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Observation of defects evolution in strained SiGe layers during strain relaxation

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ABSTRACT

Misfit defects in strained-SiGe layers grown on (100) Si-substrates by reduced pressure chemical vapor deposition (RPCVD) were investigated by using high-resolution X-ray diffraction (HRXRD) and transmission electron microscopy (TEM). While (004) omega rocking curve (ω-RC) is not sensitive to 60° misfit dislocations in a slightly strain-relaxed sample, they caused an asymmetrical shape to (113) ω-RC. On the other hand, it was found that the partial dislocations associated with stacking faults in highly strain-relaxed sample contributed to significant and symmetric peak broadening of both ω-RCs.

1. Introduction

Strained-SiGe layers play an important role in advanced devices due to their enhanced charge carriers mobility and band-gap engineering possibilities in optoelectronics [1–3]. During device fabrication processes that involve high temperature steps, strained layers could relax via defects generation, such as misfit or threading dislocations, degrading the device performance [4,5]. The stacking faults in strained layers generated during strain relaxation have been extensively studied. Kvam et al. reported general criteria for when stacking fault generation should be possible during strain relaxation as a function of substrate surface orientation [6]. Maree et al. found that the acting slip mechanism for the generation of misfit dislocations in mismatched semiconductor heterostructure showed that the dissociation of 60° dislocation into two partial dislocations was dependent of the strain types [7]. These extensive investigations to asses the relaxation of strained layers and observe the type and density of induced defects have been traditionally performed by using transmission electron microscopy (TEM). Unfortunately, despite the body of study on the defects evolution during strain relaxation, the investigation by using X-ray diffraction (XRD) techniques is deficient. Although the Ge interdiffusion at Si/SiGe interface during high temperature annealing was investigated by means of high-resolution X-ray diffraction by Zheng and Jang, the XRD study on the misfit dislocations remain relatively unclear [8,9].

We have investigated the effect of stacking faults as well as misfit dislocations on the broadening and shape of omega rocking curves (ω-RCs) of strained-SiGe layers with different Ge concentration and strain relief.

2. Experimental

$Si_{1-x}Ge_x$ layers with a nominal Ge fraction x = 0.20 and 0.25 and a thickness of 50 and 100 nm were grown on (100) Si by reduced pressure chemical vapor deposition (RPCVD) at a pressure of 10 Torr and growth temperature of 700 °C using dicholorosilane (DCS, SiH_2Cl_2) and germane (GeH_4) as silicon and germanium sources, respectively. After growth, the layers were annealed in a quartz tube furnace at 800 and 900 °C for 30 min under N_2 ambient to study the misfit defects generated during strain relaxation. A PANalytical MRD X'Pert system was employed to collect high-resolution ω-RCs. For the plan-view and cross-sectional transmission electron microscopy (TEM) images of the strained SiGe layers, a JEOL 2010F was used.

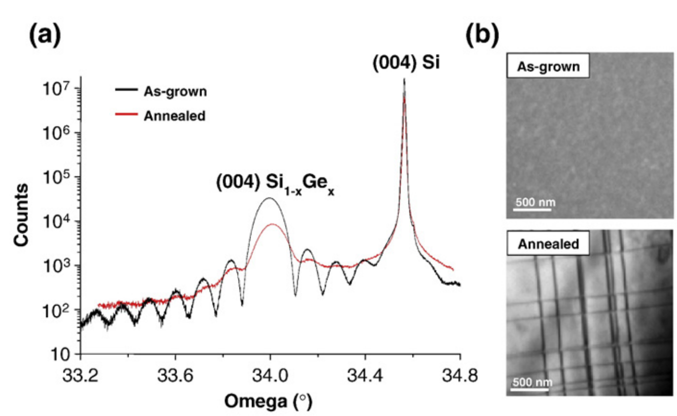

Fig. 1. (a) Omega-2theta rocking curves (ω-2θ RCs) and (b) plan-view transmission electron microscopy (PV-TEM) images of as-grown and annealed at 800 °C for 30 min $Si_{80}Ge_{20}$ films 50 nm thick.

