Study at the nanoscale of hydrogen and noble gas implantation-induced defects in semiconductors

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Context
Defects tend to modify the physical and mechanical properties of materials. Cavities (filled or not) are a major type of extended defects usually resulting from the incorporation of inert gas or hydrogen in solids by high fluence implantation or transmutation reaction in nuclear reactors. While ions implantation-induced cavities are of major interest in several domains, from materials for microelectronics and energy (nuclear and photovoltaic), to more fundamental fields (they can be key nanosystems to study plasmon excitation or nanofuidics), there are serious gaps in the understanding of their mechanisms of formation and evolution. Such an understanding is however the prerequisite to tune the characteristics and the physical properties of the cavities, which is essential for all applications. It constitutes a substantial scientific challenge. The major obstacle is related to the complex multi-scale phenomena involved in the cavity formation and evolution, ranging from the nucleation and growth of gas-vacancies clusters to the macroscopic deformation of the surface.

The studies carried out by our group are positioned in this challenging field. We mainly focus on a in-depth understanding of the physical mechanisms governing the formation and evolution under different kinds of treatments (thermal annealing, electron irradiation) of the cavities at the nanoscale with connection at the microscopic scale with the group of C. Coupeau and J. Colin (Pprime Insitut). Our studies are mainly performed using quantitative electron microscopy in different modes (EF-TEM, STEM-EELS, HR-TEM/STEM), ab initio and molecular dynamics calculations.

Recent studies carried out by the group

- Helium desorption from unique nanobubbles under the electron beam

Helium nanobubbles of about 16 nm in diameter were created in silicon and germanium by helium implantation at high fluence and subsequent annealing. Individual nanobubbles were analyzed by spatially resolved Electron Energy-loss Spectroscopy (EELS). We report on the in-situ probing and mapping of helium desorption from the nanobubbles under electron irradiation. This opens new perspectives for a more accurate determination of the helium density through spatially resolved EELS.
Helium nanobubbles in (001) Ge submitted to a He implantation at 50 keV, 7x10$^{16}$ cm$^{-2}$, followed by an annealing at 500°C during 30 min.

a) Energy filtered image (20.75-22.14 eV) showing the He chemical map. b) EELS spectra extracted from the image-spectrum: in black, inside the bubble and in red, outside the bubble. In the inset, the He K-edge has been extracted from the raw signal in black (after multivariate statistic analysis, deconvolution of plural scattering and germanium plasmon fitting). c) Helium density map clearly showing the He desorption under the e-beam during spectrum imaging. (Titan 80-300, probe corrected and monochromated, 200 keV, CCEM, Mc Master University, Hamilton (Canada))

“*In situ probing of helium desorption from individual nanobubbles under electron irradiation*”

- First-principles calculations of noble gas properties in silicon

We have investigated the stability and the migration of single noble gas atoms (He, Ne, Ar, Kr, Xe) in silicon and silicon carbide, by performing first-principles calculations combined with the use of the Nudged Elastic Band technique. The desorption of He and Ne from a well defined bubble in silicon was also studied as a function of the gas pressure inside the bubble, and compared with experiments. Our simulations revealed that at the maximum of desorption, an average pressure of 1–2 GPa is present into the bubble.

*Computed mechanism for the migration of a noble gas (NG) atom in a silicon divacancy*
High resolution transmission electron microscopy (HRTEM) experiments were performed to investigate nanoplatelets induced by ion implantation into a germanium wafer. Atomistic models were used for image simulation in order to get quantitative information from the experimental images. The geometrical phase shift analysis technique was also employed to measure the strain field induced by such defects. We discuss the limits and artefacts imposed by each approach and show how these approaches can be combined to study the atomic structure of such defects and the strain field they induce. Further, combining these results with extensive first principles calculations, we present a model for the atomic structure of (001) hydrogen-induced platelets in germanium. It involves broken Ge-Ge bonds in the [001] direction that are dihydride passivated, vacancies, and trapped H₂ molecules, showing that the species involved in platelet formation depend on the habit plane.

a) HRTEM image of a (001) hydrogen-induced platelet (HIP) in germanium. b) Ball and stick representation of the Hydrogenated vacancy-based (001) HIP structure we have proposed, with two germanium layers removed and two trapped H₂ molecules, along two perpendicular orientations (Ge, large spheres; H, small spheres).