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Characterization of Planar Defects in Annealed SiGe/Si Heterostructure

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Abstract Due to the importance of the SiGe/Si heterostructure in the fields of thermoelectric and electronic applications, SiGe/Si heterostructures have been extensively investigated. For practical applications, thermal stability of the heterostructure during the thermoelectric power generation or fabrication process of electronic devices is of great concern. In this work, we focused on the effect of thermal annealing on the defect configuration in the SiGe/Si heterostructure. The formation mechanism of planar defects in an annealed SiGe/Si heterostructure was investigated by transmission electron microscopy. Due to the interdiffusion of Si and Ge, interface migration phenomena were observed in annealed heterostructures. Because of the strain gradient in the migrated region between the original interface and the migrated interface, the glide of misfit dislocation was observed in the region and planar defects were produced by the interaction of the gliding misfit dislocations. The planar defects were confined to the migrated region, and dislocation pileup by strain gradient was the origin of the confinement of the planar defect.

Key words SiGe, strain gradient, misfit dislocation, transmission electron microscopy, thermoelectric.

1. Introduction

SiGe/Si heterostructures have been attracted much attention for various kinds of application, such as, thermoelectric generation, heterojunction bipolar transistor, field effect transistor, and optoelectronic devices.[1,2] However, because of the lattice mismatch between SiGe layer and Si substrate, thermal budget during the fabrication process for the devices can affect on the structural properties, such as defect formation and diffusion enhanced by strain potential, and these effects could severely degrade the electronic and optical properties.[3,4] Therefore, the study on the thermal stability of the SiGe/Si heterostructure is of great concern.

The strain relaxation mechanism in SiGe/Si heterostructure has been extensively investigated.[5-9] In literatures, it has been reported that dislocations initially located at the SiGe/Si heterointerface could be multiplicated by thermal annealing, and that strain exerted on the SiGe layer could be relieved by the multiplication of the dislocations.[10,11] Frank-Read source is a well-known mechanism for the multiplication, and this mechanism could induce dislocation pileup in graded SiGe/Si heterostructure.[10,12] However, although many authors have reported the defect configuration in SiGe/Si heterostructures, but the effect of strain distribution on the defect configuration in annealed SiGe/Si heterostructures has not yet been reported.

In this work, defect configuration in annealed SiGe/Si heterostructure was investigated. Annealed SiGe/Si heterostructures in the temperature range from 700 to 1000°C were characterized by high-resolution transmission electron microscopy (HRTEM), and the interface migration phenomena was confirmed from the results. The interface migration was originated from the interdiffusion of Si and Ge, and it induced strain gradient between original interface and migrated interface. The strain gradient effects on the defect configuration in annealed heterostructures were discussed, and the confinement mechanism of defects in the migrated region was also proposed.

2. Experimental Procedure

SiGe/Si layers were grown using an ASM EPSILON-ONE reduced pressure CVD system with a 125 mm, single-wafer CVD module using SiH_4 and GeH_4. The reactor has two N_2-purged load lock chambers so that the deposition chamber was not exposed to air. The wafer was supported by a SiC-coated graphite susceptor in the quartz chamber. The wafer and the susceptor were heated by two sets of tungsten-halogen lamps placed above and below the deposition chamber. The SiGe/Si layers were deposited at 650°C and a reduced pressure of 40 torr.

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The strain in the as-deposited sample was relaxed about 12.4% by misfit dislocations, and the thickness of SiGe layer was 56.6 nm. The composition and strain of the sample were measured by Rutherford backscattering spectroscopy and high-resolution x-ray diffractometer (HRXRD), respectively. After deposition, the samples were annealed in dry N_2 at temperatures from 700 to 1000°C up to 2 hr using vacuum chamber. Transmission electron microscopy (TEM) characterization was performed by using a JEM 2000 EX operating at 200 kV along a [110] zone axis.

3. Results and Discussion

Fig. 1(a) is a cross-sectional HRTEM micrograph of as-deposited $Si_{0.83}Ge_{0.17}$/Si heterostructure. There is an abrupt heterointerface at 56.6 nm from the film surface and the intermixing of Si and Ge during the deposition could be negligible. Therefore, it could be proposed that there is an abrupt Ge concentration profile at the original interface (I_O). However, in annealed sample at 750°C for 7200 min, a new interface (I_M) was produced below the original interface, as shown in Fig. 1(b). The formation mechanism of the migrated interface was the intermixing of Si and Ge atoms by strain-induced diffusion, and this result was already reported in Ref. 4. The activation energy of the strain-induced diffusivity was 0.5 eV and it was significantly lower value than that of concentration gradient diffusivity (3.0~4.7 eV). Because the strain energy in SiGe/Si heterostructure is dependent on the content of Ge, and because the strain energy could be reduced by the intermixing of Si and Ge, the abrupt concentration profile at the original interface in the as-deposited sample could be modified by the strain-induced diffusion during thermal annealing.[13,14) Furthermore, the interdiffusion of Si and Ge in SiGe/Si heterostructure by the strain-induced diffusion was also experimentally proven by using secondary mass ion spectroscopy and medium energy ion spectrometry.[15,16] Therefore, it could be proposed that the migrated interface indicates

