第 21 卷第 10 期　　半 导 体 学 报　　Vol. 21, No. 10
2000 年 10 月　　CHINESE JOURNAL OF SEMICONDUCTORS　　Oct., 2000

Annealing Behavior of $Si_{1-x}Ge_x$/Si Heterostructures*

YU Zhuo(于　卓), LI Dai-zong(李代宗), CHENG Bu-wen(成步文),
LI Cheng(李　成), LEI Zhen-lin(雷震霖)[1], HUANG Chang-jun(黄昌俊),
ZHANG Chun-hui(张春辉), YU Jin-zhong(余金中),
WANG Qi-ming(王启明) and LIANG Jun-wu(梁骏吾)

(*State Key Laboratory on Integrated Optoelectronics, Institute of Semiconductors, The Chinese Academy of Sciences, Beijing* 100083, *China*)
(1 *Shenyang Scientific Instrument Research Center, The Chinese Academy of Sciences, Shenyang* 110003, *China*)

Abstract: The behavior of $Si_{1-x}Ge_x$/Si heterostructures under different annealing conditions has been studied. It is found that while RTA treatment diminishes the point defects, it introduces the misfit dislocations into $Si_{1-x}Ge_x$ layers at same time. Higher annealing temperature will result in the propagation of misfit dislocations and then the total destruction of the crystal quality.

Key words: SiGe; heterojunction; annealing
PACC: 6855; 6170A; 8140
CLC number: TN305.99　**Document code**: A　**Article ID**: 0253-4177(2000)10-0962-04

1 Introduction

There are two reasons for people studying on the materials annealing. Firstly, devices with semiconductor heterostructure may unavoidably experience some high-temperature processes during both fabrication and operation. The thermal stability of the materials is therefore an important parameter for its application[1]; Secondly, annealing is very useful to improve the crystal qualities of the materials as well as their optical and electrical properties[2]. $Si_{1-x}Ge_x$/Si material, one of the recent focusing[3—5], with its metastable structure, it is very worthy to be paid more attention to its annealing behavior that may be af-

* Project Supported by National High Technology Research and Development (863) Program of China Under Grant No. 863-307-15-4(03) and by National Natural Science Foundation of China Under Grant No. 69896260.

YU Zhuo (于　卓) Docter, was born in 1966. His current research interests are in silicon-based material growth and optoelectronics.

LI Dai-zong(李代宗) was born in 1972. He is working for his Ph. D degree and his research interest are in relaxed SiGe growth and SiGe/Si type-II quantum wells.

CHENG Bu-wen(成步文) Associate Professor, was born in 1967. His current research interests are in silicon-based material growth and optoelectronics.

Received 1 March 2000, revised manuscript received 19 April

fected by many factors, such as the growth temperature, the growth rate, the layer thickness, the composition and the density of the defects, etc[6—9]. In this paper, we reported the annealing behavior of $Si_{1-x}Ge_x$/Si heterostructures.

2 Experiments and Analysis

220nm-$Si_{0.89}Ge_{0.11}$/Si(100) samples, grown by home-made UHV/CVD at 650℃, were required to be given the RTA (Rapid Thermal Annealing) treatment for 60s at 700, 800, 900, 1000℃, respectively. Double Crystal X-ray Diffraction (DC-XRD) and Raman spectroscopy ware employed to detect the samples before and after the annealing.

(004) X-ray diffraction results are shown in Fig. 1. The peak position of SiGe layer from as-grown samples lies at 68.528°(2θ) with a FWHM of 102 arcsec. Notice that the Pendellosung stripe representing the high crystal quality and the sharp interface can be distinctly seen here. All SiGe peaks shift nearly to the peak of Si substrate after RTA process (Fig. 2). This kind of shift is accelerated at the RTA temperature higher than 700℃ and the fastest shift is observed at 800℃. With the rise in RTA temperature, the FWHM of SiGe peaks, after a little narrowing at 700℃, begins to broaden gradually and then widen rapidly at 800℃.

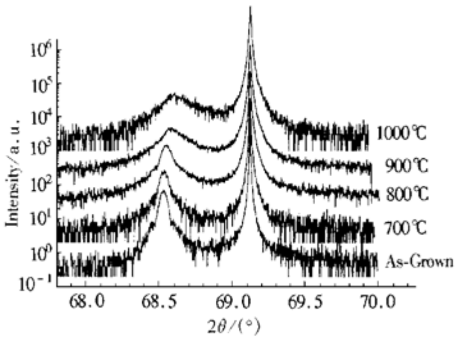

FIG. 1 (004) X-Ray Diffraction of $Si_{0.89}Ge_{0.11}$/Si Sample After Different Annealing Treatment

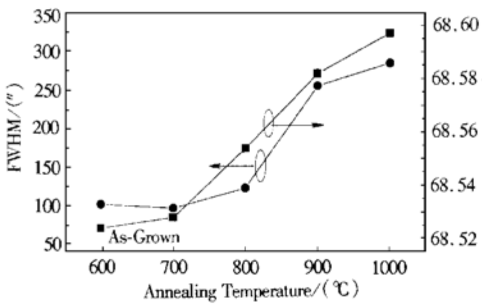

FIG. 2 Change of FWHM and Peak Position of $Si_{0.89}Ge_{0.11}$/Si Samples After RTA

