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High-resolution channeling contrast microscopy of compositionally graded $Si_{1-X}Ge_X$ layers

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Abstract

Epitaxial $Si_{1-x}Ge_x$ layers have a wide range of applications in microelectronic and optoelectronic devices. One of the possible SiGe configurations involves the growth of $Si_{1-x}Ge_x$ on a virtual substrate (VS). The VS is grown by linearly grading the Ge composition of the $Si_{1-x}Ge_x$ layer up to the final desired Ge composition for subsequent device growth. Such VSs are designed to accommodate the misfit strain between the substrate and the overlying active layer. However, a cross-hatch surface morphology often results which affects subsequent device layer growth on the VS. In this paper, we report on high-resolution channeling contrast microscopy (CCM) on such VSs. CCM measurements give both lateral and depth-resolved information on the cross-hatch features observed. The channeling RBS maps reveal a slight lattice plane bending in adjacent bands of width of ~10 μm, consistent with the relaxation of the SiGe layer. In addition, the Ge concentration distribution was imaged by proton induced X-ray emission, in order to check if the cross-hatch is associated with increased Ge concentrations.

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Keywords: Channeling contrast microscopy; SiGe; Virtual substrate

1. Introduction

Ge has a 4.17% larger lattice constant than Si, therefore lattice strain is produced when epitaxial films of Ge or $Si_{1-x}Ge_x$ are grown on a Si substrate. Strained layers offer the ability to modify the energy band gap and band offset energies. These attributes can enhance the performance range of electrical and optical devices and thus improve the performance of integrated circuits [1]. However, above a "critical thickness", large densities of misfit dislocations are formed, due to relaxation of the structure to accommodate the strain. These defects significantly reduce the carrier mobility and therefore the electronic quality of the

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material. Much effort has been geared towards the understanding of the nature of this defects and their formation in the hope of finding ways to control dislocations and to minimize their densities.

Relaxed, $Si_{1-x}Ge_x$ substrates with low densities of threading dislocations are grown by molecular beam epitaxy (MBE) or chemical vapour deposition (CVD) using the compositional grading technique [2,3]. This involves growing a linearly graded buffer up to the desired Ge concentration prior to the growth of the relaxed $Si_{1-x}Ge_x$ layer, i.e. the top of the graded layer has the bulk lattice constant of the $Si_{1-x}Ge_x$. Such substrates are termed virtual substrates (VS). A common surface feature of such VS is a cross-hatch pattern that is oriented along [1 1 0] directions with a typical periodicity of about 2 μm.

The influence of the relaxation process on the surface morphology is typically studied using atomic force microscopy (AFM) [4,5]. High resolution channeling contrast microscopy (CCM) [6], on the other hand, provides both laterally and depth resolved information, hence allowing us to extract information from the bulk of the VS. In previous work [7] on a similar VS structure, we have shown that the CCM images correspond closely to the images obtained using AFM and thus providing a better understanding of the origin of the cross-hatch morphology. In this work, we extend the range of the lattice tilt measurements and we use proton induced X-ray emission (PIXE) measurements to determine if the cross-hatch is associated with an increased Ge concentration.

2. Experimental

The investigated samples (BF1039 and BF1040) were grown using conventional gas source molecular beam epitaxy (GSMBE) [8]. The system pressure during growth is typically 10^{-5} mbar. A Si buffer layer was grown on the boron doped Si(0 0 1) substrate using GSMBE prior to the growth of the SiGe layer. Sample BF1039 and BF1040 consist of a linearly graded SiGe layer (thickness of 1 and 3 μm respectively) followed by 2 μm thick $Si_{0.7}Ge_{0.3}$ layer and Si cap layer of 5 nm to prevent oxidation of the SiGe. The Ge composition was increased from 0% to 30% for the graded layer. The growth temperature for both samples was at 650 °C.

The channeling RBS and channeling PIXE measurements were carried out using the Singletron accelerator [9] at the nuclear microscope facility at the National University of Singapore [10]. 2 MeV He^+ was used for channeling RBS and 2 MeV H^+ was used for channeling PIXE measurements. The CCM data were taken with a 300 mm^2 PIPS detector of 19 keV energy resolution at 145° scattering angle. A solid angle of 280 msr was used so that reasonable statistics could be accumulated with typically 100 pA beam current. A Si(Li) detector of 160 eV resolution was used for the PIXE measurements.

