

Probing the SiGe virtual substrate by high-resolution channeling contrast microscopy

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(Received 7 January 2002; accepted for publication 1 March 2002)

Relaxed, epitaxial SiGe layers with low densities of threading dislocations are grown by linearly grading the Ge composition. However, such compositionally graded SiGe layers (virtual substrates) often result in a cross hatch surface morphology which affects subsequent device processing. Here, we report on high-resolution channeling-contrast-microscopy (CCM) measurements on such virtual substrates grown by gas-source molecular-beam epitaxy and low-pressure chemical vapor deposition. A two-MeV He⁺ beam focused to a submicron spot is used in these CCM measurements to obtain both lateral and depth-resolved information on the cross hatch features observed and their association with a slight lattice tilt. © 2002 American Institute of Physics.

[DOI: 10.1063/1.1474597]

The “virtual substrate” (VS) concept has enabled epitaxial growth of semiconductor heterostructures on mismatched but readily available substrates¹ as well as strain-balanced structures for optoelectronic applications.² In the case of SiGe this concept also allows the manipulation of electronic structures of Si through strain and provides the basis of modulation-doped field-effect transistors^{3,4} and other devices. Utilizing a compositionally graded VS, strain relaxed SiGe substrates are obtained as a template for pseudomorphic device layers. In producing these VS, a “cross hatch” morphology is produced on the surface.⁵ While this morphology is clearly associated with the strain relaxation process occurring during the growth of VS, its origin has not been clearly identified. The influence of the relaxation process is frequently studied using atomic force microscopy (AFM)^{6,7} providing morphological information about the surface, but it is very difficult to extract information from the bulk of the VS. High-resolution channeling-contrast microscopy (CCM)⁸ provides laterally resolved information. At the same time, depth resolution arises from the fact that ions scattered at a different depth will emerge with different energies. In this letter, we report a study of such SiGe VS using CCM providing information on the tilting of the layers. The images correspond closely to the images obtained using AFM and provide a better understanding of the origin of the cross hatch morphology.

Two linearly graded VS were grown using conventional gas-source molecular-beam epitaxy (GSMBE) (sample BF832) and low-pressure chemical vapor deposition (LPCVD) (Sample BF834) in the same growth facility using a managed pumping system.⁹ The system pressure during growth is typically 10⁻⁵ and 10⁻² mbar under the GSMBE

and LPCVD mode of operation, respectively. A silicon buffer layer was grown on the B-doped Si (001) substrate using GSMBE prior to the growth of the VS under either growth technique. The VS consists of a linearly graded layer with a Ge composition increasing from 0% to 25% over 1 μm followed by a 25% constant Ge composition layer of approximately 1 μm. A thin Si cap layer was grown on top of the VS to prevent oxidation of the SiGe. The growth temperature of both layers was 550 °C but the times required are significantly different due to growth rate differences.⁹

The measurements were carried out using the recently installed 3.5 MeV Singletron accelerator¹⁰ at the nuclear microscope facility at the National University of Singapore.¹¹ This dynamitron driven accelerator provides a very high brightness beam with a stable current, typically below 1% intensity variation on a minute time scale. This allows fast alignment procedures for channeling and CCM measurements. The beam collimators were set so as to reduce the beam divergence to below 0.2° thus providing acceptable channeling conditions. Both the high brightness and the high current stability are advantages of the Singletron accelerator not easily available on conventional van de Graaff machines.

