Investigation on the strain of SiGe/Si heteroepitaxial system during high temperature annealing by RBS/Channeling

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Abstract The influence of the high temperature processing on the strain stored in SiGe hetero epilayer was studied by means of RBS/Channeling. Channeling angular scan along the < 110 > axial direction in the (100) plane was used to characterize the tetragonal distortion in the SiGe strained layer. The strained crystal structure parameters were acquired by combining the determination of strain with the elasticity theory. It is shown that the strain stored in the SiGe epilayer has significantly change (relaxation factor from 0.023 to 0.84) after high temperature annealing. The potential strain relaxation mechanisms were discussed.

Keywords Strain, SiGe epilayer, RBS/Channeling, High temperature anneals.

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1 INTRODUCTION

Silicon-germanium ($Si_{1-x}Ge_x$) is playing an increasingly important role in modern very-large scale integration (VLSI) technology, particularly in high-speed devices for future telecommunication applications.[1] When $Si_{1-x}Ge_x$ alloy films are grown epitaxially on Silicon substrates, there exists a lattice mismatch at the interface. This mismatch causes a strain in the $Si_{1-x}Ge_x$ alloy film, which is compressive in the plane of the interface and tensile perpendicular to it. The lattice misfit strains at the $Si_{1-x}Ge_x$/Si interface provides a means to adjust the valence and conduction band offset. Both the different electronic properties of Ge and the strain in the alloy layer cause a lowering of the band gap.[2,3] Besides affecting the band structure and optical properties of Si_xGe_{1-x} alloy materials, the strain also affects the morphology and growth mechanism of the epitaxial layer. As a consequence, the strain in these films is an important parameter, which affects the performance of SiGe-based devices. However, heat treatment processes are unavoidable during the device fabrication such as high temperature annealing for post-implantation, that will give rise to the strained Si_xGe_{1-x} alloy epilayer to relax through

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the injection of misfit dislocations at the interface, which will have a lethal influence on the devices. Therefore, the quantitative information on the changes of strain during high temperature processing is very valuable for Si_xGe_{1-x} -base device application.

Several investigations on the strain stored in the small lattice mismatch systems, such as $Ga_{1-x}Al_xAs/GaAs$ were reported, in which X-ray diffraction (XRD)[4,5] was used to characterize the strain and its relaxation. However, there are some limitations of the XRD technique in determining the strain stored in the highly mismatched SiGe/Si system. For example, the position of the X-ray diffraction peak is related to both the composition and the strain of epilayers. If the strain is not negligible, the composition deduced by XRD will be inaccurate, which will give rise to some difficulties in characterizing the strain stored in the SiGe epilayers. On the other hand, due to low signal-to-noise ratios for thinner epitaxial films, XRD can not be used to evaluate strain stored in thinner SiGe/Si systems accurately.[6] Fortunately, RBS /Channeling technology is a reliable and accurate method for determining the composition of an alloy and the strain stored in the epitaxial film directly and nondestructively.[7]

In the present work, the grazing RBS technique with an improved depth resolution was employed to accurately determine the Ge content in the thin SiGe/Si system. The ion channeling angular scan was used to characterize the strain change stored in very thin SiGe epilayers during high temperature processing. AFM (atomic force microscopy) was used to characterize the surface morphology of the virgin and annealed samples.

2 THE STRAIN STORED IN THE Si/SiGe/Si HETEROEPITACIAL SYSTEM

The coherent growth of a SiGe alloy film on Si substrate requires that in-plane lattice constant at the interface is equal to that of the Si substrate. The SiGe film being free of dislocations is taken by a homogeneous tetragonal distortion. The tetragonal distortion in the distorted crystal was derived from the formula[8]

$$\varepsilon_T = (a_{\parallel} - a_{\perp})/a_{bulk} = \Delta\theta/\sin\theta\cos\theta \tag{1}$$

where $a_{\parallel}$ and $a_{\perp}$ are the in-plane and normal lattice constants, respectively; a_{bulk} is the SiGe alloy bulk lattice constant; θ is the angle between the $< 100 >$ and $< 110 >$ orientation in the substrate and $\Delta\theta$ is the angular difference in the substrate and epilayer, which can also be referred to as a kink angle.[9] Fig.1[10] indicates schematically a crystal cell of the SiGe alloy epitaxial layer. The cell with a bulk lattice constant a_i can be biaxially compressed in the growth plane and partially or fully match the in-plane lattice constant of the substrate. The average in-plane strain and perpendicular strain of the SiGe alloy epitaxial layer are given by

