Highly regular self-organization of step bunches during growth of SiGe on Si(113)

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(Received 20 March 1998; accepted for publication 13 July 1998)

We have studied the structural properties of highly periodic arrays of terrace steps in a Si/SiGe multilayer grown on a miscut Si(113) substrate by atomic force microscopy, x-ray reflection and high resolution x-ray diffraction. The data reveal a regular array of step bunches with vertical correlation within the multilayer and periodic surface steps extending over lengths of several tens of microns. The (113)-faceted terraces have a lateral period of about 360 nm which is locally modulated due to a long-range waviness of the surface. © 1998 American Institute of Physics.

Heteroepitaxial growth on (113)-oriented substrate surfaces has been extensively studied in III-V material systems. As for group-IV semiconductors, the step interaction on miscut (113)-oriented Si was studied previously, but to our knowledge only very few publications concerning the growth of SiGe on Si(113) exist. Knall and Pethica have studied the initial growth behavior of low temperature molecular beam epitaxy (MBE) of pure Ge on a Si(113) substrate with a very small miscut. Rows of missing atoms parallel to (332) were observed by scanning tunneling microscopy for a Ge coverage of 3 ML, which led to the formation of long ridges with (429)-oriented sidewalls after continued deposition of Ge. Omi and Ogino reported the formation of wire-shaped nano-scale islands oriented along (332) with (519) sidewall facets during MBE growth. It was found that the wire formation is not related to the miscut direction.

We have studied the structural properties of MBE-grown Si/Si1-xGex multilayers, with x ranging from 0.25 to 0.45, grown on miscut Si(113) substrates by atomic force microscopy (AFM), x-ray reflection (XRR), and x-ray diffraction (XRD). In this letter, we report about the results obtained on one sample grown at the WSI on a Si(113) substrate with a miscut of 0.37°±0.01° in a direction 36°±2° off from [10]. The growth temperature was 550 °C, the growth rates were 0.5 Å/s for SiGe and about 0.35 Å/s for Si. The sample consists of 19 periods of nominally 10 nm Si and 2.5 nm Si0.65Ge0.35. Prior to the growth of the multilayers, a 100 nm Si buffer layer was deposited on the substrate and annealed at about 1100 °C for 10 min. The topmost SiGe layers are uncapped.

XRD experiments were performed at the ESRF-beamline ID19 using a Si(111) double monochromator and a single bounce Si(111) analyzer. Both symmetrical (113) and asymmetrical (315) reciprocal space maps (RSMs) were recorded. XRR experiments were performed at Masaryk University using a conventional x-ray source (Cu Ka) and a parabolic graded multilayer mirror. We have measured so-called ω scans, i.e., rotated the sample at fixed detector angle 2θ, for various azimuthal orientations of the sample. We have adjusted the 2θ angles so that the scan trajectories in reciprocal space cross satellite reciprocal lattice points corresponding to the superlattice periodicity in growth direction.

Figure 1 is an AFM image of the sample surface, i.e., of the topmost SiGe layer. It clearly shows the extremely periodic terraced surface profile, with the terrace edges oriented normal to the miscut direction. A statistical analysis of the surface normals obtained by AFM shows that the step terraces are (113) facets. This indicates that the measured steps result from the bunching of intrinsic steps due to miscut. A possible crystallographic orientation of the steps might occur only on a very short length scale that is not accessible by our experimental methods. Additionally, a waviness with a mean period of about 1.2 μm and the same orientation as the terraces is present. Furthermore, linear structures oriented along [21] and [12] directions can be seen. As these directions are the intersection lines of (111) glide planes of dislocations with the (113) surface, we associate them with misfit dislocations. For these dislocation directions the Burgers’ vectors point along [011] and [101], i.e., they are normal to the dislocation lines and thus provide for maximum

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strain relief. No dislocation lines along $[\bar{1}10]$ are observed, which may be due to the strong elastic anisotropy experienced by strained layers grown on the (113) surface. 8 The density of dislocations nearly parallel to the step edges is about three times lower than for dislocations with a larger angle relative to the step direction. This might be attributed to a reduction of the misfit strain due to the stepped morphology.

In Fig. 2 the two-dimensional Fourier transform (FT) of the surface profile is plotted. The sharp lines through the center are perpendicular to the dislocation lines along $[12\bar{1}]$ and $[21\bar{1}]$. The broad, weak peaks near the center (labelled W) correspond to the 1.2 $\mu$m waviness, and the other peaks are associated with the terraces. A periodic sequence of narrow peaks is visible, accompanied by weaker satellites. The distance of the main peaks (labeled $T_1, T_2, \ldots$) corresponds to the mean terrace width of $L = (360 \pm 10)$ nm. The origin of the satellites ($S_1, S_2, \ldots$) can be explained from Fig. 3. As the distance of the $S$ peaks from the $T$ peaks does not increase with the order of the $T$ peaks, they are attributed to a periodic modulation of the terrace widths. The period of this latter modulation (approx. 1.2 $\mu$m) coincides with the period of the waviness, which can be understood from the inset of Fig. 3: the waviness causes a local variation of the angle between the mean surface and the (113)-oriented terrace plateaux, which is accommodated by an according variation of the plateau widths. In the measured spectrum (Fig. 2) only the outer satellites can be observed. This asymmetry of the satellites depends on the particular modulation function of the terrace widths, e.g., a harmonic function gives such an asymmetry.

