ESRF	**Experiment title:** Dislocation-free Interfaces in Mismatched Semiconductor Heteroepitaxy	**Experiment number**: HC-2006
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Shifts: 15	**Local contact(s)**: Boesecke Peter (email: boesecke@esrf.fr)	*Received at ESRF:*

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Report:

The mismatched materials suffer from misfit (MDs) and threading (TDs) dislocations formed at the material interface and from wafer bowing during the heteroepitaxial growth. Both MDs and TDs negatively impact the electrical and optical properties of the potential device.

Recently Falub et al. achieved a breakthrough in the attempt to eliminate threading dislocations from heteroepitaxial SiGe/Si layers, realized by using a novel kind of epitaxial growth in which densely packed 3D SiGe crystals are formed on patterned Si substrates [1]. All threading dislocations stemming from the heavily defected heterointerface are forced to leave the crystals through their sidewalls, leaving the upper crystal region defect-free [2]. This method is highly effective in eliminating threading dislocations, but it does not prevent the formation of misfit dislocations at the SiGe/Si heterointerface [3]. Recently M. Salvalaglio et al. have proposed [4] an innovative approach to eliminate misfit dislocations in highly mismatched, compositionally graded SiGe/Si heterostructures. The misfit stress may be relaxed entirely elastically by choosing the appropriate crystal width and Ge grading rate [5] investigated in this work.

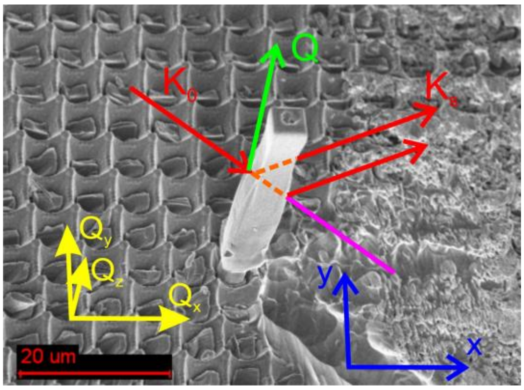

Fig. 1: *Perspective view SEM micrograph of an isolated 35 um tall graded SiGe crystal which was used for the nanodiffraction experiment. The image also shows a schematic sketch of the scattering geometry with incident beam K_0 and exit beam K_s defining the scattering vector Q. The yellow vectors define the reciprocal space coordinates (Qx;Qy;Qz) and the blue arrows indicate the xy movements of the piezo stage.*

In this experiment, we have used X-ray nanodiffraction technique performed on isolated 3D $Si_{1-x}Ge_x$ microcrystals (see Fig. 1), in which the Ge content x is linearly increased from 0 to 40%. Three types of microcrystals were measured: ones with a base size 2 μm at the low grading of 1.5% μm^{-1} (LG2), ones with a base size 5 μm at the same low grading (LG5), and ones with a base size 2 μm at the high grading rate of 6% μm^{-1} (HG2). Unpatterned (UNP) area was measured as well as a refference. Depending on the crystal width, some types of 3D SiGe crystals are expected to be completely free from misfit and threading dislocations. During the

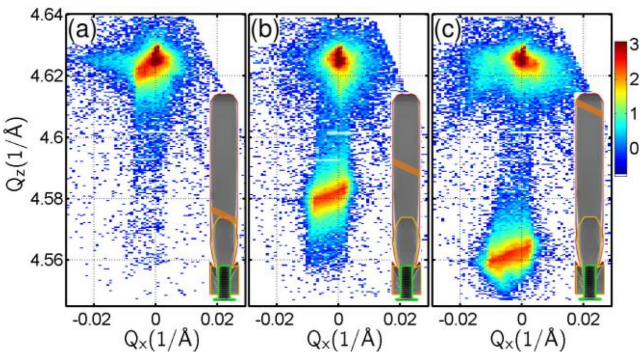

Fig. 2: *Series of QxQz RSMs projected along Qy direction as measured for various beam positions on a SiGe crystal LG2. Beam positions at the bottom, the middle and the top of the graded part are shown for the symmetric (004) diffraction (a, b, c). The inset in the right bottom corner of each RSM shows the irradiated area in the microcrystal.*

experiment we have performed series of scanning X-ray diffraction microscopy (SXDM) images for different incidence angles and for various positions of the nanobeam in the microcrystal (see Fig. 2). For series of positions in real space *(x,y,z)* 3D reciprocal space maps (RSMs) have been built (see Fig. 3). RSMs around the (004) and (115) Bragg reflections have been collected on 2D meshes for microcrystals with different Ge grading rates and different widths, and on an unpatterned area as well. From positions of maxima we could reconstruct 3D spatial maps of crystal lattice tilt depending on the Ge grading rate and crystal width, details can be found in recent publication [6]. We demonstrate that the misfit strain relaxation results in convex lattice bending and the results are in excellent agreement with finite element calculations.