3. Results and discussions

Optical images taken with Nomarski interference contrast to show the surface topography are given in Fig. 1. Cross-hatch patterns, corresponding to a network of interface dislocations, are seen, running along orthogonal ⟨1 1 0⟩ directions for both samples. The dislocations are bunched together in some regions and further apart in others. These bands of dislocations result in steps at the sample surface. There are also regions of pits with sizes ranging from 2 to 10 μm and depths from 0.1 to 0.3 μm. The sample surface roughness was determined from a number of 80 μm × 80 μm surface scans using tapping mode AFM. Sample BF1039 has a rougher surface with root mean square (rms) roughness of about 25 nm as compared to 15 nm for that of sample BF1040. The larger rms roughness for BF1039 was probably due to the large number of pits present at the surface.

In order to determine the crystalline quality of the top SiGe layer, the minimum yield χ_{min}, which gives an indication of the fraction of ions channeled through the crystal, was obtained from channeling angular scans along ⟨1 0 0⟩ axis. Sample BF1040 which has a thicker graded layer of 3 μm has a slightly lower χ_{min} of 3.5% as compared to 4% for that of sample BF1039 which has a thinner graded layer of 1 μm. This agrees well with the

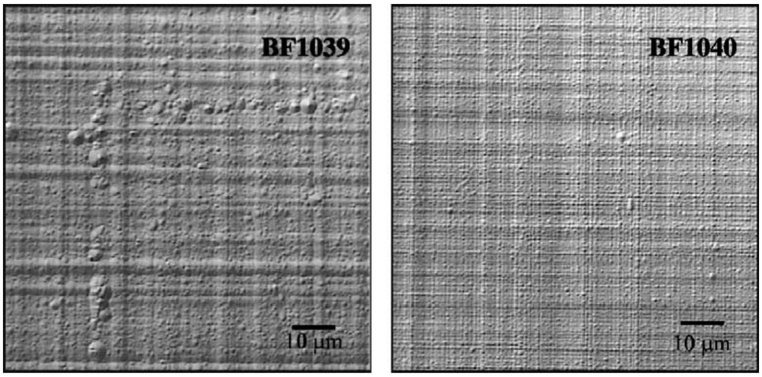

Fig. 1. Nomarski interference contrast optical images of sample BF1039 and BF1040.

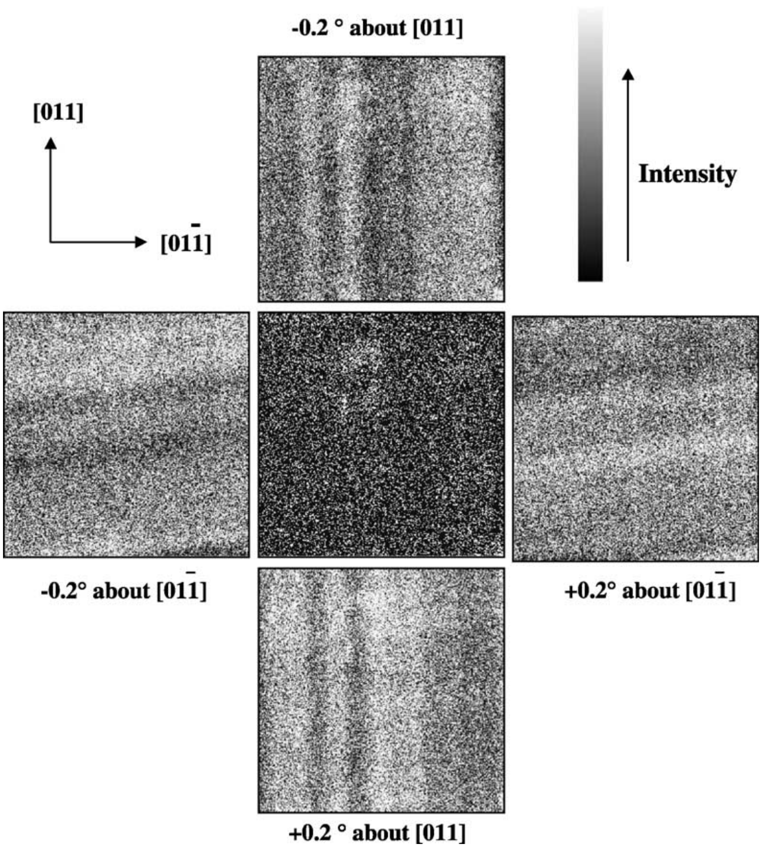

Fig. 2. 100 μm × 100 μm CCM maps of sample BF1040 for ±0.2° rotation off axial about [0 1 1] and [0 1 $\bar{1}$].