For the broad beam channeling measurements, a 2 MeV He⁺ beam of typically 5 nA and 1 mm² spot size was used. Rutherford backscattering (RBS) spectra were recorded with two 50 mm² passivated implanted planar silicon (PIPS) detectors of 14 keV energy resolution at 160° and 110° scattering angles. The CCM data were taken with a 300 mm² PIPS detector of 19 keV energy resolution at 145° scattering angle. A solid angle of 280 mstr was used so that reasonable statistics could be accumulated during the 1 h runs with typically 100 pA beam current. The samples were mounted on a eucentric goniometer which has 14 mm translation stages in both the *x* and the *y* direction and allows rotations up to 20°

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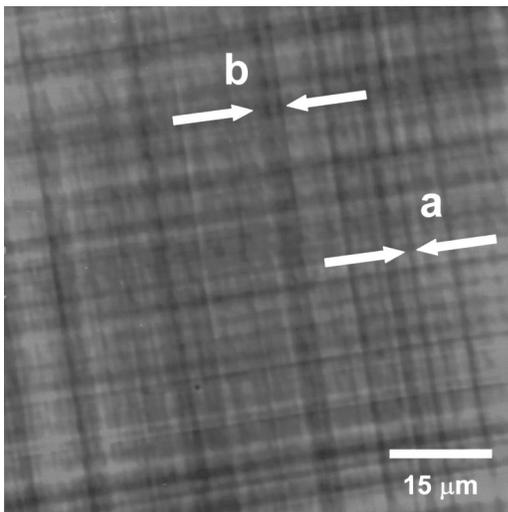


FIG. 1. 80 $\mu\text{m} \times 80 \mu\text{m}$ AFM image of surface morphology of sample BF834. The fine and large features of the cross hatch patterns with spatial frequency of $\sim 1 \mu\text{m}$ and $\sim 5 \mu\text{m}$, respectively, are labeled a and b.

about both the x and the y axis with a resolution of 0.1 mrad. The cross hatch pattern on the grown sample (BF834) is evident from the atomic force micrograph shown in Fig. 1. The root-mean-square roughness of the surface is typically a few nanometers depending on growth conditions. From broad beam $\langle 100 \rangle$ axial channeled spectra, a value of about 10% was obtained for χ_{min} , which represents the ratio of the height of the channeled spectrum to the height of the random spectrum near the surface. This χ_{min} value is significantly higher than the χ_{min} of 3.3% for a near-perfect epitaxially grown SiGe layer.¹² This indicates the presence of crystalline disorder or tilt of lattice planes in the epitaxial layer relative to the substrate. Figure 2 shows the 100 $\mu\text{m} \times 100 \mu\text{m}$ CCM maps of the same spatial location generated from three regions of a $\langle 100 \rangle$ axial channeled spectrum, corresponding to three different depths for both the Ge and Si signals, as indicated. The cross hatch contrast oriented along the orthogonal $\langle 110 \rangle$ directions with a period of a few microns is observed in all CCM maps obtained from the three energy

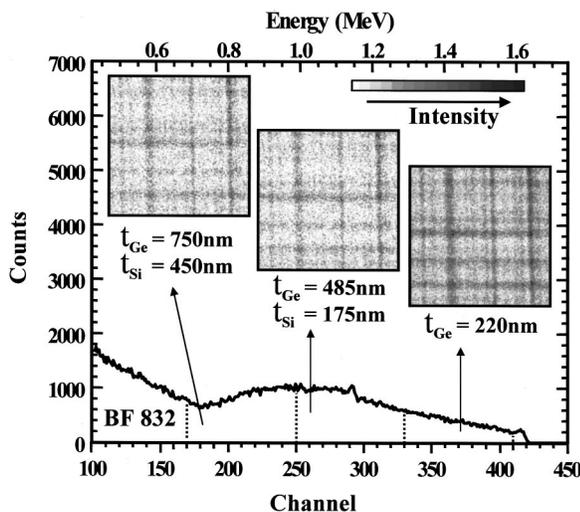


FIG. 2. 100 $\mu\text{m} \times 100 \mu\text{m}$ CCM maps taken from three regions in the channeled spectrum of sample BF832 with the corresponding depths for the Ge (t_{Ge}) and Si (t_{Si}) signals indicated.