$$\varepsilon_T = (a_{\parallel} - a_{bulk})/a_{bulk} \qquad \varepsilon_{\perp} = (a_{\parallel} - a_{bulk})/a_{bulk} \tag{2}$$

where

$$a_{||} = a_{bulk}\{[1 + (2c_{12}/c_{11})]/[(1/\tan\theta_i) + (2c_{12}/c_{11})]\} \quad (3)$$

which can be easily obtained from the lattice geometry and the elasticity theory.[11] In this formula c_{11} and c_{12} are the elastic constants of the SiGe layer. No data from reliable experimental measurements of the elastic constants of the SiGe alloys have been published to date. The data that exist suggest that the SiGe alloy elastic constants can be adequately determined using simple linear rule-of-mixtures (ROM) interpolations from the elastic constants of pure Si and pure Ge. a_{bulk} is the lattice constant of SiGe alloy bulk materials, which was obtained by using Dismukes's data.[12] The value of θ_i in Eq.3 was derived from the equation, $\theta_i = \theta - \Delta\theta$, where $\Delta\theta$ was obtained from experimental curves.

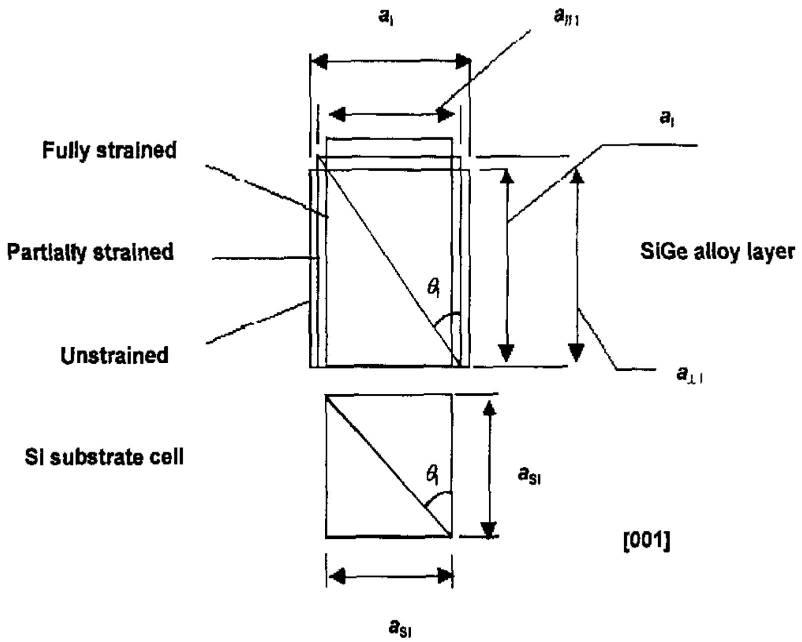

Fig.1 Schematic illustration of the SiGe alloy epilayer on the Si substrate indicating the lattice constants and angle involved in strain

Combining Eq.1 with Eq.2 or Eq.3, once $\Delta\theta_i$ was derived from the determination of dip curves for the Si/SiGe/Si< 100 > sample along the < 110 > axial direction in the (100) plane, the tetragonal distortion ε_T, parallel strain $\varepsilon_{||}$ and perpendiclar strain can be obtained. Therefore, all the information on strain and crystal geometry parameters can be obtained by means of RBS/Channeling.

3 EXPERIMENTAL

The $Si/Si_xGe_{1-x}/Si$ heteroepitaxial samples used for this study were prepared by commercial ASM Epilon 2000 chemical vapor deposition (CVD) reactor described in our another paper.[13] It consisted of the n-type (100)Si substrate with an undoped 30 nm Si buffer, followed by an undoped $Si_{1-x}Ge_x$ layer and an undoped Si cap. The sample was cut into two pieces, one is referred to as the virgin sample, the other is annealed at 950°C for 1 h in Ar inert gas ambient (henceforth we refer it as the annealed sample). The Ge content of $Si_{1-x}Ge_x$ layer was determined by 2 MeV $^4He^+$ grazing angle incident (incident angle of 700°) Rutherford backscattering spectroscopy (RBS) at the scattering angle of 170°.

