Ion Beam Induced Strain Relaxation in Pseudomorphous Epitaxial SiGe Layers

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***Abstract*-The effects of irradiation with Ge^+ and Ar^+ ions at elevated temperatures on the relaxation behavior of pseudomorphic $Si_{0.79}Ge_{0.21}$/Si heterostructures have been compared. It was found the strain relaxation in the structures implanted with Ge^+ at 400°C started already upon implantation. Post-implantation thermal annealing of this sample resulted in considerably higher degree of relaxation than that in control (non-implanted) samples as well as in samples implanted with Ar^+ both at 230 and 400°C and with Ge^+ at 230°C. This result points to a dramatic influence of both the implantation temperature and ion species on relaxation behavior of the ion-irradiated heterostructure. Two possible mechanisms for this effect are discussed.**

I. Introduction

Epitaxial growth of $Si_{1-x}Ge_x$ on Si substrates is of increasing interest because it provides a possibility to design new electronic and optical devices. A crucial issue in fabrication of electronic devices based on SiGe/Si heterostructures is eliminating threading dislocations [1], which deteriorates the electronic properties of the structures [2]. In recent years, it has been demonstrated that non-equilibrium point defects introduced into heterostructures enhance strain relaxation and can considerably reduce density of threading dislocations [3–11]. Point defects were introduced by lowering growth temperature, which led to the saturation of the growing layers with point defects [3–8], as well as by low-energy ion bombardment of layers during epitaxial growth [7–9] or after growth [10–13]. It is generally accepted that the accelerated strain relaxation is due to aggregates of point defects acting as sites for nucleation of misfit dislocations. However, particular mechanisms responsible for the strain relaxation in SiGe/Si heterostructures supersaturated with point defects are not understood. Besides, the effects of implantation species, implantation temperature, and peak position of the implanted species on the relaxation behavior of SiGe/Si heterostructures have receive rather little attention. In this paper, we report on the effect of implantation temperature and ion species on the strain relaxation in SiGe/Si heterostructures.

II. Experimental

$Si_{0.79}Ge_{0.21}$ layer was grown on Si(100) wafer doped with boron to the concentration 1.3×10^{15} cm^{-3} by solid-source MBE. The wafer was chemically precleaned *ex situ* by the standard procedure [14] and immediately introduced into the load-lock chamber of the MBE machine. A protecting SiO_2 layer was removed *in situ* by heating to 850°C in a weak Si beam followed by a temperature flash at 1000°C for 1 min. The base pressure in the growth chamber was 10^{-10} Torr, during deposition the pressure rose to 4×10^{-9} Torr. The undoped pseudomorphic $Si_{0.79}Ge_{0.21}$ layer 150 nm thick was grown at a temperature of 450°C and a rate of about 0.1 nm/s. This thickness of the SiGe layer was chosen to avoid strain relaxation during the growth. The film composition was determined by x-ray diffraction measurements. The Ge content varied over the substrate within 2%. Then, the wafer was scribed into samples about 2 x 2 cm in dimensions.

The samples were implanted with 130-keV Ar^+ or 200-keV Ge^+ ions at 230°C or 400°C to doses of 10^{14} (Ar) and 5×10^{13} (Ge) cm^{-2}, respectively. The implantation parameters were chosen so that depth profiles of radiation-induced defects were about the same for Ar^+ and Ge^+ ions. The defect profiles were calculated under the Suspre program. The peak positions of the defect profiles were within the SiGe layer, at a depth of ≅80 nm. The implanted and as-grown samples were annealed in a vacuum furnace (10^{-6} Torr) at temperatures from 450 to 550°C. The temperature was kept constant at ±2°C, the absolute temperature accuracy being of about 3°C.

Chemical Ge profiles were measured by secondary ion mass spectroscopy (SIMS) using a Cameca IMS-4f machine. The depth calibration was performed by measuring crater depths with a Taylor–Hobson Talystep profilometer.

Strain relaxation in the heterostructures was studied by double-crystal x-ray diffraction measurements (Rigaku RU-200 source) and plan-view transmission electron microscopy (TEM) using a JEOL JEM-200 CX microscope operated at 200 kV. The specimens for TEM were prepared by chemical etching from the backside of the heterostructure. From x-ray

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diffraction data, the degree of relaxation was calculated by the well-known formula $R = (a_{\perp}^{pseud} - a_{\perp}^{rel})/(a_{\perp}^{pseud} - a_c)$, where $a_{\perp}^{pseud}$ and $a_{\perp}^{rel}$ are the out-of-plane lattice constants of pseudomorphic and relaxed SiGe layers, respectively, and a_c is the lattice constant of bulk SiGe.

