JOURNAL OF RARE EARTHS
Vol. 22, Suppl., Aug. 2004, p. 026

Effect of Ion Dose on Growth of Relaxed SiGe Layer on Ion Implantation Si Substrate

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Abstract: Thin strain-relaxed $Si_{0.8}Ge_{0.2}$ films (57.6 nm) on the 30 keV Ar^+ ion implantation Si substrates for different dose (1×10^{14}, 5×10^{14}, $3 \times 10^{15}\ cm^{-2}$) were grown by ultra high vacuum chemical vapor deposition (UHVCVD) system. Rutherford backscattering/ion channeling (RBS/C), high resolution X-ray diffraction (HRXRD), Raman spectra as well as atomic force microscopy (AFM) were used to characterize these SiGe films. Investigations by RBS/C as well as HRXRD demonstrate that these thin $Si_{0.8}Ge_{0.2}$ films could indeed epitaxially grow on the Ar^+ ion implantation Si substrates. Under low dose ($1 \times 10^{14}\ cm^{-2}$) and medium dose ($5 \times 10^{14}\ cm^{-2}$) implantation conditions, the relaxation extents of SiGe films are 60.6% and 63.6%, respectively. However, high dose implantation ($3 \times 10^{15}\ cm^{-2}$) prompt the strain in epitaxial SiGe film to be close to full relaxation status (relaxation extent of 96.6%). On the other hand, determinations of RBS/C also indicate the crystalline quality of SiGe film grown on high dose implantation Si substrate is nearly identical to that grown on low dose ($1 \times 10^{14}\ cm^{-2}$) implantation Si substrate.

Key words: strain relaxation; UHVCVD; ion implantation; SiGe
CLC number: TG175; TB383 **Document code:** A **Article ID:** 1002 - 0721(2004) - 0026 - 04

Relaxed SiGe layers have gained considerable attention due to their applications for strained Si/SiGe high electron mobility transistor, metal-oxide-semiconductor field-effect transistor (MOSFET) and other devices. High-quality relaxed SiGe templates, especially those with low threading dislocation density and smooth surface, are crucial for the electrical performances of devices[1, 2]. In order to realize high-quality relaxed SiGe layer with such good characteristics, several methods have been developed, such as compositionally graded buffer layers (CGLs)[3] and low temperature (< 400 ℃) grown Si buffer layers (LT)[4]. Especially, the CGLs have already been successfully applied to various types of devices based on SiGe/Si heterostructures. However, these approaches still have some disadvantages. For example, CGLs are, in general, required to be several μm in thickness. This value is too thick for the practical monolithic integration of devices. LT method with growth temperature below 400 ℃ can not be performed in gas source growth systems such as chemical vapor deposition (CVD) and gas source molecular beam epitaxy (GSMBE), since the growth temperature higher than 400 ℃ is necessary for the decomposition of source gas. Therefore, a novel approach needs to be solved for the implementation of relaxed SiGe buffer layers.

With regard to strain relaxation of SiGe pseudormorphic layer, Holländer et al.[5] have ever reported that He^+ ion implantation into pseudomorphic $Si_{1-x}Ge_x/Si$ (100) and subsequent annealing can enhance strain in the SiGe layer to relax. According to this idea, Sawano et al.[6] have recently developed a new method (ion implantation into Si substrate before SiGe growth) as an alternative of the LT growth to fabricate thin strain-relaxed SiGe layer in solid source molecular beam epitaxy system (solid source-MBE). Considering the complexity, the cost, compatibility with widely industrial application and the low productivity of MBE equipment, UHVCVD is a good choice for epitaial growth of SiGe film. In our recent study[7], we have succeeded in fabricating strain - relaxed SiGe epitaxial film on Ar^+ ion implantation Si substrate by UHVCVD and investigate the dependence of relaxed SiGe film growth on ion implantation energy under the identical

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Received date: 2004 - 06 - 10; **revised date:** 2004 - 06 - 30
Foundation item: Project supported by National High Technology and Research Development Program (863 Program) (2002AA3Z1230)
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ion dose. Experimental results show that the relaxed SiGe film grown on low energy Ar^+ (30 keV) implantation Si substrate outperformed that grown on 45 or 60 keV implantation Si substrate, which was not observed in Ref.[6]. In the present article, we investigated the effect of different ion dose on the relaxed SiGe film grown on 30 keV Ar^+ implantation Si substrate by UHVCVD with the purpose of exploring the optimum relaxed SiGe film fabrication condition.

