Session: I2, Venue: Reithoffer Hoersaal

Advanced Coatings 2

Session Chairs: Hiroaki Nishikawa, Takayuki Ohta

I2 July-03 13:30 Keynote
*** Benzoate-based inhibitor film to prevent chloride-induced corrosion: a Molecular Dynamics study of efficiency of dry or hydrated film**
Giuseppina Raffaini
Politecnico di Milano, Milan, Italy

I2 July-03 14:00
* Synchrotron-based scanning transmission X-ray spectromicroscopy (STXM) on graphene-containing alumina thermal spray coatings
Uta Klement
Chalmers University of Technology, Gothenburg, Sweden

I2 July-03 14:20
* Thermal sprayed Fe-based metallic glass composite coating: Influence of morphology and phase evolution on corrosion and wear properties
Sapan Nayak, Tapas Laha
Indian Institute of Technology Kharagpur, India

I2 July-03 14:40
* Effect of CeO2 doped Zirconium Titanate with various Temperatures by Solid-state reaction method
Nagasravanthi M, Sudagar J, Selvakumar A
VIT-AP University, Vijayawada, India

I2 July-03 15:00
Corrosion protection of riv-bonded aluminum-magnesium joints based on plasma electrolytic oxidation coating
Josef Domitner, Jennifer Stippich, Peter Auer, Norica Godja, Zahra Silvayeh, Christian Pichler, Luka Payrits, Andreas Schindel, Rudolf Allant, Christof Sommitsch
Graz University of Technology, Austria

I2 July-03 15:20
* Establishment of transfer process for epitaxial thin films of transition metal oxides to polymers with a large area
Hiroaki Nishikawa
Kindai University, Kinokawa, Japan

I2 July-03 15:40
Grain refinement mechanism and surface mechanical performance of Ti-6Al-4V alloy by severe shot peening process
Wang Chenglin, Zhou Wenlong, Fu Xuesong, Jia Zhihong
Nanjing Tech University, China

Session I2: Advanced Coatings 2
Coffee / Tea break 16:00 to 16:30

69 Benzoate-based inhibitor film to prevent chloride-induced corrosion: A Molecular Dynamics study of efficiency of dry or hydrated film

Giuseppina Raffaini
Politecnico di Milano, Milan, Italy

Organic inhibitor films play an important role to prevent the chloride-induced corrosion process of reinforcing steel in concrete structures. Using MM and MD methods, the interaction between dry or hydrated benzoate protective film adsorbed on a completely covered γ-FeOOH lepidocrocite surface in presence of chloride ions was investigated. Using a simulation protocol proposed in previous work, the dry protective film well prevents the Cl^- adsorption on the solid surface. Benzoate molecules are perpendicular to the surface forming H-bonds interactions between the carboxylate groups and the hydroxyl groups of the γ-FeOOH surface. Only a few benzoates are parallel to the surface, exposing the negative charges to the environment. On the dry bare surface, Cl^- ions can adsorb on the unprotected solid surface, and then induce the corrosion process. In the presence of water, some chlorides pass through the hydrated film and come directly into contact with the solid surface. At longer time no other chloride ions cross the protective film. Interestingly, these adsorbed Cl^- ions induce a different arrangement in the benzoate film due to electrostatic repulsion with neighboring carboxylate groups of benzoates. This film inhomogeneity can affect its efficiency to prevent the corrosion process. It is known experimentally that chlorides at the steel/concrete interface can subsequently destroy the passive layer when adsorbed on the steel surface. Therefore, not only the number of Cl^- ions in contact with the lepidocrocite surface, but also the stability over time of dry or hydrated film must be studied theoretically as well as experimentally.

70 Digital material design guidelines for high strength alloys with resistance to hydrogen embrittlement

Vsevolod Razumovskiy, Philipp Hammer, Christian Posch, Oleg Peil, Max Hodapp, Werner Ecker
Materials Center Leoben Forschung GmbH, Leoben, Austria

New trends in the energy sector aiming at a circular and emission-free economy call for new material solutions. The modern approach for material selection and design is based on the use of predictive computer methods that are intended to replace some experiments and accelerate the material design cycle. A combination of predictive computational methods like the density functional theory (DFT) with machine learning (ML) and continuum models for segregation, diffusion and mechanical properties, allows one to bridge the time and length scales between different methods and to approach solutions for the new materials in a form of digital material design guidelines (DMDG).

In this work, we would like to demonstrate a DMDG concept for high strength alloys suffering from the hydrogen embrittlement phenomenon. The concept is based on DFT predictive calculations of the H segregation (trapping) energy distributions at available defects and interfaces and hydrogen redistribution modeling within the material microstructure during mechanical straining using the finite element method (FEM) and