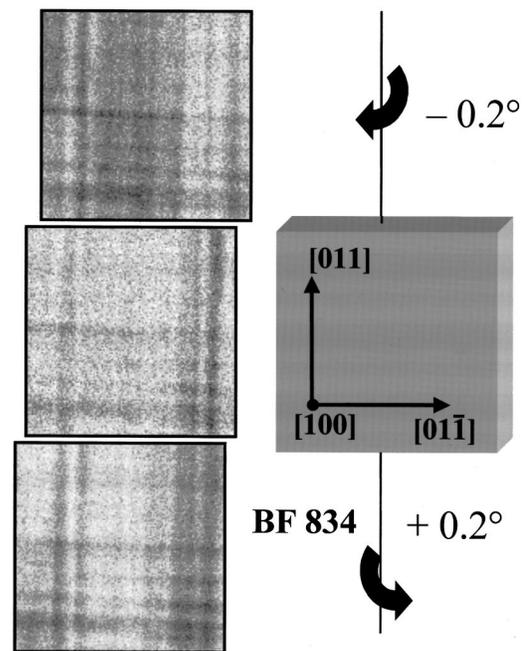


FIG. 3. 100 $\mu\text{m} \times 100 \mu\text{m}$ CCM maps generated from $[100]$ axial alignment and $\pm 0.2^\circ$ rotation off axial about the $[011]$ direction of sample BF834.

regions selected. The CCM contrast has a lower spatial frequency compared with the fine features in the AFM image (labeled a in Fig. 1) but appears to have a similar spatial frequency to the larger features (labeled b in Fig. 1) in the AFM micrograph. This confirms that features, similar to the large features in the cross hatch pattern found in the surface morphology, are present throughout the constant composition and the compositionally graded layers. If a χ_{min} value is extracted from the areas between the cross hatch bars only, χ_{min} value of 3.5% is found, comparable to that obtained for a perfect SiGe layer (3.3%). Figure 3 shows the CCM map taken from the LPCVD grown sample for the $[100]$ axial position and two CCM maps generated with $\pm 0.2^\circ$ rotation off axial about the $[011]$ direction of the sample. These maps correspond to the same area of the sample, a lateral shift of about 2 μm introduced by the rotation was corrected for by means of a marker outside the display area. A contrast reversal is observed when going from a tilt of 0.2° to -0.2° from the axial position. This indicates the presence of lattice tilt of the order of 0.5° between light and dark regions. A full angular scan is still required before any conclusion on the degree of lattice tilting can be made but the data does indicate that the CCM contrast may originate from lattice tilt produced by bunched up dislocations. By implication, the larger features observed in the surface morphology obtained by AFM may have a similar origin.

The correspondence between the features in CCM at all depths with the large features on the surface morphology obtained by AFM suggests that these features are accompanied by local tilt of lattice planes generated in the graded region. The lattice tilt may be related to the high misfit dislocation density in the graded region or the dislocation bunching. The tilt over the 5 μm period of the cross hatch features would produce a morphological undulation on the scales of $\sim 10 \text{ nm}$ as observed in the AFM micrograph. However, the smaller features observed in the surface morphol-

ogy by AFM could not be resolved spatially by the current CCM technique. These features with period of approximately $1\ \mu\text{m}$ can arise as a result of local variation of the growth rate induced by lateral Ge composition variations due to strain density waves.¹³

High-resolution CCM and channeling RBS were used to characterize the crystal and interface quality of SiGe layers grown on micron thick graded layers grown by LPCVD and GSMBE on B-doped Si(001) substrates. The RBS angular scans around the $\langle 100 \rangle$ axis give a χ_{min} value of around 10% for the linearly graded layer, up to a depth of 100 nm, indicating the presence of disorder or lattice tilts. The CCM results also reveal cross hatch pattern present in both the compositionally graded structures and the constant composition SiGe layer. There is evidence that these cross hatch structures are associated with the presence of slight lattice tilt. Our results demonstrate that the CCM technique is able to provide both laterally and depth-resolved information on submicron sized cross hatch features and their association with lattice tilts.

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