ESRF	Experiment title: Nanostructures for the deformation control of group-IV epilayers and membranes	Experiment number : HS-4672
Beamline: ID01	Date of experiment: from: 12/09/2012 to: 18/09/2012	Date of report : 14/03/2013
Shifts: 18	Local contact(s): Gilbert Chahine	Received at ESRF:
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Report:

Using high-resolution x-ray nanodiffraction, we aimed to map the local uniaxial strain fields in SiGe nanostructures patterned in a top-down manner by electron-beam lithography. Elastic redistribution of the heteroepitaxial strain resulting from the lattice mismatch between Ge and Si is expected to induce strong deformations on the sub-micron scale in either the substrate or the capping layer, if a strained two-dimensional SiGe layer is patterned into a long ridge. The strain can be measured using symmetric and asymmetric three-dimensional reciprocal space mapping, and compared with Finite Element Method (FEM) models and micro-Raman spectroscopy results.

Samples were fabricated from strained Si/Si_{1-x}Ge_x/Si(001) layers. A sample with 100 nm of Si_{0.7}Ge_{0.3} and another with 20 nm of Si_{0.6}Ge_{0.4} were prepared; in both cases the Si cap layer was 10 nm thick. As grown, the SiGe layers were fully strained, as verified by laboratory x-ray diffraction. Patterns were designed with arrays of SiGe stripes (aligned along the [110] directions) of a range of widths from 300 to 1450 nm, with a 1000 nm gap between the stripes in all cases. Scanning electron microscopy images are shown in Fig. 1. Thinner stripes should show stronger elastic relaxation effects, but would also be harder to resolve with a finite x-ray beam width, so this range of stripe widths allowed us to explore the optimum stripe widths in which to see the desired effects.

At ID01, a 8.4 keV beam was used. This energy was chosen so that the exit angle for the asymmetric (113) reflection would be extremely grazing (1.55° for Si), such that the diffracted signal would come from a region very close to the surface where the relevant effects are expected to be seen. The incidence angle for (113) was around 52°, which maintained a small beam footprint on the sample, and was close to the limit of collision between the optical microscope objective and the x-ray focusing optics. The symmetric (004) reflection was also accessible. A Fresnel zone plate was used and a spot diameter of about 500 nm was obtained. This beam width allowed stripes to be resolved, as shown in Fig. 2, in which the variation of intensity of the SiGe(113) signal can be seen as the piezo stage was scanned in the *x* direction (along the beam).



Fig. 1. Scanning-electron microscopy images of the nanostructures fabricated for the HS-4672 experiment. On the left, the whole structure can be seen, including the wide markers which allowed the beam position on the sample to be easily identified. The structure was clearly visible in the optical microscope fitted to the sample stage. In the central and right-hand images, it can that there is a range of stripe widths. This allowed individual stripes to be uniquely identified during scans.

Fig. 2. Total diffracted intensity of the SiGe(113) reflection during a scan, with each line representing a different incidence angle. The stripes can be clearly identified, with broader stripes at lower pix values. The intensity scans have been corrected for the drift of the sample with respect to the beam, which amounted to roughly 100 nm per hour.





ormalized intensity

Fig. 3. Top left: Reconstructed (113) reciprocal space map taken as the x-ray beam passes over a 950 nm wide $Si_{0.7}Ge_{0.3}$ stripe. Top right: kinematical simulation based on a 500 nm beam passing through a FEM model of the structure. The SiGe signal peaked is at $q_{ll} = 2.598 \ nm^{-1}$ (and $q_{\perp} = 5.43 \text{ nm}^{-1}$) while the Si peak is at $q_{\parallel} = 2.600 \text{ nm}^{-1}$; comparison with the FEM reveals that this is due to elastic strain relaxation rather than an error of tilt correction, and that the extension of the SiGe signal towards higher q_{\parallel} is also a real effect. The bottom panels show results (left) and simulations (right) for a beam position between two stripes. In this case the SiGe intensity is lower but not absent, indicating incomplete etching.

Figure 3 presents reconstructed (113) reciprocal space maps, and kinematical simulations of diffraction in a FEM model. Careful comparison reveals that the misalignment of the Si and SiGe peaks in $q_{||}$ is a real experimental effect rather than an error in tilt correction between the two measurements, and also that the intensity towards $q_{||} \sim 2.62 \text{nm}^{-1}$ is a real feature. Some variation in the Si peak may also be visible, corresponding to direct identification of the thin tensile-strained cap layer, but this effect will be very small.