III. Results and Discussion

X-ray diffraction measurements revealed no strain relaxation ($R = 0$) in the as-grown $Si_{0.79}Ge_{0.21}$/Si structure. The spectra of all the samples measured before and after ion implantation are similar, except for the spectrum of the sample implanted with Ge^+ at 400°C, which is noticeably broadened as compared to the spectrum of this sample measured before implantation, although the peak position remains unchanged (Fig. 1, curves 1 and 2). The SIMS data prove that this broadening cannot be explained by interdiffusion of Si and Ge at the SiGe/Si interface: the depth profile of Ge remains virtually unchanged upon implantation. Therefore, we attribute this effect to the presence of radiation-induced defect complexes or/and dislocations in the SiGe layer. Indeed, plan-view TEM study revealed a low-density network of misfit dislocations; i.e., strain relaxation started in the sample implanted with Ge^+ at 400°C upon implantation.

X-ray diffraction measurements of the samples annealed at 450°C for 15 min revealed that the degree of relaxation R of the sample implanted with Ge^+ at 400°C is as high as 0.5, whereas $R = 0$ for other samples (control sample, and the samples implanted with Ge^+ at 230°C and with Ar^+ at 230°C and 400°C). As an illustration, Fig. 2 compares plan-view TEM images of the samples implanted with Ge^+ at 230 and 400°C and then annealed at 450°C. One can see that the misfit-dislocation network in the second sample is much more dense. Dislocation arcs clearly seen in Fig.2b indicate that dislocation half-loops propagate into the substrate; i.e., the misfit-dislocation network in the sample implanted with Ge^+ at 400°C occupies three-dimensional region. Annealing of this sample at 550°C for 15 min results in the degree of relaxation of about 0.92 (according to x-ray diffraction data) as compared $R = 0.47$ for the sample implanted with Ge^+ at 230°C.

Thus, relaxation behavior of the sample implanted with Ge^+ at 400°C differs drastically from that of the other samples. In our opinion, there are two explanations for this result. First, dislocation sources existing in the as-grown heterostructure may be activated under these implantation conditions (high temperature and heavy ion species). Second, defect complexes of a specific type may form in the SiGe layer during Ge implantation at 400°C. This presumption is supported by the fact that TEM examination of the sample im-

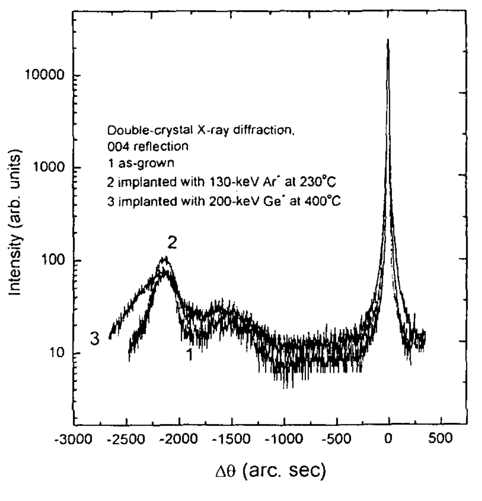

Fig. 1. X-ray diffraction spectra of (*1*) the as-grown sample, (*2*) the sample implanted with Ar^+ at 230°C, and (*3*) the sample implanted with Ge^+ at 400°C. The spectra of the samples implanted with Ar^+ at 400°C and Ge^+ at 230°C are similar to that of the as-grown sample. The weak feature around 1600 arc sec is due to nonuniform film composition.

