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Disordered Si/SiGe superlattices grown by ultrahigh vacuum chemical vapor deposition

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Abstract

A series of $Si/Si_{1-x}Ge_x$ disordered superlattices with various degrees of disorder were grown in an ultrahigh vacuum chemical vapor deposition system (UHV/CVD). High-resolution double-crystal X-ray diffraction (HRXRD), and conventional cross-sectional transmission electron microscopy were used to evaluate the crystalline quality of these superlattices. A dynamical X-ray simulation program was employed to analyze the experimental rocking curves. Excellent matches between experimental rocking curves and simulated ones were obtained for all superlattices with various degrees of disorder.

1. Introduction

Silicon is used for a variety of logic and memory integrated circuits but not for optoelectronic integrated circuits, because of its indirect band structure. Therefore, the ability to synthesize Si-based materials with new optical, photonic, and electronic properties is desired. In the indirect band $Al_{1-x}Ga_xAs/AlAs$ ($x \geqslant 0.5$) system, Sasaki had proposed a new class of semiconductors which is able to exhibit anomalously strong luminescence intensity [1]. It is referred to as a "disordered crystalline semiconductor". Disordered crystalline semiconductors are constructed artificially in such a manner that the constituent atoms are sufficiently ordered to allow epitaxial growth, but the chemical composition is disordered. The improvement in luminescence capability could be attributed to localized states created by artificial disordering. The concept of disordered crystalline semiconductors can be applied to the $Si/Si_{1-x}Ge_x$ system. In this work, a series of $Si/Si_{1-x}Ge_x$ disordered superlattices with various degree of disorder were grown in an ultrahigh vacuum chemical vapor deposition system (UHV/CVD). In order to determine and to verify the quality of the crystallinity, including the layer thickness, compositional uniformity and the structural differences between these disordered superlattices, the high-resolution double crystal X-ray diffraction (HRXRD) and cross-sectional transmission electron microscopy (XTEM) were used. A dynamical X-ray simulation program based on a solution of the Takagi–Taupin equations was employed to analyzed the experimental rocking curves [2].

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2. Experimental procedures

All of the disordered Si/Si$_{1-x}$Ge$_x$ superlattices were grown on 3 inch (001) Si substrates using the UHV/CVD system. The UHV/CVD technique was first described and developed by Meyerson. The construction and operation of our UHV/CVD system is similar to that reported in Ref. [3]. This system was designed and built at the National Chiao Tung University, ROC and has been successfully used to grow epitaxial layers of both Si and Si$_{1-x}$Ge$_x$ at temperatures as low as 550°C. Details of our UHV/CVD system are described elsewhere [4–6]. In this work, the growth temperature was kept constant at 550°C. Prior to the growth, the substrate was subjected to an $H_2SO_4:H_2O_2 = 3:1$ clean and a

