Composition of Ge/Si islands in the growth of Ge on Si(111)

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The heteroepitaxial growth of group IV semiconductors represents a field of enormous interest, due to the possibility it offers to engineer the optoelectronic properties of the resulting structures with vast flexibility^{1,2}. In particular, the Stranski-Krastanov (SK) growth mode of Ge on Si surfaces may yield a real breakthrough in the fabrication of low cost optoelectronic devices, compatible with the existing Si-based technology. The self assembly of Si/Ge islands may pave the way to the exploitation of quantum dot nanostructures, whose luminescence properties could be used to develop novel lasers, light emitting diodes and photodetectors for applications in telecommunications.

For these reasons, the growth of Ge on Si substrates has been the subject of numerous theoretical and experimental reports during the past two decades^{3,4}. Nevertheless, several critical issues are still preventing the adoption of Si/Ge nanostructures for device fabrication. Most applications require a narrow size and shape distribution of the islands; the ability to control and order the positioning of the nucleation sites on the substrate is necessary to obtain a dense array of light emitters; the thermal stability of the islands versus their kinetic ripening is a requirement of primary concern. Presently, all these problems are widely debated, yet unsolved. Further, little is known about the actual chemical composition and profile inside individual islands.

Intermixing is known to occur since the early stages of growth of Ge on Si surfaces and to affect most of the critical issues listed above. A detailed description of the chemical composition gradient inside individual dots is necessary to model the potential barriers which cause the carrier confinement inside the system. Further, mapping the Si/Ge concentration inside self-assembled islands could cast some light on the nature of the main diffusion mechanisms that cause the alloying itself, thus eventually leading to their control. In particular, this last point presently represents the focus of an extremely active debate. For these reasons, intermixing in SK resulting 3D structures represents the focus of many experimental reports, mainly addressed to related systems and mainly obtained through "side view" cross sectional techniques.

In this poster, we discuss results obtained by Low Energy Electron Microscopy (LEEM) and X-Ray Photoemission Electron Microscopy (XPEEM) on the growth of Ge on Si(111). XPEEM yields photoelectron spectra with a high lateral resolution, thus allowing for a "top view" mapping of the Si/Ge concentration in the topmost layers of the studied system. Ge was deposited by MBE on Si(111) substrates kept at temperatures ranging from 460 to 560 C. The surface morphology and quality were analyzed by LEEM and Si2p and Ge3d XPEEM core level spectra were acquired with a 25 nm lateral resolution, highlighting Si or Ge enriched areas of the sample. Some of our achievements yield a very significant progress in the understanding of the alloying dynamics in the investigated surface.

Contour plots of the Si2p photoelectrons intensity from the islands surface show a Si enriched centre with respect to their borders⁵, in agreement with diffusion models based on an important bulk mass transport between the 3D structures and the buried layers, and resulting in a partial release of the accumulated strain energy⁶ (**Fig. 1**).

An analytical framework developed *ad hoc* allowed us to obtain for the first time a quantitative estimate of the surface stoichiometry out of the contrast in the XPEEM images. A correlation was established between chemical composition and lateral dimensions of different coexisting islands⁷ (**Fig. 2**). The deposition temperature dependence of such relation indicates that alloying processes are thermally activated and kinetically limited.

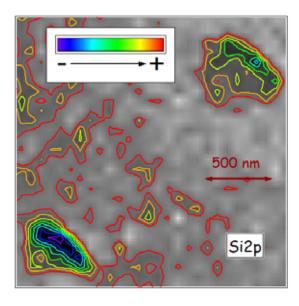


Fig. 1) $2 \times 2 \ \mu m^2$ integrated XPEEM image taken at the Si2p core level, together with the contour plots from a more (top) and a less (bottom) ripened island. Photoelectron yields are increasing from blue (lowest) to red (highest). The darkest regions in the panels are produced by the shadows of the 3D islands, due to the 16° grazing incidence angle of the X–Ray beam. The growth temperature was 530 °C. The wetting layer appears to be inhomogeneous.

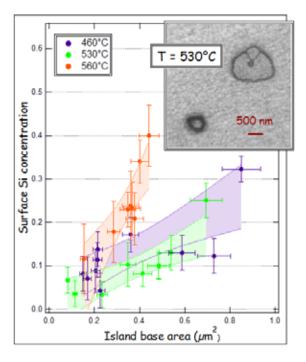


Fig. 2): Silicon surface concentration for selected islands versus their basal area, together with 90% confidence bands. Islands were grown at the indicated temperatures. Note that the 460 °C and 530 °C confidence bands overlap over the entire accessed range. Inset: $4.5 \times 4.5 \ \mu\text{m}^2$ LEEM image of a sample grown at 530 °C. Ripened *atoll like* structures coexist with smaller islands.

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