Optical studies of Ge/Si based heterostructures and Si interstitials related defects in SiGe alloys

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This work is focused on the application of photoluminescence (PL) for the study of a low dimensional structure based on the Si/Ge system and of Si interstitial related optical centers in Si and SiGe alloys. In the first part, we consider a superlattice structure with embedded Ge islands grown by molecular beam epitaxy (MBE) at 600ºC on top of a Si(001) substrate [1]. The samples were irradiated with 2.0 MeV protons to fluences in the range $2x10^{12}$ - $2x10^{14}cm^{-2}$. The structural and optical properties of the samples were investigated by cross-sectional transmission electron microscopy, X-ray reciprocal space mapping (RSM), X-ray reflection (XRR) and Rutherford backscattering/channeling. No changes to the as-grown heterostructure were observed after the irradiation in all fluences (Fig. 1). The nominal period of the superlattice was confirmed. The radiative recombination related to type-II transitions in the Si/Ge interface was observed in PL measurements additional to free and bound excitons recombination in the Si layers and substrate, near the energy band gap of Si. The PL related to the Ge islands was observed even for the highest irradiation fluence showing an extremely high radiation hardness of the studied structure, which was confirmed by the absence of changes in the structural properties (Fig. 1).

In the second part of the work, the Si interstitial related W and X centers, were studied by photoluminescence and the results compared with the ones from first-principles calculations [2]. The samples were obtained after the growth of a Si or $Si_{1-x}Ge_x$ alloy layers (x=0.0069, 0.0125) on top of a Si(001) substrate at 800ºC by MBE. For the production of the centers, irradiation with 875 keV protons (dose of 10^{16} H^+ cm^{-2}) followed by annealing of 15 min, in N_2 atmosphere, at a temperature in the range 100 – 650ºC, was performed. It was found that the annealing temperature (300ºC) that maximizes the PL intensity of the W center is independent of the Ge content, whereas for the X center, a shift was observed from the Si layer (400ºC) to the SiGe alloys (450ºC) suggesting that the minority Ge atoms delay the formation of this center. The radiative excited state in both centers comprises a pseudodonor state, where a trapped exciton combines a tightly bound hole and a diffuse electron. No acceptor level in the gap was found for either of the centers. The ionization energies of both centers were calculated from a temperature dependence of the PL intensity and the hole binding energy was extracted considering also the spectroscopic energy of the W and X lines in the spectra. The calculated change rates of donor levels with Ge content are in qualitative agreement with the hole binding energy shifts obtained from the experiments. Our results support the previous assignment of the trigonal (I_3) and tetragonal (I_4) forms of tri- and tetra-interstitial defects to the W and X centers, respectively.

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[2] J. P. Leitão, A. Carvalho, J. Coutinho, R. N. Pereira, N. M. Santos, A. O. Ankiewicz, N. A. Sobolev, M. Barroso, J. Lundsgaard Hansen, A. Nylandsted Larsen and P. R. Briddon, Phys. Rev. B 84, 165211 (2011)

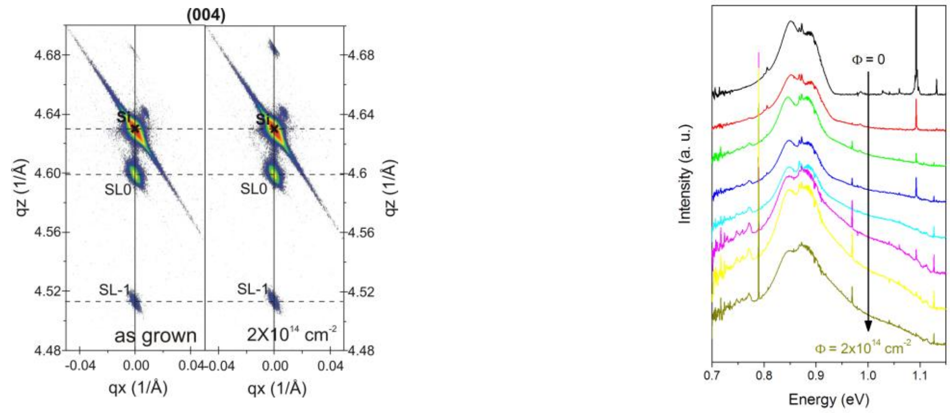

Fig. 1 a) X-ray reciprocal space map for the as-grown and irradiated to the highest fluence samples. The Si substrate and superlattice related peaks are identified. b) Photoluminescence spectra of as-grown and irradiated samples (range from $2x10^{12}$ to $2x10^{14}$ cm^{-2}).

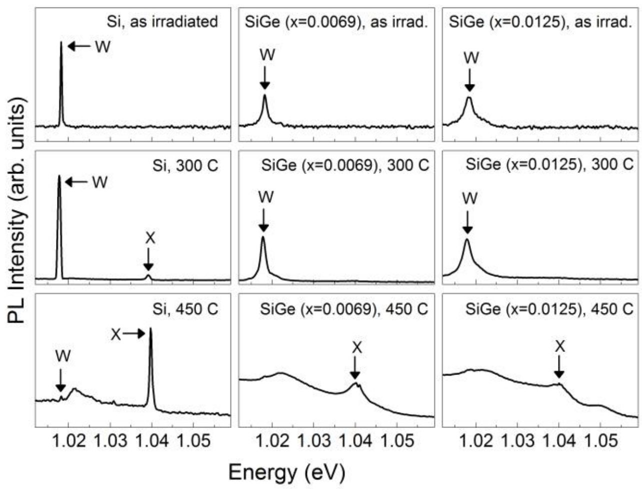

Fig. 2. PL spectra recorded at 5 K for the Si and SiGe layers as irradiated (top row), after an annealing at 300ºC (middle row), and after annealing at 450ºC (bottom row). Both W and X lines are identified in the spectra.

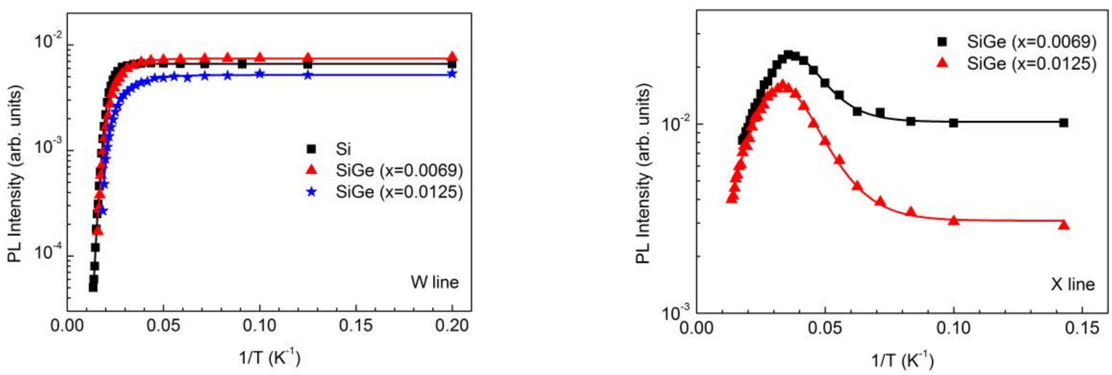

Fig. 3 Integrated PL intensity temperature dependence of the W and X lines in Si (squares) and SiGe alloys with x=0.0069, 0.0125 (triangles and stars, respectively). The lines represent the best fit to the experimental points according to the model described in Ref. [2].