	Experiment title: High brillance for three-dimensional DAFS mapping of Ge/Si(001) nano-islands.	**Experiment number**: MI-1008
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Names and affiliations of applicants (* indicates experimentalists):

Hubert Renevier (1), Marie-Ingrid Richard* (2), Vincent Favre-Nicolin* (3), Nebil Katcho* (4), Clément Leclerc* (1), Maria Grazia Proietti (5), Günther Bauer (6)*

(1) LMGP, Groupe INP - Minatec, Grenoble, France (2) Université Paul Cézanne, IM2NP, Marseille, France (3) INAC, CEA-Grenoble, France (4) IQFR-CSIC, Universidad Complutense de Madrid, Spain, (5) ICMA, CSIC-Universidad de Zaragoza, Spain (6) Johannes Kepler Universität Linz, Austria

Report:

Introduction: The aim of this experiment at beamline ID03 was to study structural properties (local composition, strain and atomic ordering) of Ge islands (either {105} faceted pyramids or dome-shaped islands) grown on nominal and nano-structured Si(001) substrates, by combining **Multiwavelength Anomalous Diffraction** (MAD) and **Diffraction Anomalous Fine Structure** (DAFS) spectroscopy. The MAD technique is nowadays well established, however, in some cases it fails to determine the chemical composition locally since it collects the measured signal from a large iso-strain volume that may include both the nanostructures and part of the substrate or the surrounding host matrix. This disadvantage is overcome by the diffraction anomalous fine-structure method (DAFS) [1] that measures the fine structure of the energy-dependent diffracted intensity, so that a space resolution is achieved inside an iso-strain volume *via* the chemical selectivity [2].

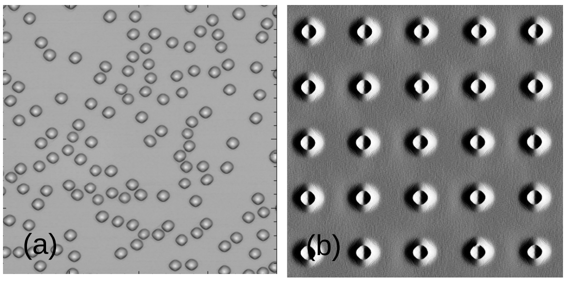

Fig.1 (a) $2\mu m^2$ atomic force microscope (AFM) image of the dome-shaped islands grown on a flat Si(001) substrate. (b) $4\mu m^2$ AFM image of {105} faceted pyramids grown on a nano-structured Si(001).

Information on the composition inside pyramids and at the basis of domes and a direct evidence for Si-Ge ordering on atomic scale *are still missing* and are necessary to provide fundamental knowledge on the coupling between intermixing, strain and morphology of SiGe nanoislands. Indeed, due to spatial resolution issues, MAD alone can not determine the composition inside pyramids and at the basis of domes.
This preliminary DAFS experiment was aimed to answer these questions and to test and implement the grazing-incidence DAFS spectroscopy technique at beamline ID03.

Experimental data and results: The experiment was performed in grazing incidence geometry to reduce the scattering contribution of the substrate. A submicron size x-ray beam (less than 100µm in vertical) was obtained with an achromatic Kirkpatrick-Baez mirror. Two samples were studied: dome-shaped islands grown at a temperature of 650°C on a flat Si(001) substrate (Fig. 1a) and {105} faceted pyramids grown at 720°C on a nano-structured Si(001) substrate (Fig. 1b).

Figures 2a and 2c display the square root of the scattered intensity (√Iexp) close to the in-plane Si(440) Bragg reflection, the modulus of the Ge and Si structure factors, as well as the Ge content, as a function of reciprocal unit *h*, for the dome-shaped islands and pyramids, respectively. The MAD results reveal a lower Ge content inside pyramids and a slight linear increase of the Ge concentration above *h*=3.96 for domes. Figures 2b and 2d show GIDAFS spectra measured for the dome-shaped islands at *h*=3.972 and *h*=3.974 and for pyramids at *h*=3.985 (*h* positions indicated by the grey arrows in Figs. 2a and 2c). In Fig. 2d, the two peaks at the energies of 11.46keV and 11.48keV are due to multiple scattering. Encouraging GIDAFS results have been obtained as shown by the good quality of the DAFS spectra of Fig. 2b. Nevertheless, beamline optimization still needs to be performed: at the end of the experiment, GIDAFS spectra were no more reproducible and low frequency distortions appeared in the spectra (see Fig. 2d).

