ESRF	**Experiment title:** Quantitative evaluation of the composition of nano-objects on flat and nano-patterned substrates.	**Experiment number**: SI-1559
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Report:

Introduction: The knowledge of strain, chemical composition, interface quality, atomic ordering, *i.e.* structural properties at the long and short range scales, are of great importance to understand the growth mechanism as well as the electronic and optical properties of hetero and nanostructures. The aim of this preliminary experiment on BM02 was to study structural properties (composition, strain and atomic ordering) of semiconductor heterostructures and nanostructures (here, GeSi islands grown on nominal and nano-structured Si(001) substrates), by combining **Multiwavelength Anomalous Diffraction** (MAD) and **Diffraction Anomalous Fine Structure** (DAFS) spectroscopy, in grazing incidence. 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) [1,2] 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 [3].

Experimental data and results: In the following, we will especially show that the combination the DAFS technique with atomic simulations reveals to be a very powerful and new approach to disentangle strain and composition and to detect *atomic ordering* inside SiGe nanostructures. As an example, Fig. 1 shows an experimental Extended DAFS spectrum (EDAFS) of SiGe dome shaped islands, grown on nominal Si surfaces, together with a number of theoretical EDAFS spectra obtained by atomistic simulations of relaxed cubic Ge-Si alloys with diamond structure. Calculations were performed using Monte Carlo (MC) simulations based on a Tersoff potential that is acknowledged to reproduce well the interatomic distances in semiconductors of group IV and III-V. Simulations have been tested on Ge-Si relaxed alloys and pure Ge, providing correct interatomic distances and EXAFS shape. One can see the EDAFS oscillations showing remarkable changes with Ge/Si relative composition, which are more evident in the low k values range due to the very different backscattering function shape of Ge and Si. The experimental EDAFS spectrum is well reproduced by atomistic simulation revealing a 50% Ge-Si relaxed alloy.

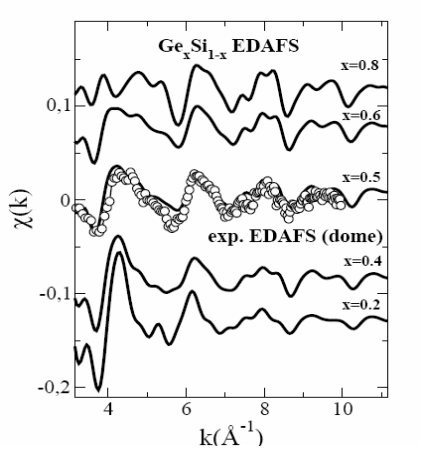

Figure 1: Experimental background-substracted EDAFS spectrum of a SiGe dome shaped island together with theoretical EDAFS spectra obtained by atomistic simulations (MC) of relaxed Ge-Si alloys [4].

In Fig. 2 we show grazing incidence EDAFS oscillations collected at BM02 corresponding to a series of samples. From top to bottom, (a, b, c) domes grown on Si nominal surface, (d) small pyramids with Si capping, (e) domes with pyramidal faceted (111) shape in the upper part. Changes in the EDAFS shape from one case to the other are quite evident, each spectrum, indeed, is qualitatively reproduced by different atomistic simulations. The different shapes are essentially reproduced by two main factors: Ge concentration and atomic ordering. The atomic ordering used in the simulations is the so-called RS3 model, that has been already observed by Malachias [5] associated to antiphase boundaries in GeSi domes. Small capped pyramids are the closest to the RS3 ordered GeSi lattice corresponding to a 50% Ge concentration. The ordering phenomenon manifests as a Ge rich-like shape due to the higher number of Ge Nearest Neighbors (3 over 4 instead of 2). At last we show EDAFS of pyramidal domes showing a mixing of ordered and random phases. Random and ordered alloys can be simulated and compared with experimental data.

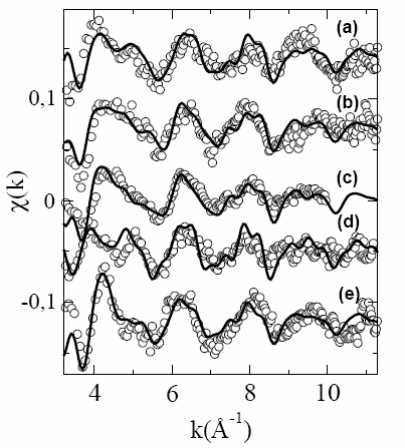

Figure 2: Grazing incidence EDAFS oscillations corresponding to a series of samples together with Monte Carlo simulations (Tersoff potential). From top to bottom, (a, b, c) domes grown on Si nominal surface (d) small pyramids with Si capping, h=7.97 (e) pyramids with dominant {111} facets in the upper part, h=3.97.

Conclusion: These preliminary results show the great potential of combining DAFS with atomistic simulations to determine the local chemical composition of free-standing Ge dots and the local atomic neighborhood of Ge atoms located at different heights in the dot volume, by combining the Iso Strain scattering method and Grazing Incidence DAFS, and to determine possible spontaneous atomic ordering of the SiGe alloy in some region of the dot volume. The further step to clarify and quantify the effects of growth conditions and morphology on the structural local properties of the QDs is performing atomistic simulation for a realistic model that can be compared to this complex mosaic of experimental results and to collect additional EDAFS spectra to confirm these observations.

References:

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Reference related to this work:

- *Structural properties of Ge/Si(001) Nano-Islands by Diffraction Anomalous Fine Structure and Multiwavelength Anomalous Diffraction*

M.-I. Richard, N.A. Katcho, M.G. Proietti, et al., 10SXNS Conference proceedings (2008), to be published.