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Report:

The replication of the interface roughness in Si/SiGe multilayers grown on (001) Si substrates, which is an important quantity for their electronic transport and optical properties, has been studied by x-ray reflectivity reciprocal space mapping.

We had previously shown [1] that for Si/SiGe multilayers grown on slightly miscut (001) Si substrates, the interface profiles are highly correlated, but the direction of the replication is inclined with respect to the growth direction. In Ref. [1], this oblique replication was explained as being caused by the influence of the inhomogeneous strain distribution around step bunches . In the mean time, the Linz group has carried out further studies on the growth of epilayers on vicinal (001) Si surfaces [2], which have shown that already in homoepitaxy, highly periodic morphological features appear, related to a kinetic growth instability. In order to discriminate between strain induced morphological instabilities and the kinetic ones, Si/SiGe multilayer samples ($x = 0.35$ %, $d_{SiGe} = 3.3$ nm, $d_{Si} = 21$ nm or $d_{Si} = 38$ nm, 10 periods) were grown on Si (001) substrates which had a miscut less than 0.14° and a miscut of 1° in the in-plane [100] direction .

Information on the interface roughnesses and their correlation were obtained from measurements of the specular and non-specular x-ray reflection in coplanar geometry using a triple bounce Si (111) monochromator and a wavelength of 1.05 Å. The divergence of the primary beam and hence the resolution in ω was approximately 0.002°. The distribution of the scattered intensity in reciprocal space (reciprocal space map) was measured $I(\boldsymbol{Q})$, where $\boldsymbol{Q} = \boldsymbol{k} - \boldsymbol{k}_o$, $\boldsymbol{k}$ and $\boldsymbol{k}_o$ are the wavevectors of the scattered and incident beams. In the figures the Q_x axis is parallel to the sample surface and the Q_z axis parallel to the surface normal.

The interface roughness and its correlation gives rise to resonant diffuse scattering accompanying the coherent superlattices satellites in the regions $Q_x > 0$ and $Q_x < 0$. For the sample with a miscut angle of the substrate of 0.14°, the resonant diffuse scattering sheets are barely visible, indicating very smooth interfaces (see Fig.1(a)). Also the top surface does not show any appreciable surface undulations, as obtained from atomic force microscopy. For the sample, which was grown at the same time on the same substrate holder, on a (001) Si substrate with 1° miscut, the reciprocal space maps are shown for three azimuthal angles ϕ in Figs. 1(b)-(d). This angle ϕ describes the orientation of the scattering plane (determined by $\boldsymbol{k}$, $\boldsymbol{k}_o$, and the surface normal) with respect to the miscut direction. For $\phi = 0°$ the scattering plane is parallel to the miscut direction and upwards the steps, which results from the step bunching process. In this case the resonant diffuse scattering (RDS) stripes are clearly inclined by an angle χ with respect to the Q_x direction, indicating the oblique replication of the surface roughness (Fig. 1(b)). The angle χ changes the sign for $\phi = 180°$ (Fig. 1(d)), proving the asserted origin. In the geometry with the scattering plane perpendicular to the miscut direction (ϕ =90° in Fig. 1(c)) the RDS stripes are parallel to the Q_x direction, as it was expected.