1 Experimental Procedure and Characterization

2 cm × 2 cm n-type Si (100) substrates with resistivity of 2 ~ 7 Ω·cm were implanted (7° tilt angle) with 30 keV Ar^+ ions at three different dose (1×10^{14}, 5×10^{14} and 3×10^{15} cm^{-2}), respectively. After completing Ar^+ ion implantation, These three Si substrate wafers were then cleaned by boiled $H_2SO_4:H_2O_2 = 4:1$ solution for 10 min, rinsed in de-ionized water and the surface was H-terminated by diluted HF/H_2O (1:10) solution dip for 45 s. Finally, these substrate samples were loaded into a 5-inch sample holder in self-developed UHVCVD system[8]. Pure silane (SiH_4) and hydrogen-diluted 15% germane (GeH_4) were used as reactant gases. The growth of SiGe film on the these substrates started from a high temperature bake at about 750 ℃ for 10 min, then reactant chamber temperature was decreased to 590 ℃ and kept stable at 590 ℃ for 4 min. Before the growth of SiGe film layer, a 15 nm thick Si buffer was grown at 590 ℃. The growth time of the SiGe film at 590 ℃ is 30 min with the flux of SiH_4 and GeH_4 kept at 6 sccm and 1.1 sccm, respectively. Finally, for convenience, SiGe films grown on various Si substrates (30 keV implantation at different dose: 1×10^{14}, 5×10^{14} and 3×10^{15} cm^{-2}) can be referred to as sample No.1, No.2 and No.3, respectively.

The thickness, Ge content and crystal quality of these $Si_{1-x}Ge_x$ films on various Si substrates were verified by RBS/C. RBS/C determination was carried out by using 2.022 MeV $^4He^+$ ions at a scattering angle of 1650 and at normal incidence by using a standard Au - Si surface barrier detector with an energy resolution of 18 keV full width at half maximum (FWHM). Analysis of RBS random spectra was carried out using SIMNRA program[9]. The characteristics of these $Si_{1-x}Ge_x$ films were also evaluated by HRXRD. Rocking curve measurements were performed on a Bruker X-ray high-resolution diffractometer with a four-bounce Ge (220) monochromator. The X-ray source was Cu Kα1 (λ = 0.154 nm). Raman scattering measurements in a backscattering geometry were used to locally probe the strain in the $Si_{1-x}Ge_x$ film. The samples were excited with the 514 nm line of an argon-ion laser. The Raman frequency shift due to the Si - Si optical phonon mode in the SiGe film was measured with an accuracy of ± 0.2 cm^{-1}. The surface roughness of SiGe films was measured by atomic force microscopy (AFM) (Digital Instruments Nano-scope Ⅲa) and the root of mean square (RMS) of the surface profile was used to characterize the surface morphology.

2 Results and Discussion

RBS spectra (random and [100] axial channeling) acquired from sample No.1, No.2 and No.3 are displayed in Figs.1 (a), (b) and (c), respectively. At first, both the thickness of $Si_{1-x}Ge_x$ and Ge content x in these three samples are nearly close to 57.6 nm and 0.20 according to RBS random spectra analyzed by SIMNRA program[9]. The [100] axial minimum yield value χ_{min} deduced from the channeled-to-random ratio of germanium signal slightly above 1500 keV energy can be used to characterize the crystal quality of SiGe film grown on the various Si substrates. These χ_{min} of sample No.1, sample No.2 and sample No.3 show in Figs.1 (a), (b) and (c) are 41.2%, 47.6% and 42.0%, respectively. This larger χ_{min} for three samples may be due to the misfit dislocations generated at the layer-substrate interface. In addition, the existence of aligned spectrum for these three samples demonstrates that thin $Si_{0.8}Ge_{0.2}$ films were epitaxially grown on the Ar^+ ion implantation Si substrates.

