

Epitaxial Growth of Strained $\text{Si}_{1-y}\text{C}_y$ Alloy on Si(100) by Ultrahigh Vacuum Chemical Vapor Deposition Using Si_2H_6 and C_2H_2

Masayuki Hiroi, Keiko Miyanaga and Toru Tatsumi

Microelectronics Research Labs., NEC Corporation
34 Miyukigaoka, Tsukuba, Ibaraki 305, Japan

Epitaxial growth of strained $\text{Si}_{1-y}\text{C}_y$ alloys on Si(100) surface was successfully achieved by cold-wall type ultrahigh vacuum chemical vapor deposition using disilane and acetylene. X-ray diffraction and transmission electron microscopy confirmed the growth of pseudomorphic tetragonally strained alloy layers with no detectable silicon carbide precipitation. The carbon concentration was proportional to the acetylene flow rate at a fixed disilane flow rate.

1. Introduction

$\text{Si}_{1-y}\text{C}_y$ alloy is a new material which has been made only in recent years.¹⁻⁵⁾ Silicon-carbon system has known to be a mixture of silicon, carbon, and silicon carbides. The growth of the $\text{Si}_{1-y}\text{C}_y$ alloy was firstly reported by Posthill *et al.* using plasma enhanced chemical vapor deposition.¹⁾ However, the grown layer was much dislocated, and most part of the carbon atoms did not situate the substitutional sites. Recently, undislocated and tetragonally strained $\text{Si}_{1-y}\text{C}_y$ alloys on silicon has been studied by S.S. Iyer and coworkers using conventional solid source molecular beam epitaxy (MBE).²⁻⁵⁾ They achieved the synthesis of $\text{Si}_{1-y}\text{C}_y/\text{Si}$ superlattices (SLSs)²⁾ below 550°C and studied its thermal stability.³⁾ They also reported strain compensation in $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ system.⁴⁾ The conventional electron beam evaporator type Si-MBE is a suitable method for the low temperature growth, but high silicon flux was required to grow the good morphology. So, it is not easy to grow the good quality $\text{Si}_{1-y}\text{C}_y$ by the solid source MBE because the crystal became defective or amorphous with the higher silicon flux at the low temperature.²⁾

We used a cold-wall type ultrahigh vacuum chemical vapor deposition (UHV-CVD) to grow the $\text{Si}_{1-y}\text{C}_y$ alloys using disilane (Si_2H_6) and acetylene (C_2H_2). The UHV-CVD system has a capability of selective epitaxial growth of silicon⁶⁾ and $\text{Si}_{1-x}\text{Ge}_x$ ⁷⁾ to fabricate the self-align devices.⁸⁾ In contrast to the solid source Si-MBE, the crystal does not become defective at low temperature and high Si_2H_6 because the growth does not proceed at lower temperature in the UHV-CVD. The growth of tetragonally strained $\text{Si}_{1-y}\text{C}_y$ alloy was successfully achieved, and strain compensated $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ could be grown by germane (GeH_4) addition.

2. Experimental

The details of the UHV-CVD system are described elsewhere.⁷⁾ The growth chamber made of stainless steel was pumped by turbo molecular pump, and its base pressure was about 1×10^{-9} Torr. Pumping speed for Si_2H_6 was about 200 l/s. Pure Si_2H_6 , pure C_2H_2 and pure GeH_4 were used as the source gases. These gases were introduced directly into the growth chamber from each nozzles without dilution after passing through the mass flow controllers. The grown samples were examined by transmission electron microscopy (TEM), secondary ion mass spectroscopy (SIMS) and X-ray diffraction (XRD).

3. Results and discussions

The undislocated $\text{Si}_{1-y}\text{C}_y$ alloys could be grown at relatively low growth temperature and low $\text{C}_2\text{H}_2/\text{Si}_2\text{H}_6$ flow ratio conditions. Because three-dimensional nucleation and island formation occurred by increasing the temperature and/or the $\text{C}_2\text{H}_2/\text{Si}_2\text{H}_6$ flow ratio. Figure 1 shows an image of transmission electron microscopy (TEM) for a Si/ $\text{Si}_{1-y}\text{C}_y$ SLS grown at 620°C . Each layers of the sample were grown with a fixed Si_2H_6 flow rate, 10 SCCM for 3 min. The $\text{Si}_{1-y}\text{C}_y$ layers were grown with increasing C_2H_2 flow rate forward to the surface. The growth rate was decreased by the C_2H_2 addition. The island formation appeared when the $\text{C}_2\text{H}_2/\text{Si}_2\text{H}_6$ flow ratio was excess 2% in this case. The islanding also depended on the growth temperature and total flow rate. If the temperature increased, the islanding occurred at lower $\text{C}_2\text{H}_2/\text{Si}_2\text{H}_6$ flow ratio.

