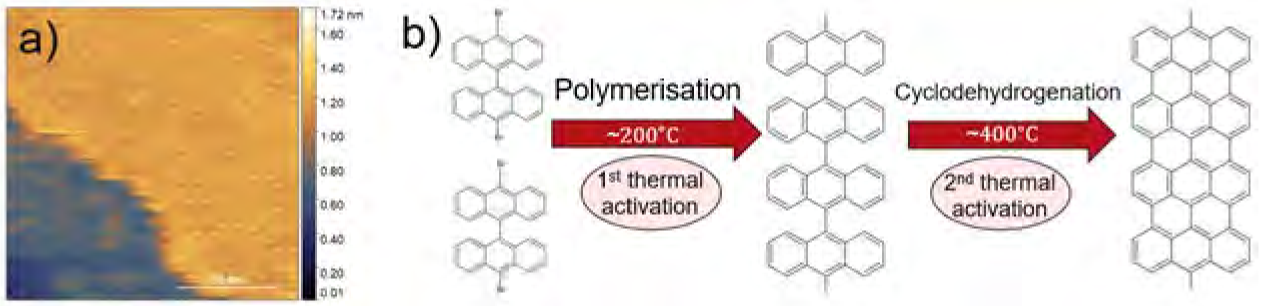

Ab initio study of Pentacene adsorption on the fivefold surface of the Tsai-type Ag-In-Yb quasicrystal

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

The Tsai-type Quasicrystals (QCs) are composed of the rhombic triacontahedral (RTH) cluster arranged in a quasiperiodic manner. The spaces between the RTH clusters are filled with the acute rhombohedron (AR). The ARs form the cog wheel complex and the stellate polyhedron [1], and there are no such structures composed of the ARs in the periodic approximant crystals. Recently, experimental studies [2, 3] of the Pentacene (Pn) adsorption on the twofold and fivefold surfaces of the Tsai-type Ag-In-Yb QC have demonstrated that Pn molecules are arranged in a quasiperiodic manner on the surfaces. In the previous study of the Pn adsorption on the twofold surface of the Tsai-type Ag-In-Yb QC by density functional theory (DFT) calculations, we revealed that Pn is stabilized on the ARs [4]. In this work, we examined the adsorption structures of Pn on the fivefold surface of the Tsai-type Ag-In-Yb QC by DFT calculations using the cluster model. We calculated the adsorption energy of Pn with its molecular axis parallel to the surface and confirmed that Pn is stabilized on the ARs. The Pn molecules placed on the ARs can form some Pn motifs observed in the experiment [2].

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An effective use of total-reflection high-energy positron diffraction (TRHEPD) for structural analysis of hydrogen atoms on a surface: its application to CeO2 (111) 1x1-H surface

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Hydrogen (H)-terminated ceria (CeO2) surface has been attracting much attention as a promotive catalyst for hydrogenation reactions due to the low activation energy [1], the highly reactive efficiency [2], and for a synthesis-gas production [3] by solar power, etc. To unravel roles of the H atoms in catalysis, it is crucial to determine the exact atomic positions on the rare-earth dioxide surface.

A diffraction method would be valuable to detect the location of the H atoms. Surface X-ray diffraction, electron diffraction, and positron diffraction are known to be surface sensitive, but have disadvantage of the lowest scattering amplitude of H. Neutron diffraction is sensitive to H, but not surface sensitive, and has disadvantage of huge background scattering from bulk atoms.

If there is any potential in these, it is the positron diffraction which has a particularly high surface selectivity. We investigated its potential and have developed a novel effective use [4] of total-reflection high-energy positron diffraction (TRHEPD) [5]. As it applied to a CeO2 (111) 1x1-H surface [4], we found some specific azimuthal angles of incidence where the TRHEPD rocking-curves (glancing-angle dependence of the 00-spot intensity) change sensitively to presence/absence of the H atoms on the topmost surface.

In this presentation, we report the determined positions of the H atoms on the ceria surface with TRHEPD. We also describe the method and discuss why the H atoms are detectable at certain incident azimuthal conditions in spite of the very low scattering amplitude of H for the positron.

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Regulating the properties of Mo thin films to form an efficient back contact for CZTSSe solar cells

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Cu2ZnSn(S,Se)$_4$ (CZTSSe) is a promising material for thin film photovoltaics, with core constituent elements that are both earth-abundant and non-toxic. Due to similar crystal properties and device architecture, CZTSSe is regarded as a sustainable analogue of Cu(In,Ga)(S,Se)$_2$ (CIGS). Similarly to CIGS, CZTSSe also employs a sputtered layer of Mo for the back contact. The back contact in substrate-type solar cells serves not only as the charge extraction layer but also as a foundation for subsequent layers in the device. During the processing of CZTSSe, a moderately-high temperature anneal is performed under a Se-rich atmosphere, inducing segregation of CZTSSe and promoting growth of a Mo(S,Se)$_2$ intermediate layer upon the Mo back contact [1]. This study details the optimisation of Mo deposition by DC sputtering in order to reduce the thickness of the somewhat resistive Mo(S,Se)$_2$ intermediate layer, as presented in the device cross-sections shown in figure 1. CZTSSe devices used in this work were fabricated using an established process based on CZTS crystalline nanoparticles [2].

It is found that the working pressure during Mo sputtering is a critical parameter for adhesion to the glass substrate and reducing the growth rate of Mo(S,Se)$_2$. Grazing incidence X-ray diffraction measurements are used to imply the orientation of Mo(S,Se)$_2$. The transition in orientation for Mo(S,Se)$_2$, from parallel-to-tilted to tilted-to-perpendicular, is found to be less pronounced for Mo films deposited under higher working pressures. This reduced transition is proposed to impede excessive growth of Mo(S,Se)$_2$. Finally, optoelectronic characterisation is performed to describe the charge transfer in the complete device. In particular, temperature dependent current-voltage measurements are used to determine the back contact barrier height, this was correlated to Mo(S,Se)$_2$ thickness.

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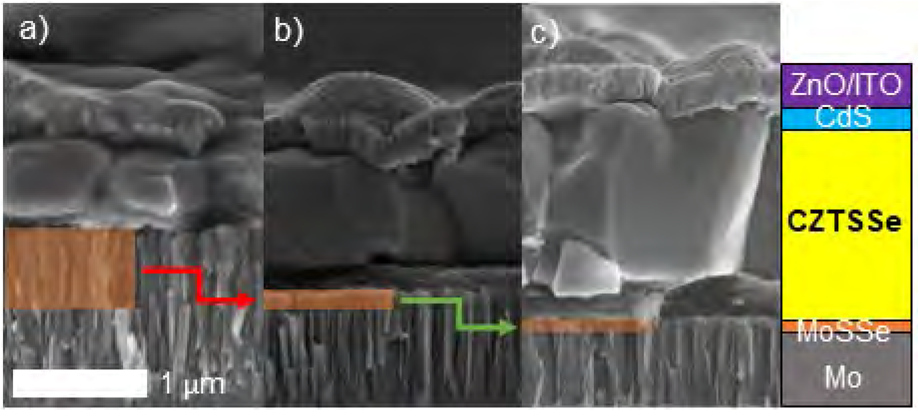

Active phases of molten alloy catalysts composed of binary or ternary alloys for catalytic methane pyrolysis at high temperatures

Jina Kim[1], Changguen Oh[1], Hyunseok Oh[1], Yukwon Kim[1]
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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Hydrogen production from hydrocarbons such as methane requires low CO_2 emission to meet the net zero emission target by 2050. One of the promising approaches employs the pyrolysis of hydrocarbons into molecular H_2 and solid C using Ni or Fe-based solid catalysts. However, the use of solid catalysts limits its industrial-scale development due to the facile accumulation of carbon. As a promising alternative technology to overcome such a limitation, we studied liquid alloy catalysts at high temperatures for catalytic pyrolysis of hydrocarbons toward H_2 and C as a large-scale H_2 production technology. Here, we have found several interesting aspects of the pyrolysis process in molten media. First, the catalytically active phases of molten alloys may be quite different from each other even when the starting composition of the alloys is the same. The homogeneity of the molten states, as well as the impurity level, are suggested to have a strong influence on the overall catalytic performance. Second, the addition of other elements, such as K, Mg, Zn, Mo, Cu, Fe, etc, into molten alloys such as NiSn (or NiBi) has a strong influence on the catalytic activity of dissolved Ni. Zn has an inhibiting effect while others have a promotional effect in the overall pyrolysis catalytic activity. The origin of the changes in the catalytic activity is explained by the charge transfer, solvation, and the formation of heterogeneous phases. Third, the presence of oxide surfaces such as zirconia in contact with the molten alloys can provide catalytically active solid surface sites for pyrolysis. Finally, we find that the approaches employing molten liquid phases can also be effective for the pyrolysis of hydrocarbons in other forms, such as plastics.

Substrate preparation for SRF thin films: Comparisons of roughness properties.

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

As part of the ASTeC SRF program, looking into the preparation of the substrate material for deposition of thin film materials.

Cavities which have defects, can lead to breakdown of the RF. These can be caused by various processes used for the formation of a SRF thin film cavity.

We study the impact of mechanical polishing, chemical polishing and heat treatment on the roughness of the substrate, as well as parameters used for thin film deposition. This was achieved by using white-light interferometry, based on measuring the average roughness found for each sample from 3 different points, where the root mean squared roughness and the arithmetic mean roughness were calculated.

These results can help in optimising the substrate preparation and improving the quality of the thin films.

First-principles study of displacive diffusion on fcc metal (110) and (100) surfaces

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Diffusion of adsorbed atoms (adatoms) on surfaces is one of the fundamental processes of crystal growth. For some adatom-surface combinations, instead of an adatom diffusing on the surface, the adatom may become embedded in the surface layer and the ejected atoms may move across the surface instead, which is sometimes called "displacive diffusion". Such substitutions between adatoms and surface atoms have been reported on the (100) and (110) faces of fcc metal surfaces by field ion microscopy (FIM) [1]. Here we applied the nudged-elastic band (NEB) method to evaluate the migration potential and theoretically investigate displacive diffusion for Ni and Cu adatoms on the Ni(110) and Ni(100) surfaces as model systems. We employed 7-layer slab model with 2×4 and 3×3 unit cells for the Ni(110) and Ni(100) surfaces, respectively. Stable atomic configurations were first evaluated by fully relax surface 3 layers and adatoms. Then transition states were evaluated using NEB method. We evaluated three paths for the Ni(110) surface. (see figure) Path A is surface diffusion without atom exchange, and paths B and C involve exchange of adatom and substrate atoms in so-called cross-channel diffusion. For a Ni adatom, the calculated diffusion barrier was 0.321 eV for path A, while 0.444 and 0 443 eV for paths B and C, respectively. We also evaluated the displacive diffusion for a Ni adatom on the Ni(100) surface. The diffusion barriers were 0.728 eV for path A without atom exchange and 1.105 eV for path B with adatom-substrate atom exchange. These values are comparable to the experimental results [1], but while experimentally there was an obvious difference in transition probabilities between paths B and C of the cross-channel diffusion, calculations showed virtually no asymmetry.