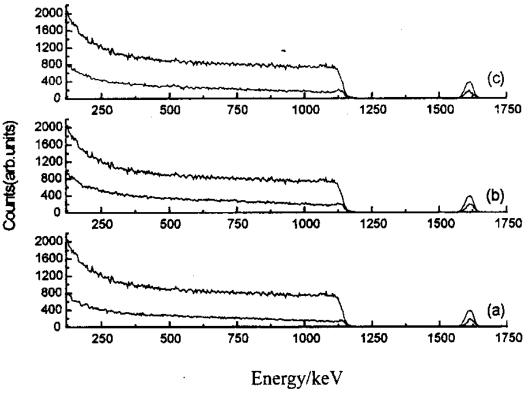

Fig.1 RBS spectra (random and [100] axial channeling) acquired from sample

(a) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ion at dose of 1×10^{14} cm^{-2}; (b) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ion at dose of 5×10^{14} cm^{-2}; (c) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ion at dose of 3×10^{15} cm^{-2}

Fig.2 shows the HRXRD spectra from Si (004) and SiGe (004) planes of sample No.1, No.2 and No.3. The appearances of SiGe peak in three samples also indicate that SiGe film can epitaxially grow on Si substrate with 30 keV Ar^+ ion implantation at three different doses, which is in good agreement with RBS/C determination. In addition, as seen in this figure, the XRD peak of SiGe layer in sample No.3 shifts to higher angles than that of sample No.1 and No.2. Because the Ge content in SiGe film for three samples is nearly identical, therefore, the strain stored in SiGe layer of sample No.3 is least.

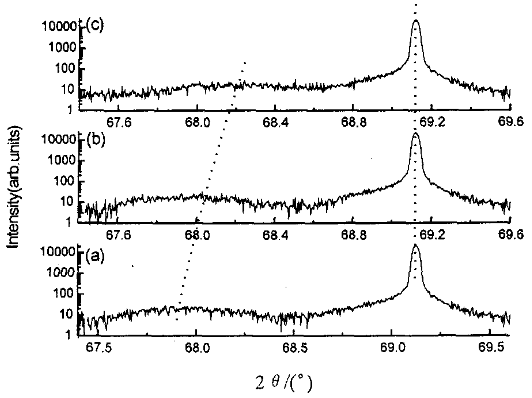

Fig.2 HRXRD (004) rocking curve for sample
(a) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ion at dose of 1×10^{14} cm^{-2}; (b) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ion at dose of 5×10^{14} cm^{-2}; (c) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ion at dose of 3×10^{15} cm^{-2}

Raman spectra of samples No.1, No.2 and No.3 are shown in Figs.3 (a), (b) and (c). The peak at 520 cm^{-1} is ascribed to the Si-Si phonon vibration mode of Si substrates. The Si-Si phonon mode of the SiGe epilayer, the specific ordering Ge-Si mode[10], Ge-Si mode and Ge-Ge mode of the SiGe epilayer for these three samples (No.1, No.2 and No.3) are shown in Table 1. According to these peak positions, it is possible to estimate the relaxation extent of the SiGe films due to the linear Ge composition dependence of the Si-Si optical phonon mode shift relative to the Si substrate for both the fully relaxed and the fully strained SiGe epilayers. Utilizing the formula of relaxation extent in SiGe described in Ref. [11], all the relaxation extents of strained SiGe layers in three samples are also listed in Table 1.

Obviously, the relaxation extent of strained SiGe layer in sample No.3 is the biggest. Thus our Raman results are quantitatively consistent with that obtained from HRXRD determinations as discussed above.

Figs.4 (a), (b) and (c) show three-dimension AFM images as well as surface root mean square (RMS) roughness of sample No.1, sample No.2 and sample No.3. The surface morphology in SiGe layers of three samples is similar, while the roughness is different. To the best of our knowledge, strain relaxation of pseudomorphic SiGe layers generally causes roughening of the surface in proportion to the amount of strain relaxation[12]. Therefore, the largest roughness of sample No.3 (RMS of 8.668 nm) compared to those of sample No.1 and No.2 (7.460 and 7.468 nm) reflects the largest strain relaxation extent, which is in good agreement with the results of strain relaxation determined by Raman spectra as well as HRXRD.

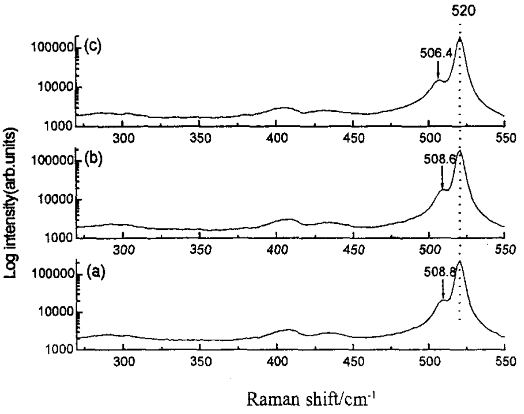

Fig.3 Raman spectra obtained from sample
(a) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ion at dose of 1×10^{14} cm^{-2}; (b) SiGe film grown on Si substrate implanted by 30keV Ar^+ ion at dose of 5×10^{14} cm^{-2}; (c) SiGe film grown on Si substrate implanted by 30keV Ar^+ ion at dose of 3×10^{15} cm^{-2}

