Thin relaxed SiGe layer grown on Ar^+ ion implanted Si substrate by ultra-high vacuum chemical vapor deposition

CHEN Chang-Chun[1*], YU Ben-Hai[1], LIU Jiang-Feng[1], CAO Jian-Qing[2], ZHU De-Zhang [2]

([1] College of Physics and Electronic Engineering, Xinyang Normal University, Xinyang 464000

[2] Shanghai Institute of Applied Physics, the Chinese Academy of Sciences, Shanghai 201800)

Abstract Thin strain-relaxed $Si_{0.81}Ge_{0.19}$ films (95 nm) on the Ar^+ ion implanted Si substrates with different energies (30 keV, 40 keV and 60 keV) at the same implanted dose ($3\times10^{15}cm^{-2}$) were grown by ultra high vacuum chemical vapor deposition (UHVCVD). Rutherford backscattering/ion channeling (RBS/C), Raman spectra as well as atomic force microscopy (AFM) were used to characterize these SiGe films. Investigations by RBS/C demonstrate that these thin $Si_{0.81}Ge_{0.19}$ films were epitaxially grown on the Ar^+ ion implanted Si substrates, although there existed lots of crystal defects. The relaxation extent of $Si_{0.81}Ge_{0.19}$ films on the Ar^+ implanted Si substrates is larger than that in the unimplanted case, which were verified by Raman spectra. Considering the relaxation extent of strain, surface roughness and crystal defects in these SiGe films, the thin relaxed SiGe film on the 30 keV Ar^+ implanted Si substrate is optimal.

Key words Strain relaxation, Ultra high vacuum chemical vapor deposition, Ion implantation, SiGe

CLC number TN32

1 Introduction

Relaxed SiGe layers have gained considerable attention due to their applications in 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 performance 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℃ cannot be performed in gas source growth systems such as chemical vapor deposition (CVD) and gas source molecular beam epitaxy (GSMBE), for 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).

Partially supported by the National Natural Sciences Foundation of China (No.10075072)

* Corresponding author. E-mail address: changchunchen@hotmail.com

Received date: 2004-12-17

Considering the complexity, cost, compatibility with wide industrial application and the low productivity of MBE equipment, UHVCVD is a good choice for epitaxial growth of SiGe film. In this study, we have utilized gas source growth system—UHVCVD system to grow thin relaxed SiGe layer on Ar^+ ion implanted Si substrate.

2 Experimental procedure and characterization

n-type Si (100) substrates with resistivity of 2~7 Ω • cm were implanted (7° tilt angle) with Ar^+ ions at three different energies (30, 40 and 60 keV) to a dose of 3×10^{15} cm^{-2}. After completing Ar^+ ion implantation, all implanted Si substrates were cut into pieces with a size of 2 cm × 2 cm. These 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. Subsequently, these substrate samples together with a 2 cm × 2 cm n-type Si (100) wafer (as a control) rinsed by the same procedure were loaded into a 5-inch sample holder in self-developed UHVCVD system.[7] Pure silane (SiH_4) and hydrogen-diluted 15% germane (GeH_4) were used as reactant gases. The growth of SiGe film on the above-mentioned substrates started from a high temperature bake at about 750℃ for 10 min, and 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 5.8 sccm and 1.2 sccm, respectively. Finally, for convenience, SiGe films grown on various Si substrates (unimplanted Si substrate, Si substrates implanted by 30 keV, 40 keV or 60 keV Ar^+ ions) were referred to as Sample No.1, No.2, No.3 and No.4, 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 was carried out by using 2.022 MeV $^4He^+$ ions at a scattering angle of 165° and at normal incidence by using a standard Au-Si surface barrier detector with an energy resolution of 18 keV (FWHM). Analysis of RBS random spectra was carried out using SIMNRA program.[8] Raman scattering measurements in a backscattering geometry were made 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.

3 Results and discussion

RBS spectra (random and [100] axial channeling) acquired from Samples No.1, No.2, No.3 and No.4 are displayed in Fig.1 (a), (b), (c) and (d), respectively. At first, both thickness of $Si_{1-x}Ge_x$ and Ge content x in these four samples are nearly close to 95 nm and 0.19 according to RBS random spectra analyzed by SIMNRA program.[8] The [100] axial minimum yield value χ_{min} deduced from the channeled-to-random ratio of germanium signal slightly above 1500 keV can be used to characterize the crystal quality of SiGe film grown on various Si substrates. The χ_{min} values of Samples No.1, No.2, No.3 and No.4 shown in Fig.1 (a), (b), (c) and (d) are 6.42%, 46.3%, 62.9% and 92.8%, respectively. The relatively high [100] axial minimum yield values χ_{min} for Samples No.2, No.3 and No.4 indicate the presence of crystal defects in these SiGe films. In addition, these [100] axial channeling spectra of Si signal of Samples No.2, No.3 and No.4 show a pronounced peak, as a result of

