Hole-doped Ge-rich $Si_{1-x}Ge_x$ parabolic quantum wells for mid-infrared photonics

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***Abstract*—The design, growth and characterization of hole-doped Ge-rich $Si_{1-x}Ge_x$ parabolic quantum wells are discussed. The heterostructures were epitaxially grown by low-energy plasma-enhanced chemical vapor deposition and characterized by secondary ion mass spectroscopy, scanning transmission electron microscopy and X-ray diffraction measurements. Fourier-transform infrared spectroscopy revealed an almost temperature- and doping-independent intersubband transition at around 120 meV which is stable up to room temperature, making these heterostructures promising candidates for the realization of optoelectronic devices working in the fingerprint region.**

I. INTRODUCTION

THE ability to generate, manipulate and detect mid-infrared (MIR) light is crucial in countless applications such as material recognition, sensing and imaging and, in this context, group-IV semiconductors are being considered for the realization of cheap and compact Si-compatible devices working in the fingerprint region which could eventually replace most of nowadays available devices relying on III-V semiconductors. In particular, hole-doped $Si_{1-x}Ge_x$ multiple quantum wells (QWs) integrated on silicon substrates represent a viable solution for the realization of MIR-active tunable devices exploiting intersubband (ISB) transitions.

Among the possible QWs, those exhibiting a quadratic variation of the compositional profile are immune to electron-electron interaction and thus exhibit almost doping-independent ISB transitions [1] and, for this reason, they have been identified as optimal candidates for the investigation of the ISB strong coupling regime. Digital alloying was historically employed to mimic the harmonic compositional profile and only recently high-quality continuously graded parabolic QWs (PQWs) were demonstrated both in III-V [2] and silicon-germanium [3-5] alloy semiconductors, however featuring ISB transitions in the THz spectral region.

As a preliminary study towards the exploitation of PQWs in actual devices, potentially working in the strong coupling regime, we report on the structural and optical characterization of p-doped $Si_{1-x}Ge_x$ multiple QWs designed to have an ISB transition lying in the MIR.

II. RESULTS

The heterostructure was designed by means of the 8-band k-dot-p Schrödinger-Poisson solver, as implemented by the nextnano software. Each period nominally consists of 8 nm-thick $Si_{1-x}Ge_x$ parabolic wells, where the germanium content x is varied between 60 and 100 %, enclosed between 4 nm-thick $Si_{0.4}Ge_{0.6}$ barriers.

The investigated samples were grown by low-energy plasma-enhanced chemical vapor deposition [6] on Si(001) wafers. The first part of the stack consists of a forward graded buffer (GB), where the germanium concentration linearly increases from 0 to 78 %, followed by a fully-relaxed 2 µm-thick $Si_{0.22}Ge_{0.78}$ layer serving as virtual substrate (VS) for the QWs as pictorially depicted in Fig. 1(a). The QWs were *in situ* doped in their center adding B_2H_6 as precursor gas for boron during the growth.

The structural properties of the samples were studied by scanning transmission electron microscopy (STEM), secondary ion mass spectroscopy (SIMS) and high-resolution X-ray diffraction (XRD) measurements. A STEM image showing part of the GB, the VS and the PQWs is reported in Fig. 1(b) while a detailed view of the QWs region is shown in Fig. 1(c). A truly parabolic variation of the compositional profile was revealed by SIMS measurements and confirmed by STEM. However, when approaching the barriers, the entropic interdiffusion typical of random alloys such as silicon-germanium prevails smearing-out the nominal profile. As the obtained average germanium content does not match the one retrieved from XRD measurements, the SIMS profile was fed into the dynamical Darwin model simulation and optimized eventually managing

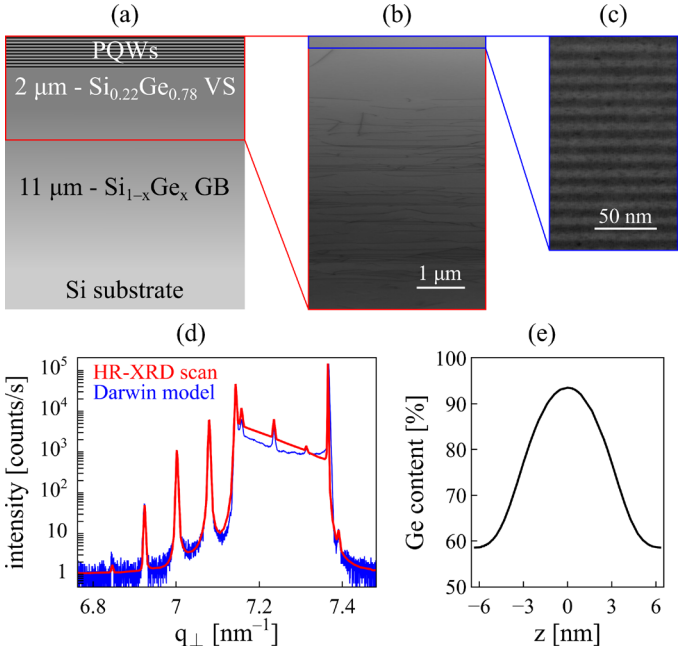

Fig. 1. (a) Schematic representation of the detailed epitaxial steps including the GB, the VS and the PQWs. (b) STEM image showing part of the GB, the VS and the PQWs. (c) High-resolution STEM image focusing on the QWs region. (d) ω-2θ XRD scan of the investigated heterostructure and best fitting curve obtained by dynamical Darwin model simulation. (e) Germanium content profile retrieved by SIMS and refined fitting the ω-2θ XRD scans.