postulate that a thicker graded layer can accommodate the dislocation nucleation that results from growth beyond the critical thickness, and therefore results in a better crystalline layer grown above. It is thus concluded that the surface crystalline quality of the top 2 μm thick relaxed $Si_{0.7}Ge_{0.3}$ layer is as good as that of a thin epitaxially grown $Si_{0.7}Ge_{0.3}$ layer despite problems of a rough surface and presence of cross-hatch patterns.

Fig. 2 shows the CCM maps taken from sample BF1040 for ⟨0 0 1⟩ axial alignment and ±0.2° rotations off axial about [0 1 1] and [0 1 $\bar{1}$]. At the axial channeling alignment, no significant contrast was observed from the dislocation bands. The relatively large half angle, $\Psi_{1/2}$ of 0.49° for the Si⟨1 0 0⟩ axis renders axial channeling less sensitive to the dechanneling from disruptions in lattice structure, as compared to planar channeling ($\Psi_{1/2} = 0.12°$ for Si(1 0 0)) [6]. At ±0.2° rotations off ⟨0 0 1⟩ axial alignment, regions of bright and dark bands along orthogonal ⟨1 1 0⟩ directions were observed. The larger width of these bands compared to those observed in the optical image implies that each band encompasses several of the densely spaced dislocation. Similar bands of dark and bright contrast were also observed for sample BF1039 (not shown).

For the vertical bands, tilting from +0.2° to −0.2° about the [0 1 1] direction results in a reversal of the contrast in the CCM images but little or no contrast change is observed for the horizontally running bands. Similarly, contrast reversal was observed for the horizontal bands and little or no contrast changes were observed for the vertically running bands when tilting about the [0 1 $\bar{1}$] direction. This contrast reversal indicates the presence of a lattice tilt, consistent with the relaxation of the SiGe layer. The results are consistent with previous work on strain relaxation by 60° misfit dislocations [11].

In order to investigate the origin of the cross-hatch features, channeling maps from different depth regions were extracted. Fig. 3 shows the CCM maps taken at the same spatial location but generated from different regions of the RBS spectrum with the sample BF1040 rotated +0.2° off ⟨0 0 1⟩ axial alignment about the [0 1 1] direction. The intensity profiles across the horizontal direction for each maps are also given. The depth scales for the Ge and Si backscattered yield are given. Cross-hatch contrast was observed in all the CCM maps obtained from the selected energy windows. This confirms that the wider bands encompassing many densely packed dislocations are present throughout the constant composition layer up to a depth of approximately 1.5 μm.

Further measurements were carried out to determine if the cross-hatch contrast observed from the channeling maps could be due to accumulation of Ge atoms along these dislocation bands. PIXE and RBS measurements were taken with 2 MeV protons on a same region for both channeling and random incidence direction. PIXE was used here

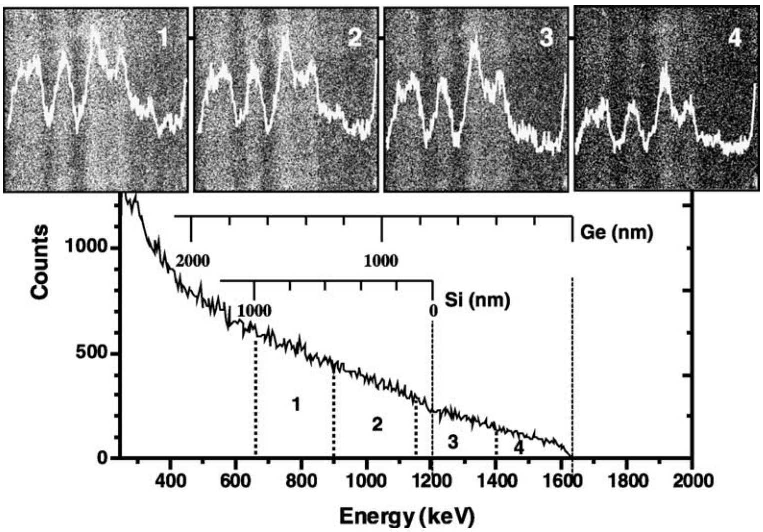

Fig. 3. 100 μm × 100 μm CCM maps of the same spatial location, generated from four energy windows with sample BF1040 rotated +0.2° off axial about the [0 1 1] direction. The intensity profiles across the horizontal direction for each map are given.