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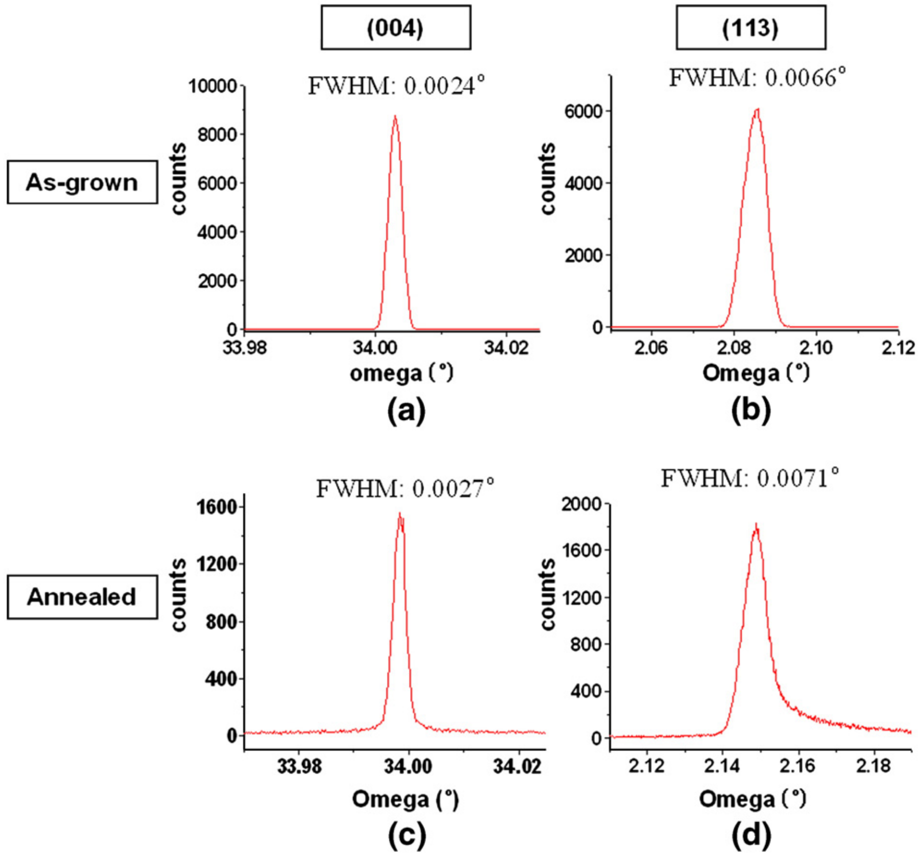

Fig. 2. (004) and (113) omega rocking curves (ω-RCs) acquired from the as-grown and annealed strained $Si_{80}Ge_{20}$ layers.

