Optical characterization of as-prepared and rapid thermal oxidized partially strain compensated $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ films

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Abstract

The optical properties of as-prepared and rapid thermal oxidized (RTO) heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ alloys grown on Si substrate have been characterized using spectroscopic ellipsometry. The critical points $E_1$, $E_0$, $E_2$ band gaps were determined by line shape fitting in the second derivative spectra of the pseudo-dielectric functions. For as-prepared films, the $E_1$ gap increases with C concentration and a linear dependence on C content was observed. However, the $E_2$ gap decreases as the C concentration increases. For the RTO samples, the amplitude of $E_2$ transition reduces rapidly and the $E_1$ transition shifts to a lower energy. The reduction in the amplitude of $E_2$ transitions is due to the presence of oxide layer. A high Ge content layer and the low C content in the RTO films account for the $E_1$ shift to lower energy and the increase of the refractive indices. © 2002 Elsevier Science Ltd. All rights reserved.

Keywords: $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$; Spectroscopy ellipsometry; Pseudo-dielectric functions; Refractive indices

1. Introduction

The addition of C into substitutional sites in $\text{Si}_{1-x-y}\text{Ge}_x$ films allows one to tailor the strain in the film [1] and changes its band structure [2]. This may overcome the critical thickness limitation imposed on $\text{Si}_{1-x-y}\text{Ge}_x$ films grown epitaxially on Si [1]. We notice that there are only a few optical studies on strained $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ films that examine the band structure of the material [3–5]. There is also, to the best of our knowledge, no report on the dielectric properties of rapid thermal oxides (RTO) grown on $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ substrate. As SiGe-based materials have been proposed in applications in very high frequency electronics [6,7], it is important to investigate the influence of C on the dielectric properties of the as-prepared and rapid thermal oxidized $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ films.

2. Experiment

The $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ samples were grown on n-type (100) Si substrate in a rapid thermal chemical vapour deposition (RTCVD) system. The growth temperature and pressure were set at 600 °C and 1.5 Torr, respectively. The flow rates of the silane, germane and hydrogen were fixed at 80, 2, 1000 sccm, respectively. The flow rate of methylsilane was varied from 0 to 1.75 sccm to prepare alloys with different C contents. The exact amount of Ge (11.3 at%) and C (0.59, 1.32 and 1.84 at%) were determined by SIMS analysis. Rapid thermal oxidation was carried out in a dry oxygen ambient using an AST SHS 10 rapid thermal processor. The oxidation was performed at 1000 °C for 270 s with a gas flow of 2 slm for all the samples. Further details of the RTO process can be found in our previous paper [8].

The spectroscopic ellipsometry (SE) experiments were performed using a spectroscopic phase modulated ellipsometer (UVSEL) with an energy range of 1.5–4.5 eV. The rotating polarizer and tracking analyser were set at 70°. The energy increment and integration time for the SE experiments were set at...
0.01 eV and 2 s, respectively. The critical point energy ($E_{cp}$) and broadening factor ($\Gamma$) were obtained by fitting the second derivative of the dielectric constant ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) versus the energy curve using least-square method.

3. Results and discussion

Fig. 1 shows the experimental pseudo-dielectric function versus the photon energy curves for the as-prepared Si$_{0.887}$Ge$_{0.113}$ and Si$_{0.887-y}$Ge$_{0.113}$C$_y$ alloys. The large amplitudes of $E_1$ and $E_2$ gaps of these samples indicate good crystallinity of the films. The energy and peak values of $\varepsilon_2$ for Si$_{0.887}$Ge$_{0.113}$ are comparable to strained SiGe films [9]. The amplitudes of $\varepsilon_2$ at $E_1$ and $E_2$ gaps decrease with an increase in C concentration. This is due to the alloying effect and the stoichiometric deformation of the films. The humps at the lower edge of the $E_1$ gap at 2.6, 2.4 and 2.3 eV for Si$_{0.8811}$Ge$_{0.113}$C$_{0.0059}$, Si$_{0.8738}$Ge$_{0.113}$C$_{0.0132}$ and Si$_{0.8686}$Ge$_{0.113}$C$_{0.0184}$ films may be due to C-related band gaps.

Fig. 2(a) shows the energy dependence of the second derivatives of $\varepsilon_1$ and $\varepsilon_2$ for the as-prepared samples. The results are fitted using the lineshape formula developed by Aspne [10] by assuming two critical points at $E_1$ and $E_0'$. In general, good agreement is obtained between the experimental and the simulated results. Fig. 3(a) shows the peak positions of $E_1$ and $E_0'$ as a function of C concentration for the as-prepared samples. The $E_1$ transition increases linearly with increasing C concentration. However, the $E_0'$ transition is independent of the C concentration. The broadening factor of $E_1$ transition for Si$_{0.887}$Ge$_{0.113}$ is 0.137 eV and increases to 0.149, 0.157 and 0.197 eV with the C concentration equal to 0.59, 1.32 and 1.84 at%, respectively. For the Si$_{0.887-y}$Ge$_{0.113}$C$_y$ alloys, the $E_2$ peak also broadened but shifts to lower energy. The broadening and shifting of the $E_1$ and the $E_2$ peaks may be attributed to the distortion near the carbon atoms and the internal splitting of electronic bands [11].