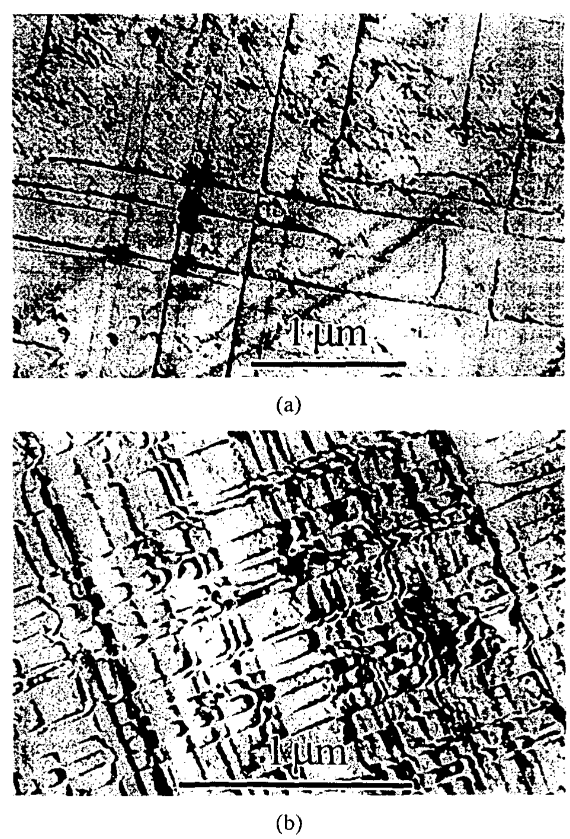

Fig. 2. Plan-view TEM images of the samples implanted with Ge^+ at (a) 230°C and (b) 400°C and annealed at 450°C. According to x-ray diffraction data, $R = 0$ for the first sample, and $R = 0.5$ for the second.

planted with Ge^+ at 400°C and then annealed at 450°C revealed the presence of V-shaped defects consisted of two threading 60°-dislocations (Fig. 3). These defects were observed at various depths in the SiGe film. Such a configuration can arise, if these dislocations nucleated on some defects (presumably, complexes of implantation-induced point defects). It seems likely that the defect complexes, which are located at the SiGe/Si interface, can promote the formation of misfit-dislocation network, thus enhancing strain relaxation. Although the depth profiles of radiation-induced point defects are the same for all the samples studied, the V-shaped defects are observed only in the sample implanted with Ge^+ at 400°C. This allows us to conclude that rather heavy ions producing dense cascades and sufficiently high implantation temperature providing high diffusion mobility of radiation-induced point defects are essential for the formation of the complexes responsible for the V-shaped defects. Further investigations are needed to clarify the nature of these complexes. It is not improbable that the two proposed mechanisms operate concurrently.

IV. Conclusion

The relaxation behavior of pseudomorphic $Si_{0.79}Ge_{0.21}$/Si heterostructures implanted with Ge^+ or Ar^+ ions at 230°C or 400°C was studied. It was found that the rate of strain relaxation in the sample implanted with Ge^+ at 400°C is noticeably higher than in other samples. Two possible mechanisms for the enhanced relaxation were proposed: (1) activation of existing dislocation sources under ion implantation with heavy ions at elevated temperature and (2) formation of specific defect complexes acting as nucleation sites for V-shaped dislocations and promoting the formation of the misfit-dislocation network. In both cases, heavy ion species and elevated implantation temperature are required to accelerate strain relaxation.

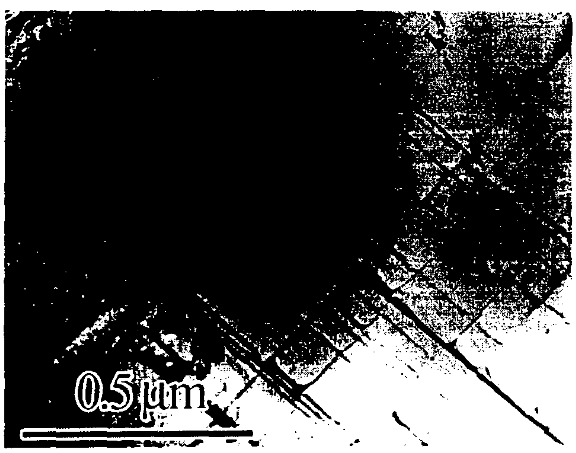

Fig. 3. Plan-view TEM image of the sample implanted with Ge^+ at 400°C and annealed at 450°C. The micrograph was taken from the region of the oblique section, where the misfit-dislocation network was removed almost completely during the sample preparation. Therefore, the network of misfit dislocations seems less dense than that in Fig. 2b. V-shaped defects consisted of two threading 60°-dislocations are clearly seen in the micrograph.

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