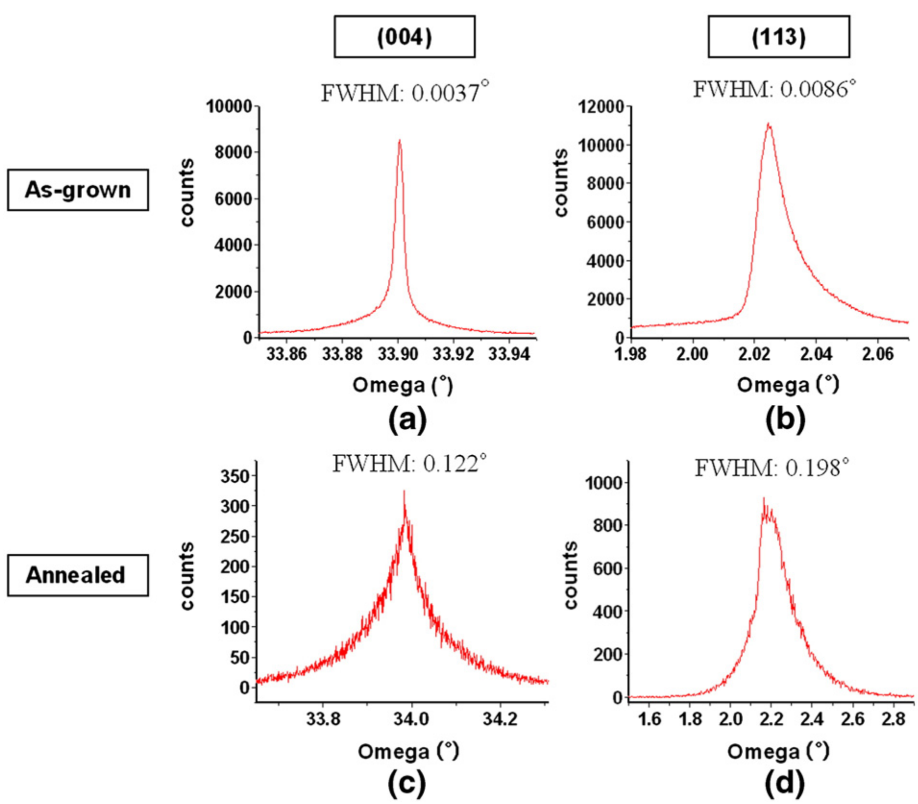

Fig. 3. (004) and (113) ω-RCs acquired from the as-grown and annealed at 900 °C for 30 min $Si_{75}Ge_{25}$ 100 nm thick.

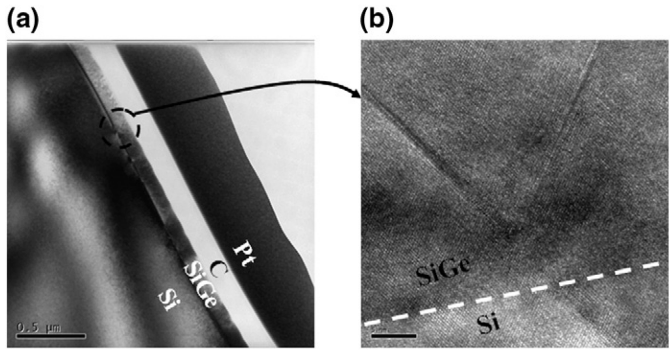

Fig. 4. (a) Cross-sectional and (b) high resolution TEM images in <110> projection of 100 nm thick strained $Si_{75}Ge_{25}$ annealed at 900 °C for 30 min.

Plan-view and cross-sectional samples were prepared by the jet electro-polishing and focused ion beam (FIB) methods, respectively.

3. Results and discussion

Fig. 1 (a) shows (004) omega-2theta rocking curves (ω-2θ RCs) of as-grown and annealed at 800 °C for 30 min $Si_{80}Ge_{20}$ films 50 nm thick. The RC of as-grown sample shows the well-defined thickness fringes which indicate the formation of an abrupt interface between Si substrate and strained $Si_{80}Ge_{20}$ layer. From the simulation of the acquired ω-2θ RC, the film thickness and Ge composition of strained $Si_{1-x}Ge_x$ layer were found to be 46.8 nm and 21%, respectively. However, the RC of $Si_{80}Ge_{20}$ layer annealed at 800 °C for 30 min is different from that of as-grown sample. The intensity of annealed $Si_{1-x}Ge_x$ layer was reduced and the thickness oscillation was dampened, compared to as-grown sample. In addition, the Bragg peak position of strained layer slightly shifts towards Si-substrate position. These changes indicate a strain relaxation accompanied by misfit defects generation and Ge interdiffusion near the interface [8]. Fig. 1 (b) shows plan-view transmission electron microscopy (PV-TEM) images of as-grown and annealed $Si_{80}Ge_{20}$ samples. As-grown sample does not show any misfit dislocations, indicating that the strained layer was pseudomorphically grown and the interface was abrupt, which is consistent with the results of ω-2θ RC of as-grown sample. However, the annealed sample shows many misfit dislocations with a cross-hatching pattern which consist of perfect 60° dislocations, $\frac{1}{2}\langle 110\rangle\{111\}$ Burgers vector and slip plane [10,11].

The omega rocking curve (ω-RC) investigation was performed to study the effect of misfit dislocations on the peak broadening. A full width at half maximum (FWHM) value of ω-RC has been used as a figure of merit (FOM) for the crystalline quality. Very small FWHM values, similar to the instrument resolution limit of 0.0021° measured from a high quality Si wafer, and symmetric profile shapes of (004) and (113) ω-RCs acquired from the as-grown $Si_{80}Ge_{20}$ layer displayed in Fig. 2 (a) and (b) indicate that the strained layer is a perfect single crystal. The FWHM values of ω-RCs acquired from annealed sample shown in Fig. 2 (c) and (d) were also similar to those of as-grown sample. However, it needs to be noted that the shape of (113) ω-RC of annealed sample is asymmetric while (004) ω-RC is symmetric. Therefore, it is found that while (004) ω-RC is not sensitive to the presence of 60° misfit dislocations within the annealed strained layer as shown by TEM results, the profile shape of (113) ω-RC is.

