ESRF	**Experiment title:** **Nano-diffraction mapping and predictive modelling of the strain in single artificial SiGe nanostructures**	**Experiment number**: SI-1873
Beamline: ID13	**Date of experiment**: from: 02/07/2009 to: 07/07/2009	**Date of report**: 01/09/2009
Shifts: 15	**Local contact(s)**: S. Schoeder	*Received at ESRF:*

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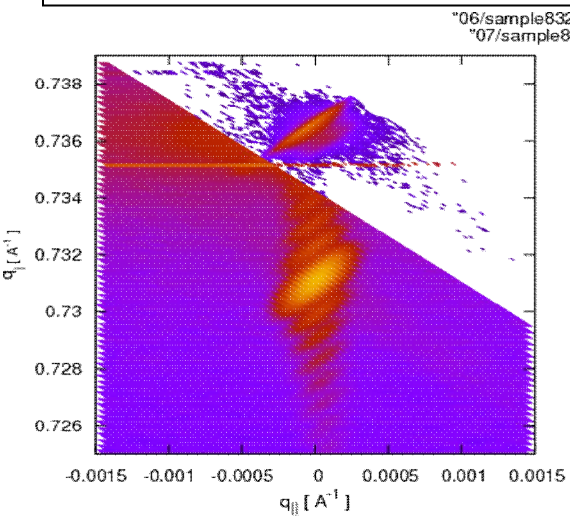

Figure 1: Reciprocal space map, taken in an unetched region, reconstructed from two separate scans of 101 images each. The Si peak is at $q_{\perp}$ = 4/(5.4310 Å) = 0.7365 $Å^{-1}$ (and $q_{||}$ = 0 $Å^{-1}$) with the $Si_{1-x}Ge_x$ peak below; the fringes vertically above and below the peak relate to the finite thickness of the $Si_{1-x}Ge_x$ layer, and the sharp horizontal $Si_{1-x}Ge_x$/Si interface and $Si_{1-x}Ge_x$ surface. Diagonal elongation of each peak is related to the ~1 mrad beam divergence.

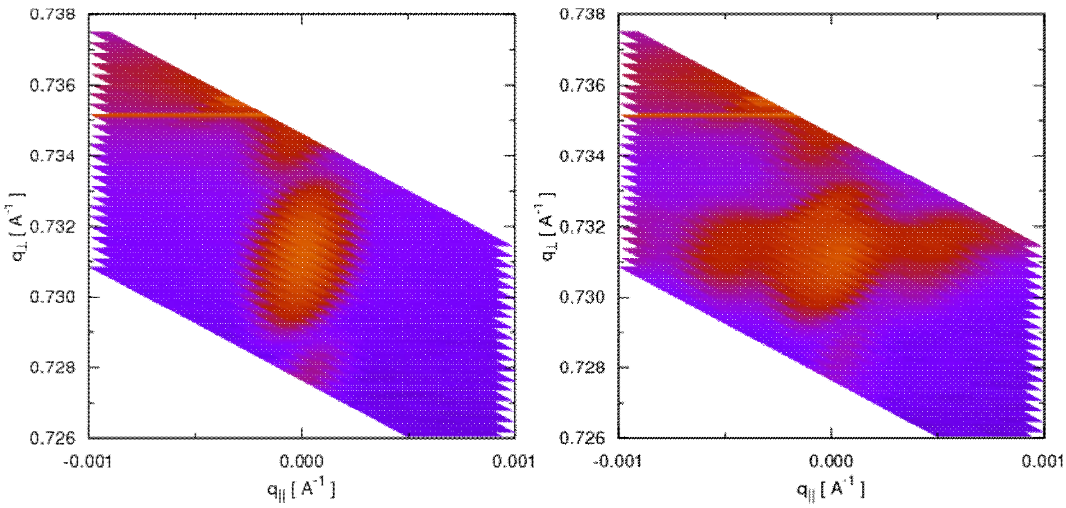

Figure 2: Reciprocal space maps around (004) taken on an etched $Si_{1-x}Ge_x$ region (left) and passing over a $Si_{1-x}Ge_x$ ridge. Lateral fringes appear as the spot passes over the ridge. The peak intensity moves slightly upwards, indicating a change in the relaxation state of the ridge with respect to etched or planar unetched regions.