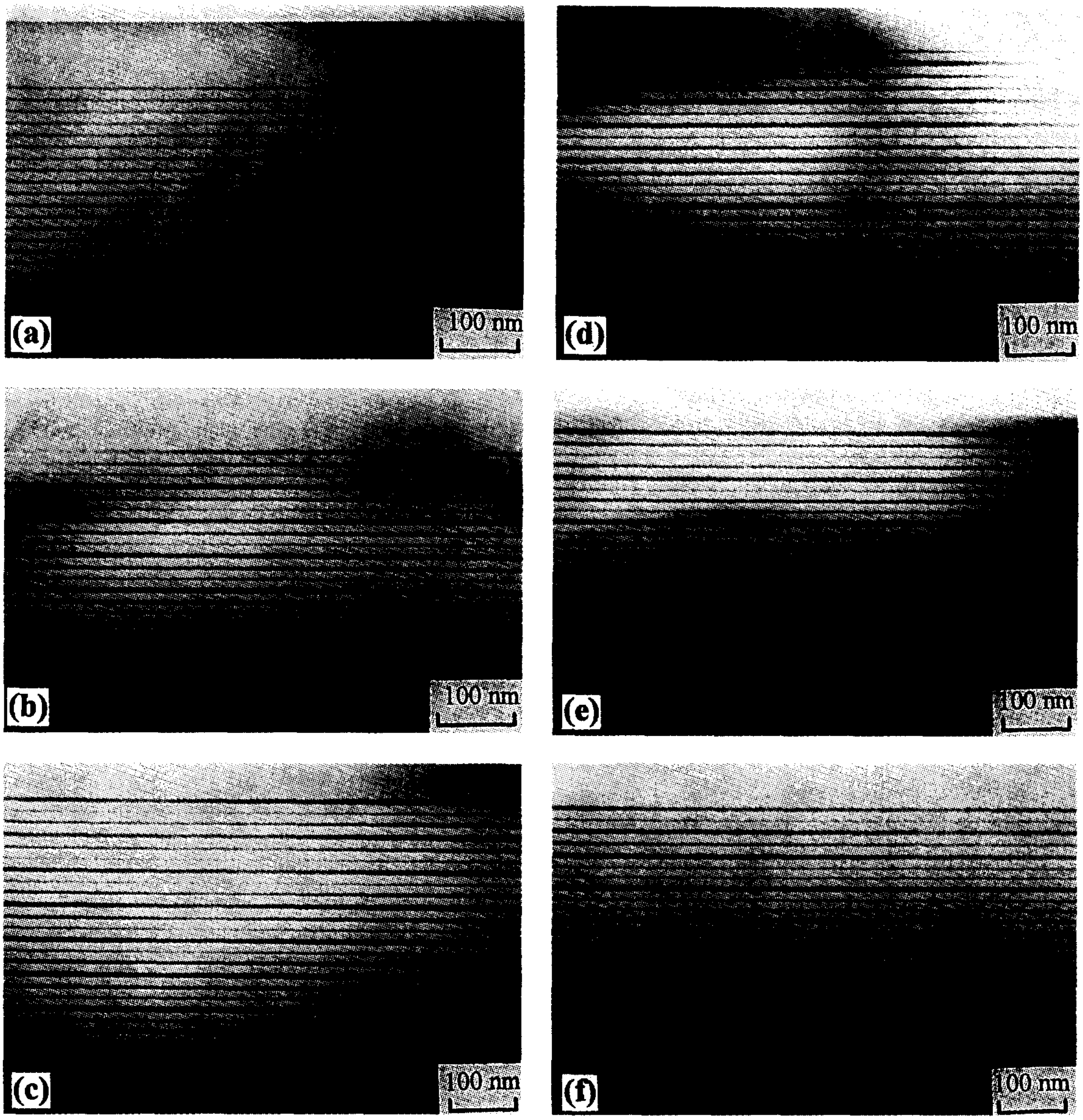

Fig. 1. (a), (b), (c), (d), (e), and (f) show the XTEM micrographs of ordered (Ord), Dis-3, Dis-6, Dis-12, Dis-24, and Ran-24 superlattices, respectively.

10% HF dip. Silane ($\mathrm{SiH_4}$) and 10% germane ($\mathrm{GeH_4}$) in hydrogen were used as reactant gases. The base pressure of the system was maintained at about 2×10^{-8} Torr in the growth chamber. During growth, the system was operated at about 1.0 mTorr.

HRXRD was used to determine the structural quality of these superlattices. X-ray rocking curves were obtained by using a Phillips DCD-3 double crystal diffractometer. The system was operated in parallel $(+, -)$ diffraction geometry using Cu Kα radiation. A Si single crystal with (004) symmetric reflection was used for the first reflection. A dynamical X-ray simulation program was used to aid the determination of the perfection, interfacial abruptness, layer thickness and Ge composition of these superlattices. Cross-sectional transmission electron microscopy was performed to examine the crystal quality and interfacial abruptness.

