	Experiment title: Si surface nanopatterning and quantum dot relaxation	**Experiment number:** Si-983
Beamline: ID01	**Date of experiment:** from: 05.11.2003 to: 10.11.2003	**Date of report:** 26.02.2004
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Report:

In-plane reciprocal space mapping and anomalous x-ray diffraction has been employed to study the structural and compositional properties of a Ge deposit onto a prepatterned Si-substrate.

The prepatterned substrate is obtained in the following way: a single Si (001) wafer is cut into "twin" slices with an implantation plus a separation process, then we bond the "twin" surfaces again with a controlled relative in-plane rotation (1° in the analysed sample). This twist leads to a regular square grid of srew dislocations [1], and a chemical etching of the sample leads to a square mesa array with a periodicity of about 22 nm [2]. Two samples have been characterized before and after a Ge-deposition of 9 Å (6.4 ML) on top of the mesa array. In-plane reciprocal space maps in the vicinity of the Si (440) reflection of these samples are shown in Fig. 1 for the corrugated Si surface (a) and for the sample after Ge deposit (b). Note that the reciprocal axes are labelled in reciprocal lattice units of the mesa-array. The mesas are oriented along the "average" crystalline <110> direction and the periodic spacing is determined to be 218.8 Å. The Si (440) reflection can be found at the (228 0) reciprocal lattice point of the 2D mesa array with commensurate model.

The radial directions for the (440) reflection of the underlying substrate and the ultrathin twisted coverlayer are indicated. Inbetween these lies the reciprocal direction of the mesa array. This situation is sketched in Fig. 1 (d). Figure 1 (c) presents a similar in-plane map for a Stranski-Krastanov type of growth of Ge on nominal Si (001). The dramatic difference in the degree of relaxation between the standard reference and the Ge deposited sample is clearly visible. For the mesa-array, the size of the long-range ordered domains could be estimated via the rocking width of the sattelites visible in Fig. 1(a). It extends over 500 nm thus containing about 24 periods of the mesa grid. Concerning the epitaxial relation between the deposited Ge and the underlying crystal, an *unconconventional type of growth* can be observed. The radial direction of the Ge(440) reflection does not follow the one of the upper Si layers. It rather lies in between the radial direction of the bonded layer and the radial direction of the mesa grid. This could be one possible reason for the unusually high degree of relaxation in the Ge-nano-crystals.

To evaluate the Ge-concentration in the crystals, anomalous diffraction was performed at the (440) reflection [3]. The scan along the radial direction is shown in Fig. 2 for an x-ray energy of 11042 eV (black symbols). The concentration as a function of momentum transfer is plotted as a red line. It amounts up to 85 % at its maximum. The lateral size of the Ge-islands can be estimated from the width of the diffuse signal in Fig. 1 (b). It turns out to be of the order of 50 Å and thus is significantly smaller than one mesa size. This small size limits the concentration resolution in reciprocal space due to the large overlap of the formfactor in the radial direction. This value is in close agreement with STM measurements obtained on the same sample showing 4 to 5 dots / mesa.