An angular scan along the (100) planes through $< 110 >$ orientation of the sample was used to characterize the strain stored in the SiGe heteroepitaxial system. In order to obtain the correct angular difference between the $< 110 >$ axial direction of the SiGe alloy layer and the Si substrate, the position of the dip centroid in the angular scans was extracted using a cubic spline fit.[14,15]

4 RESULTS AND DISCUSSION

Fig.2 shows an experimental 70°-grazing incident RBS spectrum of the virgin sample and a computer simulation one by RUMP program. The simulated RBS spectrum verified that the sample structure is 12 nm Si/13 nm $Si_{0.79}Ge_{0.21}$/Si substrate. The Si signal from the surface and the Ge signal from the buried layer can be clearly seen. Arrows indicated the surface scattering positions of Si and Ge.

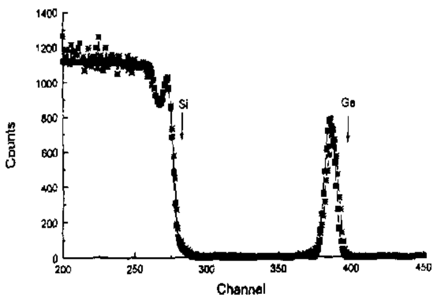

Fig.2 RBS spectrum of 2MeV He⁺ at the incidence angle of 70° and scattering angle of 170° from the virgin sample.
The starred line is an experimental spectrum and the squared line is a computer simulation

Fig.3 and Fig.4 show channeling angular scanning curves along the inclined $< 110 >$ axial direction from the virgin sample and the annealed sample, respectively. A shift of minimum yield between the SiGe epilayer and Si substrate, a direct measurement of strain, was obtained. For the virgin sample, the angular difference of $\Delta\theta = -0.40°$ shown in Fig.3 was obtained. Identically, the angular difference of $\Delta\theta = -0.0630$ between the SiGe epilayer and the Si substrate of the annealed sample was also inferred from Fig.4. The related strain and structure parameters of the virgin and the annealed sample are tabulated in Table 1.

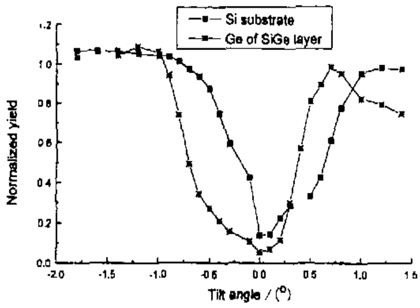

Fig.3 Angular scan of the virgin sample (Si/SiGe/Si < 100 >) along the < 110 > axial direction

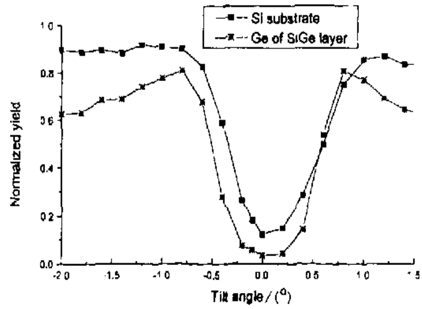

Fig.4 Angular scan of the annealed sample (Si/SiGe/Si < 100 >) along the < 110 > axial direction

Table 1 Structure parameters and magnitudes of the strain derived from RBS/Channeling measurements

	$a_{\parallel}$ /nm	$a_{\perp}$ /nm	$\varepsilon_{\parallel}$ /10^{-3}	$\varepsilon_{\perp}$ /10^{-3}	ε_T /10^{-3}	R	χ_{min} /%	FWHM of the Ge peak by RBS/keV
The virgin sample	0.5432	0.5508	-7.85	6.11	-14	0.023	2.7	30
The annealed sample	0.5468	0.5480	-1.28	0.920	2.2	0.84	3.4	42

For the virgin sample, the theoretical value of tetragonal distortion is -0.015 derived from the formula,[16] $\varepsilon_T = f \times (1 + \nu)/(1 - \nu)$, where ν is the Poisson ratio. The experimental value is in good agreement with the theoretical value. The relaxation factor R defined as $(a_{\parallel} - a_{Si})/(a_{bulk} - a_{Si})$ is equal to zero if the epilayer is fully strained and $R = 1$ if it is unstrained. The relaxation factor R of the virgin sample is 0.023. Hence the virgin sample is fully strained and the SiGe alloy film coherently grows on Si substrate. The relaxation factor R of the annealed sample is 0.84, which indicates that strain was mostly relieved when the virgin sample is annealed at 950°C for 1 h in Ar inert gas ambient.