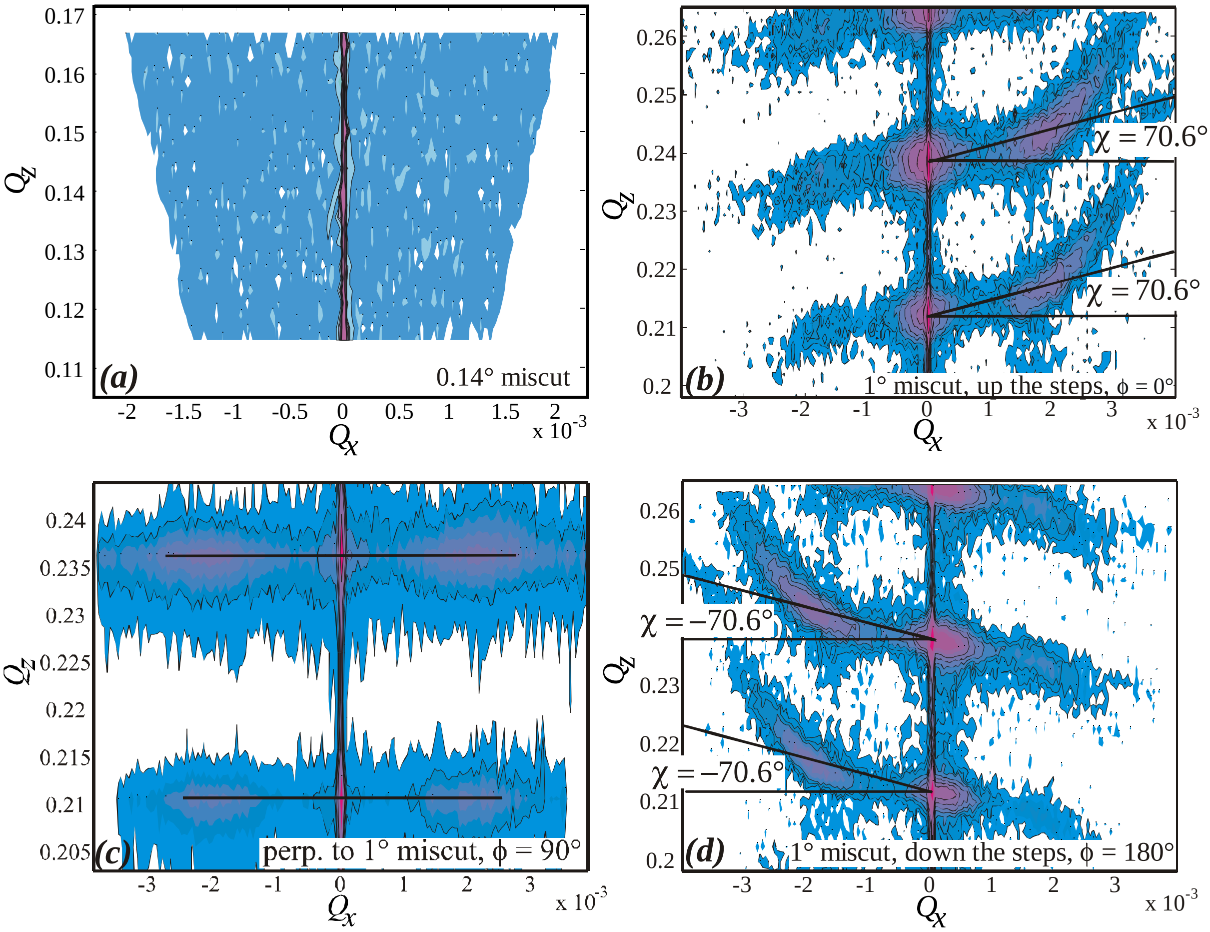

Figure 1: RDS stripes of a sample with 0.14° miscut (a) and 1° miscut (b)-(d) in different azimuths.

The increase the width of the Si layers in the SiGe/Si superlattices decreases the strain modulation at the growth front. For a sample similar to the one shown in Fig. 1(b)-(d), but with d_{Si} = 38 nm instead of 21 nm , oblique replication with essentially a similar angle *c*, as the one shown in Fig. 1(b)-(d), is still present.

The analysis of the reflectivity data is still in progress, but the following conclusions can be made right now:

(i) on flat Si (001) surfaces strained Si/SiGe multilayers with Ge contents of about 35% and SiGe layer thicknesses around 3.5 nm grown at 495°C do not exhibit appreciable interface roughening;

(ii) identical Si/SiGe multilayers, grown under the same conditions on miscut, i.e. vicinal Si substrates do show step bunching instabilities, with an oblique replication of the interface roughness;

(iii) from the experiments carried out at the OPTICS beamline, the oblique replication is related to strained Si/SiGe layer growth on already corrugated Si buffer layers.

In order to finally discriminate between strain induced surface roughness and kinetically induced step bunching instabilities, samples have to be grown on vicinal Si substrates, but using for the Si buffer growth temperatures in excess of 650°C, where no kinetic roughening occurs. Such samples would provide rather flat Si buffer layer surfaces for the subsequent growth of the strained Si/SiGe multilayers.

Additional, we measured the Ge depth profile of different SiGe heterobipolar transistors (HBT) on structured 8 inch wafers in monitoring areas of less than 500 x 500 μm^2 in size across the whole wafer. This results in a quantification of the lateral homogeneity of the SiGe epitaxy in a 0.25 µm BiCMOS technology. The results are also important for the calibration of routine in-line measurements with a conventional X-ray diffractometer.

[1] V. Holý, A.A. Darhuber, J. Stangl, G. Bauer, J. Nützel, G. Abstreiter, Phys.Rev.B **57**, 12 435 (1998).

[2] C. Schelling, G. Springholz, F. Schäffler, Phys.Rev.Lett. **83**, 995 (1999).