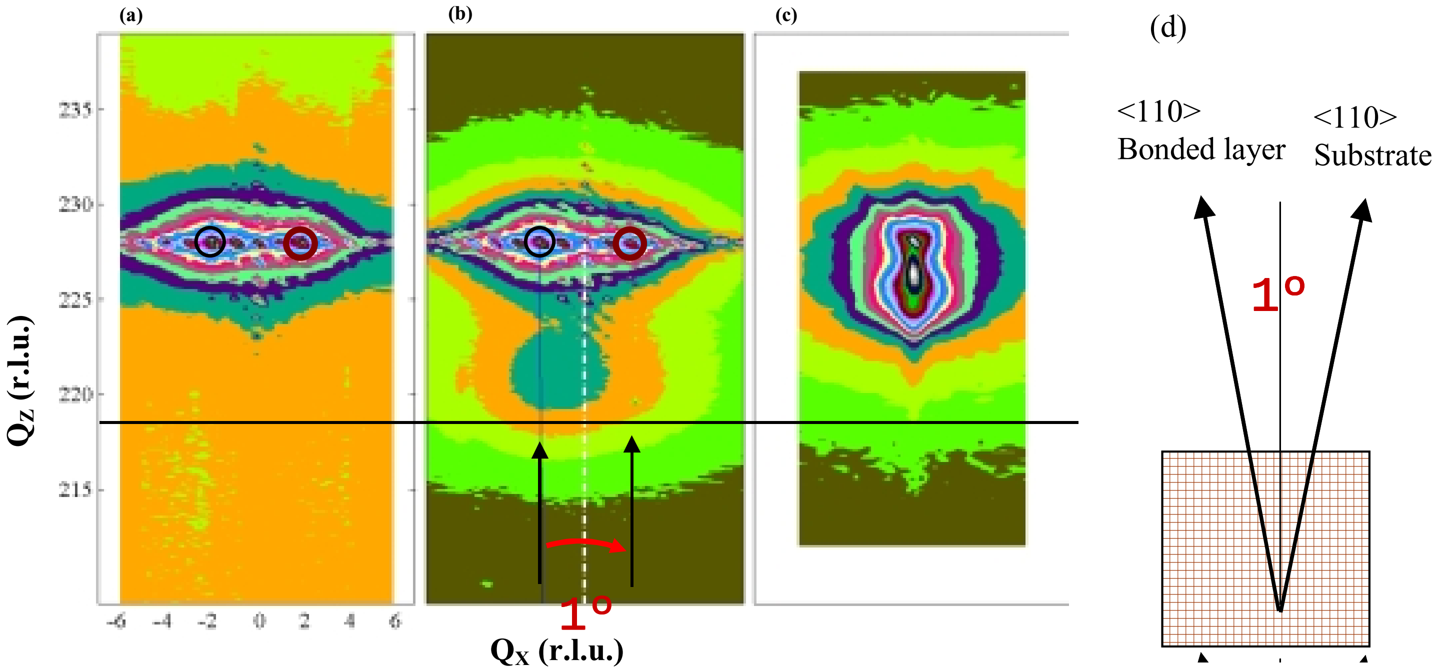

Fig.1: Reciprocal space maps in the vicinity of the Si(440) reflection. All maps are plotted on the same scale of reciprocal lattice units that correspond to reciprocal lattice of the 2D cubic array of mesas with 218.8 Å periodicity. (a) represents the pure Si surface with the meas array. (b) shows the same sample after deposition of 8 ML Ge and (c) shows the same map for a Stranski-Krastanow grown sample. Black arrows in (b) describe the radial <110> directions for substrate and twisted bonded coverlayer as sketched in (d). The white dashed line traces the <1 0> direction of the mesa array. A horizontal black line marks the reciprocal space position for pure, relaxed Ge.

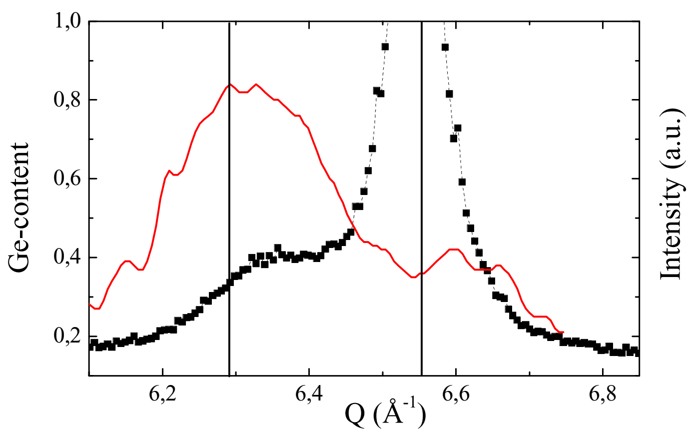

Fig.2: Radial scan at an X-ray energy of 11042 eV (black squares) across the (440) reflection from the 50 large Ge crystallites and the Si-surface reflection (truncated peak). The red line discribes the Ge-content as determined from anomalous diffraction. Perpendicular lines mark the reciprocal positions corresponding to the lattice parameters of pure Si and Ge.

In addition to these results, radial and tangential scans close to the (220) have been performed, they will be quantitatively analysed with kinematical theory including atomic positions perturbed by the elastic displacement field of the dislocation networks [4]. We found "new" superlattice peaks at half order positions (for example (113.4 k 0) scans) that are currently under study.

References

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