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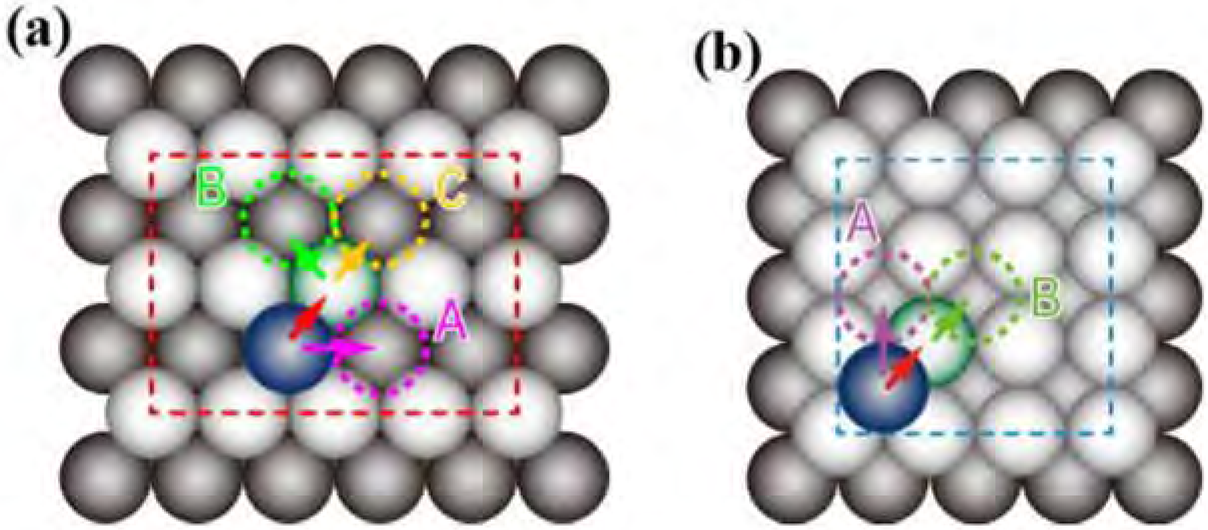

Fig. 1: Adatom migration pathways for (a) Ni(110) and Ni(100) surfaces. The unit cells used in the structural calculation are shown by the dotted lines. Initial adatom position is indicated by blue circle, and path A, B, and C on the Ni(110) surface and path A and B on the Ni(100) surface are indicated by purple, green, and yellow, respectively.

One-dimensional fluctuation of Ag overlayers on the Ni(110) surface

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[1]*Osaka Metropolitan University, Japan*

Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

The immiscible combination of metal thin film heterostructures has great potential to synthesize a new class of two-dimensional alloys that are unparalleled to their bulk counterparts and to realize a new type of catalysis and novel mechanical properties. Silver on nickel is one such immiscible metal combination, but only a limited number of studies have previously been performed on Ag/Ni(110) surfaces. Here we address the initial Ag thin film formation on the Ni(110) surface with Ag coverage 0.4-1.5 ML and the substrate temperature between RT-400°C studied by STM and LEED under UHV.

The STM image of 0.9 ML-Ag deposited at room temperature shows a stripe structure (A) along the [001] direction consisting of the epitaxially aligned Ag rows in the close-packed [1-10] row, and periodic grooves (C) with a depression of about 120 pm, indicating the absence of Ag atoms within the groove. In addition to the regular Ag stripes, we find a fussy region (B) connecting the stripes. This structure seems to be one-dimensional random motion of adsorbed Ag running within a [1-10] row. On the Ag/Ni(110) surface prepared at 200°C, it was confirmed that Ag was not alloyed with the Ni atoms of the substrate and that Ag formed a stripe structure over a wide area. Despite the high surface energy of the substrate, the second Ag layer was grown before the first layer was completed, and the stripe structure remained. This is due to the effect that Ag atoms are less likely to associate with Ni(110) substrate due to lattice mismatch, and a barrier is formed at the ends of the Ag row to prevent adsorption, resulting in a decrease in adsorption.

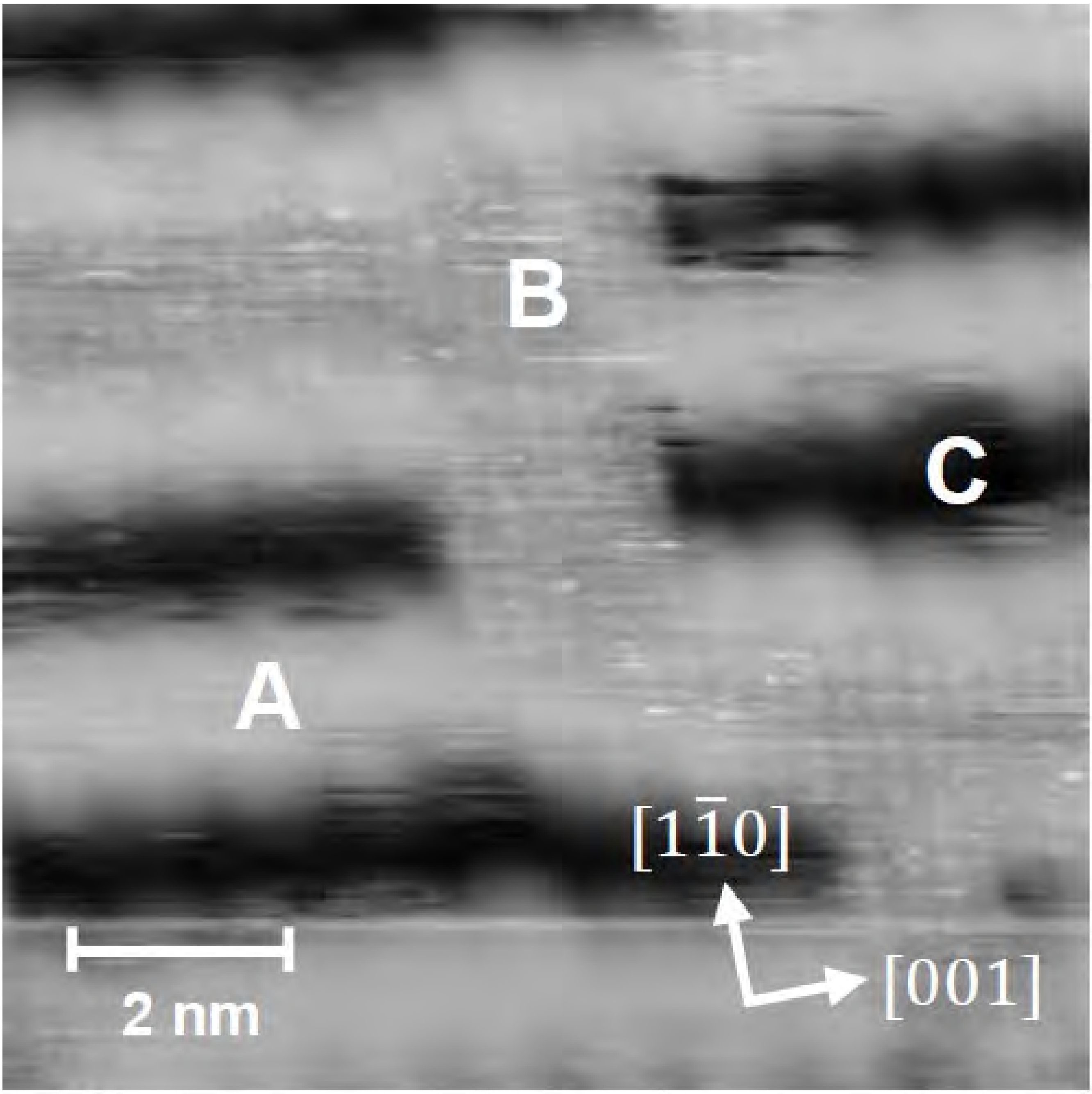

Figure: STM image of Ni(110) surface with 0.9 ML-Ag deposited at room temperature.

Advancements in Surface Analysis: 3D ToF-SIMS with Gas Cluster Ion Beams

Dr. Sam Lambrick[1,2], Nick von Jeinsen[1,2], Naoko Sano[2], Fauzy Nasher[3], Jonah Messinger[1], Kate McHardy[2], David Ward[1,2]

[1] University Of Cambridge, United Kingdom, [2] Ionoptika Ltd, United Kingdom, [3] London School of Health and Tropical Medicine, United Kingdom

Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) stands as a robust technique for surface analysis, offering spatial resolution coupled with high mass accuracy. The utilization of gas cluster ion beams (GCIB), particularly those employing large water clusters, has significantly expanded the scope of samples compatible with ToF-SIMS analysis[1]. This expansion is owed to enhanced ionization yields and the detection of molecular fragment ions with water GCIB beams.

The Ionoptika J105 instrument integrates a GCIB source with the capability for performing 3D tomographic ToF-SIMS measurements using a single DC ion source for both analysis and sputtering. In this poster, we present case studies employing 3D ToF-SIMS GCIB measurements on both biological and technological samples, demonstrating the 3D capabilities of technique.

[1] H. Tian, et al., “Multiomics Imaging Using High-Energy Water Gas Cluster Ion Beam Secondary Ion Mass Spectrometry [(H2O)n-GCIB-SIMS] of Frozen-Hydrated Cells and Tissue,” Anal. Chem., vol. 93, no. 22, pp. 7808–7814, Jun. 2021, doi: 10.1021/acs.analchem.0c05210.

Recent research on NEG coatings for HALF vacuum systems

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

The Hefei Advanced Light Facility (HALF), a new-generation diffraction-limited storage ring with a beam energy of 2.2 GeV, is currently under construction. It comprises 20 arcs and straight sections, each with unique geometries. To mitigate photon-stimulated desorption (PSD) and ensure distributed pumping within the narrow 26 mm aperture vacuum chambers, a decision has been made to coat most of these chambers with a non-evaporable getter (NEG) film. The NEG films were deposited using specialized DC magnetron sputtering equipment with a Ti-Zr-V alloy target. Extensive studies have been conducted on the microstructure, thermal activation characteristics, pumping properties, and PSD behavior of the NEG films. Additionally, the activation process, storage, and lifetime of the NEG have been thoroughly evaluated.

