Strain Relaxation Enhancement of Ge_{1-x-y}Si_xSn_y Epitaxial Layer on Ge Substrate Using Ion-Implantation Method

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Abstract

We demonstrated that the strain relaxation enhancement of both $Ge_{1-x-y}Si_xSn_y$ and $Ge_{1-x}Sn_x$ epitaxial layers on ion-implanted Ge substrate and the reduction of critical energy for strain relaxation. This fact supports a mechanism of reducing a static friction from substrate side by ion implantation. This possibility is discussed based on Raman spectroscopy analysis.

1. Introduction

Ge_{1-x-y}Si_xSn_y/Ge_{1-x}Sn_x double heterostructure with type-I energy band structure and direct transition Ge_{1-x}Sn_x are promising structure for future optoelectronic and transistor applications [1,2]. We previously demonstrated the enhancement of the photoluminescence intensity of a Ge_{1-x}Sn_x layer formed by Ge_{1-x-y}Si_xSn_y/Ge_{1-x}Sn_x/Ge_{1-x-y}Si_xSn_y double heterostructure pseudomorphically grown on Ge substrate. However, the Ge_{1-x}Sn_x layer is still indirect transition due to a large compressive strain. It looks generally difficult to form a direct transition Ge_{1-x}Sn_x with the pseudomorphic growth on Ge substrate since a very high Sn content more than 16% is required to a compressive-strained Ge_{1-x}Sn_x [3]. To decrease the required Sn content, the increase of a lattice constant of under layer to reduce the strain of Ge_{1-x}Sn_x is a possible solution.

Since the $Ge_{1-x}Sn_x$ layer is grown on a $Ge_{1-x-y}Si_xSn_y$ layer, the strain relaxation method of $Ge_{1-x-y}Si_xSn_y$ layer is examined in this study. It was reported that the ion implantation to Si substrate successfully enhance the strain relaxation of $Si_{1-x}Ge_x$ epitaxial layer on Si substrate [4]. Thus, we examined ion-implantation method to Ge substrate before $Ge_{1-x-y}Si_xSn_y$ growth. As a result, the strain relaxation of $Ge_{1-x-y}Si_xSn_y$ layer is sufficiently enhanced on an ion-implanted Ge substrate [5]. In this report, to obtain a general guideline for controlling the strain relaxation of group-IV semiconductor materials, we also discussed the mechanism of the strain relaxation enhancement of not only $Ge_{1-x-y}Si_xSn_y$ but also $Ge_{1-x}Sn_x$ epitaxial layers on ion-implanted Ge substrate.

2. Experimental

B ions were implanted on Ge(001) substrate after removing surface native-oxide. Ion doses were 1×10^{14} cm⁻² and 3×10^{14} cm⁻² and the ion implantation energy was 20 keV. Subsequently, the ion-implanted Ge(001) wafer was cleaned with chemical solutions and then thermally cleaned at 430 °C in ultrahigh vacuum. A 100-nm-thick Ge_{1-x}-vSi_xSn_y or Ge_{1-x}Sn_x

layer was grown on the substrate at 100 °C using molecular beam epitaxy system. The target Si and Sn contents in $Ge_{1-x-y}Si_xSn_y$ layer were 10% and 13%, respectively. The Sn content in $Ge_{1-x}Sn_x$ layer was ranging from 5% to 12%. The crystalline structure was characterized with X-ray diffraction 2-dimensional reciprocal space mapping (XRD-2DRSM). Also, Raman spectroscopy measurement was performed to analyze the effect of ion implantation on the strength of Ge-Ge bonds.

3. Results and discussion

Figure 1 shows XRD-2DRSM results for the $Ge_{1-x-y}Si_xSn_y$ layer grown on (a) Ge substrate without ion implantation and (b) Ge substrate after the ion implantation of an ion dose of 3×10^{14} cm⁻². The strain relaxation is clearly observed for the $Ge_{1-x-y}Si_xSn_y$ layer grown on the ion-implanted substrate, while not for the sample without ion-implantation.

From XRD-2DRSM results, the in-plane lattice constant and the degree of strain relaxation (DSR) were esti-



Fig. 1. XRD-2DRSM results around the Ge reciprocal lattice for samples of $\text{Ge}_{1-x-y}\text{Si}_x\text{Sn}_y$ grown on (a) un-implanted and (b) ion-implanted substrate. The ion dose was $3 \times 10^{14} \text{ cm}^{-2}$.



