The Loss Kinetics of Substitutional Carbon in Si$_{1-x}$C$_x$ Regrown by Solid Phase Epitaxy

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Epitaxial layers of Si$_{1-x}$C$_x$ ($x = 0.016$) were synthesized using ion implantation and solid phase epitaxy (SPE), and the loss kinetics of substitutional carbon was investigated. As annealing temperature and time increase, more carbon atoms were found to diffuse from substitutional to interstitial sites. The activation energy for the loss of substitutional carbon into interstitial sites was obtained over the temperature range, 700–1040°C, by furnace annealing. In addition, SPE layers regrown by rapid thermal annealing (RTA) were shown to have better crystalline quality than those regrown by furnace annealing.

KEYWORDS: Si$_{1-x}$C$_x$, SPE, substitutional carbon, activation energy, loss kinetics

1. Introduction

Group IV heteroepitaxial materials grown on Si substrates have been investigated for use as bandgap engineering materials. In particular, Si$_{1-x}$Ge$_x$ epitaxial layers have been investigated the most because of their significant potential in the fabrication of high-speed devices and for optoelectronic device applications. However, Si$_{1-x}$Ge$_x$ exhibits some severe limitations. The first is a critical thickness against misfit-dislocation formation due to the lattice mismatch between the epitaxial layer and Si. The second is that the main band-offset appears at the valence band. Hence, Si$_{1-x}$Ge$_x$ is better suited as a hole channel than as an electron channel. Thirdly, Si$_{1-x}$Ge$_x$ has some difficulty in controlling dopant diffusion, similar to Si devices.

Recently, it was shown that the incorporation of carbon into the substitutional sites could overcome some of the limitations. Ion implantation and solid phase epitaxy (SPE) have been used successfully to incorporate carbon into the substitutional sites. However, due to the low solubility of carbon in Si, β-SiC can be formed during epitaxial regrowth. Moreover, because carbon retards the SPE rates, a higher regrowth temperature is necessary. Despite these conflicting problems, Strane et al. have shown that carbon can be successfully incorporated into the substitutional sites using ion implantation followed by SPE.

However, the activation energy for the loss of substitutional carbon into the interstitial sites is not known in Si$_{1-x}$C$_x$ epitaxial layers regrown by SPE. In this article, the loss kinetics of substitutional carbon in Si$_{0.984}$C$_{0.016}$ epitaxial layers regrown by SPE is discussed. The effects of annealing temperature and time are also studied by comparing conventional furnace annealing with rapid thermal annealing (RTA).

2. Experimental Details

The Si$_{0.984}$C$_{0.016}$ layers were epitaxially grown on ~6 Ω-cm Si (100) substrates. Double-side polished wafers were used to reduce both the background signal and noise during the Fourier transform infrared spectroscopy (FTIR) measurements, and ion implantation was performed at room temperature. Before carbon implantation, the Si (100) surface was preamorphized by Si$^+$ with 50 and 100 keV at 2 × 10$^{15}$ and 8 × 10$^{15}$ Si/cm$^2$, respectively. The carbon implantation energies and doses, designed to obtain a uniform carbon profile, were 15 and 29 keV at 2 × 10$^{15}$ and 7.2 × 10$^{15}$ C/cm$^2$, respectively, for relatively flat 1.6 at. % carbon in a region of approximately 80 nm.

Annealing was performed in a fused silica tube furnace under 1 × 10$^{-6}$ Torr or RTA under a constant N$_2$ flow. The Si$^+$ and C$^+$ implanted samples were regrown epitaxially after a sequential two-step annealing process, the first step at 500°C for 30 min followed by 700°C for 30 min. After epitaxial regrowth, the samples were annealed between 700°C and 900°C by a conventional furnace, and RTA was performed between 910°C and 1040°C.

High-resolution X-ray diffraction (HR-XRD) measurements with dynamic simulations were used to characterize the lattice strain and substitutional-carbon concentration. FTIR measurements were performed in a vacuum (<0.1 Torr) to minimize absorption by the ambient gases, and all measurements were performed at room temperature. To accurately obtain the substitutional carbon content from FTIR at ~607 cm$^{-1}$, the signal was subtracted from a reference sample without ion implantation. To minimize the background error due to potential surface oxidation, each reference sample was annealed under the same conditions.