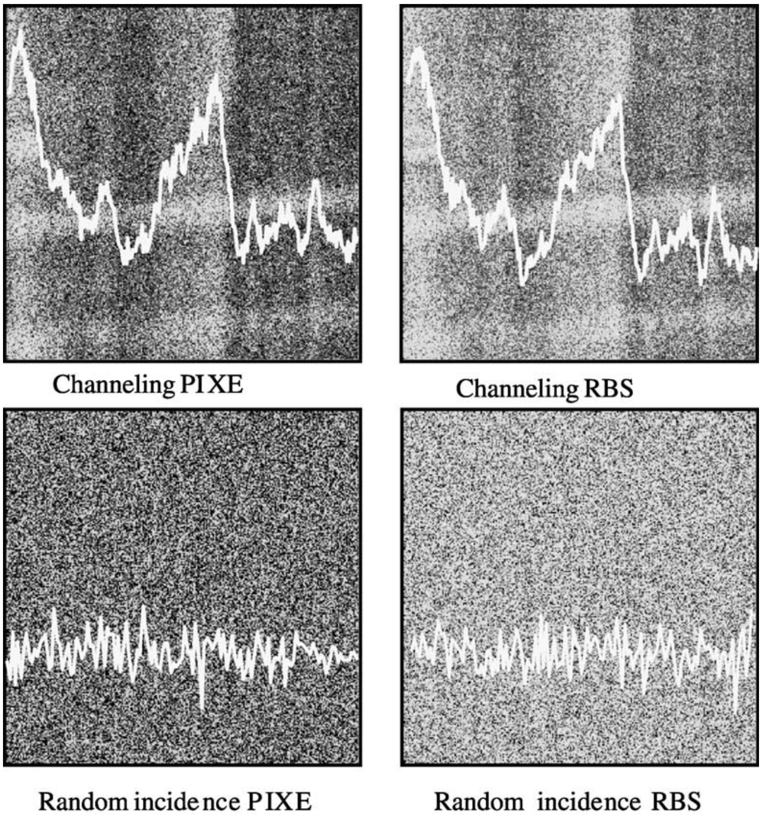

Fig. 4. 100 μm × 100 μm channeling and random incidence PIXE and RBS maps of sample BF1040. The intensity profiles across the horizontal direction for each map are given.

because of its higher sensitivity to the elemental distribution. An 8 μm thick Al absorber was used to attenuate the contribution of the X-rays from Si, thus transmitting most of the X-rays from Ge. Proton induced Ge L X-rays from the SiGe layer (both the constant and graded layer) were used to generate the PIXE maps. Horizontal line scans across the 100 μm × 100 μm PIXE maps for both samples under channeling and random directions were also extracted.

The line scans for the channeling and random incidence PIXE and RBS maps are given in Fig. 4. Axial channeling PIXE and RBS maps correspond well indicating that the contrast seen in the PIXE images were also due to the dechanneling effect at the network of dislocations. Under random incidence, PIXE maps show the Ge density distribution. From the line scan, no significant changes in the intensity within the statistical variation was observed for random orientation as compared to channeling direction. This suggests that there is no accumulation of Ge atoms along the dislocation lines within the experimental uncertainty of ±0.3%.

4. Conclusion

High resolution CCM and channeling RBS were used to characterize SiGe layers incorporating a VS. The RBS angular scans give χ_{min} values of around 3.5% and 4% for the constant composition layer, indicating a highly ordered active layer. The CCM results also reveal cross-hatch patterns present throughout the constant composition SiGe layer. The PIXE results suggest that there is no accumulation of Ge atoms along the dislocations bands within the experimental uncertainty of ±0.3%.

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