Report:

Experiment SI1873 took place at the Nanofocus extension of the ID13 beamline. The energy of the x-ray beam was 15.25 keV, giving a wavelength of 0.8130 Å. The ID13 nanofocus extensions is able to realize a spot size of ~ 100 nm using diffractive and refractive optics.

The aim was to measure the strain states in artificially made $Si_{1-x}Ge_x$ nanostructures grown on Si(100).

We performed diffraction about the (004) and (440) Bragg peaks, the former being a standard symmetric reflection geometry and the latter involving transmission *through* the sample.

$Si_{1-x}Ge_x$ layers were deposited epitaxially on Si(100) substrates by low-energy plasma-enhanced chemical vapour deposition (LEPECVD) [1,2], and nanostructures were then fabricated by e-beam lithography [3] and reactive ion etching. Layers with two different *x* and two different thickness were grown; the thinner layers were designed to be fully strained. The nanostructures comprised ridges, aligned along the <110> directions corresponding to the edges of the cleaved samples, of various widths between a few microns and about 200 nm; relatively large square areas were also left unetched. The $Si_{1-x}Ge_x$ epilayer was not completely etched away in between the structures, so that strain changes close to outside edges of the structures could also be evaluated.

Experimental

The sample was mounted such that its edges, corresponding to <110> directions, were as close to horizontal and vertical as possible. This alignment had to be carried out by using an optical microscope during the mounting step on the sample holder, since the sample stage was not able to rotate or tilt the sample about the horizontal axes. The normal to the (001) surface (and therefore the plane containing the incoming and outgoing wavevectors) was horizontal. The MAXIPIX detector was mounted at a distance of just over 1 m from the sample, positioned using an alignment laser system in order to collect diffracted intensity from either (004) or (440). *In-situ* optical microscopy and x-ray fluorescence was also used in order to locate the nanostructures.

Results

Figure 1 shows a map of reciprocal space (RSM), taken in a plane in which the [110] direction is horizontal and the [001] direction is vertical, around the (004) reflection. This map was reconstructed from 202 detector images taken as the angle θ between sample surface and indicent beam was scanned. The undulator was detuned during the scan over the Si peak (θ_{Si} = 17.42°) to avoid saturating the MAXIPIX detector. With the detector (256 × 256 pixels, 1.41 cm width) at a distance of 1.1 m, the pixel width of 55 µm corresponded to a relative precision in the determination of the perpendicular lattice constant $a_{\perp}$ better than 10^{-4}. The ~1 mrad divergence of the nanofocused beam did not reduce this precision, since as can be seen from the RSM, this divergence elongates the diffraction peaks obliquely with respect to the reciprocal space axes.

Figure 2 shows two RSMs about the (004) reflection of the $Si_{1-x}Ge_x$ layer, each reconstructed from scans over θ, taken in different positions on the sample. On the left, diffraction is from the thin etched $Si_{1-x}Ge_x$ layer, while on the right the x-ray spot is passing over a nanolithographically defined ridge with width of less than 200 nm. Analysis of the diffraction peak reveals that the component corresponding to the ridge has shifted in position, corresponding to a local elastic strain relief. This effect was also seen at the edge of the large planar region; in addition, elastic deformation of the $Si_{1-x}Ge_x$ close to the outside edges of the structures was observed.

In order to unambiguously determine both the composition and the strain of the $Si_{1-x}Ge_x$ layers, a reflection (*hkl*) with $h \neq 0$ and $k \neq 0$ (and most conveniently with $h = k$) needed to be measured. However, this required movement of the detector to a new position, which had to be determined and then performed by hand without disturbing the alignment of the rest of the experiment, since the detector was not part of the goniometer. Mapping about the (440) reflection involved transmission through the sample; the $Si_{1-x}Ge_x$ layer (440) peak is coincident with the substrate (440) peak in the case of full strain, however, and this generally meant that the $Si_{1-x}Ge_x$ layer (440) peak was not in fact visible.

Conclusion

Using the ~100 nm spot size available at the ID13 Nanofocus extension, we were able to map the perpedicular lattice constant in nanopatterned $Si_{1-x}Ge_x$ structures with a precision better than 10^{-4} and a lateral resolution

comparable to the spot size. These results go beyond the spatial resolution attainable using µ-Raman [4] and relate to artificially patterned rather than self-assembled [5] nanostructures. Elastic deformation of $Si_{1-x}Ge_x$ ridges and edges was observed.

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