Increase of the total flow rate suppressed the island formation at a fixed $\text{C}_2\text{H}_2/\text{Si}_2\text{H}_6$ flow ratio. It is noted that the growth temperature in this study was

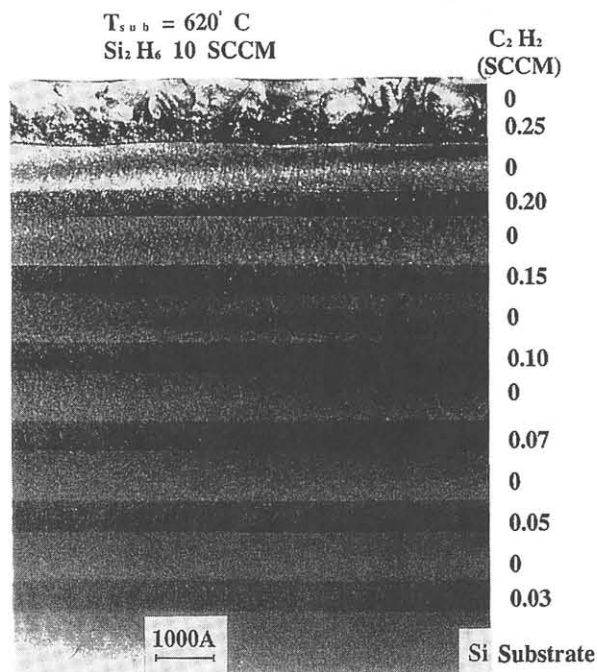


Fig. 1. Cross sectional TEM image of a $\text{Si}_{1-y}\text{C}_y/\text{Si}$ superlattices grown at 620°C . Si_2H_6 flow rate was fixed at 10 SCCM.

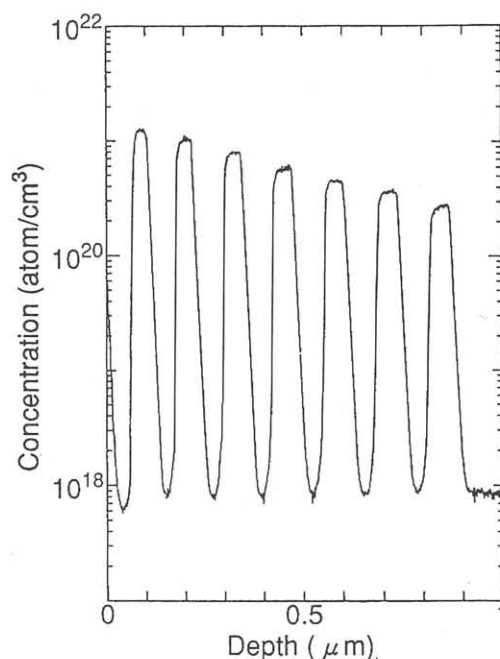


Fig. 2. Carbon concentration profile of the sample shown in Fig. 1, obtained by SIMS.

higher than in the solid source MBE. Iyer *et al.* reported that the alloy growth could be achieved only below 550°C by the solid source MBE.²⁾ In contrast, the flat surface of $\text{Si}_{0.99}\text{C}_{0.01}$ could be obtained above 700°C in the UHV-CVD under high flow rate conditions. Since the growing surface is considered to be covered with hydrogen under the high Si_2H_6 flow rate conditions,⁹⁻¹¹⁾ we think that the island formation suppression is due to the surfactant effect of hydrogen; repression of surface migration, in addition to the effect of the high growth rate, i.e., high incorporation rate.

The carbon concentration in the epitaxial layer could be controlled with the C_2H_2 flow rate at fixed Si_2H_6 flow rate. Figure 2 shows a SIMS profile for the carbon concentration of the sample shown in figure 1. The profile was very sharp at the both interfaces of $\text{Si}/\text{Si}_{1-y}\text{C}_y$ and $\text{Si}_{1-y}\text{C}_y/\text{Si}$. The carbon concentrations in the each $\text{Si}_{1-y}\text{C}_y$ layer were proportional to the C_2H_2 flow rates ($\approx \text{C}_2\text{H}_2/\text{Si}_2\text{H}_6$ flow ratio $\approx \text{C}_2\text{H}_2$ flow rate/total flow rate). The carbon content y was nearly equal to the C_2H_2 content in the total flow, for example, $\text{Si}_{0.99}\text{C}_{0.01}$ was obtained with about 1% C_2H_2 and 99% Si_2H_6 . It is noted that the carbon concentrations in the epitaxial Si layers were very low, mostly equal to the Si substrate, as shown in Fig. 2.