For further study on the defects evolution during strain relaxation, 100 nm thick strained $Si_{75}Ge_{25}$ layers with higher strain energy areal density (E_S) than 50 nm thick strained $Si_{80}Ge_{20}$ samples were grown and then annealed at 900 °C for 30 min. This strain energy areal density can be given as $E_S=\varepsilon^2 Bh$, where ε is the in-plane strain, B is the Burgers vector and h is the strained layer thickness [12]. The (113) reciprocal space map (not shown here) acquired from the as-grown 100 nm thick $Si_{75}Ge_{25}$ sample indicated a slight strain-relaxation, less than 1.0%, while strain relaxation of annealed sample was 19.1%. The defect structure of as-grown and annealed strained $Si_{75}Ge_{25}$ samples has been also studied by using ω-RC as shown in Fig. 3. It is found that the ω-RCs of as-grown $Si_{75}Ge_{25}$ are very similar to those recorded from annealed $Si_{80}Ge_{20}$ layer, as shown in Fig. 2 (c) and (d) because the layer thickness of strained $Si_{75}Ge_{25}$ is much thicker than the critical thickness for the pseudomorphic growth indicating the generation of 60° misfit dislocations. On the other hand, ω-RCs of annealed $Si_{75}Ge_{25}$ sample show a different behavior compared to slightly strain-relaxed sample with 60° misfit dislocations. First of all, it is clearly that the FWHM values of (004) as well as (113) ω-RCs of 100 nm thick $Si_{75}Ge_{25}$ annealed at 900 °C for 30 min are much larger than those of slightly strain-relaxed samples. The previous results showed that the (004) ω-RC was not sensitive to 60° misfit dislocations. It is suggested that the misfit defects in annealed strained $Si_{75}Ge_{25}$ layer with higher strain energy areal density should be different from 60° misfit dislocations. Second, the shape of both (004) and (113) ω-RCs of annealed sample is almost symmetric. Therefore, it is inferred that the defect structure of highly strain-relaxed SiGe sample is different from that of slightly strain-relaxed sample.

Fig. 4 shows cross-sectional transmission electron microscopy (CS-TEM) images of 100 nm thick $Si_{75}Ge_{25}$ annealed at 900 °C for 30 min. The strained-SiGe/Si interface is apparently seen and the misfit dislocations lying at the interface and stacking faults in the strained SiGe layer are also shown in Fig. 4 (a). Fig. 4(b) shows a high-resolution TEM lattice image of annealed sample. Typical 60° dislocations present in FCC crystal structure have Burgers vectors $\vec{b}_{60°}=1/2\langle 110\rangle$ gliding on the {111} closed packed plane. It was experimentally and theoretically described that 60° dislocations were dissociated into two partial dislocations in order to lower strain energy [13,14]. The Burgers vectors of these partial dislocations are $\vec{b}_\theta=1/6\langle 2\bar{1}\bar{1}\rangle$ and $\vec{b}_\theta=1/6\langle 11\bar{2}\rangle$ (θ=30° or 90°), where θ can be defined as the angle between the dislocation line and its Burgers vector. In addition, it was reported that the dissociation of 60° dislocations leaded to a different geometry in a strain relaxation for the tensile and compressively strained films [7]. Fig. 4 (b) shows stacking faults on {111} planes near the interface which are bounded by partial dislocations. Therefore, the peak broadening of ω-RCs of 100 nm thick strained $Si_{75}Ge_{25}$ annealed at 900 °C for 30 min, as shown in Fig. 3 (c) and (d), is due to these partial dislocations associated with the stacking faults.

4. Conclusions

In summary, the defect structure in strained-SiGe films with different strain relaxation was studied by using high-resolution ω-RCs. The result showed that the 60° dislocations generated from slightly strain-relaxed SiGe layers had an influenced on the profile shape of (113) ω-RC while they did not contribute to the peak broadening of (004) ω-RC. On the other hand, stacking faults bounded by two different partial dislocations made both ω-RCs symmetrically broad. Since the presence of the stacking faults in compressively stressed films are abnormal [6], this observation of the stacking faults by using ω-RC contributes to understanding of defects evolution and process design for high quality strained layer.

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