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Fabrication and Characterization of GeSi Superlattices

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Ge$_n$Si$_m$ strained-layer superlattices were grown on Si(001) substrate by molecular beam epitaxy using phase-locked epitaxy method. A Ge$_4$Si$_{12}$ superlattice showed intense photoluminescence peaks in the near-infrared region, and its absorption coefficient followed the $(h\nu-E_g)^{1/2}$ law, where $h\nu$ is the energy of incident light and $E_g$ is the band gap energy. These results suggest that the Ge$_4$Si$_{12}$ sample has a direct band gap.

I. Introduction

In Ge-Si alloy and strained-layer superlattices (SLS's), the band gap and the type of band alignment can be controlled by the lattice strain $^1)$. It has been theoretically predicted that Ge$_n$Si$_m$ SLS's with particular superlattice structures may possess a direct band gap $^2)$. Pearsall et al have observed new transition peaks at 0.76eV and 1.25eV in electroreflectance measurement on (Ge$_4$Si$_4$)$_5$/Si(001) superlattice structure $^3)$. Several theoretical works $^4$-$^9$ were done to explain above experimental results, however, their conclusions are controversial.

On the other hand, Zachai et al have recently observed intense emission at around 0.84eV in photoluminescence measurement of Ge$_4$Si$_{16}$ SLS on GeSi alloy (001) substrate, which suggests the direct transition $^{10})$. Thus more systematic experimental works should be necessary to make clear the above discussions.

In this paper, we report the fabrication and the characterization of Ge/Si SLS's on Si (001) substrates.

II. Experimental

Ge/Si SLS's were grown by MBE method at the temperature of 400°C. The substrates used were well oriented Si(001) ($<0.1^\circ$) and prepared to form a 2x1 single-domain structure $^{11})$. During the growth of Ge and Si layers, RHEED intensity oscillations were observed to control layer thickness precisely. The total numbers of atomic layer of SLS's were about 1200 monatomic layers (ML), which correspond to the thickness of 1600-1700Å. To protect SLS layers from oxidation, Si cap layer of 100 ML were subsequently grown on the SLS's. Details of the optical measurement conditions have been described elsewhere $^{12,13})$.

III. Results and Discussion

Figure 1 shows typical RHEED intensity oscillations observed during the growth of a Ge$_4$Si$_{16}$ SLS $^{11})$. The oscillation damping during Ge growth and recovery during Si growth were observed sequentially. This fact suggests that the roughened surface caused by the 3-D growth of Ge was smoothed by the Si over growth. With the help of
this oscillation recovery effect, the phase-locked epitaxial method can be applied for Ge₄Si₁₆ SLS's up to a total thickness of about 240 ML (~33nm).

Figure 2 shows the Raman spectra below 200 cm⁻¹ for (Ge₄Si₄₅)(n=2, 4 and 6) SLS's. The spectra exhibit the peaks assigned to such zone folded modes. The measured peak frequencies agree with the calculated ones quite well. This result indicates that the long range periodicity due to the SLS structures are properly formed as designed.

Ge₃Si₄ SLS's were characterized using electroreflectance (ER) and photoreflectance (PR) method. In Fig. 3, the ER data for the SLS's of n+m=8, i.e., (Ge₄Si₄)₅, (Ge₃Si₅)₅ and (Ge₂Si₆)₅, at 300 K are shown in the energy range 0.7-4.0 eV. The ER spectrum of (Ge₄Si₄)₅ is similar in general features to that of the previous study. However, we observed three prominent peaks at 0.76, 1.03, and 1.27 eV in the energy range 0.7-1.3 eV. The transition at 0.76 and 1.03 eV are assigned to indirect, whereas the transition at 1.27 eV is assigned to zone-folded quasi-direct. These three peaks appear in all samples of n+m=8, and they

Fig.1 RHEED intensity oscillations observed during growth of Ge₄Si₁₆ SLS.

Fig.2 Raman spectra below 200 cm⁻¹ for (Ge₂Si₈), (Ge₄Si₁₆) and (Ge₆Si₂₄) SLS's.

