ESRF	**Experiment title: Facet-dependent diffusion and atomic ordering inside SiGe nano-islands grown on vicinal surfaces**	**Experiment number**: HC618
Beamline: ID01	**Date of experiment**: from: 10 May 2013 to: 14 May 2013	**Date of report**: 29/08/2013
Shifts: 12	**Local contact(s)**: M.-I. RICHARD	*Received at ESRF:*

Names and affiliations of applicants **(* indicates experimentalists):**

Dr. Angelo Malachias* (Universidade Federal de Minas Gerais Departamento de Fisica, Brazil)

Dr. Luca Persichetti* (Universita di Roma, Italia)

Dr. Anna Sgarlata* (Universita di Roma, Italia)

Dr. Marie-Ingrid Richard* (IM2NP/CNRS, ESRF)

Report:

Introduction:

The aim of this experiment at ID01 was to study structural properties (composition, atomic ordering and strain) of SiGe nano-islands grown on vicinal Si(001) surfaces, by combining Grazing Incidence Diffraction (GID) and Multiwavelength Anomalous Diffraction (MAD). In order to provide a clean scenario where surface diffusion and faceting can play distinct roles in the atomic order process, experiment was performed in self-assembled Ge islands grown in substrates with different surface orientation, producing total facet area ratios modified with respect to what obtained in Si(001) surfaces, as well as strong changes in surface diffusion. The experiment should provide an improved understanding of the local atomic arrangement and formation of antiphase-boundaries, ordering mechanisms and surface induced intermixing processes, which are still poorly understood in the extensively studied SiGe system.

Experimental data and results:

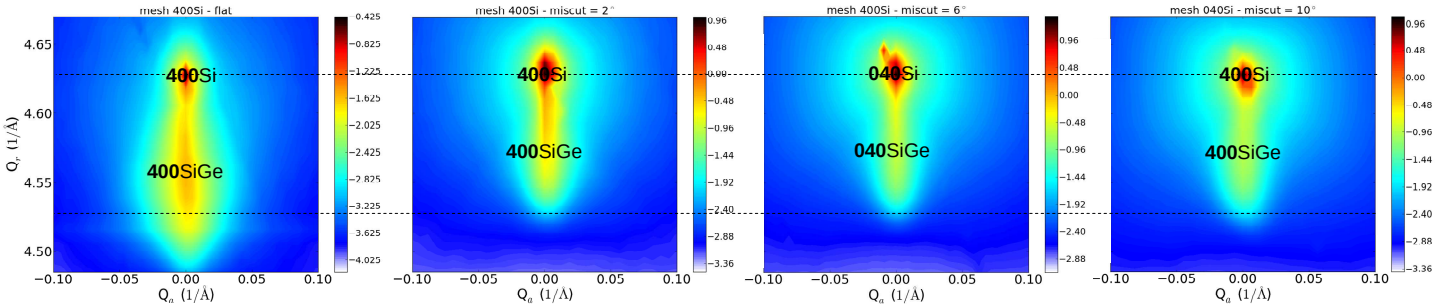

Fig. 1. From left to right: **400**Si or **040**Si reciprocal space maps of SiGe islands grown on 0, 2, 6 and 10° miscut angle samples. The positions of the Si and SiGe Bragg peaks are indicated on the maps.

13 MLs of Ge were deposited at a temperature of 600°C during 45 min on four Si(001) samples showing different miscut angles (0, 2, 6 and 10°). After growth, horizontal (vertical) steps were observed on the samples having a miscut angle of 2 and 10° (6°, respectively). The old monochromator of ID01 was used to work in grazing angle geometry. Unfortunately, at the beginning of the experiment, we observed that the old monochromator was not properly set to energy scans. The optics motors were no more following the energy changes. We decided to perform only GID measurements at a fixed energy of 11.07 keV (λ = 1.120 Å) around several Bragg reflections. Figure 1 displays **400**Si or **040**Si maps recorded for the four samples. Q_r (=

$4\pi\sin(2\theta/2)/\lambda)$ is the radial scattering vector, where 2θ is the scattering angle. Scans along Q_r are sensitive to the strain and composition of the sample, since for each value of 2θ, regions of the island with different lattice parameters are probed.

Interestingly, the elongation of the **400/040**SiGe Bragg peak along the radial direction is similar for the samples showing a non-zero miscut angle and larger for the flat sample. This may imply that the SiGe islands are less Si intermixed or more relaxed than the ones grown on surfaces with non-zero miscut angles. Q_a (= $Q_r \sin(2\theta/2 - \omega)$) is the angular scattering vector, where ω is the sample rotation. Scans along Q_a are size sensitive, since the size, D, of the region can be inferred from the width of the Q_a scan profile ($D = 2\pi/\Delta Q_a$). Figure 2 displays the lateral size of a given region of the nano-islands diffracting at a certain Q_r (= 4.565 Å^{-1}) along the <110> and <100> directions. An asymmetry of the morphology of the grown islands is observed as a function of the miscut angle in agreement with Ref. [2].

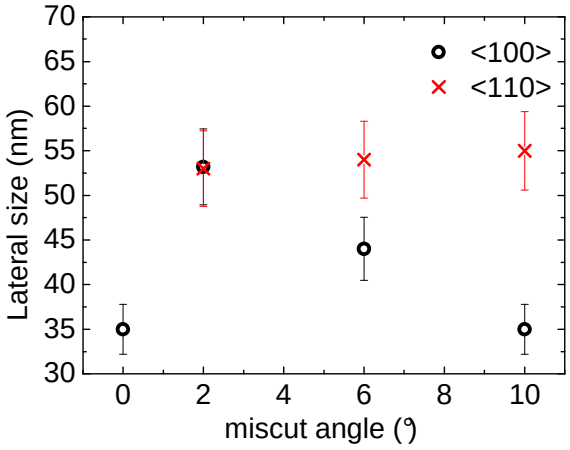

Fig. 2. Lateral size of a given region of the nano-islands diffracting at a certain Q_r (= 4.565 Å^{-1}) along the <110> and <100> directions.

200 Si reciprocal space maps were also acquired. A double-peak feature along the Q_a transversal direction was only observed in the case of the flat sample. The structure was previously described [1] as the signature of chemically ordered alloys in SiGe islands, which are separated by antiphase boundaries. This indicates that ordering only occurs in nano-islands grown on the flat sample.

Conclusion:

Grazing incidence diffraction reveals a clear anisotropy of the islands' shape as a function of the miscut angle whereas no change is observed along Q_r in the reciprocal space (see Fig. 1 – miscut angle from 2 to 10°). It would be beneficial to perform multiwavelength anomalous diffraction on these samples to disentangle strain and composition. It will allow determining whether the composition profile on misoriented substrates becomes anisotropic as the shape are modified due to surface diffusion differences (in vicinal substrates ripples with {1 0 5} orientation are formed in the surface prior to dome nucleation).

Reference:

[1] A. Malachias *et al.*, Phys. Rev. B **72**, 165315 (2005).
[2] L. Persichetti, A. Sgarlata, M. Fanfoni, and A. Balzarotti, Phys. Rev. B **82**, 121309(R) (2010).