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Influence of Carbon in *in-situ* Carbon-Doped SiGe (SiGe:C) Films on Si (001) Substrates on Epitaxial Growth Characteristics

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1. Introduction

Recently, growth of carbon-doped SiGe (SiGe:C) crystal on Si has received considerable attention, because it facilitates the control of the diffusion of boron [1-3]. It can be used around the source-drain region of pMOSFET having eSiGe structure to minimize short-channel effects [4]. However, there are some issues and difficulties needed to be addressed in using carbon. One is that doping of carbon results in an increase of surface roughness [5]. The other issue is that C atoms are incorporated not only in the substitutional but also in the interstitial sites because of its relatively low solubility in SiGe [6, 7]. With high Ge concentration, the question of which sites the carbon atoms prefer is currently not fully understood. In this work, we performed a systematic experiment of growth of SiGe:C and carried out measurements to determine the surface roughness and preferred sites of carbon atoms as functions of C source flow, Ge concentration, growth temperatures and growth rate.

2. Experimental

SiGe:C films were grown on p-type Si (001) substrates of 1-2 Ωcm by Reduced Pressure Chemical Vapor Deposition (RP-CVD). The precursor of Si, Ge, and C were SiH_4, GeH_4, and SiH_3CH_3, respectively. The carrier gas employed was H_2, and the total pressure during deposition was 5 Torr. The growth temperature range was from 575°C to 625°C. Carbon composition in the SiGe:C crystals was evaluated by secondary ion mass spectrometry (SIMS). Substitutional C concentration was determined by high-resolution X-ray diffractometry (HR-XRD) assuming that all the Ge atoms were at the substitutional sites. The surface morphology was investigated by atomic force microscope (AFM) and transmission electron microscopy (TEM).

3. Results and Discussion

Surface roughness of the epitaxially grown SiGe:C films increased with the increase of the C gas source flow as shown in Fig. 1. The sample grown with C gas flow ratio of $R_{SiH3CH3}$=0.0055, where $R_{SiH3CH3}$ = SiH_3CH_3 / (SiH_4 + GeH_4 + SiH_3CH_3), showed good crystalline quality and flat surface. By increasing $R_{SiH3CH3}$, surface was roughened with some defects in the SiGe:C layer. When $R_{SiH3CH3}$=0.0180, growth was suppressed at some portions as shown in Fig. 1 (c). TEM observation of the initial stages of the growth with high C gas flow, small separated islands were first grown as shown in Fig. 2 (a). As these islands become bigger with longer growth time, they eventually meet one another and merge into a continuous film as shown in Fig. 2 (b) and (c).

Influence of C on the increase of surface roughness well corresponded to the site of C atoms. Increase of the interstitial C atoms was observed with the roughening of the surface of SiGe:C film. When $R_{SiH3CH3}$ is low, the SiGe:C (004) diffraction peak was shifted towards higher Bragg angle with increasing $R_{SiH3CH3}$ as shown in Fig. 4, which indicates the decrease of lattice constant. However, for the sample grown with $R_{SiH3CH3}$ = 0.0091, the SiGe:C (004) diffraction peak was shifted towards the opposite direction. The surface of this sample was rough as shown in Fig. 1 (b) with Ra value of 0.59 nm as measured by AFM shown in Fig. 3 (b).

Surface roughness and the site of C atoms depend on the growth conditions, such as growth rate (Figs. 5 and 6) and temperature (Figs. 7 and 8). High growth rate and/or low growth temperature is preferable for smooth surface and high substitutional C concentration. Such deposition condition is suited for the formation of metastable state of high substitutional C concentration, because excess migration of the C atoms can be suppressed.

These results suggest that the surface roughness originates from the localization of adsorbed C atoms. Lattice constant around C rich region would be small and adsorption of bigger Ge atoms is suppressed as shown in Fig. 9. Thus, the roughness coincides with the decrease of substitutional C atoms as shown in Figs. from 1 to 4.

It might be easily anticipated that Ge atoms could increase the substitutional C concentration, because Ge and C have bigger and smaller covalent radius than Si, respectively. However, the above results suggest another mechanism of interaction between C and Ge. Experimental results with various Ge concentrations clearly showed two opposite behaviors due to Ge and C as shown in Figs. 10 and 11.