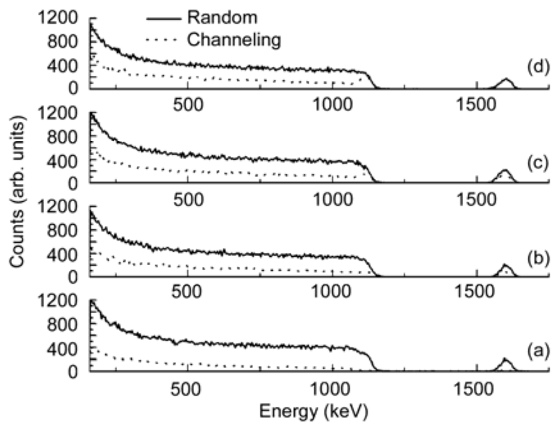

Fig.1 RBS spectra (random and [100] axial channeling) acquired from samples: (a) SiGe film grown on unimplanted Si substrate; (b) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ions; (c) SiGe film grown on Si substrate implanted by 40 keV Ar^+ ions; (d) SiGe film grown on Si substrate implanted by 60 keV Ar^+ ions.

de-channeling, which can be attributed to a network of misfit dislocations at the interface between SiGe layer and Si substrate. This is an obvious evidence of the presence of a large number of crystalline defects. Among three samples, there are the most crystalline defects in Sample No.4.

Raman spectra of samples are shown in Fig.2. The peak at 520 cm^{-1} is assigned to the Si-Si phonon vibration mode of Si substrates. The Si-Si phonon mode, the specific ordering Ge-Si mode,[9] Ge-Si mode and Ge-Ge mode of the SiGe epilayer for these four samples are shown in Table 1. From 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:[10]

$$\Delta_r = 69.0x\ (\mathrm{cm}^{-1})\ \text{(fully relaxed)} \quad (1)$$

$$\Delta_s = 36.0x\ (\mathrm{cm}^{-1})\ \text{(fully strained)} \quad (2)$$

while the extent of strain relaxation was defined as:

$$\gamma = (\Delta_{exp} - \Delta_s) / (\Delta_r - \Delta_s) \quad (3)$$

where Δ_r and Δ_s are Raman peak shifts of fully relaxed and fully strained epilayers from Si substrate, respectively, Δ_{exp} is the measured shift and x is Ge composition in SiGe layer, which can be determined by RBS random spectrum.

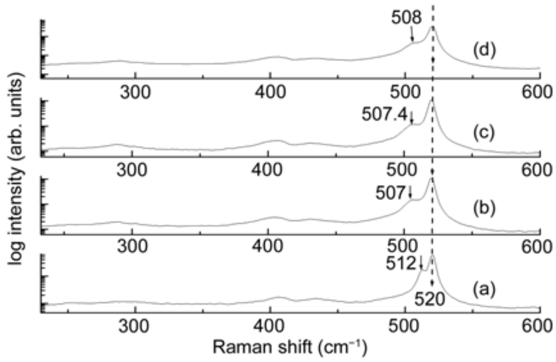

Fig.2 Raman spectra obtained from samples: (a) SiGe film grown on unimplanted Si substrate; (b) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ions; (c) SiGe film grown on Si substrate implanted by 40 keV Ar^+ ions; (d) SiGe film grown on Si substrate implanted by 60 keV Ar^+ ions.

Table 1 Peak frequencies for main Raman spectra for all four samples and the corresponding extent of strain relaxation

Sample	Peaks of SiGe epi-layer (cm^{-1})				Peak of substrate (cm^{-1})	Relaxation extent
	Ge-Ge	Si-Ge	Specific ordering	Si-Si mode	Si-Si mode	
No.1	291	406	433	512	520	18.5%
No.2	288	404	433	508	520	82.3%
No.3	289	408	430	507.4	520	91.8%
No.4	287	404	431	507	520	98.2%

The relaxation extents calculated from Eqs. (1)~(3) are shown in the last column of Table 1. Obviously, the relaxation extents of Samples No.2, No.3 and No.4 are larger than that of Sample No.1.

Fig.3 show three-dimensional AFM images and surface root mean square (RMS) roughness of the four samples. The surface morphologies of the implanted samples (No.2, No.3 and No.4) as well as the un-implanted sample (No.1) are similar, while their roughnesses are 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.[11] Therefore, the larger roughness of the implanted samples (RMS of Sample No.2, No.3 and No.4 are 3.836 nm, 5.885 nm and 6.391 nm, respectively) compared to that of the un-implanted sample No.1 (0.842 nm) is thought to reflect the larger strain relaxation, which is in good agreement with the results of strain relaxation determined by Raman spectra.