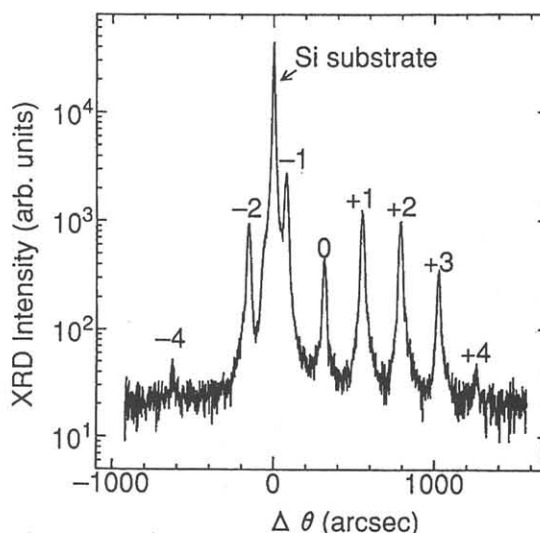


Fig. 3. Double-crystal diffractometer rocking curve of a $\text{Si}_{1-y}\text{C}_y$, Cu $K\alpha$ radiation, 400 reflection.

These results shows the good controllability of the UHV-CVD for the fabrication of the fine structures.

The lattice constant decreasing by the C_2H_2 addition was confirmed by XRD. Figure 3 shows a typical XRD spectrum of 400 reflection peaks of $\text{Si}_{1-y}\text{C}_y/\text{Si}$ SLS on Si(100) using Cu $K\alpha$ line. The SLS has 11 periods of 30 nm $\text{Si}_{0.992}\text{C}_{0.008}/$ 600 nm Si. The

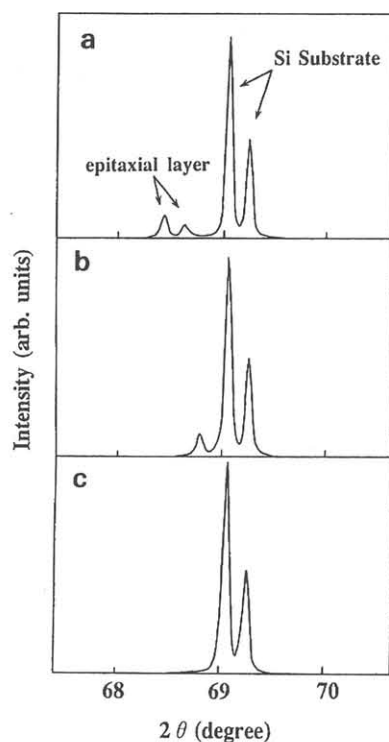


Fig. 4. 2θ - θ scanned XRD spectrum of $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y/\text{Si}$ grown at 500°C , Si_2H_6 10 SCCM, GeH_4 5 SCCM, C_2H_2 a) without addition, b) 0.1 SCCM, c) 0.2 SCCM.

measured lattice constants and tetragonal distortions of the samples, which were grown at low temperature and high flow rate, were good accordance with the Vegard's Law using the elastic moduli of silicon, $c_{11}=16.577$ and $c_{12}=6.393$.¹²⁾ Additionally, these samples gave no reflections which indicated the presence of other phase, such as 111 reflections of silicon and silicon carbide, which were observed from the samples grown at high temperature with low flow rates. These results indicate the incorporation of the carbon atoms into the substitutional sites.

The growth of $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ alloy was also achieved by GeH_4 addition. Figure 4 shows XRD spectrum of the $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y/\text{Si}(100)$ samples. With the flow rates of Si_2H_6 10 SCCM and GeH_4 5 SCCM, $\text{Si}_{0.9}\text{Ge}_{0.1}$ was obtained. As the C_2H_2 flow rate increased, the 400 reflection peaks of the epitaxial layer shifted to higher angles. It indicates the strain compensation of the ternally alloy system. As shown in Fig. 4 (c), the $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ whose lattice constant was close to the Si substrate could be obtained. We note that the $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ growth required lower growth temperature than that for the $\text{Si}_{1-y}\text{C}_y$ growth because of the island formation enhancement by the

GeH_4 addition. Thus, the island formation could not be suppressed only by the lattice compensation in the epitaxial layer and by the high incorporation rate, because the GeH_4 addition also enhanced the growth rate at the low temperature. We think that the repression of the surface migration is need to keep the good morphology during the growth.

4. Conclusion

In summary, we achieved the epitaxial growth of $\text{Si}_{1-y}\text{C}_y$ alloy on $\text{Si}(100)$ by UHV-CVD using pure Si_2H_6 and pure C_2H_2 . The tetragonally strained $\text{Si}_{1-y}\text{C}_y$ alloy layer could be grown at relatively low temperature and low $\text{C}_2\text{H}_2/\text{Si}_2\text{H}_6$ flow ratio, and high total flow rate. No evidence for the silicon carbide precipitation was observed by TEM and XRD. The carbon concentration could be controlled by $\text{C}_2\text{H}_2/\text{Si}_2\text{H}_6$ flow ratio.

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