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| ESRF | Experiment title: **Ordering, shape, strain and epitaxial orientation of Ge quantum dots during their organized growth on patterned Si(001) substrates: a combination of *in-situ* Anomalous X-ray diffraction and GISAXS studies.** | **Experiment number**: 32-03-636 |
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## Report:

A combination of *in situ* Anomalous X-ray diffraction and Anomalous Grazing Incidence Small Angle X-Ray Scattering measurements was used during growth to analyze the growth mode of Ge islands on Si nanopatterned substrates and on nominal Si substrates, 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 ESRF. Anomalous X-Ray experiments were done at twelve different x-ray energies around the Ge K-edge, 11103 eV, in order to be more sensitive to the Ge content of the islands. Two-dimensional GISAXS patterns were recorded with a Princeton CCD detector. The Si nanopatterned substrates present small mesa with a periodicity of 20nm and were produced by a procedure called twisted wafer bonding performed by the CEA-Leti.
The deposition was followed monolayer (ML) by monolayer.

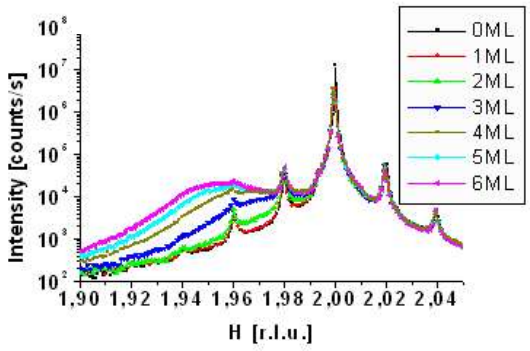


Fig. 1 Radial scans in GID geometry in the vicinity of the Si(220) reciprocal lattice point for different deposits (0 to 6ML) of Ge on a nanopatterned Si substrate.

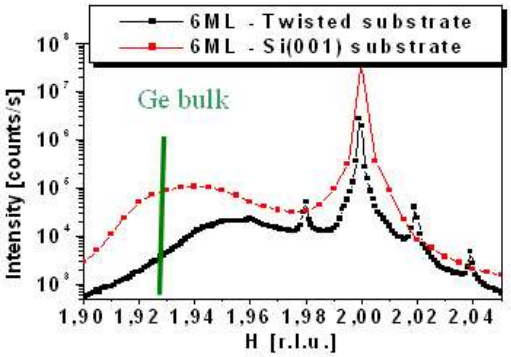


Fig.2 Radial scans in GID geometry in the vicinity of the Si(220) Bragg peak for a deposit of 6ML of Ge in the case of a twisted substrate (black line) and of a Si(001) substrate. The position of the Ge Bragg peak is indicated with a green line.

Grazing Incidence x-ray Diffraction (GID) measurements (Fig.1) showed that on these patterned substrates, at 500°C, the pseudomorphic wetting layer thickness is limited to one equivalent monolayer (instead of 4 on a nominal susbtrate), and the onset of formation of islands start at 2ML. Above 2 ML, the maximum of the

scattered intensity progressively shifts to lower H values, which indicates an increasing strain relaxation within or below the islands. This strain relaxation is found to be considerably smaller (Fig. 2) than on nominal substrates at the same temperature, which may correspond either to a larger diffusion of Si inside the Ge islands or to an effect induced by the presence below the surface of a network of screw dislocations generated by the twist between the two Si wafers.
Anomalous GID using the MAD (Multiwavelength Anomalous Diffraction) method was also performed to extract the Ge and Si partial structure factors, $F_{Ge}$ and $F_{Si}$, for each Ge deposit. Fig. 3 shows their evolution for a growth temperature of 500°C.
A significant contribution of Si is clearly found below the islands peak, which may either be attributed to the diffusion of Si into the islands, or to a strain below the Si surface, that would be induced induced by the Ge islands. As at a temperature of 550°C, the interdiffusion of Si into Ge islands is very small for nominal substrates, the last explanation seems more likely. Simulations are planned to address this question in more details.

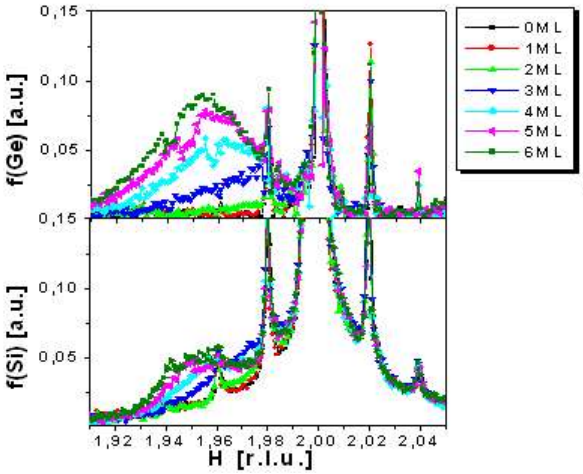


Fig. 3 Extracted anomalous structure factor, $F_{Ge}$ (up) and non-anomalous structure factor, $F_{Si}$ (down) for different deposits of Ge during the growth. The intensity was collected using radial scans along the [220] direction, in the vicinity of the Ge absorption edge

Moreover, GISAXS combined to Anomalous scattering allowed to investigate the organization of the Ge islands on the Si nanopatterned substrate. By subtracting two GISAXS images at and below the Ge absorption edge, we can reveal the localisation of Ge for a section of a GISAXS image (Fig. 4). The observed intensity corresponds to the contribution of Ge. The fact, that the Ge is located at the position of the rods of the dislocation network means that small Ge islands are organized on the patterned substrates, which was confirmed by SEM measurements (Fig. 4).

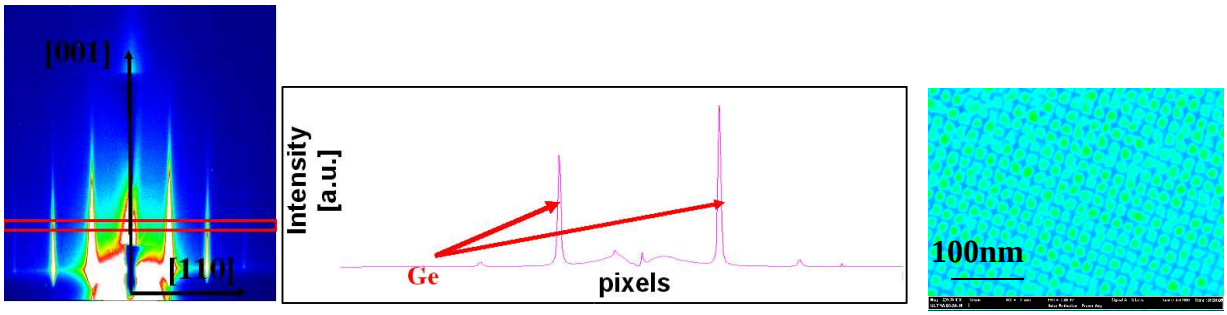


Fig. 4 GISAXS image along the <110> azimuth and below the Ge absorption edge (left). Graph obtained by subtracting the red cross section of two GISAXS images at and below the Ge absorption edge (middle). SEM measurements after 6 deposited MLs of Ge. An organization of the Ge islands on the nanopatterned substrate can be observed.

The in situ monitoring of Anomalous GISAXS and Anomalous scattering data during Ge island growth give so far knowledge on how the size and shape of the islands are connected to strain relaxation and Si interdiffusion.