Judging from the experimental results of RBS/C, Raman and AFM for SiGe film grown on Si substrate implanted and un-implanted by UHVCVD, the top region of all the ion-implanted Si substrates indeed has compliant effect,[12] which enhances the strain in SiGe layer to relax. In Ref. [6], Sawano et al. pointed out that such a compliant effect for ion implantation at 25 keV is not distinct due to the too shallow defective region. However, in this study, the favorable implantation condition is chosen at 30 keV for the formation of relaxed SiGe film with the least defect density, compared to other implantation condition. The deposition of 15 nm thick Si buffer layer prior to the SiGe film growth in UHVCVD system may be one reason that makes our experimental results obviously differ from that in Ref. [6]. Although such experimental results

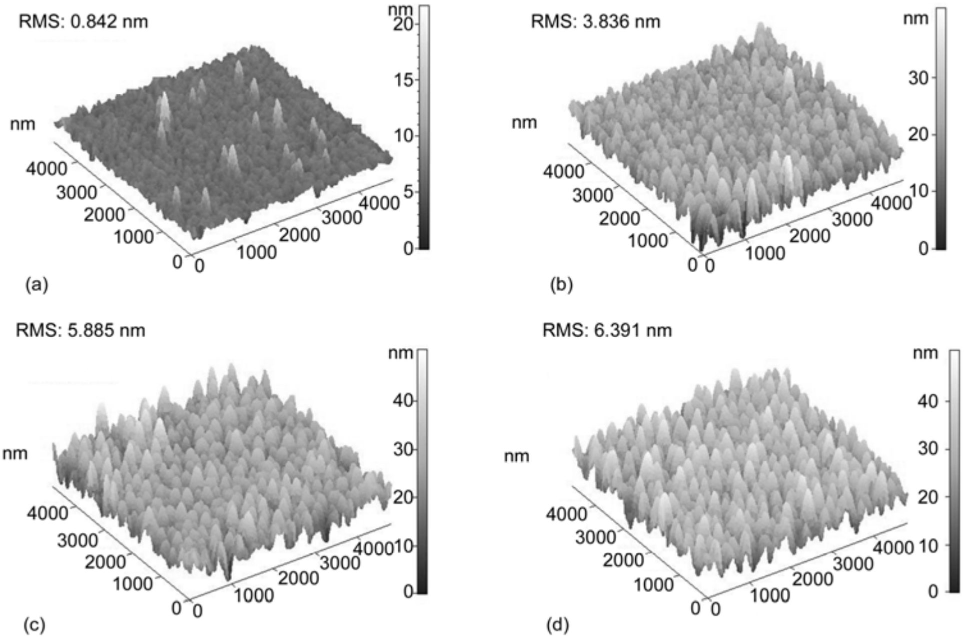

Fig.3 Three-dimensional AFM images of sample: (a) SiGe film grown on Si substrate without implantation; (b) SiGe film grown on Si substrate implanted by 30 keV Ar^+ ions; (c) SiGe film grown on Si substrate implanted by 40 keV Ar^+ ions; (d) SiGe film grown on Si substrate implanted by 60 keV Ar^+ ions.

were obtained, in order to fabricate device-grade SiGe film with fully strain-relaxation and low defect density by using UHVCVD, further investigation on the optimization of ion implantation condition (energy and dose) and epitaxy condition is under way.

4 Conclusions

We have successfully grown the thin relaxed $Si_{0.81}Ge_{0.19}$ films on Si substrate implanted by Ar^+ ion using a self-developed UHVCVD system. These SiGe films were detailedly characterized by RBS/C together with Raman spectra. Almost fully relaxed $Si_{0.81}Ge_{0.19}$ layer with thickness of 95 nm was obtained. It was demonstrated that the top region of ion-implanted Si substrate indeed had compliant effect to facilitate $Si_{0.81}Ge_{0.19}$ film above the defective region to release its strain energy during the SiGe film growth. Compared to other implantation condition (40 keV and 60 keV), the relaxed SiGe film grown on Si substrate implanted by 30 keV at dose of 3×10^{15} cm^{-2} has the least defect density. This work would provide a solid basis for the growth of relaxed SiGe films by UHVCVD in place of MBE and its realistic applications.

References

1 Mii Y J, Xie Y H, Fitzgerald E A *et al*. Appl Phys Lett, 1991, **59**: 1161-1163

2 Monroe D, Xie Y H, Fitzgerald E A *et al*. J Vac Sci Technol, 1993, **B11**: 1731-1736

3 Fitzgerald E A, Xie Y H, Green M L et al. Appl Phys Lett, 1991, **59**: 811-813

4 Linder K K, Zhang F C, Rieh J S *et al*. Appl Phys Lett, 1997, **70**: 3224-3226

5 Holländer B, Mantl S, Liedtke R *et al*. Nucl Instru Methods, 1999, **B148**: 200-205

6 Sawano K, Koh S, Hirose Y *et al*. Appl Sur Sci, 2004, **224**: 99-103

7 CHEN Changchun, HUANG Wentao, LIU Zhihong *et al*. Metals and Materials International, 2004, **10**(3): 281-284

8 Mayer M, SIMNRA User’s Guide, Technical Report IPP 9/113, Max-Planck-Institüt für Plasmaphysik, Garching, Germany, 1997

9 Lockwood D J, Baribeau J M. Phys Rev, 1992, **B 45**: 8565-8570

10 Perry C H, Lu F, Namarar F. Solid State Commun, 1993, **88**: 13-16

11 Christiansen S, Albrecht M, Michler J *et al*. Phys Stat Sol (a), 1996, **156**: 129-131

12 Powell A, Iyer S S, LeGoues F K. Appl Phys Lett, 1994, **64**: 1856-1859