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Strain-induced anisotropic Ge diffusion in SiGe/Si superlattices

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Anisotropic diffusion of Ge induced by nonuniform strain in SiGe/Si interfaces in the range of 700–850 °C is directly observed with medium-energy ion-scattering spectroscopy through its composition and strain profiles of atomic-layer depth resolution. For SiGe/Si interfaces with identical composition profiles but with different strain distributions, the anisotropic diffusion of Ge can be clearly correlated with the anisotropic relaxation of the nonuniform strain in the near-surface layer of several nm depth. The results suggest that atomic-scale strain control is critical to maintain abrupt SiGe/Si interfaces under thermal budget. © *2002 American Institute of Physics.*
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SiGe/Si heterostructures have been intensively studied due to the increasing interest in optoelectronic devices and quantum wells.[1] Interface abruptness is important for a variety of device applications but interface strain due to a large lattice mismatch of about 4% between Ge and Si strongly influences the various structural properties such as defect formation, self-assembled structure, and interface diffusion.[2–8] Atomic flux in a diffusion couple is linearly proportional to the concentration gradient in the absence of additional effects. However, for strained SiGe/Si heterostructures, there have been reports that diffusion and alloy formation are enhanced by the misfit.[4–7] Cowern *et al.* reported an exponential increase in diffusion of Ge as a function of strain, indicating a strong dependence of activation energy on strain.[5] Strain-induced diffusion and alloying have also been reported in self-assembled Ge/Si heterostructures.[6,7] Our recent report on strain-induced diffusion shows that the diffusion under strain does not follow the Fickian model with a constant diffusivity.[9] However, no direct correlation between the diffusion and the strain based on separate composition and strain profiles with atomic-layer depth resolution has been reported for SiGe/Si interfaces to clearly demonstrate the extent of the nm scale Ge diffusion induced by strain.

Here, we report the direct measurement of the Ge composition distribution and the strain distribution in a strained SiGe/Si superlattice by medium-energy ion-scattering spectroscopy (MEIS). MEIS can provide direct compositional and structural information in real space with atomic-layer depth resolution through energy and angular distribution analysis of scattered protons.[10,11] Even though a uniform composition profile in SiGe is obtained, a nonuniform strain profile is observed in the near-surface region. The diffusivity is found to strongly correlate with the strain profile in this layer.

A $Si_{0.91}Ge_{0.09}/Si$ superlattice with seven periods was grown on a Si(001) wafer by reduced-pressure chemical-vapor deposition at 650 °C, and the composition and strain of the as-deposited sample were measured by high-resolution x-ray diffraction. After deposition, the sample was annealed in dry N_2 at temperatures from 700 to 850 °C for 30 min, using a vacuum furnace. The transmission electron microscopy (TEM) characterization was performed in a JEM 2000EX operating at 200 kV along the [110] zone axis. In MEIS analysis, a 101 keV H^+ ion beam was aligned to the [111] direction in the (110) plane and 11° rotated azimuthally along the [001] axis to achieve random energy spectra, and the protons scattered from Si and Ge atoms around the $[00\bar{1}]$ direction were analyzed. For strain profile measurements, protons are incident along the [001] direction in the (110) plane with 5° polar rotation and the scattered protons were measured around the $[11\bar{1}]$ direction in the (110) plane to measure the blocking dip shift. Ge profiles in the SiGe/Si interfaces were analyzed with low-energy secondary ion mass spectroscopy (SIMS) using 650 eV O_2^+ ions under an incidence angle of 80° from the surface normal using a modified Cameca 4f to be compared with the MEIS results.