From XRR $\omega$ scans information on the morphology can be obtained as well. However, XRR is sensitive to the profile of all interfaces in the multilayer, whereas AFM only probes the top surface. Figure 4 shows $\omega$ scans measured in azimuths parallel and perpendicular to the terrace edges. The $2\theta$ angles were adjusted so that the scan trajectories crossed the third, fourth, and fifth superlattice satellite. The $\omega$ scans measured in the azimuth parallel to the step edges (lowest curve in Fig. 4) do not exhibit any nonspecular peaks, therefore, the interface roughness in this azimuth can be described by a usual fractal model. 9

In the scans taken in an azimuth perpendicular to the edges (upper three curves), a double-peak structure similar to that in Fig. 2 is present. However, in contrast to the FT of the AFM image, the pattern is asymmetric with respect to $q_x$. If we rotate the sample by 180°, the patterns are reversed with the terrace steps, through the fifth, fourth, and third superlattice satellite. The lowest, dashed, curve is a scan across the fifth superlattice satellite taken in an azimuth perpendicular to the miscut (across the terrace edges).
which are again attributed to the 1.2 μm scans, broad slightly asymmetric maxima in the data indicate that the step structure becomes more regular in the multilayer, and AFM probes only the topmost surface, up to the third order. Since XRR is sensitive to all interfaces, order T peaks are visible, whereas in Fig. 2 they can be seen in comparison with AFM. However, in XRR only the first can also be resolved, due to the larger area probed by XRR
dence to the AFM data. In the XRR curve, the inner S peaks with various 2u occur, due to the asymmetric terrace shape.10 The peak positions in the scans with various 2θ coincide. From these peak positions a mean terrace width of 360±10 nm and a modulation period of the terrace widths of about 1.2 μm follow, in good correspon-
dence to the AFM data. In the XRR curve, the inner S peaks can also be resolved, due to the larger area probed by XRR in comparison with AFM. However, in XRR only the first order T peaks are visible, whereas in Fig. 2 they can be seen up to the third order. Since XRR is sensitive to all interfaces in the multilayer, and AFM probes only the topmost surface, the data indicate that the step structure becomes more regular towards the surface. Additionally, close to the center of the scans, broad slightly asymmetric maxima (marked W) occur, which are again attributed to the 1.2 μm waviness of the surface.

High angle XRD data are presented in Fig. 5. Panel (a) displays the RSM around the symmetric (113) Bragg reflection measured in the azimuth parallel to the miscut direction (across the terrace steps). The main peak, i.e., the zero-order superlattice satellite, is accompanied by a series of side peaks along qx due to the terrace structure of the interfaces, corresponding to the T peaks described above. In contrast to XRR, XRD is sensitive not only to the geometric sample structure, but also to the strain distribution in the multilayer. The envelope of the lateral satellites as well as the diffusely scattered intensity between them is shifted towards positive qx values due to the asymmetry of the strain distribution caused by the asymmetric terrace shape.

In Fig. 5(b) the intensity distribution has been simulated by means of kinematical diffraction theory. The simulation does not include the dynamical, coherent truncation rod. In the calculations we have used the elastic Green function for the evaluation of the deformation field of a terrace edge similar to the ones presented in Ref. 11. Using this approach, we have restricted ourselves to isotropic elasticity, and we have neglected the difference in the elastic constants between Si and SiGe. A good correspondence between measurement and calculation has been achieved for a mean terrace width of L = 360 nm and its root mean square deviation σ = 50 nm.

In conclusion, we have studied a terraced Si/SiGe multilayer by means of AFM, XRR, and XRD and observed a highly regular surface structure. From the comparison of XRR and AFM results it follows that this structure is present in all interfaces, but becomes more regular towards the sample surface, i.e., with increasing number of grown bilayers. Besides the terrace structure with a mean period of 360 nm and (113)-oriented terrace plateaux, a less regular structure with a wavelength of about 1.2 μm is present, which leads to a modulation of the terrace period. From XRD the strain fields also associated with the terraces were detected.

This work was supported by GMe, BMWV ("Nanostructures"), FWF, GACR (202/97/0003), MŠČR (VS96102), BmBF (M2953 B2), and VW-Stiftung.

6Results on the whole series of samples will be presented elsewhere.