Fig.3 ER and PR spectra for (a) (Ge₄Si₄)₅, (b) (Ge₃Si₅)₅ and (c) (Ge₂Si₆)₅. The fitted critical point energies are indicated by arrows.
show a blue shift with decreasing Ge fraction. This shift may be due to the structure of the SLS and also due to the strain involved in the SLS.

In Fig. 4, the photoluminescence spectra measured for the Ge$_4$Si$_{12}$ and Ge$_4$Si$_{16}$ samples are shown. The emission at around 1100 meV is due to the Si substrate. Regarding the Ge$_4$Si$_{12}$ sample, the emission between 750 and 1000 meV with multiple structures is the signal from SLS layer. Although the thickness of the SLS layer is around 1600 Å, the emission from the SLS layer is stronger than that of Si substrate. Intense sharp peaks are observed at 800 meV and 865 meV. The other Ge$_n$Si$_m$ SLS's we examined exhibited only weak broad emission band, as shown in Fig. 4(b). If the stronger emission of the Ge$_4$Si$_{12}$ sample is due to impurities or structural defects, then a similar strong emission should be observed for all the SLS samples. The differences among the Ge$_n$Si$_m$ SLS samples indicate that the intense and sharp emission of Ge$_4$Si$_{12}$ cannot be attributed to an extrinsic effect such as the presence of impurities, but must be caused by an intrinsic effect originating from its particular superlattice structure.

The optical absorption spectrum measured for the Ge$_4$Si$_{12}$ sample is shown in Fig. 5. The absorption coefficient $\alpha$ was obtained from the thickness of the SLS layer and the transmittance of the sample. The absorption coefficient $\alpha$ increases above approximately 790 meV. The other Ge$_n$Si$_m$ SLS's examined did not exhibit such an increase of $\alpha$. In Fig. 5, the arrow shows the energy position where the strongest emission peak is observed in Fig. 4. That energy position is located just above the rising position of the absorption spectrum. The measured values of $\alpha$ (10$^{-3}$/cm) are one order of magnitude larger than those of indirect semiconductors (10-10$^2$/cm).

The energy dependence of $\alpha$ is generally formalized differently for the cases of

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![Fig. 4 Photoluminescence spectra at 4.2 K for (a) Ge$_4$/Si$_{12}$ SLS, and (b) Ge$_4$/Si$_{16}$ SLS.](image)

![Fig. 5 Optical absorption spectrum of (Ge$_4$/Si$_{18}$)$_{69}$ SLS measured at 2.8 K. The arrow indicates the energy position of the strongest photoluminescence emission line observed in Fig. 4. The dashed line indicates the best fitted curve calculated for absorption coefficient according to eq. (1). The relations of $(h\nu \cdot \alpha)^2$ vs $h\nu$ is shown in the inset.](image)
optical direct and indirect transitions, as follows\textsuperscript{16}.

\begin{align*}
\alpha &= C_d (h\nu - E_g)^{1/2}/h\nu; \text{direct} \quad (1) \\
\alpha &= C_i (h\nu - E_g)^2; \text{indirect} \quad (2)
\end{align*}

where \(C_d\) and \(C_i\) are constants, \(h\): Planck's constant, \(\nu\): the frequency of the incident light, and \(E_g\): the band gap energy of the sample. In the inset of Fig.5, the relation of \((h\nu - \alpha)^2\) vs \(h\nu\) is shown. A linear relation is seen which indicates that the observed spectrum agrees quite well with eq. (1) rather than eq. (2). The experimental results described above indicate that some optical transition occurs in the Ge\(_4\)Si\(_{12}\) SLS sample above 790 meV.

In conclusion, we have successfully grown the Ge\(_n\)Si\(_m\) SLS's on Si(001) substrate using the phase-locked epitaxy method. We observed for the first time that the Ge\(_4\)Si\(_{12}\) SLS sample exhibits the luminescent and optical absorption properties typical of direct band gap transition. The structural conditions for producing such properties should be investigated in further studies in order to clarify the possible occurrence of direct band gap transition caused by zone-folding.

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References