Fig. 4 compares the $\varepsilon_2$ values of the as-prepared and RTO samples. The intensity of the $E_1$ and $E_2$ transitions decreases for all the RTO samples. As the light penetration in the $E_2$ energy range transition is ~8 nm, the large reduction in $\varepsilon_2$ intensity at $E_2$ of the RTO samples is due to the presence of an oxide layer of 10–16 nm thick. Fig. 4 also shows that the $E_1$ transition
shifts towards the lower energy direction for the RTO samples. This means that the transition occurs from a higher Ge content layer in the samples. The higher Ge content layer may be due to the Ge pile-up at the SiO$_2$/substrate interface as a result of RTO. As the $E_1$ peak for samples Si$_{0.887}$Ge$_{0.113}$ and Si$_{0.887-\delta}$Ge$_{0.113}$C$_{\delta}$ are located at 3.07 eV, this means that the RTO process has reduced most of the C in Si$_{0.887-\delta}$Ge$_{0.113}$C$_{\delta}$. For samples Si$_{0.8738}$Ge$_{0.113}$C$_{0.0132}$ and Si$_{0.8686}$Ge$_{0.113}$C$_{0.0184}$, the $E_1$ transitions are located at 3.13 and 3.15 eV, respectively. These values are lower than the as-prepared samples. This may be due to a lower C concentration in the RTO samples as we have shown [8] from our SIMS results that the oxidized Si$_{0.8686}$Ge$_{0.113}$C$_{0.0184}$ had only 0.6% C left at the surface region. During oxidation, we suggest that the substitutional C can react with oxygen to form CO or CO$_2$. This reduces the chance of SiC precipitation.

Fig. 2. The second derivative of pseudo-dielectric function of (a) as-prepared and (b) RTO films with oxide etched away for Si$_{0.887}$Ge$_{0.113}$ and Si$_{0.887-\delta}$Ge$_{0.113}$C$_{\delta}$ alloys.

![Fig. 2](image1)

Fig. 3. Energy of the $E_1$ and $E_0'$ critical points of (a) as-prepared and (b) RTO samples with oxide etched away for Si$_{0.887}$Ge$_{0.113}$ and Si$_{0.887-\delta}$Ge$_{0.113}$C$_{\delta}$ alloys.

![Fig. 3](image2)
To study the effect of oxidation on our samples, SE measurements were done after the oxide was etched away. The second derivatives of the pseudo-dielectric function versus photon energy curves of the etched samples are shown in Fig. 2(b). As compared to the as-prepared samples (Fig. 2(a)), an even better fit between

Fig. 4. Imaginary part of pseudo-dielectric function of the as-prepared and RTO Si_{0.887}Ge_{0.113} and Si_{0.887-\gamma}Ge_{0.113}C_\gamma alloys.

Fig. 5. Refractive indices of the as-prepared and RTO Si_{0.887}Ge_{0.113} and Si_{0.887-\gamma}Ge_{0.113}C_\gamma alloys.
the experimental and theoretical results is obtained for the etched samples. Fig. 3(b) shows that the $E_1$ transition is weakly dependent on the C concentration for the etched samples. This is reasonable as the C concentration in the sample significantly reduced after RTO. In general, the $E'_0$ transition of the etched sample is independent of C content in the film. Fig. 5 shows the refractive indices of the as-prepared and etched samples. It is clear for the etched samples that the refractive index increases with an increase in the incident radiation ($<3.2$ eV). During oxidation Ge pile-up at the oxide/epilayer interface [8, 12]. This will make the surface region ($\sim 20$ nm) of the Si$_{1-x-y}$Ge$_x$$_y$ to be Ge rich. This Ge rich layer (with oxide etched away) is detectable by the SE measurements. The higher Ge content leads to a higher refractive index for the etched samples.

4. Conclusion

The pseudo-dielectric functions of the as-prepared and RTO Si$_{1-x-y}$Ge$_x$$_y$ films were studied using spectroscopic ellipsometry. The energy of transition gaps, $E_1$ and $E_2$, were obtained by performing lineshape analyses on the second derivative of the pseudo-dielectric functions. The results show that the $E_1$ gap increases and $E_2$ gap decreases as the C concentration increases. For the RTO samples, the amplitude of $E_2$ transitions reduces rapidly and the $E_1$ transition shifts to a lower energy. The reduction of the amplitude of $E_2$ transitions is due to the presence of oxide layer. The values of refractive index of the RTO samples (after etched away the top oxide layer) are higher compared to as-prepared films. A high Ge content layer and the low C content in the RTO films is used to account for the $E_1$ shift to lower energy and the increase of the refractive index.

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