3. Results and Discussion

Figure 1(a) shows the x-ray rocking curves for samples annealed at 850°C in a vacuum furnace. The displacement of the smaller satellite peaks due to the epilayer is proportional to the lattice strain between the Si substrate and epilayer. As the annealing time was increased at 850°C, the difference in diffraction angle between Si (004) and satellite peak got reduced. This is due to the diffusion of substitutional carbon to interstitial sites. For the Si$_{0.984}$C$_{0.016}$ layer annealed at 910°C by RTA, the lattice strain is similar to the layer regrown in the vacuum furnace, as shown in Fig. 1(b). These results indicate that in the early stages, most of the carbon atoms incorporated in Si remain in the substitutional sites. Another result observed in Fig. 1(b) is that the interference fringes in the diffraction peaks for the layers regrown by RTA are more
remarkable compared to Fig. 1(a). Because the interference fringe reflects the quality of the epilayer, it is inferred that the layers regrown by RTA have greater crystalline quality than layers regrown by vacuum-furnace annealing. To quantify the lattice strain and substitutional-carbon concentration, several different concentration profiles were simulated by dynamic diffraction, and the best fitting simulation results were chosen to extract the nonuniform substitutional-carbon distribution (as shown in Fig. 2). For the relationship between lattice strain and substitutional-carbon concentration, Vegard’s law between Si and diamond was used.

The relationship between the substitutional-carbon concentration and annealing time is shown in Figs. 3(a) and 3(b), and is fitted by the following exponential decay equation:

\[ \alpha \propto \exp \left( -\frac{t}{\tau} \right), \quad (1) \]

where \( \tau \) is the decay constant.\(^{17}\) Figure 4 shows the temperature dependence for the decay constants \( 1/\tau \) representing the loss of substitutional carbon over the temperature range, 700–900°C in vacuum-furnace annealing, and 910–1040°C in RTA. An Arrhenius plot of the experimental data yielded activation energies of 3.00±0.11 eV and 3.05±0.10 eV, respectively, for furnace annealing and RTA. This represents the loss kinetics of substitutional carbon, as shown in Fig. 4. These values are close to the activation energy for the diffusion of substitutional carbon in Si: 3.2 eV over the temperature range 1050°C to 1400°C.\(^{18,19}\) However, Kulik et al.\(^{17}\) reported that the activation energy for the transformation of substitutional carbon to the interstitial sites in the Si\(_{0.992}\)C\(_{0.008}\) alloy grown by molecular-beam epitaxy (MBE) was 4.45±0.15 eV. This discrepancy may be due to differences in film quality between SPE and MBE. Other results observed in Fig. 4 show that the loss kinetics for substitutional carbon to the interstitial sites during RTA is faster, by approximately a factor of 3, than vacuum-furnace annealing, although the activation energies are similar. While enhanced phase transformations by RTA compared to furnace annealing have been observed in many different systems,\(^{20,21}\) such as dopant diffusion, a sili-
Fig. 3. The relationship between substitutional carbon concentration and annealing time. (a) vacuum furnace at 700, 800, 850, and 900°C, and (b) RTA at 910, 960, 1000, and 1040°C.

Fig. 4. Arrhenius plot for the decay constant $1/\tau$ from x-ray diffraction for vacuum-furnace annealing (700–900°C) and RTA (910–1040°C).

Fig. 5. FTIR absorption spectra for Si$_{0.984}$C$_{0.016}$ alloy layer (a) after 900°C annealing in a vacuum furnace, and (b) after 1040°C annealing by RTA.

The activation energies for the loss of substitutional carbon from FTIR data are 2.81 ± 0.17 eV and 2.97 ± 0.12 eV, respectively, by furnace annealing and RTA, as shown in Fig. 6. These activation energies obtained by FTIR measurements for 240 min by furnace annealing, the absorbance at 607 cm$^{-1}$ is low while that of 810 cm$^{-1}$ peak increases remarkably [Fig. 5(a)]. It is expected that carbon atoms diffuse from substitutional sites to interstitial sites, and this will lead to the formation of nano-sized SiC precipitates. In the case of RTA at 1040°C, the small absorbance of SiC precipitates starts to appear after 100 s annealing [Fig. 5(b)].
are in good agreement with the HR-XRD results (Fig. 4). Therefore, we are confident that the activation energy for the loss of substitutional carbon to interstitial sites is \( \sim 3 \) eV over a temperature range of 700–1040°C.

4. Conclusions

The loss kinetics of substitutional carbon in the \( \text{Si}_{0.984}\text{C}_{0.016} \) system regrown by SPE was investigated using both X-ray diffraction and infrared absorption. The activation energy for the diffusion of substitutional carbon to interstitial sites is \( \sim 3 \) eV over a temperature range of 700–1040°C. Furthermore, RTA appears better suited for the SPE regrowth of \( \text{Si}_{1-x}\text{C}_x \) than vacuum furnace annealing, leading to greater structural perfection for the regrowth of implanted layers.

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