Figures 1(a) and 1(b) are the bright-field TEM micrograph of the as-deposited SiGe/Si superlattice and an enlarged high-resolution TEM micrograph of the first SiGe layer of the superlattice, respectively. To avoid intermixing by the Ar^+-ion beam during ion milling for electron transparency, the observed TEM specimen was prepared only by mechanical polishing. Each layer is clearly defined by atomic number contrast, and the thicknesses of the SiGe and Si layers were 5.7 and 4.8 nm, respectively. However, due to the 2.7 nm native oxide layer, the thickness of the first Si layer decreased to 3.5 nm. From the TEM images, considerable

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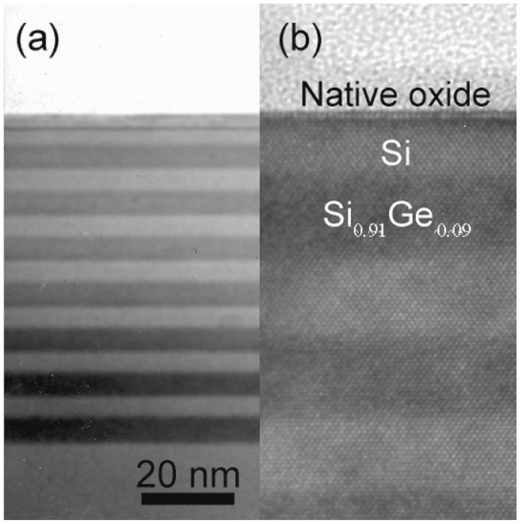

FIG. 1. (a) Bright-field TEM image of the $Si_{0.91}Ge_{0.09}$/Si superlattice and (b) enlarged HRTEM image of the superlattice. Operating voltage is 200 kV and the image is taken along the [110] zone axis.

intermixing of Si and Ge atoms is not visible and the compositional distribution at both interfaces of each SiGe layer appears identical.

Figure 2 shows the Ge peaks of random MEIS energy spectra from the first SiGe layer. MEIS is a quantitative and direct profiling technique with atomic-layer depth resolution based on binary scattering and linear electronic energy loss with little ion-surface charge exchange.[10,11] Therefore, the energy spectrum of the as-deposited sample shows that the Ge distribution in the first 5.7 nm SiGe layer is quite uniform with a full width at half maximum (FWHM) of 1.77 keV. To reconfirm that the Ge distribution in the SiGe layer is uniform, 650 eV O_2^+ low-energy SIMS with 80° grazing incidence was used, which can minimize the depth resolution degradation less than 1 nm. The $SiGe^+$ low-energy SIMS profile of Ge from the first 5.7 nm SiGe layer is shown in the inset, which shows that the Ge distributions at the two interfaces are almost identical, consistent with the high-resolution TEM (HRTEM) and MEIS results. From the viewpoint of the concentration gradient, the uniform SiGe layer with two surrounding Si layers can be regarded as a diffusion couple with two identical interfaces, and the flux of Ge atoms toward both interfaces during thermal annealing is expected to be the same. However, in the spectrum of the 700 °C annealed sample in Fig. 2, anisotropic diffusion across the lower interface is clearly shown, while diffusion across the upper Si layer is not observed at all. The tendency of the anisotropy decreases with increasing annealing temperature. The diffusion into the upper Si layer is observed even though the diffusion into the lower interface is still dominant after 850 °C annealing.

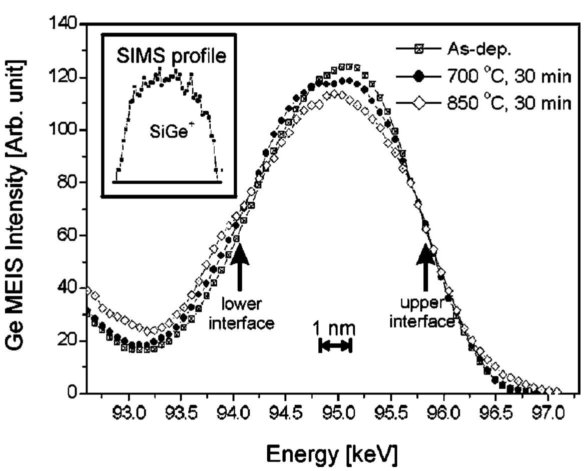

FIG. 2. Ge peaks of random MEIS energy spectra from the first 5.7 nm SiGe layer after deposition, 700 °C annealing, and 850 °C annealing for 30 min. $SiGe^+$ low-energy SIMS depth profile of the first SiGe layer after deposition is shown in the inset.

