Measurements of Anisotropic Biaxial Stresses in x = 0.15 and $0.30 \text{ Si}_{1-x}\text{Ge}_x$ Nanostructures by Oil-Immersion Raman Spectroscopy

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1. Introduction

SiGe is one of the promising candidates for the channel materials of field-effect transistors (FET) because the mobilities of electrons and holes are higher than those of Si [1]. Combination of the SiGe channel and strain technology is considered effective for improving FET performance. Fin-type and nanowire structures have also emerged as techniques to accomplish high efficiency FETs. However, the strain (stress) states in the SiGe nanostructures are complicated and localized at extremely small region. Therefore, accurate stress measurements in the SiGe nanostructures are strongly desired.

High-numerical-aperture (NA) liquid-immersion Raman spectroscopy has so far been proposed to measure anisotropic stress states in strained Si with high spatial resolution [2,3]. However, the stress measurements for SiGe are considered difficult, compared to those in Si, because several necessary parameters are unknown for SiGe [e.g., Ge concentration, Raman shift of stress-free SiGe, and phonon deformation potentials (PDPs)]. Hence, in this study, we investigated the possibility of the complicated stress measurements for the SiGe nanostructures using oil-immersion Raman spectroscopy.

2. Experimental procedure

SiGe were epitaxially grown on Si substrates. The Ge concentrations were approximately 15% and 30%. Subsequently, the SiGe nanostructures were fabricated by electron beam lithography and reactive ion etching. Figure 1(a) and (b) show the images of transmission electron microscopy (TEM) and schematic for the SiGe nanostructures, respectively. A recess structure of approximately 77 nm is observed in Fig. 1(a). The widths (*W*s) of the SiGe nanostructures were 1.0, 0.5, 0.2, 0.1, and 0.05 μ m, while the length (*L*) remains constant of 5.0 μ m, as shown in Fig1. (b). The coordinate system are *x*: [110], *y*: [110], and *z*: [001] shown in Fig. 1(b).

The wavelength of the excitation laser was 532 nm. NA and the refractive index n of the oil were 1.4 and 1.5, respectively, for oil-immersion Raman spectroscopy. The TO phonon modes can be obtained due to z-polarization obtained by high-NA lens. Using the TO and LO phonon modes of Si-Si in SiGe, the anisotropic biaxial stress states in strained SiGe can be measured similar to those of strained Si, because SiGe is also a diamond-type crystal.

3. Results and Discussion

Figure 2(a) and (b) show the out-of-plane and in-plane X-ray diffractions (XRDs) from 15% and 30% SiGe on (001) Si. From the results of in-plane XRD, it was found that the SiGe layers were epitaxially grown on the Si substrates. According to the Vegard's law, Ge concentrations (xs) were calculated to be 0.136 and 0.278, respectively. On the other hand, considering second-order correction from the Vegard's law, xs were 0.151 and 0.303, respectively [4]. Figure 3 shows the depth profiles of atomic ratio in SiGe obtained by Rutherford back scattering (RBS). From RBS, *xs* were 0.153 and 0.297, respectively. As a result, *xs* obtained by XRD with the consideration of the second-order correction and RBS were consistent with each other (Table 1).

Figure 4 shows the Raman spectra from the 15% and 30% SiGe nanostructures with L = 5.0 and $W = 1.0 \mu m$. The subtractions of the Si substrate peaks (denoted by dashed lines) from the raw data were performed for analyzing the spectra accurately. For both of the 15% and 30% SiGe nanostructures, the TO and LO phonon modes were clearly separated. The Raman shifts of TO and LO in the SiGe nanostructures as a function of W are shown in Fig. 5. As a result, the clear dependences of the Raman shifts on x and W were confirmed. It should be noted that the Raman shifts of TO and LO approach with the decrease in W. This result indicates that the stress states change from biaxial-like to uniaxial-like, explained as follows.

The relationship between wavenumber shifts and biaxial stresses in x = 0.297 SiGe is represented by;

$$\begin{pmatrix} \Delta \omega_{TO} \\ \Delta \omega_{LO} \end{pmatrix} = \begin{pmatrix} -3.22 & -0.66 \\ -2.60 & -2.60 \end{pmatrix} \cdot \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \end{pmatrix}.$$
(1)

In Eq. (1), PDPs of Si-Si in SiGe are considered to be equal to those of Si-Si in Si, i.e., $p/\omega_0^2 = -1.85$, $q/\omega_0^2 = -2.31$, and $r/\omega_0^2 = -0.71$, respectively [5]. Using Eq. (1), the wavenumber shifts of $\Delta \omega_{\Gamma O}$ and $\Delta \omega_{LO}$ from stress-free SiGe as a function of σ_{yy} (σ_{xx} remais -1.9 GPa) are shown in Fig. 6. The wavenumber shifts approach one another with the decrease in the compressive stress.

As a result, the biaxial stresses σ_{xx} and σ_{yy} in the 15% and 30% SiGe nanostructures were calculated using $\Delta \omega_{\Gamma O}$ and $\Delta \omega_{LO}$. Figure 7(a) shows σ_{xx} and σ_{yy} in 30% SiGe. Circles and triangles denote σ_{xx} and σ_{yy} , respectively. The red symbols with the line and the green symbols with the line denote the data using the Raman shifts of stress-free SiGe, ω_{0SiGe} s, proposed by Tsang *et al.* [6] and Alonso *et al.* [7], respectively. The former value seems to be accurate because the calculated stresses are close to the value of completely strained SiGe, -1.94 GPa. On the other hand, for 15% SiGe, the stresses calculated with ω_{0SiGe} proposed by Alonso *et al.* are close to the value of completely strained SiGe, -0.99 GPa, as shown in Fig. 7(b). Therefore, it is needed to use different ω_{0SiGe} s for different *xs*. Furthermore, there is a large underestimation in the case of using the Vegard's law, as shown in Figs. 7(a) and (b). Using appropriate vales of ω_{0SiGe} s and *xs*, clear dependences of σ_{xx} and σ_{yy} on *W* were obtained for the 15% and 30% SiGe nanostructures.

4. Conclusions

The measurements of the anisotropic biaxial stress states in the 15% and 30% SiGe nanostructures were

performed by oil-immersion Raman spectroscopy. We demonstrated the clear separation of TO and LO phonon modes in strained SiGe and the obvious biaxial stress dependence on W for the first time. The difference between stress states in 15% and 30% SiGe were shown.

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Fig. 1 (a) TEM image of SiGe nanostructure and (b) Schematic.



Fig. 3 Depth profiles of Atomic ratio in SiGe obtained by RBS.





Fig. 5 Raman shift dependences on SiGe nanostructure width.

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Fig. 2 (a) Out-of-plane and (b) in-plane XRD diffractions from (001) SiGe with x = approximately 0.15 and 0.3.





Fig. 4 Raman spectra from 15% and 30% SiGe nanostructures with $L = 5.0 \ \mu\text{m}$ and $W = 1.0 \ \mu\text{m}$.

Fig. 6 Calculation of wavenumber shift dependence on σ_{yy} (σ_{xx} remains constant of -1.9 GPa).



Fig. 7 Dependences of biaxial stresses σ_{xx} and σ_{yy} on nanostructure width for (a) 30% SiGe and (b) 15% SiGe, respectively.