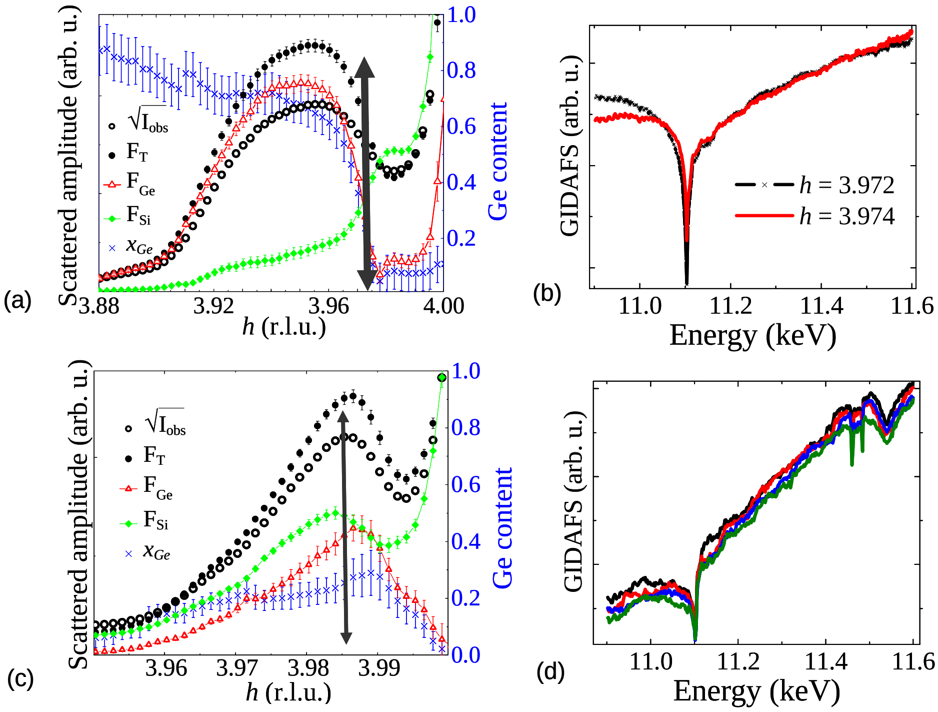

Fig.2 √Iexp measured at 11.053keV (50eV below Ge K-edge), |FGe|, |FSi| and Ge composition xGe plotted as a function of h around Si(440) for dome-shaped islands (a) and pyramids (c). GIDAFS spectra measured for the dome-shaped islands at h=3.972 and h=3.974 (b) and for pyramids at h=3.985 (d).

Analysis of the DAFS edge shape close to the Ge K-edge can give information about the Ge and Si relative composition inside different in-plane iso-strain regions of the Ge islands. The Ge occupation factor is dependent on the curvature and depth of the cusp before and at the edge. Figure 2b shows GIDAFS spectra measured at two slightly different iso-strain *h* values. The curvature and depth of the cusp are different, suggesting a different Ge composition as observed by MAD. However, the oscillations in the region above the Ge K-edge can be superimposed, revealing that the local atomic environment of the Ge atoms and thus the chemical composition in these two iso-strain regions of the dome are identical. This clearly demonstrates that the MAD technique fails to determine the chemical composition in these regions due to the scattering contribution of strained Si substrate beneath the islands. From recent atomistic simulation results [3], this implies that the dome-shaped islands display an abrupt composition profile at the interface.

<u>Conclusion:</u> These preliminary results show the great potential of the DAFS technique to unambiguously determine the composition inside strained islands. The analysis of the Extended DAFS spectra is under progress. Encouraging GIDAFS results have been obtained at ID03. Optimizations still need to be performed. Because of the low intensity of the diffracted signal and the need for a very good Extented DAFS signal-to-noise ratio (> 1000), a high brilliant source, such as the one delivered at ESRF–ID03 is mandatory for DAFS measurements inside nanostructures.

<u>References:</u>

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