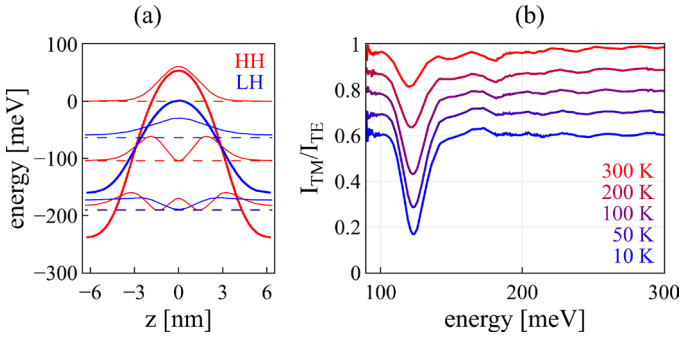

Fig. 2. (a) Calculated valence-band-structure showing the HH and LH potential energy profiles and the wavefunctions associated with the main energy levels. (b) Temperature-dependent FTIR dichroic transmission spectra of a sample exhibiting sheet hole density around 1.2×10^{12} cm^{-2}. The spectra were offset for the sake of clarity.

to nicely reproduce the ω-2θ XRD scan reported in Fig. 1(d). The XRD-corrected profile is shown in Fig. 1(e) where it can be noticed that, while the germanium content in the barriers indeed approaches the nominal value, it never reaches 100 % in the wells but is limited to 93.5 %.

The calculated valence-band potential energy profiles of the heavy- (HH) and light-hole (LH) subbands are shown in Fig. 2(a) together with the wavefunctions associated with the main electronic states. It is noteworthy that the HH-LH degeneracy at the Γ point is lifted because of the biaxial tensile strain acting in the center of the wells so that the ground state of the system belongs to the HH subband. Moreover, the HH subband confines three energy levels, which are separated by an energy of around 105 meV, while the LH subband is only capable of confining a single energy level lying 65 meV below the ground state HH_0 which, even at room temperature, is basically the only populated one because of the energy spacing separating it and the excited states being larger than the thermal energy.

A Fourier-transform infrared (FTIR) spectrometer equipped with a closed-circuit He-flow cryostat was employed to study the MIR optical response of the heterostructure between 90 and 300 meV, specifically focusing on two samples with doping levels differing by a factor of two. To promote the excitation of ISB transitions, which require light polarized along the growth direction, the samples were shaped in the single-pass prism-like waveguide geometry with 70° facets after having evaporated a metallic film (Ti/Au 10/150 nm) on top of the QWs. Fig. 2(b) shows the FTIR dichroic transmission spectra of the most doped sample acquired at temperatures ranging from 10 K up to room temperature. In all cases, a single TM-polarized absorption feature, appearing as a pronounced dip superimposed to an otherwise flat background, can be appreciated around 120 meV, which was ascribed to ISB transitions occurring within the HH subband between HH_0 and HH_1. The peak position red-shifts by 2.6 meV with increasing temperature, thus suggesting that the parabolic confining potential does not perfectly compensate for the electron-electron interaction. Furthermore, a Voigt-profile lineshape was employed to extract the linewidth (FWHM) of the resonances finding that it increases with temperature from 14 to 20 meV. In the less doped sample, a slightly narrower absorption dip appears at the same energy at all temperatures which only red-shifts by 2 meV when heating the sample from cryogenic to room temperature.

The two-dimensional absorption coefficient can be readily calculated starting from the dichroic transmission spectra, therefore also allowing for an estimate of the sheet hole density involved in the ISB transitions. At low temperature the two samples exhibit carrier densities of around 1.2×10^{12} and 6×10^{11} cm^{-2} which gradually decrease with increasing temperature reaching, at room temperature, 5×10^{11} and 3×10^{11} cm^{-2} respectively. This peculiar trend was already observed in similar MIR-active heterostructures however featuring square QWs [7].

III. Summary

In this work we demonstrated continuously-graded Ge-rich $Si_{1-x}Ge_x$ PQWs which exhibit ISB transitions in the MIR spectral range at around 120 meV. Thorough structural characterizations showed that, despite the unavoidable entropic interdiffusion, the parabolic shape is preserved in the well region. A strong and stable absorption feature was observed by FTIR spectroscopy up to room temperature which is essentially unaffected by the doping level, therefore confirming the effectiveness of the parabolic confining potential in hampering electron-electron interaction. This study hence paves the way for the realization of similar heterostructures which can be carefully optimized in order to provide robust and tunable material platforms for the implementation of Si-compatible MIR optoelectronic devices relying on ISB transitions.

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