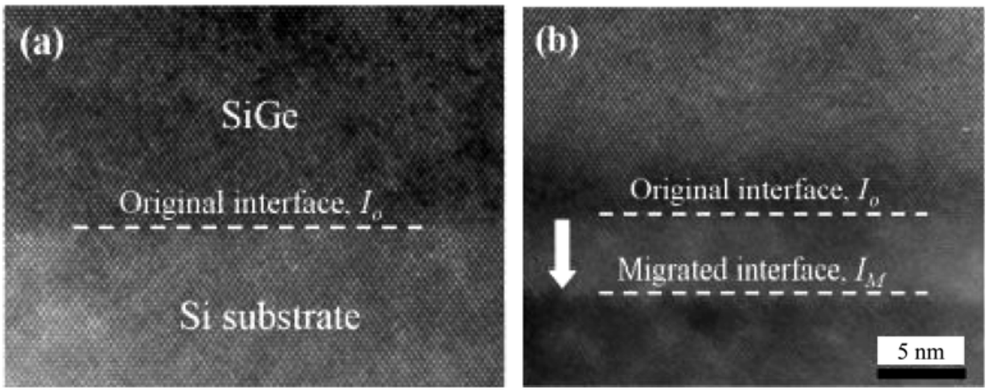

Fig. 1. Cross-sectional HRTEM micrograph of (a) as-deposited $Si_{0.83}Ge_{0.17}$/Si and (b) the $Si_{0.83}Ge_{0.17}$/Si annealed at 750°C in a dry N_2 ambient for 2 hr. I_O and I_M are the original interface and migrated interface, respectively.

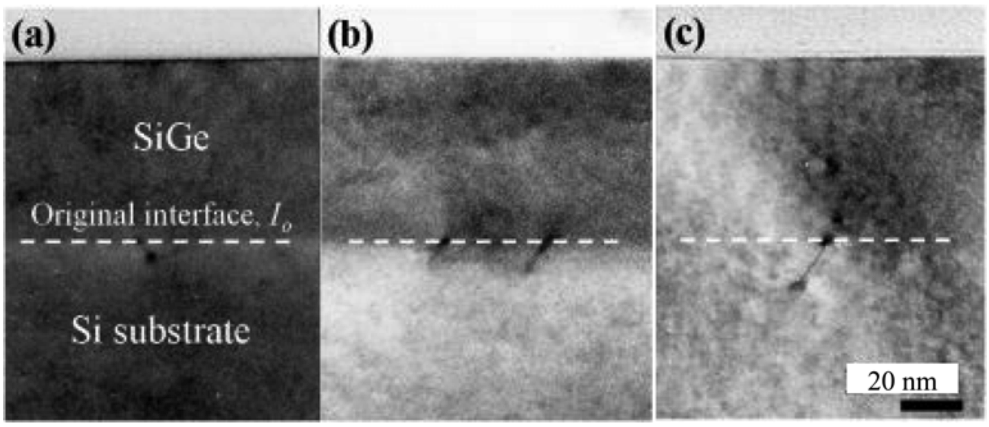

Fig. 2. Bright-field TEM micrographs of SiGe/Si heterostructures annealed at (a) 900°C for 30 min, (b) 900°C for 7200 min, and (c) 1000°C for 6300 min.

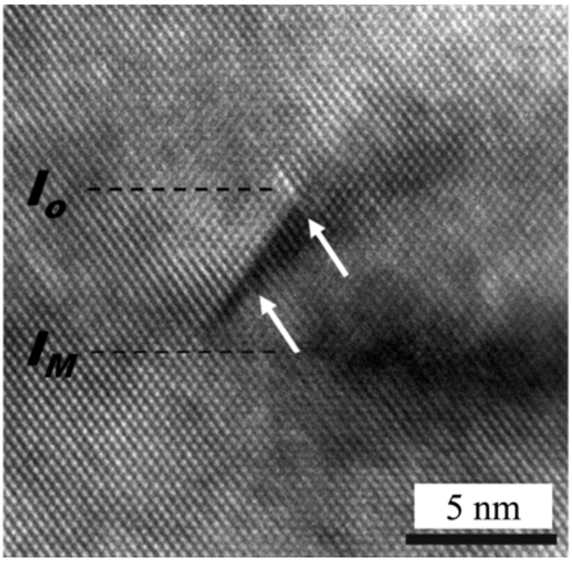

Fig. 3. A HRTEM micrograph of the planar defects confined in the migrated region between I_O and I_M.

