In-situ study of the nucleation behaviour of SiGe islands on Si(001) (SI1121)

A combination of *in situ* Grazing Incidence Small Angle X-ray Scattering (GISAXS) and X-ray Diffraction (GIXD) measurements was used during growth to analyze the growth mode of Ge islands on Si(001) with respect to their size and shape, and furthermore with respect to their composition and strain. The measurements were performed using the SUV instrument of the BM32 beamline at the ESRF. Two-dimensional GISAXS patterns were recorded with a Princeton CCD detector.
The deposition was followed monolayer (ML) by monolayer. GISAXS measurements provide the detailed evolution of the shape of the grown Ge QDs. The in-situ GISAXS experiments give information on the shape transformation from pyramids with {105} facets to domes with steeper {113} for a deposit of 6 – 7 ML of Ge (see Fig.1) and finally the appearance of {15 3 23} facets is documented.

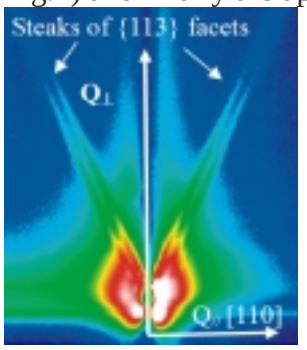

Fig. 1 GISAXS image in <110> azimuth showing the appearance of {113} facets for a deposit of 6 ML Ge on unpatterned Si (001) substrate.

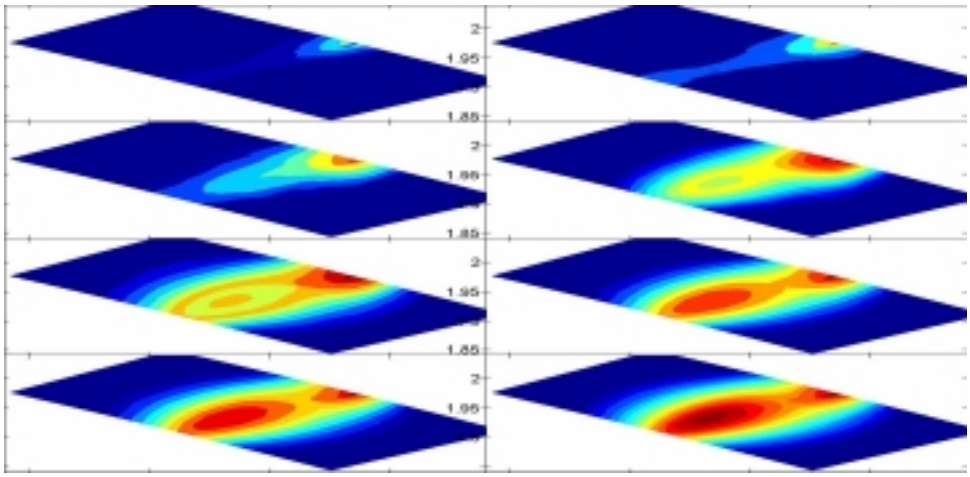

Fig. 2 Sequence of in-plane maps around (220) reciprocal lattice point for 1,4,5,6,7,8,9,10 ML of Ge deposit.

Inplane reciprocal space maps (Fig. 2) recorded in grazing incidence diffraction (GIXD) geometry allow monitoring the growth of the Ge 2D pseudomorphic wetting layer (up to 3 deposited MLs for a growth-temperature of 600°C) and the onset of formation of 3D islands at 4 ML becomes visible in the radial scans (see Fig.3). Then, a change of the relaxation behaviour between 4 and 5 deposited MLs appears accompanied by a change of the island morphology as evidenced by the GISAXS experiments. In addition to the shift of the maximum of the scattered intensity to lower values of the radial wave vector Q_r, which indicates the increasing strain

relaxation within the islands, the intensity distribution close to the peak resulting from the Si substrate shows the appearance of both compressively and tensile strained Si regions.

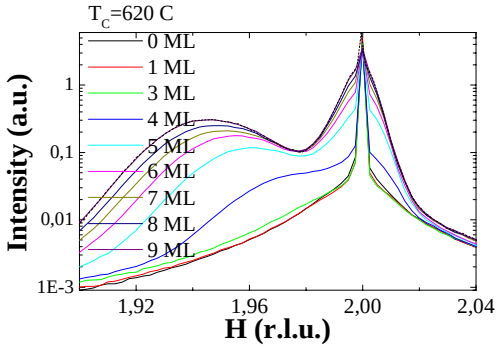

Fig.3 Radial scan in GIXD geometry in the vicinity of the Si (220) reciprocal lattice point for different deposits (0 to 9 ML) of Ge.

In order to separate the influence of the strain relaxation from that of the Ge content on the distribution of the diffracted intensities from the islands, in a forthcoming beamtime anomalous diffraction experiments are planned.

The contribution of the wetting-layer to the formation of the islands has also been studied by GIXD. The amount of Ge from the wetting layer that diffuses into the islands could be estimated using the following procedure. For each added monolayer, the intensity scattered by the partially relaxed Ge islands was integrated over all three directions of the reciprocal space maps. This integrated intensity is proportional to the number of Ge atoms inside the islands. After the onset of islands formation, this intensity should just increase linearly with the deposited amount, if no material from the Ge wetting layer is transformed into 3D islands. For a deposition temperature of 550°C, a deviation from this linear behaviour was observed between 4 and 6 ML which shows that the equivalent of about one atomic layer is transported from the 4 ML thick wetting layer into the islands. After growth AFM measurements show trenches surrounding each island, probably linked to this mechanism of material transport discovered in the GIXD data.

The in-situ monitoring of GISAXS and GIXD data during Ge island growth gives so far unprecedented knowledge on how the size and shape transformations are connected to strain relaxation and thus will serve as a valuable input for realistic simulations of the Stranski-Krastanow type of island growth.

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