A framework for multiscale thermal simulations of batteries

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Battery degradation is temperature dependent. Indeed, despite the widespread usage of battery management systems to regulate the average battery pack temperature, thermal gradients still occur due to uneven heat dissipation [1]. This is especially true in high-performance applications such as EVs, particularly during fast charging, and causes uneven degradation, reducing performance and cyclic life [2].

Batteries consist of unit cells, each with two electrodes, anode and cathode, each flanked by a current collector, and an electrical separator soaked in a liquid electrolyte. Pouch cell batteries in smartphones, for instance, have approximately fifty unit cells. Heat is primarily generated in the electrodes [3] and dissipates outward through the current collectors to the external circuit, a phenomenon which is not adequately accounted for in existing models.

Traditional models based on the heat equation are usually 2D, not parallelised, and often resort to partial or full homogenised geometries to reduce the computational cost, hampering accuracy. An accurate temperature field is crucial to better inform performance and mechanical stress simulations, to improve cooling system design, and to better predict and prevent degradation. We propose a finite element thermal model that accurately captures the physics across the full heterogeneous unit cell and up to the full battery scale at reasonable computational cost. This model will be informed by a surrogate model trained on PyBaMM, which incorporates the surface lithiation between electrode particles and liquid electrolyte. Future plans include GPU optimisations and simulations of prismatic, pouch and cylinder cells.

Understanding of battery technology by auto-manufacturers has historically been limited to the pack level. However, the move towards electrification has increased the pressure to optimise designs at the unit cell level. We believe that multiscale models, such as the one presented here, would accelerate the development of more efficient battery packs.

[1] https://doi.org/10.1149/2.0791702jes
[2] https://doi.org/10.1038/s44172-022-00005-8
[3] https://doi.org/10.1002/ente.202000915

On the application of components manufactured with stereolithographic 3D printing in high vacuum systems

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

We report on a method for using stereolithographic (SLA) additive manufacturing to rapidly and cheaply prototype components for use in high-vacuum environments. We demonstrate the primary vacuum contaminant from freshly printed SLA plastics is water with no evidence of polymers out-gassing from the material and thus the vacuum performance can be controlled with simple treatments which do not involve surface sealing. An unbaked vacuum system containing SLA printed parts achieved 1.9e-8 mbar base pressure whilst retaining structural integrity and manufacturing accuracy. Preliminary results indicate that our method can be extended to achieve ultrahigh-vacuum compatibility by baking at higher temperatures. We further report on the effect of atmospheric exposure to components and present evidence to suggest that re-wetting occurs exclusively in the component skin layer, by showing that the bulk mass changes of the material is irreversible on the timescale investigated (< 2 weeks).

Multi messenger imaging of bacterial biofilm composition and topography

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Here we present recent work related to the study of biofilms; Microbial communities embedded in a 3D extracellular matrix. The matrix is composed of a complex array of extracellular polymeric substances that contribute to the unique attributes of biofilm lifestyle. Samples of bacteria and the biofilms they evolve are prepared and the growth arrested after a set period, with the resulting sample analysed with distinct imaging techniques. We present data from Ionoptika's water cluster secondary ion [SIMS] which offers a mass and depth resolution to aid understanding of the spatial composition of the biofilm by visualising the 3D structures within. In addition, we present the first images of bacteria using a completely surface sensitive neutral beam microscopy technique (SHeM).

A key benefit of water cluster SIMS is its ability to achieve high depth resolution due to the low kinetic energy of the water clusters, which allows for the analysis of surface and subsurface structures with a high degree of precision [1]. The use of water clusters as the primary ion source also minimises sample damage and fragmentation of high m/z species which are common issues with other ion beams [2,3]. Water cluster SIMS was used in Ionoptika's J105 system with a beam spot size of down to 1.5um.

[1] Tian, Hua, et al. "Multiomics imaging using high-energy water gas cluster ion beam secondary ion mass spectrometry [(H2O) n-GCIB-SIMS] of frozen-hydrated cells and tissue." Analytical Chemistry 93.22 (2021): 7808-7814.
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Exploring diffractive contrast in scanning helium microscopy

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Scanning Helium Microscopy (SHeM) has recently demonstrated its efficacy as a surface microscopy technique utilizing neutral helium atoms as probe particles, capable of acquiring helium atom diffraction patterns on a microscopic scale [1]. This advancement has unveiled new contrast mechanisms, notably diffraction and specular contrast. In this study, we investigate monolayer MoS2, alongside bulk MoS2, hBN, and SiO2, to explore these novel contrast mechanisms.

Our results reveal distinct spatial contrasts between various substances (e.g., MoS2 to hBN and MoS2 to SiO2) when interacting with helium atoms, highlighting the potential of SHeM in material characterization. Furthermore, we conduct simulation work, using a ray tracing based framework to complement experimental findings, assessing the capability of SHeM for polycrystalline samples of different types and the mapping of different phases of 2D materials.

[1] 2D Helium Atom Diffraction from a Microscopic Spot
Nick A. von Jeinsen, Sam M. Lambrick, Matthew Bergin, Aleksandar Radić, Boyao Liu, Dan Seremet, Andrew P. Jardine, and David J. Ward
Phys. Rev. Lett. 131, 236202 – Published 6 December 2023

An experimental and theoretical study of Zinc Ferrite Single Crystals

Charlotte Hall[1,2], Dr Ivan da Silva[3], Professor Frank de Groot[4], Professor Bo Iversen[5], Dr Peter Bencok[1], Dr Santosh Kumar[1], Professor Georg Held[1,2], Dr David Grinter[1], Dr Pilar Ferrer[1], Dr Ricardo Grau-Crespo[2]
[1]Diamond Light Source, United Kingdom, [2]University of Reading, United Kingdom, [3]ISIS Neutron and Muon Source, United Kingdom, [4]Utrecht University, The Netherlands, [5]Aarhus University, Denmark

Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Zinc ferrite (ZFO) is a metal oxide with a spinel structure, (Zn1-xFex)[Fe2-xZnx]O4, where () represents the tetrahedral sites, [] represents the octahedral sites, and x is the degree of inversion ($0 \leq x \leq 1$). Due to its compositional diversity, ZFO has been identified as a potential catalyst for photocatalytic water splitting. The photocatalytic activity is influenced by its electronic structure, which changes with a varied degree of inversion. Therefore, understanding the cation distribution at the surface is crucial in catalysis studies.

Bulk ZFO is generally reported as a normal spinel ($x = 0$), however in nanoparticle form the cation distribution increases and can be easily influenced by factors such as preparation method or thermal treatment. Studies into nanoparticle and single crystal (111) ZFO samples were completed to understand the surface and bulk effects on the cation distribution and oxidation states. A combination of experimental techniques (x-ray diffraction and spectroscopy techniques) and advanced computational methods (DFT and semi-empirical methods) have been used.

Surface Characterisation of Thin Film V3Si deposition using HiPIMS

Christopher Benjamin[1,2], Reza Valizadeh[1,2], Stephane Simon[4], Liam Smith[1,2], Daniel Seal[1,2,3], Oleg Malyshev[1,2], Graeme Burt[3]

[1]STFC ASTeC, United Kingdom, [2]Cockcroft Institute, United Kingdom, [3]University of Lancaster, United Kingdom, [4]University of Liverpool, United Kingdom

Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

V3Si is one of a few materials currently marked as a potential alternative to Nb in next generation thin film SRF cavities. The relatively high critical temperature (Tc) could allow for operation at higher temperatures (≥ 4 K) reducing the complexity of the cryogenic system. Furthermore, V3Si can achieve a higher critical field leading to higher accelerating gradients. We explore thin film deposition of V3Si films using HiPIMS and Bipolar HiPIMS techniques on a single alloy target. The films are characterised by cryogenic four point probe, X-ray diffraction, secondary ion mass spectroscopy and energy dispersive X-ray spectroscopy.

Novel photocathode production method for CsTe Photocathodes via Cs Ion beam sputtering

Christopher Benjamin[1,2], Reza Valizadeh[1,2], Lee Jones[1,2], Hugh Churn[1,2]
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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Thin film Caesium Telluride (CsTe) is a widely used as the photocathode material driving many accelerators. It is typically chosen for its high quantum efficiency (QE) and its relatively long operational lifetime compared to other alkali based alternatives. Current production methods rely on Cs dispensers that are usually limited to the deposition of a few thin film cathodes per dispenser. Furthermore, Cs dispensers are typically loaded with an air stable compound which decomposes when heated to produce the film which may introduce a low level of contamination. We demonstrate a novel production method for CsTe photocathodes via Cs ion beam and ion beam sputtering of a high purity Te target, allowing for fine control of film thickness and composition. The cathodes are characterised using X-ray photoelectron spectroscopy and QE measurements.

Optimisation Of Niobium Thin Film Depositions For Superconducting Radiofrequency Accelerating Cavities

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Particle accelerators use superconducting radio frequency (SRF) cavities because of their extremely low surface resistance, allowing for continuous wave operation and low beam losses. For over 50 years, the majority of SRF cavities have been made from bulk niobium. However, in recent years niobium thin films (TF) coated on copper have been used instead. This has importantly allowed for lower material costs, creating a pathway to more sustainable accelerators. To accelerate the progression of TF development it is desirable to optimise deposition parameters on small, flat samples. For these samples, RF measurements are the most important characterisation technique, but this requires bespoke, non-commercial facilities. At Daresbury Laboratory, a high-throughput RF facility was commissioned that uses a novel 7.8 GHz choke cavity. The facility can evaluate the RF performance of planar-coated TF samples at low peak magnetic fields with a high throughput rate of up to 3 samples per week. Using this facility, an optimisation study of the deposition parameters of TF niobium samples deposited by HiPIMS has been performed. This study presents details on the deposition process used, DC and RF measurements, and results from surface analysis, such as XRD, SIMS, SEM and roughness measurements.