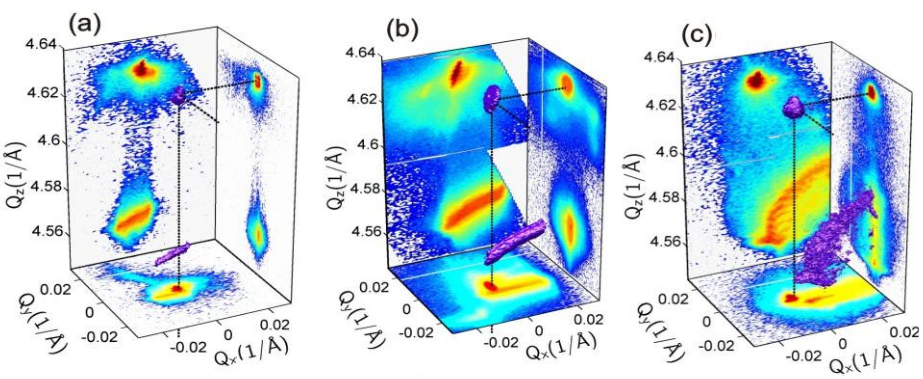

Fig. 3: A *series of 3D RSMs with all 3 projections recorded with beam positions at the top of the microcrystal. Crystals LG2 (a), LG5 (b) and HG2 (c) are shown.*

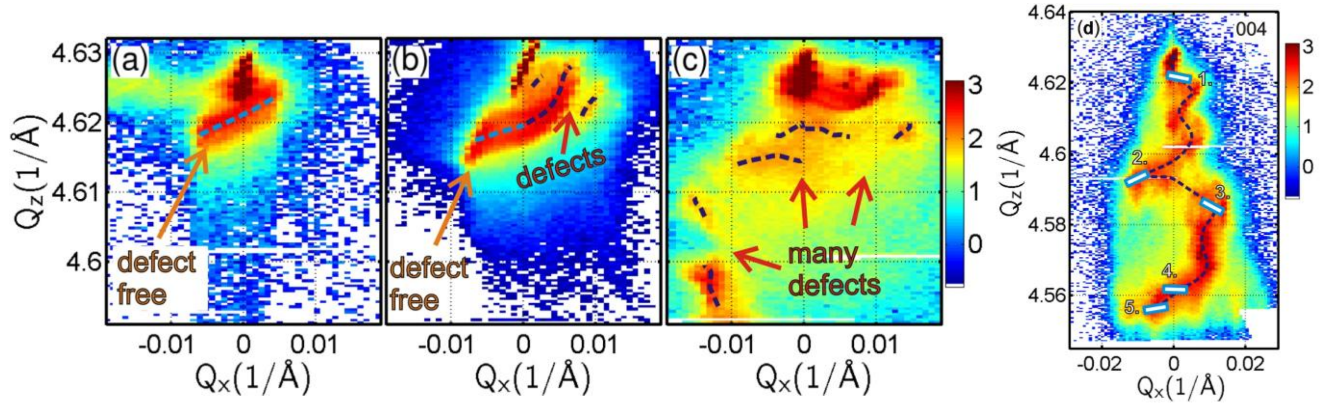

Fig. 4: *Details of the RSMs recorded close to the Si substrate peak when the beam penetrates the starting layers close to the crystal bottom with low Ge content (top of 8 μm buffer layer). Pure elasticity (parabolic bending) is observed in the SiGe crystal LG2 (a), deviations from parabolic bending is observed at SiGe peak already in the bottom part of the SiGe crystal LG5 (b) and random nonparabolic lattice bending caused by many irregular splits of the SiGe peak is observed in the SiGe crystal HG2 in most of the crystal volume (c). No defects in RSM (a) are detected, the light blue line corresponding to pure elasticity. For RSM in (b), defects are present only at very crystal bottom, combination of light blue (defect free top) and dark blue line (defects at interface). For RSM in (c) many defects are present. An RSM measured in the unpatterned planar layer (d). A series of mosaic crystal blocks with random tilts of about +-0.2deg is detected.*

In Fig. 4 we observe that the details of the RSMs which confirm that the microcrystals with a narrow size and shallow Ge grading rate are purely elastically relaxed, i.e. no defects are nucleated. Conversely, wider crystals or crystals grown at a higher grading rate are plastically relaxed. Misfit and threading dislocations are mainly introduced close to the heterointerface. The unpatterned planar layer contains several dislocations and grain boundaries. Much more details can be found in corresponding publication [6].

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