3. Results and discussion

Six samples (Ord, Dis-3, Dis-6, Dis-12, Dis-24, Ran-24) were prepared, one was a ordered superlattice (Ord) and the others were disordered superlattices with different degree of disorder. The ordered superlattice (Ord) consists of a total of 20 periods of Si/Si$_{0.815}$Ge$_{0.185}$ layers (one period contains a Si layer of 12.6 nm and a SiGe layer of 5 nm) and a p$^+$-Si cap layer of about 96 nm. The sample Dis-3 consists of 8 periods of Si/Si$_{0.815}$Ge$_{0.185}$ = 12.6/2.5/12.6/5.0/12.6/7.5 nm and a p$^+$-Si cap layer of about 96 nm. The width of the Si$_{1-x}$Ge$_x$ well was not constant in this Dis-3 superlattice. However, there were equal probabilities among the three Si$_{1-x}$Ge$_x$ well, i.e., P(2.5 nm) = P(5.0 nm) = P(7.5 nm). Therefore, the average width of the Si$_{1-x}$Ge$_x$ well was 5.0 nm which equaled to the well width of ordered superlattice as described above. Figs. 1a and 1b show the XTEM micrographs of Ord and Dis-3 superlattices, respectively. In this figure, Si and SiGe layers correspond to regions with bright and dark contrasts, respectively. No misfit dislocations were observed in these superlattices. The thicknesses of Si and SiGe layers of the ordered superlattice were measured to be 12.6 ± 0.5 and 5.0 ± 0.5 nm, respectively. However, there are three different layer thicknesses of SiGe in the Dis-3 superlattice, as shown in Fig. 1b. Similarly, sample Dis-6 consists of 4 periods of Si/Si$_{0.815}$Ge$_{0.185}$ = 12.6/2.5/12.6/5.0/12.6/7.5/12.6/5.0/12.6/2.5/12.6/7.5 nm and a p$^+$-Si cap layer of about 96 nm, as shown in Fig. 1c. The total layers of SiGe of Dis-6 equal that of sample Dis-3. However, the degree of disorder of Dis-6 is higher than that of Dis-3. Fig. 1d shows the XTEM micrograph of Dis-12 superlattices. Dis-12 consists of 2 periods of Si/Si$_{0.815}$Ge$_{0.185}$ = 12.6/2.5/12.6/5.0/12.6/7.5/12.6/5.0/12.6/2.5/12.6/7.5/12.6/2.5/12.6/7.5/12.6/5.0/12.6/5.0/12.6/7.5/12.6/2.5 nm and a p$^+$-Si cap layer of about 96 nm. Figs. 1e and 1f show the XTEM micrographs of Dis-24 and Ran-24 superlattices, respectively. The degree of disorder is Ran-24 > Dis-24 > Dis-12 > Dis-6 > Dis-3 > Ord superlattice.

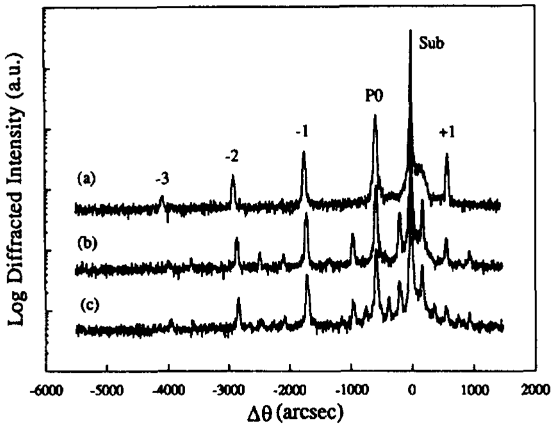

Fig. 2. (a), (b), and (c) show the HRXRD rocking curves obtained for samples Ord, Dis-3, and Dis-6 superlattices, respectively.