Substitutional C concentration indicates the two opposite interaction between Ge and C (Fig. 10). Higher substitutional C concentration can be obtained by increasing Ge concentration at constant $R_{SiH3CH3}$ of less than 0.005. This is due to the compensation of stress by Ge and C. However, the maximum substitutional C concentration is decreased, as is shown when $R_{SiH3CH3}$ =0.01. This is the results of localized C atoms discussed in the previous section. Thus, flat surface was obtained only when the Ge concentration was adequate (Fig.11).

4. Conclusions

SiGe:C thin films were epitaxially grown on Si (001) substrates by RP-CVD method. Detailed investigation of the films based on the systematic experiments revealed that the site of C, substitutional C or interstitial C, has strong impact on the epitaxial growth characteristics. Surface of the SiGe:C film is rough when most of the C atoms occupy interstitial sites. Interstitial C atoms inhibit flat epitaxial growth, because the sticking probability is low on the region where interstitial C atoms are localized. Site of C atoms is strongly affected by Ge concentration. Small amount of Ge atoms increase the substitutional C concentration due to the stress compensation, while high concentration Ge induce the interstitial localized C atoms.

In order to achieve high crystalline quality for SiGe:C films with high Ge composition, there is a need to control on what sites C atoms would occupy. Deposition condition should be carefully fixed for high substitutional C concentration.

References

[1] S. Nishikawa et al., Appl. Phys. Lett. **60** (18), 2270 (1992).
[2] L. D. Lanzerotti et al, IEDM1996, 249 (1996).
[3] H. Rucker et al., Appl. Phys. Lett. **73** (12), 1682 (1998).
[4] S. Kuppurao et al., ECS Trans. **16** (10), 415 (2008).
[5] V. LeThanh et al., Mater. Sci. Eng. B **89**, 246 (2002).
[6] Y. Kanzawa et al., Appl. Phys. Lett. **77** (24), 3962 (2000).
[7] V. Loup et al., J. Vac. Sci. Technol. B **20**(3), 1048 (2002).

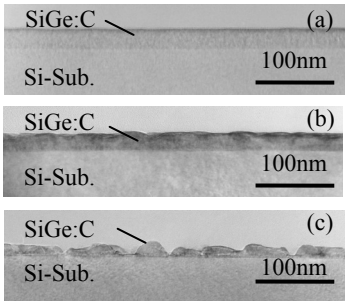

Fig. 1 Cross-sectional TEM of SiGe:C / Si samples of various C concentration. Ge concentration is 23.0%. The growth temperature is 600°C. $R_{SiH3CH3}$ was (a) 0.0055, (b) 0.0091, and (c) 0.0180.

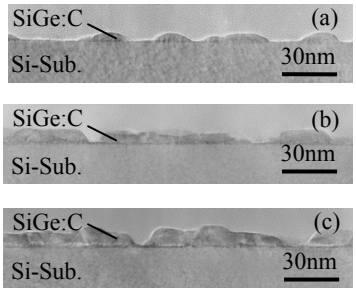

Fig. 2 Cross-sectional TEM of SiGe:C / Si of various growth time. $R_{SiH3CH3}$= 0.0180 and Ge concentration was 23.0%. The growth temperature was 600°C. The growth time was (a) 20s, (b) 51s and (c) 57s.

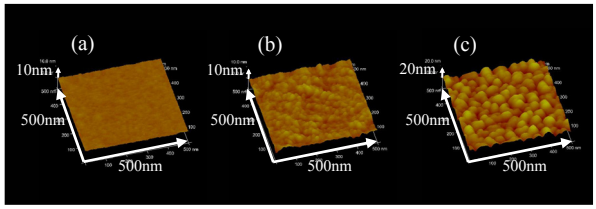

Fig. 3 AFM images of the SiGe:C layers for Ge concentration of 23.0 %. The growth temperature is constant at 600°C. $R_{SiH3CH3}$ was (a) 0.0027 (b) 0.0091 and (c) 0.0180. Height scale is (a) 10 nm (b) 10 nm and (c) 20 nm. Ra was (a) 0.23 nm, (b) 0.59 nm and (c) 2.15 nm.