Table 1 Peak frequencies for main Raman for all three samples (sample No.1, sample No.2 and sample No.3) and the corresponding extent of strain relaxation

Sample	Peaks of SiGe epi-layer/cm^{-1}				Peak of substrate/cm^{-1}	Relaxation extent/%
	Ge-Ge mode	Si-Ge mode	Specific ordering Si-Ge mode	Si-Si mode	Si-Si mode	
No.1	291.6	408.7	435	508.8	520	60.6
No.2	297.5	409	434.5	508.6	520	63.6
No.3	297	405.6	431.4	506.4	520	96.9

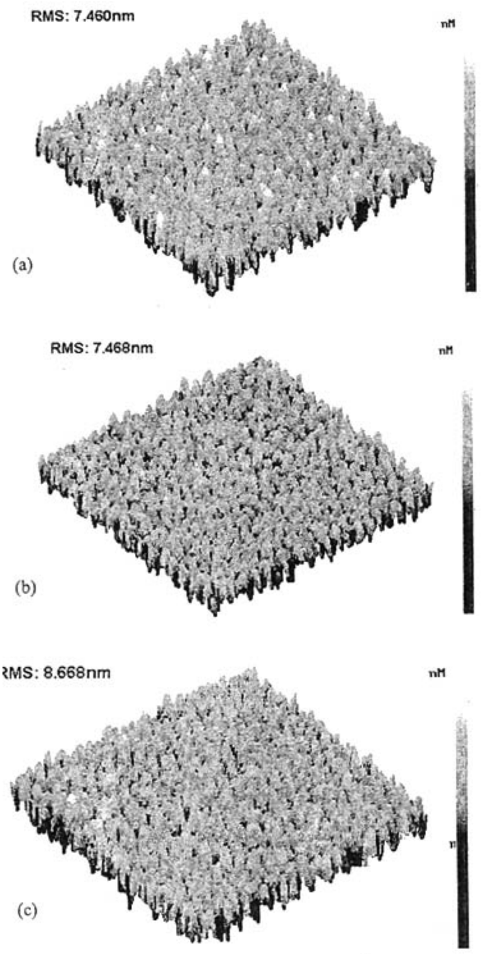

Fig.4 Three dimension AFM images of sample
(a) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ion at dose of 1×10^{14} cm^{-2}; (b) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ion at dose of 5×10^{14} cm^{-2}; (c) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ion at dose of 3×10^{15} cm^{-2}

3 Conclusion

We used UHVCVD system to have grown 57.6 nm $Si_{0.8}Ge_{0.2}$ films on the 30 keV Ar^+ ion implantation Si substrates under three different implantation doses (1×10^{14}, 5×10^{14}, 3×10^{15} cm^{-2}) condition. These SiGe films were characterized by RBS/C, HRXRD, Raman spectra together with AFM. Determinations of RBS/C as well as HRXRD demonstrate these $Si_{0.8}Ge_{0.2}$ films are epitaxially grown ion implantation Si substrate. The crystalline quality of $Si_{0.8}Ge_{0.2}$ film grown on high dose (3×10^{15} cm^{-2}) implantation Si substrate is close to that on medium (5×10^{14} cm^{-2}) and low dose (1×10^{14} cm^{-2}) implantation Si substrate. The 96.9% of relaxation extent in $Si_{0.8}Ge_{0.2}$ film grown on high dose (3×10^{15} cm^{-2}) implantation Si substrate is far larger than that in $Si_{0.8}Ge_{0.2}$ film grown on medium (5×10^{14} cm^{-2}) or low dose (1×10^{14} cm^{-2}) implantation Si substrate. Considering from relaxation extent of strain and crystalline quality of SiGe films for these samples, the thin relaxed SiGe film grown on high dose (3×10^{15} cm^{-2}) implantation Si substrate is optimal. This work would provide a solid basis for the growth of relaxed SiGe films by UHVCVD in place of MBE and its realistic device applications.

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刊名：稀土学报（英文版）ISTIC EI SCI

英文刊名：JOURNAL OF RARE EARTHS

年，卷(期)：2004,22(z2)

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