According to the theory of X-ray diffraction, the change of defect density will directly affect the FWHM of diffracted peak[10]. It is reasonable to assume the defect behavior in materials during the RTA process as follows. A large quantity of point defects in the as-grown $Si_{1-x}Ge_x$/Si samples will be diminished because of the position rearrangement of quickly heated atoms; at the same time the misfit dislocations will be dereased by interaction. On the other hand, the relaxation of strain in $Si_{1-x}Ge_x$ layers will induce the propagation of dislocations, as leads to the reduction of $Si_{1-x}Ge_x$ lattice parameter $a_\perp$ and then a shift of SiGe peak in X-ray diffraction spectrum to a smaller angles. These two kinds of mechanisms decide the variation of SiGe peak, while a of a little narrowing FWHM during

RTA at 700℃ is decided, only by the former mechanism, then FWHM broadens behind the position shift at 800℃ because of both the initiation of strain relaxation and the continuation of point defects elimination. At last, FWHM broadens rapidly at higher temperature due to the main operation of the misfit dislocations.

The diffusion at the interface can also be investigated in Fig. 1. Interference stripe that represents high crystal quality can be seen clearly from the as-grown samples. It remains unchanged after RTA at 700℃ and turns vague at 800℃ because the diffusion in the samples has already occurred. RTA at 900℃ results in the disappearance of stripe due to more serious diffusion. It is also found that the diffraction background on the right of SiGe peak has risen to a certain extent after RTA at 800℃. We contribute this phenomenon to the formation of low-Ge region due to the diffusion at the interface. When the RTA temperature goes higher, the diffraction background will rise up gradually because the diffusion has been aggravated step by step.

The relaxation of SiGe layers can be represented by coherent factor f_{coh}

$$f_{coh} = \frac{a_r - a_{/\!/}}{a_r - a_c} \quad (1)$$

where a_c, a_r and $a_{/\!/}$ are the lattice constant of Si substrate, the lattice constant of fully relaxed $Si_{1-x}Ge_x$ and the in-plane lattice constant, respectively. Formula (1) can also be written as

$$f_{coh} = \frac{a_\perp - a_r}{a_r - a_c} = \frac{4d_{(004)} - a_r}{a_r - a_c} \quad (2)$$

where $d_{(004)}$ is the spacing between the neighboring (004) crystal plane. f_{coh} has been reduced to 0.77 after RTA at 800℃ and further to 0.6 after RTA at 1000℃.

According to the experimental results, the conclusion can be drawn that RTA below 800℃ will not affect the crystal quality seriously, while RTA above 800℃ will introduce lots of bred dislocations and seriously interface diffusion, as suggests that $Si_{1-x}Ge_x$/Si structure should not be treated a thermal process at 800℃ in any circumstances.

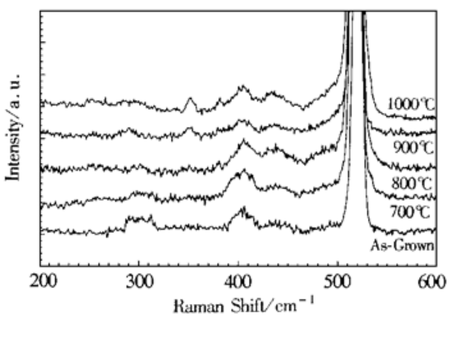

FIG. 3 Raman Spectra of $Si_{0.89}Ge_{0.11}$/Si Samples After Annealing

Raman spectroscopy provides a strong confirmation of the conclusions above. $Si_{0.89}Ge_{0.11}$/Si samples after RTA at different temperatures show obvious changes in Raman detection in Fig. 3. Red shift of Si-Ge local mode indicates the increase of strain relaxation, which is given in table 1 together with the changes of stress.

It should be notice that though serious interface diffusion has occurred after RTA at 1000℃, the stress within $Si_{1-x}Ge_x$ layer still remains. According to Dietrich[11], there exists a minimum of stress, σ_{min}, in the $Si_{1-x}Ge_x$ layer during annealing. Further annealing treatment, for longer time or higher temperature, will become invalid in reducing the stress because the energy of the epitaxial layer has reached its minimum. σ_{min} having been discussed by Houghton[12], is a function of the thickness h, which is higher in thinner layers.

Table 1 Change of Stress and Strain with RTA Temperature in $Si_{0.89}Ge_{0.11}$/Si Samples

T/℃	$\Delta\omega$/cm^{-1}	ϵ/‰	τ/kbar
As-Grown	3.5	7.70	13.51
700	3.2	7.03	12.35
800	2.5	5.71	9.65
900	1.5	3.30	5.79
1000	1.0	2.20	3.86

The intensity of Si-Ge phonon mode, which can indicate the state of crystal structure, varies correspondingly during RTA. RTA above 700℃ will enhance it because of the improvement of crystal quality with the elimination of point defects.

A strange phenomenon of Raman mode appearance at 352cm^{-1} is also observed in Fig. 4, which will not appear until the RTA temperature rises to higher than 900℃. We contribute it to the Si-LA like phonon mode, though no strong evidences have been obtained[13].

3 Conclusion

The behavior of $Si_{1-x}Ge_x$/Si heterostructures under different annealing conditions has been studied in this paper. RTA process can affect the crystal quality by reducing the point defects and propagating the misfit dislocations. The change of strain and stress in $Si_{1-x}Ge_x$ layers are detected by DC-XRD and Raman spectroscopy. It has been found that the crystal quality will be greatly decreased when the annealing temperature is higher than 800℃.

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