Figs. 2a–2c and Figs. 3a–3c show the HRXRD rocking curves obtained for the samples Ord, Dis-3, Dis-6, Dis-12, Dis-24, Ran-24 superlattices, respectively. In these figures, peak Sub represents the Si substrate reflection, peak P0 the zeroth-order superlattice reflection (main peak), and other main peaks are nth-order satellite peaks $(+1, -1, -2, -3)$, resulting from the periodicity of the superlattice. The intensities of all the main satellite peaks $(+1, \mathrm{P0}, -1, -2, -3)$ decrease with increasing degree of disorder, as shown in Figs. 2 and 3. The disordered structure would cause destructive X-ray diffraction. As a result, the intensity of all main peaks (which resulted from constructive diffraction from ordered layered structures) reduces with the

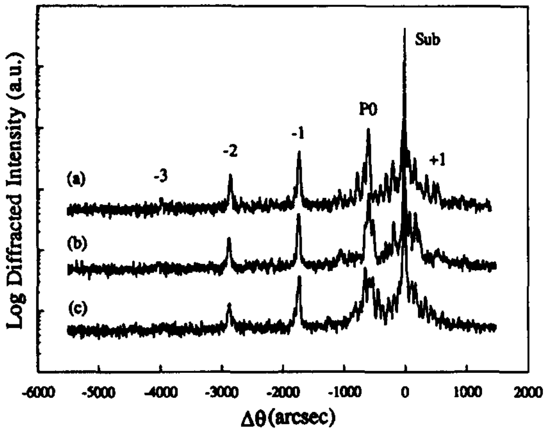

Fig. 3. (a), (b), and (c) show the HRXRD rocking curves obtained for samples Dis-12, Dis-24, and Ran-24, respectively.

increase of the degree of disorder. In addition, some extra peaks with low intensity were observed among the main satellite peaks. The number of these extra peaks increases with increasing degree of disorder; however, the intensities of these extra peaks reduce with the increase of the degree of disorder. These extra peaks result from the extra periodic structure with a larger period.

Fig. 4a shows the HRXRD rocking curve obtained for the ordered superlattice (Ord) with a Si first crystal while Fig. 4b shows the simulated rocking curve for a full-strained $Si_{1-x}Ge_x/Si$ superlattice of 20 periods with $x = 0.185$, Si 12.6 nm, SiGe 5.0 nm. In this simulated rocking curve, the effect of diffused scattering from the first crystal and substrate has been considered [5]. Upon comparison, excellent matches between experiment and simulation in terms of peak position, peak intensity, and full width at half maximum (FWHM) of each main peak are clearly observed. The layer thicknesses of Si and SiGe layers well agree with the layer thickness measured from the TEM photograph. In this figure, the peak C is diffracted from the heavily boron-doped Si cap on the superlattice structure.

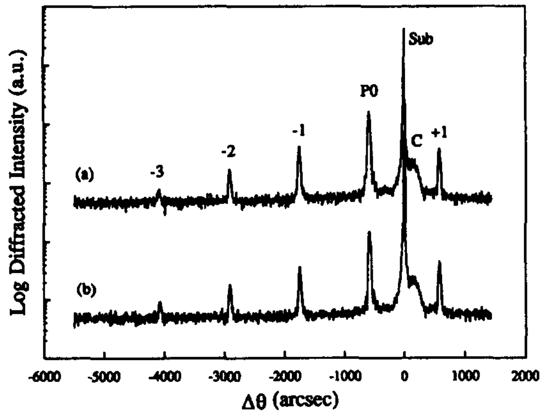

Fig. 4. (a) shows the HRXRD rocking curve obtained for ordered superlattice (Ord) with a Si first crystal; (b) the simulated rocking curve for a full-strained $Si_{1-x}Ge_x/Si$ superlattice of 20 periods with $x = 0.185$, Si 12.6 nm, SiGe 5.0 nm.