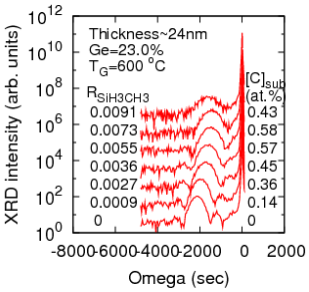

Fig. 4 HR-XRD (004) rocking curve scans for samples grown using different $R_{SiH3CH3}$ at 600°C with Ge concentration of 23.0%. $R_{SiH3CH3}$ was varied between 0 and 0.0091.

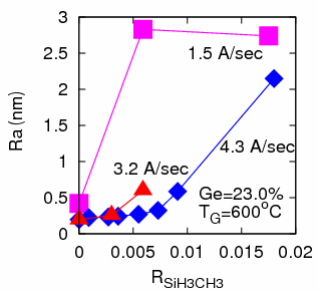

Fig. 5 Ra of the SiGe:C layers as a function of $R_{SiH3CH3}$ for various growth rates. Ra becomes higher as growth rate is higher. Growth rate was varied by changing the flow rate of precursors.

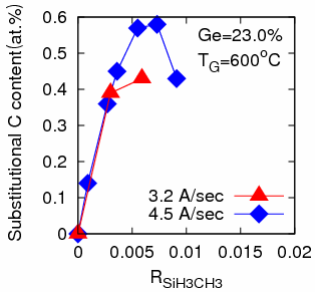

Fig. 6 Substitutional C concentration of the SiGe:C layers as a function of $R_{SiH3CH3}$ for growth rates. Maximum of substitutional C concentration becomes higher as growth rate is higher.

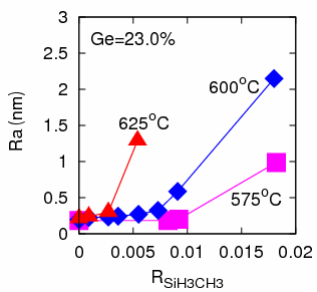

Fig. 7 Ra of the SiGe:C layers as a function of $R_{SiH3CH3}$, for various growth temperatures. Surface becomes rough as growth temperature is higher.

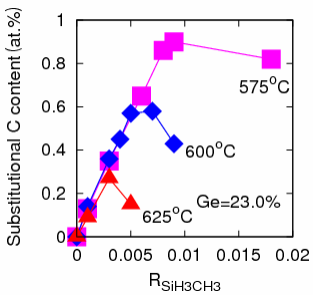

Fig. 8 Substitutional C concentration as a function of $R_{SiH3CH3}$, for various growth temperatures. Maximum of substitutional C concentration becomes higher as growth temperature is lower.

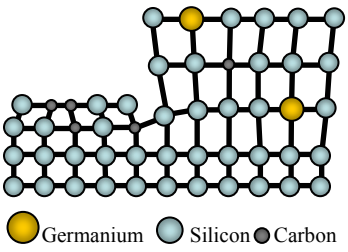

Fig. 9 Schematic illustration which explains the mechanism of defect formation. Localized C atoms are formed. Lattice constant around C rich region would be small and adsorption of bigger Ge atoms are suppressed.

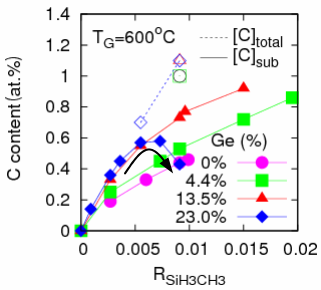

Fig. 10 Total and substitutional C percentage incorporated in the SiGe:C layers as a function of $R_{SiH3CH3}$, for various Ge concentrations.

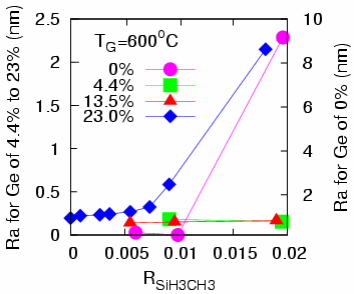

Fig. 11 Ra of the SiGe:C layers as a function of $R_{SiH3CH3}$, for various Ge concentrations.