Cryogenic Facilities For Superconducting Thin Film Characterisation

Mr Daniel Seal[1,2,3], Dr Christopher Benjamin[1,2], Professor Graeme Burt[2,3], Mr Nathan Leicester[2,3], Dr Oleg Malyshev[1,2], Mr Kam Sian[1], Dr Taaj Sian[1,2], Mr Liam Smith[1,2], Dr Reza Valizadeh[1,2], Mr James Wilson[1]
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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

There is a growing desire for thin film (TF) coated superconducting radio frequency (SRF) cavities to improve the sustainability of current and future particle accelerators. Optimisation of thin film (TF) coating parameters for these cavities first requires rapid testing of various superconducting properties on small, planar samples. In addition, TF analysis on cavity-like geometry is possible on recently developed split-6 GHz cavities. For testing, three cryogenic vacuum facilities, based on liquid helium free cryocoolers, are in operation at Daresbury Laboratory. These allow for multiple sample tests per week under DC and RF conditions:

(1) A dedicated multiprobe facility. This has vacuum tubular inserts where the sample probe can be loaded and cooled with He gas. Experimental inserts allow for measurements of critical temperature, residual resistance ratio and magnetic field measurements of samples up to 10 x 10 mm2 at a rate of 2 per day.

(2) A magnetic field penetration facility allows for characterisation of planar samples up to 100 mm diameter and split 6 GHz cavities under DC magnetic field conditions at a rate of 3 per week.

(3) An RF facility allows for characterisation of planar samples up to 100 mm diameter under low field RF conditions and split 6 GHz cavities at a rate of 3 per week.

Synthesis and characterization of graphite anode with more stability and wettability by coating alumina layer from aluminium salt

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

The most essential indications of electric vehicle performance are safety, charging speed, and battery capacity. Wettability is critical to the rapid charging and stability of lithium batteries. In this paper, graphite coated by alumina are synthesized using a simple solution method without toxic gas produced to improve wettability and battery stability. To prevent a decrease in electrical conductivity, the alumina extent is limited. The TEM shows alumina layer applied to the graphite has a thickness ranging only from 7nm to 30nm. Graphite coated by 0.5wt% alumina exhibits reversible specific capacity 318 mAh g-1 at current density 50 mA/g and only dropped from to 308 mAh g-1 when current density increased to 2000 mA/g. Electrochemical impedance spectroscopy analysis reveal the wettability of anode is increased after alumina introduced. The cycle performance for both half-cell and full-cell reveal the introduction of alumina improved the stability of anode. Overall, this work provides a practical and environmentally friendly method to obtain graphite anode with more stability and wettability for lithium-ion batteries.

Modification of CdZnTe crystal surface properties by femtosecond laser pulses

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Experimental study of the peculiarities of CdZnTe crystal surface modification by ultrashort laser pulses has been carried out at low laser fluencies (near the visual modification threshold) to determine changes in the semiconductor surface properties. Laser irradiation was carried out by femtosecond laser pulses at a wavelength of 1.030 µm and a pulse duration of 300 fs, which corresponds to the transparency region of CdZnTe crystal [1]. The modified surface is analyzed by optical, micro-Raman spectroscopy and low temperature photoluminescence. Detailed analysis of optical images did not reveal the occurrence of dislocations due to heating of the crystal lattice by infrared radiation. A shift of the 122 cm-1 peak to the red region up to 120 cm-1 (Fig.1) was detected in the Raman spectrum, which was attributed to the reduction of mechanical stress around the Te inclusions in the CdZnTe matrix [2]. Photoluminescence measurements at low temperature showed that no change in the intensity of the A0X peak and the appearance of the Y dislocation band were observed in the samples irradiated with laser intensities below the visible surface modification levels

Fig.1. Raman shift of CdZnTe after laser irradiation

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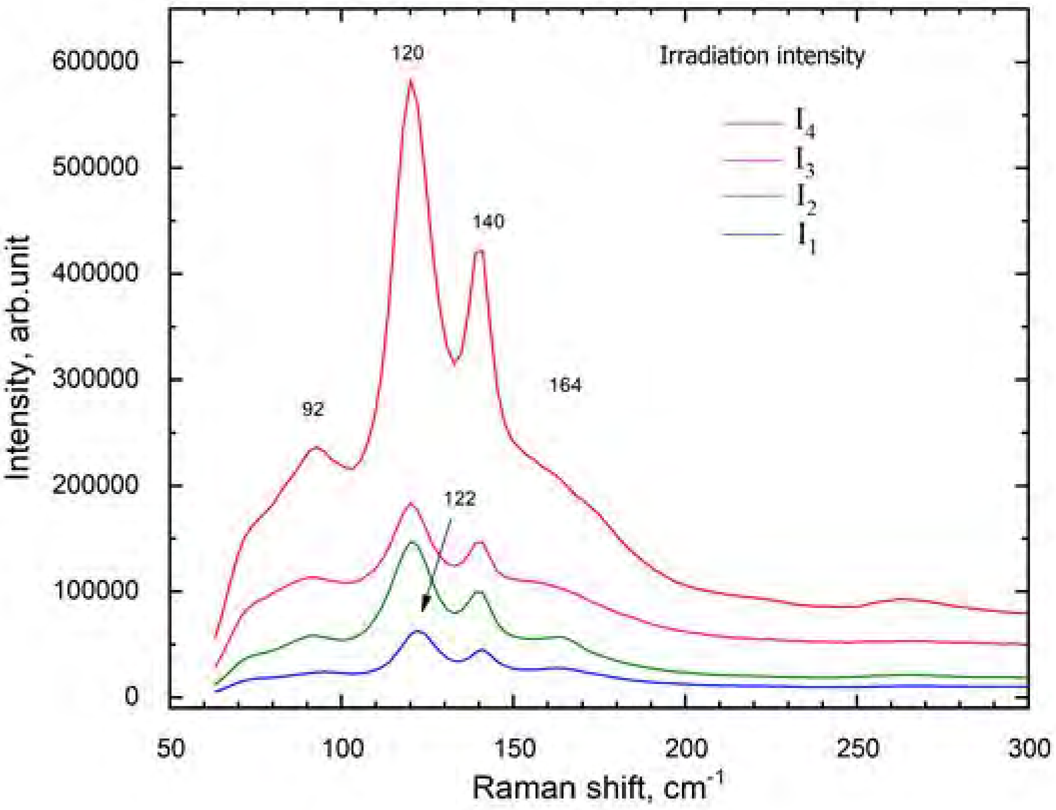
Irradiation intensity
I_4
I_3
I_2
I_1
120
140
92
164
122
600000
500000
400000
300000
200000
100000
0
Intensity, arb.unit
50
100
150
200
250
300
Raman shift, cm^{-1}

In-situ Near-Ambient Pressure Scanning Tunneling Microscopy Study of MoS2 for Hydrodeoxygenation Applications

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

More than 20% of greenhouse gas emissions in the EU are produced by the heavy transport and aviation sector. Pyrolysis oil derived from biomass is a realistic and promising replacement for fossil fuels for aviation and heavy transport applications, as currently there are no suitable electric or fuel cell alternatives. Fast pyrolysis is a process of decomposing biomass into pyrolysis oil by rapidly heating it in an oxygen-free atmosphere. An advantage of pyrolysis oil derived from biomass is that it is compatible with the existing infrastructure that is used in the catalysis and distillation of jet fuels and diesel. However, the oxygen content in pyrolysis oil derived from biomass is unacceptably high (up to 50%) and can lead to corrosion and instability [1].

To produce useful and efficient hydrocarbons from the pyrolysis oil, a pre-treatment and hydrodeoxygenation (HDO) step is required to be added to the refining process. Molybdenum disulphide (MoS_2) has previously demonstrated its effectiveness as a catalyst in hydrodesulphurisation (HDS) and has further shown to be a promising candidate as a catalyst in HDO and is therefore the primary material of interest in this study [2].

To develop atomistic structure determination of the catalyst and elucidate the reaction pathways for oxygen-containing molecules during HDO, model studies are required. In this study, model MoS_2, supported by gold, has been exposed to oxygen-containing molecules and characterised using the surface-sensitive techniques, near-ambient pressure scanning tunnelling microscopy (NAP-STM), and near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS). By using these complementary techniques, we can gain insight into both the chemical and physical changes of MoS_2 upon exposure to oxygen-containing compounds.

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Out-of-plane growth of 2D molybdenum diselenide nanosheets on ultrafast laser-structured substrates

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

In out-of-plane configuration, TMDs exhibit roughness and high specific surface area along with a strong bonding to the surface through boundary atoms in the 2D plane and at the substrate. This latter feature adds complexity to the properties since the monolayers/multilayers acquire an interface-induced asymmetry. These, and other kinds of porous TMDs are key in applications calling for ion or gas exchange, as in many catalytic, energy storage or sensing applications [1, 2].

In this study, we explore the morphology and orientation of molybdenum diselenide, a Van der Waals 2D material, through isothermal closed space vapor deposition on both pristine and laser-structured substrates. Laser structuring is conducted on dielectric (sapphire), semiconductor (silicon), and conductive (titanium nitride) substrates using ultrashort laser pulses, resulting in smooth topographic changes such as laser-induced periodic surface structures (LIPSS) or selective ablation. Scanning electron microscopy (SEM) reveals the pivotal role of surface structuring in the growth of out-of-plane $MoSe2$ nanosheets. This effect is particularly pronounced on crystalline substrates like sapphire and silicon, exhibiting in-plane growth on pristine substrates. Additionally, Raman spectroscopy not only confirms the vertical orientation of flakes on structured substrates but also highlights the presence of active edge sites by demonstrating an increased abundance of deposited material. Overall, our findings emphasize the controllability of directing the growth of $MoSe2$ flakes through appropriate pre-treatment of the substrate, with potential applications in various fields, including Surface-Enhanced Raman Scattering (SERS). Furthermore, the scalability, reproducibility, and applicability to any substrate make ultrashort laser structuration a highly promising general strategy for orienting 2D materials.