It is well established that the strain relaxation can be mainly accommodated by means of misfit dislocations, inter-diffusion and surface roughness for the strained epitaxial system.[17] The strain relaxation by misfit dislocations occurs only for epilayer thickness greater than the critical thickness. In our study, because the Ge concentration in the SiGe samples is relatively low, the thickness of $Si_{0.79}Ge_{0.21}$ alloy epitaxial layer is less than the critical thickness according to the Matthews–Blakeslee mechanical equilibrium curve.[18] Hence, misfit dislocation will not be introduced into the SiGe/Si interface during the epitaxial growth of SiGe alloy film. The strain relieves by means of surface roughness can occur for any epitaxial layer thickness,[1] which are also evidenced in our study. Fig.5 shows the image of AFM for the virgin sample. The surface of the virgin sample is very smooth. The image of AFM for the annealed sample is shown in Fig.6, indicating that the sample surface becomes roughness. It is evidenced that the relaxation via surface roughening is a factor of strain relief in our SiGe/Si heteroepitaxial system at elevated temperature annealing. The strain relaxation via inter-diffusion is not a significant mechanism at the growth temperatures used in MBE or CVD, but it would be conceivably significant at elevated temperature processing involved to device fabrications.[18] Comparing the RBS random spectra between the annealed sample and the virgin sample (not shown in this article), it is found that the Ge peak is lower and broader for the annealed sample than for the virgin sample (the FWHM of Ge peak changes from 30 to 42 keV), which indicates a pronounced Ge out-diffusion from the $Si_{1-x}Ge_x$ layer in one annealing duration. The out-diffusion of Ge seems to relief the stored strain energy and thereby minimizes the dislocation generation. The surface roughening favors the reduction of the energetic barriers for dislocation nucleation, which is associated with surface morphology. During the high temperature processing, the misfit dislocations introduced at interface between the SiGe layer and substrate will be significantly reduced. The (110) planar channeling spectra of the virgin and annealed samples shown in our another paper[13] have insignificantly change. It also verified that even if the misfit dislocation is generated during the 950°C high temperature annealing, it will be insignificant. Hence the pronounced strain relaxations in the annealed sample are mainly attributed to the out-diffusion of Ge from the $Si_{1-x}Ge_x$ layer and surface roughness.

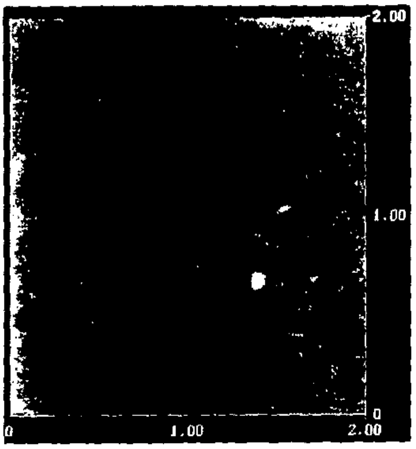

Fig.5 Surface morphology of the virgin sample determined by AFM

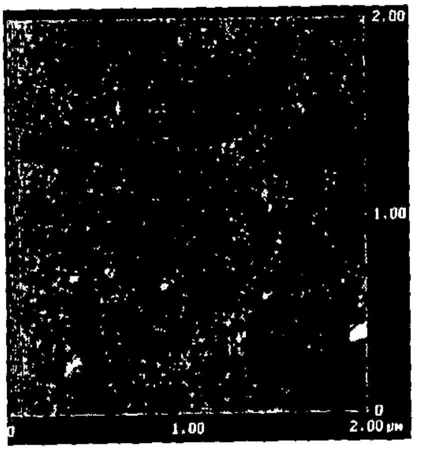

Fig.6 Surface morphology of the annealed sample determined by AFM

5 CONCLUSIONS

Channeling angular scans were used to characterize the strain stored in the Si/SiGe/Si epitaxail system. Subjected to high temperature annealing, the tetragonal distortion of SiGe epitaxial system changes from -0.014 to -0.0022. The strained crystal structure parameters are obtained combining the channeling angular scans with the elasticity theory. The SiGe epilayer keep considerably good crystal quality pre- and post-annealing (channeling minimum yield from 2.7% to 3.4%). Out-diffusion of Ge, surface roughness rather than formation of misfit dislocations give rise to the pronounced strain relaxation in the annealed sample.

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