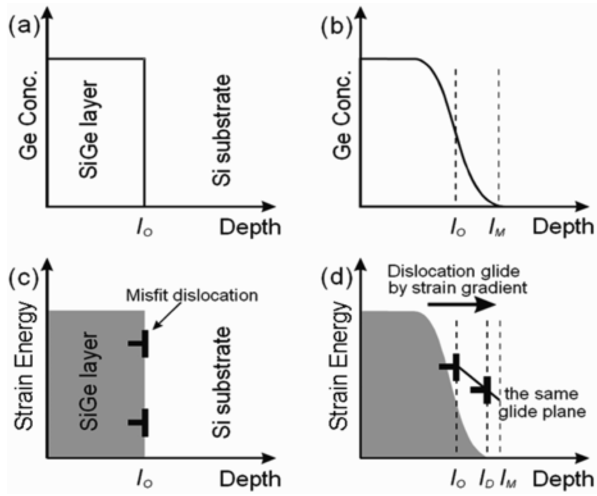

Fig. 4. Schematic diagrams of the glide of misfit dislocations by strain gradient.

the modified concentration of Ge near the SiGe/Si heterointerface during thermal annealing, and that there is a concentration gradient in the migrated region between I_O and I_M.[17)]

Fig. 2(a)~(c) show bright-field TEM micrographs of SiGe/Si heterostructures annealed at 900°C for 30 min, 900°C for 7200 min, and 1000°C for 6300 min, respectively. In all annealed samples, planar defects which propagating from the original interface toward Si substrate could be clearly observed. The angle between the planar defect and the interface was almost 54°, so that the planar defect is supposed to be {111} planar defect. Because the length of the planar defect increased with increasing annealing time and temperature, the propagation of the planar defect toward Si substrate is a thermally activated process, which has a strong relation with the strain relaxation and interface migration.

Fig. 3 shows a HRTEM micrograph of the planar defect in the sample annealed at 900°C for 30 min. In this figure, two 60° misfit dislocations are located in the region between I_O and I_M. Upper misfit dislocation was located at the original interface, and lower misfit dislocation was located close to the migrated interface. In general, misfit dislocations are inserted at SiGe/Si heterointerface to minimize the strain energy after critical thickness, and the glide of misfit dislocation toward Si substrate is energetically unfavorable. However, in the annealed sample, misfit dislocation was clearly observed in between I_O and I_M, as shown in Fig. 3. It means that this configuration of misfit dislocations is energetically favorable in the annealed SiGe/Si hetetostructure, and that the strain gradient in the region acts as the driving force of the glide motion. Therefore, the strain energy exerted on the SiGe/Si heterostructure could be reduced by the glide of misfit dislocations toward I_M.[18)]

However, the upper misfit dislocation is still in unstable state. Because the glide of upper misfit dislocation could relax the strain energy further, the strain gradient might be the driving force of the glide of the upper misfit dislocation. In this case, because the lower misfit dislocation acts as an obstacle against the glide, the glide of the upper misfit dislocation is suppressed. Therefore, there is a dislocation pileup in the migrated region. Because the migrated region is severely distorted by the stress field of the pileup, some new defects could be produced in the region.[19)] Therefore, this stress field made the glide plane a planar defect and the planar defect was confined in the migrated region, as shown in Fig. 2 and 3. In our experiment, all observed planar defects were confined in the migrated region, and they consisted of two 60° misfit dislocations. Therefore, it was confirmed that the formation of the planar defects is originated from the glide of misfit dislocation by strain gradient and also from the stress field of dislocation pileup.

The schematic diagram of the above mechanism is drawn in Fig. 4. Fig. 4(a) and (b) are the concentration profiles of Ge in the as-deposited and annealed sample, respectively. The Ge concentration in the as-deposited SiGe layer is constant, and that in the annealed sample varies significantly with depth in the migrated region. Fig. 4(c) and (d) are the strain energy profiles in the as-deposited and annealed sample, respectively. Because the strain energy is proportional to the square of the strain, the strain energy decreases more rapidly than Ge concentration in the migrated region. Therefore, glide of misfit dislocation is limited to I_D as shown in Fig. 3. However, although the lower misfit dislocation glided only to I_D, the planar defects propagated to I_M as shown in Fig. 2 and Fig. 3. The origin is still unclear but it is expected to be the stress field concentrated on the leading dislocation.

4. Conclusion

Defect configuration in annealed SiGe/Si heterostructures was investigated. In the temperature range from 700 to 1000°C, interface migration phenomena due to the interdiffusion of Si and Ge atoms was confirmed by transmission electron microscopy. Because of the interdiffusion, there was a strain gradient in migrated region between original interface and migrated interface, and the glide of misfit dislocations was induced by the strain gradient. Dislocation pileup by strain gradient was observed and the pileup was the origin of the planar defect confined in the migrated region.

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