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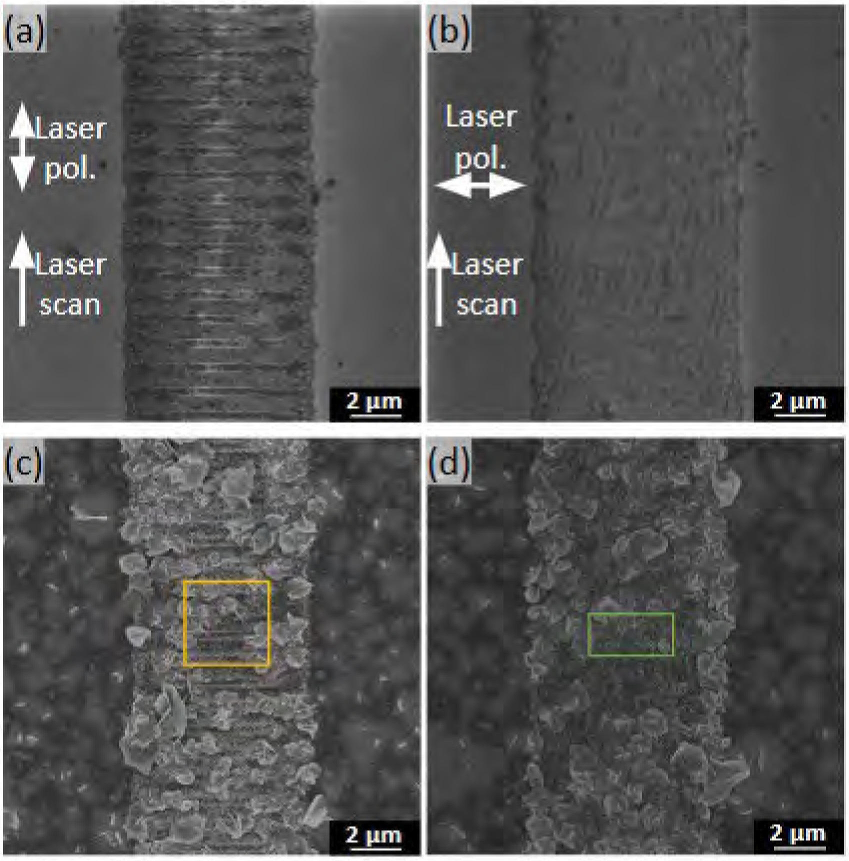
(a)
Laser pol.
Laser scan
2 µm
(b)
Laser pol.
Laser scan
2 µm
(c)
2 µm
(d)
2 µm

Multi-detector scanning helium microscopy

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Multi-detector scanning helium microscopy

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Scanning helium microscopy (SHeM)[1-2] is an emerging surface imaging technique that uses neutral helium atoms as the probe particles. The low energy and unique surface sensitivity of neutral atoms makes SHeM suitable for characterizing a wide range of materials without any concerns of beam damage. A 2nd generation of SHeM has been built in Cambridge, with a key advantage of multiple detectors, designed and developed for both topographical and diffracted contrast imaging. We explore some of the key advantages and uses of multi-detector scanning helium microscopy, such as 3D imaging, via heliometric stereo[3], mixed gas experiments, and simultaneous measurement with different imaging modes, e.g. forwards and backwards scattering. The mixed gas experiments utilised a combined He-Ar beam demonstrated for both topographic and diffractive contast.

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Improving operational stability of thin film perovskite solar cells in extreme humidity and thermal environments using ultra-thin hydrophilic polymer films.

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Since the emergence of third-generation thin film solar cells, represented by organic-inorganic hybrid perovskite solar cells (PSCs), there has been a notable interest in improving their performance using simple, accessible polymers. While some research focuses on hydrophilic polymers in PSCs, investigation into the operational stability hydrophilic polymer-bound PSCs under extreme conditions is limited, and the precise mechanisms of stability remain unclear.

This study investigates the role of ultra-thin hydrophilic polymer films in enhancing PSC stability. Utilizing advanced X-ray photoelectron spectroscopy techniques (XPS), including in situ XPS and hard XPS (HAX-PES), we elucidate the stability mechanisms of ultra-thin hydrophilic polymer layers in mitigating challenges posed by high humidity and temperature. Moreover, we delve into the contribution of these layers in passivating defect sites and bolstering PSC stability under practical application pressures.

Optical tests reveal that introducing an ultra-thin hydrophilic polymer monolayer during perovskite crystallization effectively reduces defect site density in PSCs. The interaction between the polymer films and perovskite not only fills grain boundaries, minimizing pinhole formation, but also encapsulates perovskite microcrystals in situ. This is confirmed by further XPS quantitative and angle-resolved HAXPES depth analyses, validating polymer penetration into the crystal interior and its advantage in resisting moisture and thermal pressures. In situ XPS demonstrates that hydrophilic materials significantly delay PSC degradation induced by water and heat in ultra vacuum.

Notably, devices with added polymer hydrophilic films exhibit nearly a 10% increase in maximum power conversion efficiency (PCE) compared to untreated ones. After ~500 hours at 80% relative humidity, these devices retain about 90% of their optimum efficiency, while untreated ones drop to about 60%. In a 400-second high-temperature exposure test, modified devices retain 80% of their initial efficiency, while untreated ones retain only 50%, affirming the significant role of polymer hydrophilic films in enhancing PSC stability.

Revealing the Role of Magnesium in Mitigating the Properties of BCNO Material for Dye Adsorption, Antibacterial Activity : Experimental and Theoretical Investigation

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

Water is often exposed to many pollutants ranging from the presence of dye waste (physical and chemical) to pathogenic bacteria (biological). In the meantime, BCNO material appears as one of the promising solutions in wastewater treatment because it has high chemical and structural stability, is nontoxic, corrosion resistant, and its band gap energy can be regulated with the addition of dopants. Dopant Mg is proven to improve the physicochemical properties of semiconductor materials and can increase the concentration of superoxide (O_2^(•-)) which effectively damages the bacterial cell wall. Therefore, the synthesis of Mg-BCNO was carried out to analyze the effect of adding dopant on adsorption, photocatalytic and antibacterial activity, using the one pot - solid state method based on green chemistry and then applied to the degradation of methyl green dye by adsorption first, then photocatalysis which is destructive for the dye. The results of the XRD characterization of the Mg-BCNO material showed a higher peak intensity in the BN and BCN phases than BCNO. TEM results are in line with SEM-EDS results, showed a more even distribution of Mg-BCNO (hexagonal) particles compared to BCNO (turbostratic). UV-Vis DRS characterization showed a smaller band gap energy for Mg-BCNO, 3.95 eV. The PL characterization of Mg-BCNO material showed a high purple emission peak (367 nm) with a band gap of 3.38 eV; as well as a moderate and broad peak around the green emission (493 nm), with a band gap value of 2.50 eV. The adsorption test results showed a better performance on Mg-BCNO, 77,59 mg/g (90th minutes). Mg-BCNO was also shown to be active against E. coli and S. aureus with the average diameters of inhibition zone are 6.45 and 12.08 mm. These results indicate that Mg-BCNO has the potential as a good adsorbent, photocatalyst, and an antibacterial agent.

Synthesis of TiS_2 Nanoclusters on Au(111) Surface as a Model Platform for CO_2 Conversion

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

The utilization of (waste) carbon dioxide as a carbon source is attractive because it not only improves the atomic economics of that process but also leads to a quicker amortization of for example plant investments, especially in view of CO2 prize strategy in Europe. Hence, investigations on the thermal, photochemical or electrochemical utilization of carbon dioxide (CCU) become more and more important.[1] As shown in the literature, TiS2 reveals a high reactivity in CO2 conversion, for example in electrochemical cells.[2] However, a suitable model platform to understand the atomic-level details of the structure and the catalytic behaviour of TiS2 is widely missing except for one special case, which is limited by the use of an oxidizing sulfur source forming an AuSx precursor state and thus appears non-transferable to other relevant supports, such as oxides.[3]
Herein, we present such a model system consisting of TiS2 nanoparticles on Au(111) surfaces, rendering it suitable for atomic-level microscopy and spectroscopy techniques. A direct TiS2 synthesis route was developed based on the established protocol of other 2D transition metal dichalcogenides (TMDCs).[4] Our method involves titanium deposition onto Au(111) surfaces in the presence of different (organic) non-oxidizing sulfur sources. The resulting materials were characterized by combined scanning tunneling microscope (STM, see Figure 1) and X-ray photoelectron spectroscopy (XPS).

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A comparative X-ray spectroscopic study of on-surface synthesised 2D & 1D porphyrin-derived nanostructures on Au surfaces

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

High resolution C 1s, N1s and Br3d X-ray photoemission spectroscopy (XPS), carbon and nitrogen K-edge Near Edge X-ray Absorption Fine-structure Spectroscopy (NEXAFS) together with Scanning Tunnelling Microscopy (STM) have been used to study the on-surface synthesis of a variety of two-dimensional porphyrin-derived nanostructured networks and one-dimensional porphyrin-derived nanostructures on vicinal and flat gold surfaces. Precursors such as 5,10,15,20-tetrakis-(4-bromo,-2,3,5,6-tetramethyl-phenyl)-21H,23H-porphine (H2-T(BrTMeP)P), Ni-(5,15-dibromo-10,20-diphenyl) porphyrin (NiDBrDPP) are deposited at sub monolayer coverages on Au (788) and Au (111) crystals. Annealing induces dehalogenation of molecules, dehalogenation from substrate, progressive Ullmann coupling, and finally cyclo-dehydrogenation. The resultant cyclo-dehydrogenated nanostructures exhibit intrinsically different connectivity of the adjacent porphyrin macrocycles, whether as 2D networks with porphyrins covalently coupled to each other through intermediate structures or in the 1D case through triply-fused direct connections between adjacent porphyrin macrocycles within the tape. The on-surface synthesis is studied as a function of the annealing temperature via continuous monitoring of C 1s and Br 3d XPS signals. High resolution C 1s, N1s XPS and C and N K-edge NEXAFS is obtained from the as deposited stage; at the intermediate oligomer stage after full debromination and Ullmann coupling; and from the final cyclo-dehydrogenated linked 2D network and 1D tape nanostructures. Several distinct spectroscopic changes are noted between each stage for both systems studied on the Au(111) and Au(788) surfaces. Spectroscopic and STM results indicate successful formation of flattened π conjugated 2D networks and 1D tapes. The contrast in the observed NEXAFS and the resultant electronic structure is elucidated by density functional theory simulations of these molecules, networks, tapes and their XPS and NEXAFS.

Growth of Si-Ag-Tl thin films for self-assembly of organic molecules

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Organic-inorganic hybrid nanoelectronics has the potential to combine the unique electronic properties of new 2D materials with the adaptable nature of organic molecules. They can be used in various practical applications, including electronics, photonics, spintronics, solar cells, chemistry, catalysis, medicine, and many others. The 2D materials are of particular interest to our research from the point of view investigating quantum phenomena.

