Future roads for group-IV defect-enhanced quantum dot light-emitters for silicon photonics

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Abstract—Optical and optoelectronic properties of all-group-IV quantum dot light-emitters for which the optical properties are enhanced by in-situ implantation of heavy ions (DEQDs) are investigated and discussed. Research directions towards more efficient light-emission from DEQDs as well as considerations towards the microstructural investigation of the nature of DEQD-defects are elaborated.

Keywords—Nanostructures, Low dimensional structures, Epitaxy, Ion-implantation, Germanium, Optoelectronics

I. INTRODUCTION

The intensified research efforts for efficient on-chip, group-IV-based light-emitters that preserve their optical properties well above room-temperature (RT) and that can be fabricated directly on Si are ongoing. Clearly essential for their CMOS-compatible integration are possibilities of electrical charge carrier injection and convenient coupling to other Si photonics components on standard SOI platforms, e.g. waveguides, detectors, etc.. Epitaxially-grown quantum dots (QDs) [1-4] offer benefits of charge carrier confinement and an all-crystalline matrix material, important for doping of e.g. light emitting diodes (LEDs) and laser diodes. A new class of all-group-IV light-emitters was discovered recently consisting of epitaxial Ge on Si QDs containing extended point defects, intentionally introduced upon low-energy ion-implantation [5-7]. In contrast to conventional Ge/Si QDs [2-4], for such defect-enhanced quantum dots (DEQDs), charge carriers are confined *within* the QD by two zero-dimensional but fundamentally different mechanisms [5,6]. Holes experience quantum confinement due to the large band-offsets between Ge and Si, while electrons are trapped by the introduced defects [6]. The most prominent features of DEQDs are clear signs for optically-pumped lasing [5,7], absence of thermal quenching of the photoluminescence (PL) emission up to RT [5-9], and the demonstration of LEDs working at 100°C, grown directly on Si without the need of micrometer-thick buffer layers [9]. Nevertheless, in view of the intriguing but still poorly explored properties of these DEQD-based light-emitters and the perspectives of using them for Silicon-based photonics, strategies have to be developed towards (1) improvement of their light-emission efficiency, (2) understanding the microstructural and energetic nature of the defects-states upon their formation, robustness, optical properties, strain, etc. and (3) fostering the potential of DEQDs concerning devices in the field of optoelectronics and beyond.

II. EXPERIMENTAL RESULTS AND MODELING

A. DEQD-fabrication procedure and optical properties

In this work, Ge QDs are grown on Si(001) substrates by molecular beam epitaxy by depositing 8 Å of Ge at 500°C on a 45 nm thick crystalline Si buffer layer. For DEQD

formation in-situ Ge ion-implantation was applied during the whole deposition time of Ge. The ion-implantation depth was matched to the QD height, i.e. ~2 nm, corresponding to Ge ion energies of ~1.5 keV. For optical characterization, QD-overgrowth with crystalline Si is mandatory. A Si capping layer of 70 nm thickness was deposited at a growth temperature T_G of 475°C. Significantly lower and higher T_G result into incomplete solid phase epitaxial regrowth and defect-complex migration out of the QD, respectively, both to be avoided by any means [6,7]. More details on the growth procedure can be found in [5-9].

In Fig. 1 the light-emission enhancement upon DEQD treatment is depicted by PL-spectra recorded at sample temperatures T_S of 77 K, 222 K and 300 K, respectively. At $T_S = 77$ K the DEQD sample (green) exhibit a ~40 times higher emission intensity as compared to reference QDs without Ge ion bombardment (black). This discrepancy increases for elevated T_S . While reference Ge/Si QDs do not emit light at RT, the emission intensity of DEQDs recorded at 300 K is more than 200 times higher than the one of reference QDs at $T_S = 222$ K.

B. Theoretical modeling

First insights into the nature of the defect-structure of DEQDs were found in [6]. There, the minimum energy configuration of an amorphous Ge structure with one atom in excess of that for a perfect crystal of the same domain size upon annealing was calculated by density functional theory [5]. The atom reconfiguration upon annealing resulted in an extended defect structure known as a split-[110] interstitial which is surrounded by a neighborhood of ~45 displaced atoms. This defect-structure in the QD causes a downward shift of the lowest conduction band (CB) by ~72 meV. It also results in a significant change in the CB-alignment.

Fig. 1. Photoluminescence spectra of a DEQD-sample and a reference QD sample without additional Ge ion implantation. At $T_S = 222$ K, a PL-intensity increase of DEQDs as compared to unimplanted QDs can be observed. Gray spectra are magnified by a factor of 10.