Fig. 2. In-plane lattice constants and DSR of $Ge_{1-x-y}Si_xSn_y$ layers as a function of the ion dose.

mated. **Figure 2** shows the in-plane lattice constant of $Ge_{1-x-y}Si_xSn_y$ layers as a function of the ion dose. The in-plane lattice constants of Ge and $Ge_{0.9}Sn_{0.1}$ are indicated with dotted lines. The DSR value of each $Ge_{1-x-y}Si_xSn_y$ layer is also shown in **Fig. 2**. It is observable that both the in-plane lattice constant and DSR of $Ge_{1-x-y}Si_xSn_y$ layer increase with the ion dose. For the ion dose of 3×10^{14} cm⁻², we achieved a large DSR value of 92% and large in-plane lattice constant more than 5.74 Å, which is comparable to the lattice constant of $Ge_{0.9}Sn_{0.1}$.

Next, we discuss the strain relaxation mechanism of $Ge_{1-x-y}Si_xSn_y$ layer on ion-implanted Ge substrate from the macroscopic viewpoint that is a strain energy. According to our previous work [6], there is a critical strain energy for the strain relaxation of $Ge_{1-x}Sn_x$ on Ge substrate ($E_{c,GeSn}$), which was roughly estimated to be $3\sim 5 \text{ J/m}^2$. This value is independent on the substrate orientation regardless that strain relaxation mechanisms of $Ge_{1-x}Sn_x$ such as Sn precipitation and dislocation propagation should be complexly related each other. Thus, we investigated the effect of the ion-implantation method on $E_{c,GeSn}$. To discuss that, we examined to grow a $Ge_{1-x}Sn_x$ layer on the ion-implanted Ge substrate with an ion-dose of 3×10^{14} cm⁻². Figure 3 shows the DSR of $Ge_{1-x}Sn_x$ layers on ion-implanted and un-implanted Ge substrates as a function of the Sn content. The strain energy, E_{strain} of $\text{Ge}_{1-x}\text{Sn}_x$ layer was estimated with the following equation,



Fig. 3. DSR of $\text{Ge}_{1-x}\text{Sn}_x$ grown on un-implanted and ion-implanted Ge substrates as a function of the Sn content, corresponding to the strain energy. The ion dose was 3×10^{14} cm⁻².



Fig. 4. Raman spectra of un-implanted and ion-implanted Ge substrate with ion dose is 3×10^{14} cm⁻².

$$E_{\text{strain}} = M_{001} \varepsilon^2 h \tag{1}$$

Here, M_{001} is the biaxial modulus of 001 orientation, *h* is the thickness of Ge_{1-x}Sn_x layer, ε is the strain estimated from the Sn content assumed by the pseudomorphic growth of Ge_{1-x}Sn_x on Ge, respectively. As shown in **Fig. 3**, the strain relaxation of Ge_{1-x}Sn_x on the ion-implanted substrate occurs with increasing the Sn content higher than 5%, while that on the Ge substrate without ion implantation still does not even at a Sn content of 12%. This result indicates that $E_{c,GeSn}$ is effectively reduced to be less than 1 J/m² by ion implantation. We expected that the decrease of $E_{c,GeSn}$ is due to the reduction of the static friction from the Ge surface.

Finally, to investigate the effect of ion-implantation on the static friction, Raman spectroscopy analysis was carried out. Figure 4 shows Raman spectra of Ge substrate without and with the ion implantation with an ion dose of 3×10^{14} cm⁻². The peak position of the ion-implanted Ge substrate shifts by 0.5 cm⁻¹ from that without ion implantation. Also, the full width of half maximum value increases from 2.4 to 2.8 cm^{-1} by the ion-implantation. We confirmed that peak shift and broadening are located only at the surface side by combining chemical etching method (not shown). If this peak shift is caused by only the strain, the tensile strain with 1.0% is applied to Ge substrate. But the estimated strain value from XRD is just 0.5%, meaning that the observed Raman peak shift is not only from the strain. The remained possible mechanisms are crystal damage or softening of Ge-Ge bonds. Although we have not distinguished these two mechanisms yet, the similar Raman peak shift and broadening are verified for heavily Ga-doped Ge formed by the in-situ doping technique (not shown). Since Ge-Ge bond softening can be caused by increasing hole carrier concentration [7], this result is reasonable. In our presentation, we will also discuss the $Ge_{1-x-y}Si_xSn_y$ growth on a p⁺-Ge substrate.

4. Conclusions

We demonstrated that the formation of 92% strain-relaxed $Ge_{1-x-y}Si_xSn_y$ epitaxial layer with a lattice constant of 5.74 Å. Also, we found that $E_{c,GeSn}$ is reduced to be less than ~1 J/m² on the ion-implanted Ge substrate. This mechanism is expected to be the reduction of the static friction of the substrate side due to the crystal damage or softening of Ge-Ge bonds according to Raman spectroscopy analysis, which have not been distinguished yet. The possibility of phonon softening induced strain relaxation is a worth to be further investigated to realize the growth of strain-relaxed $Ge_{1-x-y}Si_xSn_y$ layer with a high crystallinity for the practical applications.

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