For study of molecular nanostructures, flat, relatively large (≥ 100 x 100 nm2), and well-defined surfaces are necessary. Metals grown on silicon substrates usually provide such surfaces. In our study we focus on Tl bi-layer on flat Ag islands formed on the Si(111) surface [1]. In the case of bi-layer materials with global inversion symmetry, locally broken inversion symmetry can generate degenerate spin-polarized bands, in which the spins in each layer are oppositely polarized. This fact could be utilized in the development of spintronic devices. In addition, the layer has the potential to transition into a superconducting state at temperatures below 0.9 K [1].

Deposition of few monolayers of Ag on the Si(111) substrate at room or higher temperature does not produce surfaces with the required properties [2]. We found a way to enlarge the flat islands of Ag by using Tl as a surfactant. Our thin films were observed by the scanning tunneling microscope, which confirmed the structure of Tl bi-layer on large-enough Ag islands. Further we observed molecular nanopatterning formed after deposition of organic molecules onto the surface.

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Ab initio calculation of matter wave interactions with strained surfaces

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Helium atom microscopy is a new form of microscopy that has been shown to exhibit unique contrast compared with other imaging techniques. It offers an ultimate resolution approaching charged beams while being totally surface sensitive and due to the low energy in the beam – completely non-destructive [1]. We extend the contrast mechanisms of scanning helium microscopy to include imaging of mechanical properties such as strain. The diffraction from the surface potential of the (001) plane of an α-quartz crystal was calculated using a combination of density functional approach and close-coupled scattering calculations. A systematic theoretical study of the formation of surface structures and domains previously investigated using helium atom scattering is presented [2]. The strain response of the α-quartz surface in an external static electric field is studied in the framework of perturbative density functional theory. The atomic displacements when a macroscopic field of 1 kV/mm is applied along the crystallographic axis are in good agreement with experimental data obtained from x-ray scattering intensity variations. In this work, we calculate the variation of diffraction intensity and corrugation with piezoelectric strain in different external electric fields.

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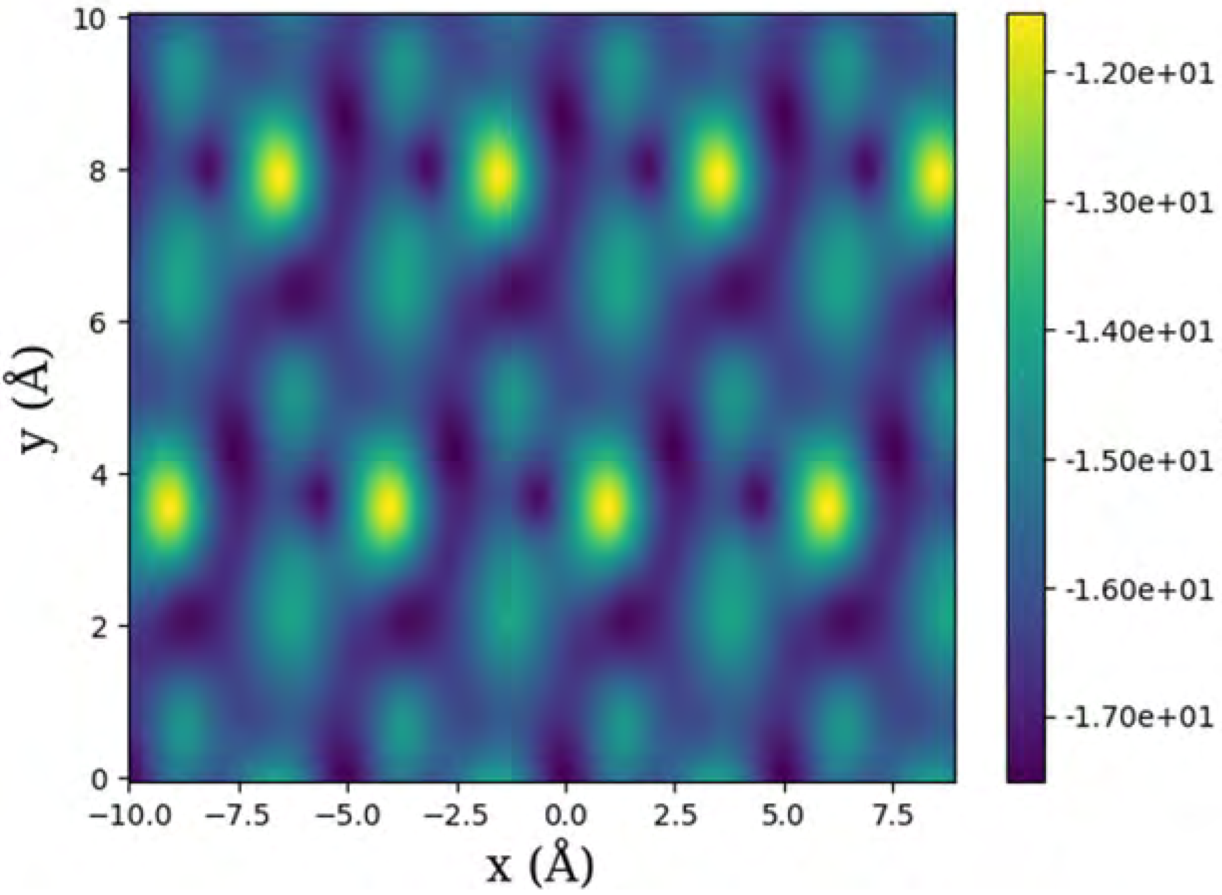

Design of the Vacuum System for the High-Energy Beam Transport Section of RAON

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

The heavy-ion accelerator (RAON) currently under construction in Daejeon is an experimental facility capable of accelerating heavy ions such as uranium to produce various rare isotopes. It is designed to accelerate ions ranging from protons to uranium, obtaining beam energy (200MeV, beam power 400kW). Currently, the construction of the low-energy acceleration section (SCL3, Superconductor LINAC 3) has been completed, and successful primary beam extraction experiments have been conducted. Beams passing through the low-energy acceleration section are provided to the experimental facility via the high-energy acceleration section. To deliver the accelerated high-energy beam to each experimental facility without beam loss, the establishment of ultra-high vacuum system is necessary. In this paper, we will discuss the design of the vacuum system for the high-energy beam transport section.

Computational Prediction of Material Properties for New and Improved Superalloys

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Superalloys have been investigated and used over the past several decades and are known for their corrosion and high temperature resistance, high strength, and hardness. These properties are advantageous for both automotive and aerospace applications, and more specifically are vital for the development of efficient and robust gas turbine engines as they enable safer and more reliable engines whilst resisting thermal fatigue. For Ni superalloys to exhibit specific required properties, they must be synthesised through sophisticated metallurgical processes such as heat treatment in a specific heat range using an elemental composition in well-defined ranges. The challenge of optimising these superalloys is the existence of multiple phases within the material some of which are responsible for superalloy performance at high temperatures, but which can transition into other phases as temperature increases. A methodology that can computationally predict the performance of different compositions of superalloys is CALPHAD (CALculation of PHAse Diagrams), which can account for the thermodynamic interaction of multiple phases. CALPHAD depends on databases that are not always available for complex materials or are not open source. In this work, we will develop a CALPHAD toolkit for the prediction of phase diagrams and thermodynamic properties of Ni-superalloys, laying the foundation upon which we can build in the future for the design of other superalloys. The fundamental physics-based models will be explored and developed for analysis and modelling purposes and to generate the databases. In addition, the statistical models will be used to quantify the uncertainties of the results and optimize the assessments. The toolkit will enable the prediction of new, improved Ni-superalloys for use in energy and transportation, by predicting performance measures of new compositions both in the bulk and on surfaces or even interfaces with various materials.

Effect of subsurface hydrogen on formation and stabilisation of enol form of 2-acetylpyridine

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

The stability of the C=O bond makes hydrogenation of carbonyl compounds challenging and thus requires effective catalysts. There is an ongoing discussion on a possible low-temperature hydrogenation pathway proceeding via formation of enol form of a carbonyl compound followed by H insertion into the newly formed olefinic bond. This two-step process was theoretically predicted to proceed via significantly lower activation barriers as compared to the direct hydrogen insertion into the C=O bond. The major challenge of this mechanism is the low stability of enol species that – if not deliberately stabilised – would readily convert to ketone under the reactive conditions.

In this contribution, we present a mechanistic study on keto-enol tautomerisation of a carbonyl compound 2-acetylpyridine (APy) performed by a combination of infrared reflection absorption spectroscopy (IRAS), molecular beam techniques and scanning tunneling microscopy (STM) to investigate its adsorption behaviour and formation of the enol form on Pd(111) in presence of hydrogen. The main focus lies on the understanding of the role of different hydrogen species – Hsurf adsorbed on the surface vs. Hsub absorbed in the subsurface region of Pd – on the formation and stabilisation of enol form of APy. Particularly, we show spectroscopically that APy can readily convert to the enol form on all types of Pd surfaces, however, the largest amounts of the enol species were detected in the presence of subsurface Hsub. Complementarily, the STM results indicate that the enhanced evolution of enol species on Hsub-containing Pd is accompanied by formation of the specific acetyl-acetyl dimers, interacting via the acetyl groups. This specific interaction is most likely responsible for the efficient formation and stabilisation of the enol species.

Electrostatic properties of POM by frequency modulated EFM combined with Fowler-Nordheim tunneling spectroscopy

Masahiro Nakayama[1], Ryo Tsunashima[2], Hiroshi Ohoyama[1], Takuya Matsumoto[1]
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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Polyoxometalates (POM) are polynuclear molecular clusters whose basic unit is a 4-7 coordinated polyhedral structure of oxygen atoms on a transition metal. POM is known to exhibit unique electronic properties due to its high electron acceptive and redox-induced mixed valance state with delocalized electrons in the cluster. Understanding the electronic properties of POM requires essential knowledge of its energy level positions and dielectric constants. However, due to its large cluster size, quantum chemical simulation of dielectric constants is infeasible. Previously, the LUMO conduction and dielectric constant of Ru complexes arranged in multilayers have been reported by Electrostatic force microscopy (EFM) combined with Fowler-Nordheim tunneling spectroscopy[1]. In this study, we employed a type of POM known as {Mo154/152}-ring[2] and determined dielectric constants using EFM combined with Fowler-Nordheim tunneling spectroscopy (Fig. 1).

In sample preparation, Au(111) film grown on a mica substrate was immersed in ethanol solutions (1 mM) of 6-amino-1-hexanthiol (6-AHT) for two hours. Subsequently, they were immersed in a solution of {Mo154/152}-ring for one hour.