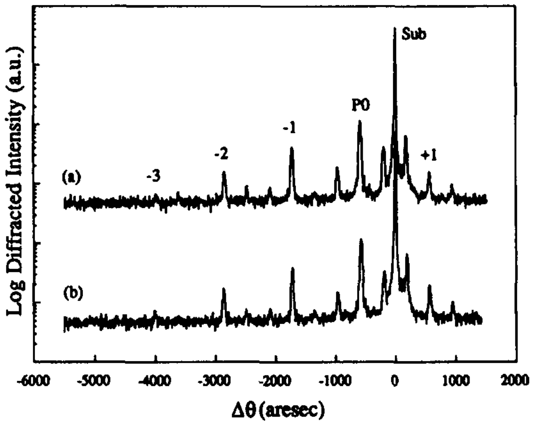

Fig. 5. (a) shows the HRXRD rocking curve obtained for sample Dis-3 with a Si first crystal; (b) the simulated rocking curve for a full-strained $Si_{1-x}Ge_x/Si$ superlattice which consists of 8 periods of $Si/Si_{0.815}Ge_{0.185} = 12.6/2.5/12.6/5.0/12.6/7.5$ nm and p^+-Si cap layer about 96 nm.

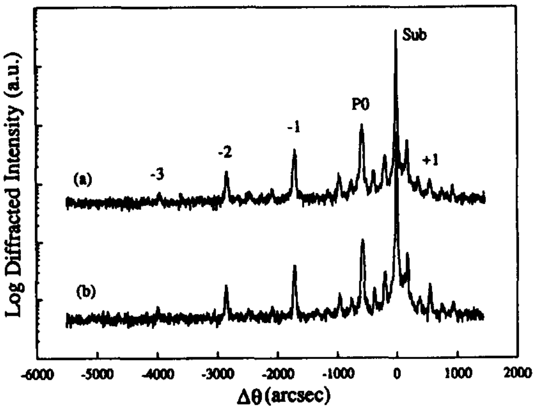

Fig. 6. (a) shows the HRXRD rocking curve obtained for sample Dis-6; (b) shows the simulated rocking curve for sample Dis-6.

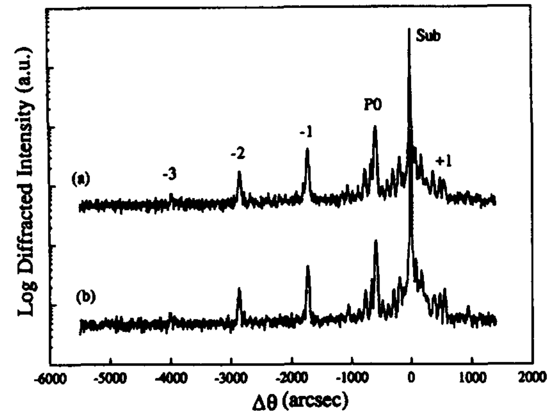

Fig. 7. (a) shows the HRXRD rocking curve obtained for sample Dis-12; (b) shows the simulated rocking curve for sample Dis-12.

Similarly, Fig. 5a shows the HRXRD rocking curve obtained for sample Dis-3 with a Si first crystal. Fig. 5b is the simulated rocking curve for a full-strained $Si_{1-x}Ge_x/Si$ superlattice which consists of 8 periods of $Si/Si_{0.815}Ge_{0.185}$ = 12.6/2.5/12.6/5.0/12.6/7.5 nm and a p^+-Si cap layer of about 96 nm. Upon comparison, excellent matches between experiment and simulation in terms of peak position, peak intensity, and FWHM of each main satellite peaks are clearly observed. In addition, the peak position, peak intensity, and FWHM of each extra satellite peaks of the experimental rocking curve also well match those of the simulated rocking curve, as shown in Figs. 5a and 5b.

Figs. 6a and Fig. 7a show the HRXRD rocking curves obtained for samples Dis-6 and Dis-12, respectively. Fig. 6b and Fig. 7b show the simulated rocking curves for samples Dis-6 and Dis-12, respectively. Comparison of the experimental rocking curves with the simulates ones, shows an excellent match between experiment and simulation in terms of peak position, peak intensity, and FWHM of each main and extra satellite peak. The results of XTEM and HRXRD indicate that high quality disordered Si/SiGe superlattices with various degrees of disorder can be achieved by the UHV/CVD system.

4. Conclusion

We have grown a series of Si/SiGe disordered superlattices with various degrees of disorder by using the UHV/CVD. The results of XTEM and HRXRD indicate that high quality disordered Si/SiGe superlattices can be achieved.

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