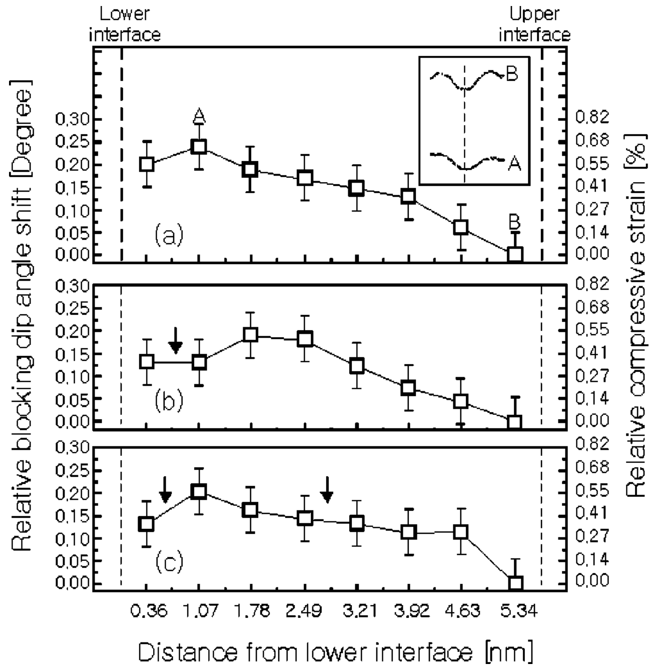

FIG. 3. Compressive strain distribution in the first SiGe layer relative to the upper interface: (a) as deposited, (b) annealed at 700 °C for 30 min, and (c) annealed at 850 °C for 30 min. A typical blocking dip shift is shown in the inset.

For interfaces with the identical compositional distribution, the Ge concentration profile will follow the Fickian diffusion law. The observed anisotropy in the diffusion couple suggests that there is an additional driving force for the diffusion, besides the concentration gradient. Since the SiGe layer is strained, a nonuniform strain distribution might be the origin of the observed anisotropic diffusion. This can be directly measured by the blocking dip position in the angular distributions of the MEIS intensity.[10,11] Figure 3(a) shows the $[11\bar{1}]$ blocking dips in the first SiGe layer of the as-deposited superlattice taken at eight intervals between the lower and upper interfaces. The blocking dip shift shows that the strain distribution in the first SiGe layer is nonuniform, while the Ge concentration is almost uniform, as shown in Figs. 1 and 2. It shows that the lower interface side has ~0.6% higher compressive strain than the upper interface side, which is calculated from the blocking dip shift, ~0.2° to the higher scattering angle with a simple trigonometry and Poisson's ratio of 0.2. The blocking dip angle shift has been estimated to be reproducible within 0.1°. The observed strain change corresponds to a composition difference of ~15%, which is not present in the Ge layer according to the MEIS and SIMS results, as shown in Fig. 2. Even though it cannot be clearly understood at present, the strain seems to relax near the surface in the depth of several nm. A dependence of the Ge strain distribution on the first capping Si layer thickness has also been observed, details of which will be discussed elsewhere.

In the 700 °C annealed sample, while the strain distribution near the upper interface does not change, the relative strain near the lower interface decreases to ~0.3%, as shown in Fig. 3(b). The anisotropic strain relaxation indicates that the diffusive strain relaxation preferentially occurred at the highly strained region, and that the main driving force of the diffusion is the strain energy reduction by the diffusive relaxation mechanism. Therefore, it is shown that the anisotropy observed in Fig. 2 is induced by the anisotropic diffusive relaxation to reduce the strain energy.[4] The relative strain distribution in the 850 °C annealed sample shows that the strain distribution in the layer becomes more uniform by diffusive strain relaxation.

In conclusion, direct observation of strain-induced diffusion is reported for a SiGe/Si superlattice based on the Ge composition and strain profiles with atomic-layer depth resolution. Nonuniform strain distribution and subsequent anisotropic diffusion were clearly observed for interfaces located several nm near surface even though the composition profiles are identical. Precise control of the strain distribution could be important to protect nm scale active regions of various devices with abrupt SiGe/Si heterostructures from thermal budget.

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