EFM spectra of POM/6-AHT/Au indicates electrostatic energy loss around ±5 V. The value of energy, ξ, plotted against external bias voltage in the negative region is fitted well with Simmons' equation [3], showing a Fowler-Nordheim tunneling process. The coefficient β representing the split field between POM and 6-AHT revealed huge the dielectric constant of ca. 50.

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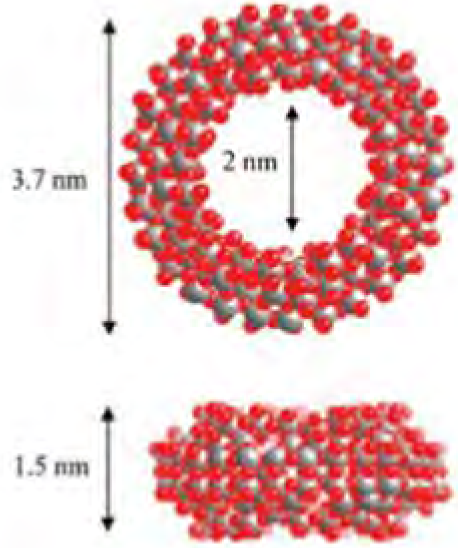
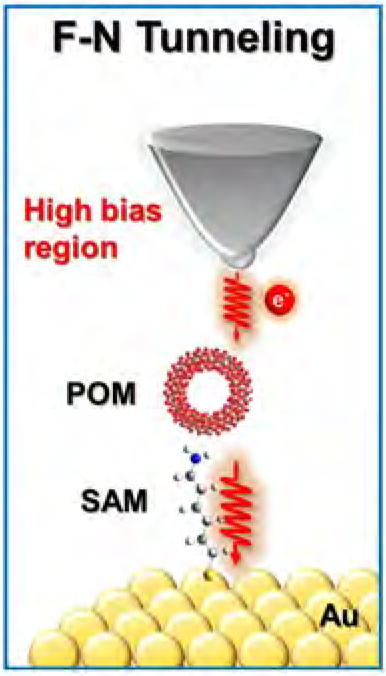

3.7 nm
2 nm
1.5 nm


F-N Tunneling
High bias region
e-
POM
SAM
Au

Fabrication of Clean-Surface Microcrystals by Field Ion Beam for Surface Spectroscopy

Fumio Komori[1,2], Yanze Guan[1], Masafumi Horio[1], Atsushi Fukuda[2], Yuki Tsujikawa[1], Kenichi Ozawa[3], Masao Kamiko[2], Daisuke Hamane[1], Taizo Kawauchi[2], Katsuyuki Fukutani[2], Yuki Tokumoto[2], Keiichi Edagawa[2], Ryuji Tamura[4], Iwao Matsuda[1]

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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

There are plenty of interesting single crystals on the micrometer scale. Recent developments of microscopy technique have made it possible to use them for microspectroscopy. In the case of high-resolution surface-sensitive electron spectroscopy such as angle-resolved photoelectron spectroscopy (ARPES), it is important to keep the surface clean and ordered. By cleaving the sample in situ in an ultra-high vacuum, electronic properties of microcrystals have been studied with such micro-spectroscopic methods. However, there are many small single crystals for which simple cleavage is not directly applicable.

In the present study, we develop a new microfabrication method for fixing small crystals to solid substrates based on focused ion beam (FIB)-scanning electron microscopy (SEM) to study their electronic properties in detail using surface-sensitive methods. [1] Microfabrication using FIB-SEM has been widely used for preparing small samples. The surface of the sample prepared by FIB is, however, usually contaminated and/or amorphized by the focused ions. It has been difficult to use them directly for the surface-sensitive analyses. Here, using highly oriented pyrolytic graphite, we show the FIB milling process with keeping the surface clean and ordered. We prepared tens micrometer scale graphite attached firmly on Si or Cu substrates through tungsten deposition in FIB-SEM. We evaluated the cleanliness of the surface using SEM with energy dispersive X-ray spectroscopy, and microbeam X-ray photoelectron spectroscopy. Our microbeam ARPES measurements successfully obtained the bulk band structure of the single-domain micrographite.

The present fabrication method offers a new solution to realize detailed characterization by surface-sensitive electron spectroscopy for newly discovered interesting micromaterials. In particular, the target is those grown on non-flat surface, synthesized as a mixture of microcrystals with various orientations, or mixed with other materials.

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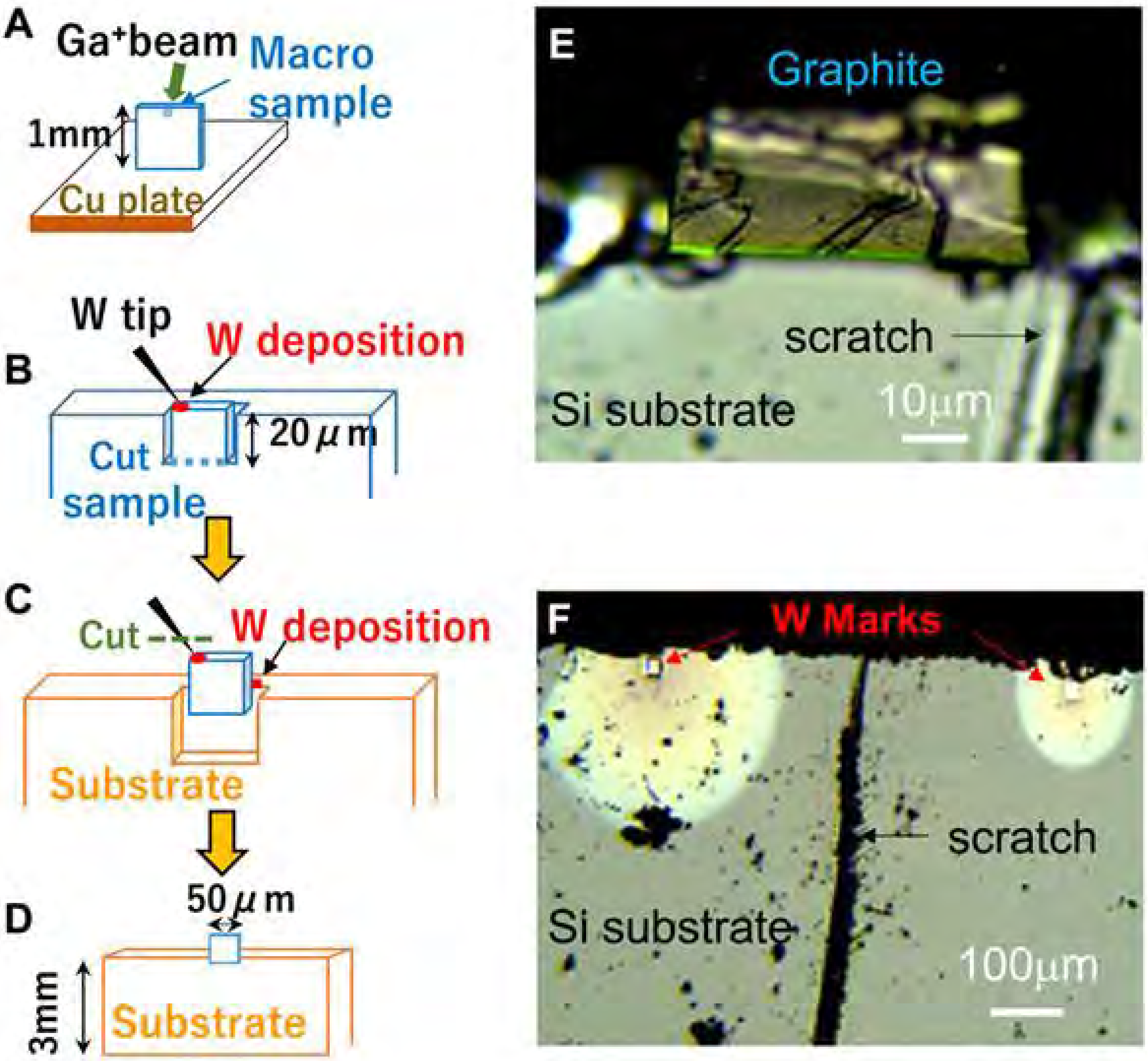

Figure 1: (A-D) Sample preparation process in FIB-SEM. (E,F) Optical microscope images of the micro-sample on the Si substrate.

Spectroscopic studies of on-surface synthesis of chiral graphene nanoribbons on Ag (111)

Dr. Igor Chunin[1], Mr. Lee Gannon[1], Prof. Attilio A. Cafolla[2], Prof. Valentina De Renzi[3], Dr. Nicola Cavani[3], Dr. Alexei Preobrajenski[4], Dr. Alexander Generalov[4], Dr. Nikolay Vinogradov[4], Dr. Stefan Appelfeller[4], Dr. Zongping Chen[5], Prof. Akimitsu Narita[5], Prof. Klaus Muellen[5], **Prof Cormac McGuinness**[1]

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Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

The building blocks or precursor materials for on-surface synthesis of all-types of graphene nanoribbons (GNRs) and other nanostructures have increased very rapidly in recent years. Graphene nanoribbons synthesised on different metallic surfaces under ultrahigh vacuum (UHV) conditions through thermal dehalogenation, Ullmann coupling and dehydrogenation have led to bandgap engineering and new molecular electronics. The most extensively investigated have been armchair edge GNRs starting with on 10,10´-dibromo-9,9´-bianthracene (DBBA) [1] molecular precursors on many surfaces. More recently interesting heteroatom doped (4,1)-chiral GNR were demonstrated arising from the 6,16-dibromo-9,10,19,20-tetraoxa-9a,19a-diboratetra-benzo[a,f,j,o]perylene monomer [2], which embeds O-B-O motifs along the GNR edge as observed on Au(111) by scanning tunneling microscopy (STM). Spectroscopic studies of their on-surface synthesis has been extended to the formation of these (4,1)-chiral GNRs on Ag(111). This has been through temperature dependent synchrotron based core level x-ray photoemission spectroscopy (XPS) of the C 1s, O 1s, B 1s and Br 3d core levels and measurements of the C, B and O K-edge near-edge x-ray absorption fine structure (NEXAFS) spectra, combined with in-situ scanning tunnelling microscopy (STM) studies. This spectroscopic data is presented for each stage of the on-surface synthesis: 1) precursor molecules; 2) polymerised chains and 3) fully formed cyclodehydrogenated chiral (4,1)-OBO-GNRs; all simulated through density functional theory (DFT) using the StoBe implementation3. Comparison is made between the simulated and observed high-resolution core-level SXPS during the temperature-dependent on-surface synthesis. NEXAFS data presented here correlates with the final STM and XPS measurements. The interaction with the Ag substrate and Ag adatoms via intermediate organometallic chains is discussed..