We acknowledge funding by: Austrian Science Funds (FWF): P29137-N36 Linz Institute of Technology (LIT): LIT-2016-1-YOU-002 and QuantERA, co-funded under Horizon 2020, Grant Agreement No 731473.

In particular, the first band above the CB edge is localized at the defect at its Γ -point. For these calculations, the resulting calculated density of states (DOS) for DEQD-electron- and hole-states (magenta) are plotted with respect to the undisturbed Ge lattice (black) in Fig. 2. The original bandgap is indicated in yellow. Immediate conclusions from Fig. 2 are (1) that the DOS for electrons is increased (2) the bandgap is reduced as compared to crystalline Ge without split-[110] interstitial, and (3) hole-states are largely unaffected by the defect structure, albeit there still exist hole-states within the bandgap of the nanostructure.

III. DISCUSSION AND OUTLOOK

Even though both, initial experimental and theoretical investigations were reported, overall the understanding of the DEQD platform, its optoelectronic properties, atomistic configuration, band structure and functionalization to devices is still at a rather basic level. Here, we want to draw a non-exclusive, coarse roadmap of what is necessary to advance the DEQD-platform.

A. Enhancing the optical properties of DEQDs

For any kind of optoelectronic application, the optical properties of DEQDs have to be advanced, e.g. light-emission from the single defect centers in QDs has to be optimized, non-radiative emission reduced, wave-function overlaps and optical matrix elements enhanced and the sheet density of active emission centers increased e.g. by vertical stacking of QDs [8]. Such goals can be targeted by changing the QD growth parameters to ensure formation of even smaller QDs, changes of the chemical composition of the QD and or matrix material to ensure optimum band alignment in the system and by changing the nature of the defect structure itself, see point IIIB. Furthermore, Hydrogen-treatment and advanced annealing techniques promise to reduce non-radiative recombination by saturation of unwanted defects created in the Si matrix. Thereby, the optical yield has to be monitored quantitatively, possibly by making use of integrating spheres and/or comparing DEQDs to emitters with well-known optical properties e.g. InAs/GaAs QDs [1].

B. Defect alphabet and light-emission

The split-[110] self-interstitial seems to be a minimum energy configuration for DEQDs considering implantation of Ge ions. Nonetheless, the question is valid if there exist other low-energy defect-configurations. This can become of particular importance considering the implantation of

Fig. 2. Calculated DEQD electron- and hole-states (magenta) with respect to the undisturbed, relaxed Ge lattice (black). Note that DFT-results usually underestimate bandgap energies (here 0.34 eV) while energy differences of the states close to the band edges are rather accurately predicted.

different ions than Ge for DEQDs. Although in previous studies only Ge ions were used for implantation, it is a priori not clear that a Ge ion should be the ideal candidate concerning the resulting optical properties of DEQDs. Also, the role of strain in the Ge QD crystal was not evaluated so far. The calculations in [6] were performed using a relaxed Ge crystal. In reality, it is, however, clear that the Ge film (QD) is pseudomorphically strained to almost 4% when deposited on Si(001). Thus, what happens to the defect configuration and the optical transitions if the strain status of the QD is changed? Experimentally this can be achieved either by changing the QD architecture [3], the growth of SiGe alloys on Si, or deposition of Ge on a relaxed SiGe pseudo-substrate, etc.. Furthermore, the influence of potential hole-traps (Fig. 2) on the optical properties of DEQDs was not investigated so far. Can transitions involving defect-states for holes or, alternatively, the incorporation of heavier ions such as Sn or Sb into the QD contribute to a shift of the optical transitions further to the mid-infrared or THz, regions that are highly important for sensing applications?

C. DEQD-devices

The realization of an electrically-driven DEQD-laser is a major milestone to be reached. However, the full potential of DEQDs has still to be unfolded. Applications towards DEQD-based detectors, sensors or other electronic or thermoelectric devices were not considered at all by now. Given the additional degree of freedom in the system, caused by the ion implantation into epitaxial QDs, we expect that the true potential of DEQDs as compared to fully crystalline QDs has yet to be unfolded.

IV. SUMMARY

In this work, we have presented upcoming routes in the research of defect-enhanced quantum dots (DEQDs). The coexistence of crystalline regions and ones with disturbed crystallinity allows us to envision device applications beyond conventional optoelectronics, but also in other fields of electronics e.g. as thermoelectric coolers.

ACKNOWLEDGMENT

The authors thank M. Grydlik, T. Fromherz, P. Rauter, F. Schäffler and A. Rastelli for fruitful discussions.

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