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Origin of various appearance of oxidation in ambient-stable β- InSe

Eunji Sim[1,2], Dongwook Kim[3], Thi Huong Nguyen[4,5], Jehan Kim[1], Ha Eun Cho[1,4], Somang Koo[1], Sunglae Cho[4], Ji Hoon Shim[3], Seong Chu Lim[2], Kyuwook Ihm[1]

[1]Pohang Accelerator Laboratory, South Korea, [2]Sungkyunkwan University, South Korea, [3]Pohang University of Science and Technology, South Korea, [4]University of Ulsan, South Korea, [5]Nha Trang University, Vietnam

Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Understanding and controlling the oxidation of layered materials remains a key interest in the final stage toward practical device applications of them. Although layered materials with broken inversion symmetry have a band gap, but the oxidation process became more complicated. Representively, InSe has drawn a lot of attentions because it shows not only high charge-mobility but also a Si like bandgap. However, the oxidaton process of this material is not understood in a consistent way. Including contrasting evaluations of oxidation susceptibility, conflicting observation such as oxidation through Se and through In have been reported. Here, we report in-situ spectroscopy results showing the origin why different pathways of oxidation appear depending on the experimental conditions. We observed that, at low defect-density regime, the reduced reaction barrier of InSe by Se vacancy causes oxygen adsorption, while, as the defects increases, the lower electronegativity of In rises as a new path for oxidation. At low defect-density the bulk layer was more energetically favored for oxygen adsorption, which allows oxygen diffusing to a depth sufficient to build pseudo-hetero junctions and makes the surface layer seemingly resistant to oxidation. Our results provides the answer why the phenomenologically diverse oxidation and resulting diversity of optical responses has been observed, as well as strategies to achieve gas stability.

Dynamics and long-range ordering of perylene on Ag(110).

Dr Kirill Bobrov[1], Dr Lionel Amiaud[1], Dr Céline Dablemont[1], Dr Anne Lafosse[1], Dr Laurent Guillemot[1]
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Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

One of the challenges in molecular nanoelectronics is the integration of the bottom-up nanofabrication process into nanomanufacturing. The integration requires fabrication of arrays of functional organic molecules spatially ordered over an arbitrary large surface area and being in registry with the underlying substrate. Despite significant progress in the surface-templated nanofabrication, fabrication of the molecular arrays ordered at meso- or macroscale has not been achieved yet.

We present a room temperature STM and HREELS study of dynamics of the quasi-liquid perylene- Ag(110) interface driven by molecule recognition of specific substrate sites. Analysis of the STM topographies indicates that the atomically flat substrate provides memory to the molecular motion. The distinct motion modes, in turn, generate dynamically a compact two-dimensional (2D) quasi-liquid monolayer. Fourier transform (FT) unravels the long-range spatial correlations and epitaxial character of the quasi-liquid state. Analysis of the HREEL spectra indicates that the site recognition occurs via interfacial dynamic charge transfer. We show that the dynamic dipoles emerging within the interface under decay of the intramolecular vibrational C-C-H modes play a central role in the heterogeneous dynamics. We demonstrate that the quasi-liquid state possesses, therefore, dynamics, characteristic of a liquid, and long-range order, characteristic of a crystalline solid.

We anticipate that this duality, unattainable under conventional nanofabrication, opens perspectives to fabricate epitaxial long-range ordered nanostructures of arbitrary lateral size.

Physically Unclonable Functions Based on Heterostructured 2D Molybdenum Disulfide and Tungsten Disulfide

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[1]Korea Research Institute of Standards and Science, South Korea, [2]University of Science and Technology, South Korea

Poster Session 1 and Drinks Reception, June 17, 2024, 17:35 - 19:30

In the age of fifth-generation mobile networks, Internet of Things (IoT), and edge computing, a hyper-connected society demands real-time data transmission and secure identification and authentication. Physically unclonable functions (PUFs) offer a hardware-based cryptography solution to address these challenges. This study presents a novel electrical PUF that takes advantage of the considerable device-to-device variability in field-effect transistors (FETs) with laterally-heterostructured two-dimensional transition metal dichalcogenide channels as entropy sources. The variability originates from the inherent randomness of physical disorders, such as stochastic electrode contacts, heterostructure interface defects, molybdenum disulfide and tungsten disulfide (MoS_2/WS_2) layer count variations, nanoflake density and distribution, and fabrication imperfections. Cryptographic keys are generated from multiple challenge-response pairings using a bit extraction process. To assess the viability of this hardware security method, we evaluate PUF performance metrics, including bit uniformity, reproducibility, uniqueness, randomness, false rates, and reliability. The growth of laterally-heterostructured MoS_2/WS_2 delivers exceptional randomness and unpredictable security keys in PUF systems, showcasing a promising security strategy for identification and authentication processes.

3D MS imaging using Cluster SIMS (Ar, CO2, H2O, C60) for various types of analytes: How to select an efficient sputter beam for a specific material?

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[1]*Ionoptika Ltd, United Kingdom*

Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

Gas Cluster Ion Beams (GCIBs) are a low-damaging, highly versatile ion source used predominantly for surface analysis of organic and biological samples. Ionised clusters of atoms/molecules accelerated to high energies (keV) are highly efficient at sputtering intact molecules from surfaces with reduced damage, making them suitable for applications from fundamental biology to materials science especially using large H2O cluster beams.
Meanwhile, use of smaller-cluster GCIBs has also been reported as an efficient technique to provide chemical information in depth profiling of inorganic and organic hybrid multilayer semiconductor materials such as OLEDs, perovskite solar cells, and nano/micro-structured films. Smaller-cluster GCIBs have the feature of combining the strengths of monoatomic ion beam and large-cluster beams for depth profiles on hybrid materials.

In this work, we demonstrate examples of 3D MS imaging and depth profiling using different cluster species to see efficient cluster conditions for various types of analyte materials.

A new lead-free low-temperature hermetic edge seal for the fabrication of vacuum glazing

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Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

High performance low-cost vacuum glazing is a key development in realising more energy-efficient buildings. Vacuum glazing consists of two parallel glass sheets separated by a narrow, 0.15-0.3 mm wide vacuum gap. The glass sheets are separated and supported by an array of small pillars, required to maintain the vacuum gap against atmospheric pressure incident on the external surfaces of the two glass sheets. The vacuum gap with a pressure of less than 0.1Pa, sealed by a contiguous edge seal, minimizes heat transfer by conduction and convection across the glazing. Low-E coatings on the glass surfaces reduce IR heat transfer through the gap. Improved hermetic edge-sealing materials are required to address the challenges of cost, use of hazardous substances and issues of complexity of manufacturing of vacuum glazing. This work reports the use of a new lead-free alloy made of Sn-Zn-Al+Ti+Si+Cu+Er+Ce in the ratio 96:3:1 by weight % (Cerasolzer- GS-217), with a melting point of 217°C, to form a hermetic vacuum glazing edge seal. The design, construction, and performance of vacuum glazing prototypes of three different dimensions are reported. Sample A- 150mm x 150mm achieved a vacuum pressure of 0.02Pa, Sample B- 300mm x 300mm achieved a vacuum pressure of 0.03Pa, and Sample C- 500mm x 500mm achieved a vacuum pressure of 0.02Pa. The developed vacuum glazing edge seal uses J-B Weld epoxy-steel resin as a secondary seal to improve glazing robustness. A guarded hot box calorimeter was used to experimentally determine the thermal performance of the vacuum glazing. The experimentally determined overall heat transfer coefficient and temperature profiles along the central line of the vacuum glazing are in good agreement with predictions made using 3-D models.

Distributed Pumping and Seamless Flanges for the 120 km UHV Tubes of the Einstein Telescope

Charlotte Marie Benning[1], Stefan Krischer[1], Maike Kuehler[1], Jan Lamkin[2], Oliver Pooth[1], Purnalingam Revathi[1], Ralf Schleichert[3], Frans Slangen[2], Achim Stahl[1]
[1]Physics Institute IIIB, RWTH Aachen University, Germany, [2]SBE Piping, Machine- Apparatenbouw B.V, Netherlands, [3]Forschungszentrum Jülich GmbH, Nuclear Physics Institute, Germany

Poster Session 3 and Drinks Reception, June 19, 2024, 17:30 - 19:30

The Einstein Telescope will be the next European gravitational wave detector. It requires about 120 km of vacuum tubes with a diameter of 1 m for a laser beam of multiple kW to achieve the design sensitivity. A pressure below 10^{-10} mbar is necessary to minimize the residual gas noise. The current baseline design of the vacuum system foresees welding together ~20 m sections of stainless-steel tubes and connecting them to pumping stations every few hundred meters. Achieving UHV in these tubes requires high pumping capacities and long bake-out times of the tubes.

This poster discusses two possible improvements over the baseline design: Integrating non-evaporable getter (NEG) surfaces into the inside of the tubes to reduce costs and aiming for a more homogeneous distribution of pumping power (distributed pumping). Furthermore, we are investigating forming seamless flanges from the pipe material to eliminate the need for welding, which is especially relevant for the underground environment of the Einstein Telescope.

An Extended Hueckel Approach to Modelling Molecular Self-Assembly

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[1]School of Physics and Astronomy, University of Nottingham, United Kingdom

Poster Session 2 and Drinks Reception, June 18, 2024, 17:30 - 19:30

Semi-empirical techniques such as the Hueckel method [1] aim to tread the middle ground between ab initio simulations and lower computational cost analyses (e.g. force-field approaches) by maintaining a quantum mechanical basis but using some empirical parameters to simplify the calculation process. Over the last twenty years or so, the Hueckel method has unfortunately been rather overlooked with the advent of new and improved ab initio techniques, particularly the many recent variants of density functional theory (DFT) . Here we show that the Huckel method, despite its relative simplicity, is a powerful, yet computationally inexpensive, tool for modelling molecular self-assembly. Our Huckel method simulations of phthalocyanines on solid surfaces compare very favourably with DFT approaches, despite their much lower cost.

Poster Presentations

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7	Jose	Brandao-neto	Poster Session 1 - Monday 17 June
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13	Ranferi	Cancino	Poster Session 1 - Monday 17 June
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19	Karthikeyan	Chockalingam	Poster Session 1 - Monday 17 June
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5	Rezwan	Ahmed	Poster Session 2 - Tuesday 18 June
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