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Observation of Direct Band Gap in Ge_nSi_m Strained-Layer Superlattices

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Photoluminescence and optical absorption measurements were carried out for Ge_nSi_m strained-layer superlattices grown by molecular beam epitaxy. A Ge_4Si_{12} superlattice showed intense emission in the near-infrared region, and its absorption coefficient followed $(h\nu\text{-}Eg)^{1/2}$. These results indicate that the Ge_4Si_{12} sample has a direct band gap.

It has been theoretically predicted that the band structures of proper Ge_nSi_m superlattices are direct band gap type.[1] Up to now, the observation of some optical transitions for Ge/Si strained-layer superlattices (SLS's) depending on the superlattice structure have been reported by several researchers.[2,3] However, decisive proofs of direct transition in Ge_nSi_m SLS's have not been explicitly shown yet. To obtain the superlattice structure expected to have a direct band gap, it is required to control the thickness of each component layer in an atomic scale. Using phase-locked epitaxy (PLE) technique, we succeeded in preparing Ge_nSi_m SLS's with periods of several nm.[4] In this paper, the results of photoluminescence and optical absorption measurements of such Ge_nSi_m SLS's are reported. It is shown that Ge_4Si_{12} SLS has a remarkable optical transition, and its transition type is discussed.

$(Ge_nSi_m)_N$ SLS's were fabricated on well-oriented Si (001) substrates showing 2x1 single-domain surface. The SLS layers were grown at 400°C by PLE monitoring the RHEED intensity oscillation. Total numbers of atomic layers of the SLS's were around 1200 monatomic layers(1600-1700Å). Details of the growth procedure have been described elsewhere.[4] X-ray diffraction patterns of the samples indicate the designed superlattices to be formed properly. Photoluminescence and optical absorption measurements were carried out at 4.2K and 2.8K, respectively. In the photoluminescence measurements, the 488nm line of an Ar laser was used as an excitation light, and signals were detected by a Ge detector. In the optical absorption measurements, a W-lamp light source and a PbS cell detector were used.

In Fig.1, the photoluminescence spectra measured for the Ge_4Si_{12} and Ge_4Si_{16} samples are shown. Regarding the Ge_4Si_{12} sample, the emission between 750 and 1000meV with multiple structures is the signal from the SLS layer. Intense sharp peaks are observed at 800 and 865 meV. The energy region where the emission is observed is between the band gap energy of Si and that of Ge lattice-matched to Si. The emission peak at the lower energy side has the stronger intensity. While, Ge_nSi_m SLS's with the other superlattice structures exhibit only so weak broad emission band as shown by Fig.1(b) in the spectral region between 700 and 900meV, although they were prepared by similar procedure in the same MBE system as Ge_4Si_{12} sample. Compared with Fig.1(b), the emission intensity of Fig.1(a) is more than one order of magnitude higher, and the peak widths are quite small. If the band gap of the sample is direct type as predicted theoretically, increase of transition probability and enhancement of emission intensity should be expected, with which the result is consistent.

The optical absorption spectrum measured for the Ge_4Si_{12} sample is shown in Fig.2. Above around 790meV, increase of the absorption coefficient α is seen. Ge_nSi_m SLS's having the other superlattice structures did not exhibit such increase in the measured spectral region. The energy corresponding to the strongest emission peak in Fig.1(a) is located just above the rising position of α. Considering these results together, the rising point of absorption coefficient is considered to correspond to the band gap energy. Above this rising point, the measured values of the absorption coefficients are in the order of $10^3 cm^{-1}$. This values of α is too large for band-to-band transition in optical indirect semiconductors. On the contrary, as large α as observed is expected for optical direct semiconductors, because transition can occur without phonon assistance. In the case of direct transition, the exponent of energy dependence for α is generally 1/2. In the inset of Fig.2, the relation between $(h\nu\,\alpha)^2$ and hν is shown. The linear relation shown in the inset indicates that the observed α follows the typical energy dependence for direct transition quite well, and that the optical direct transition occurs in the Ge_4Si_{12} SLS sample above 790meV.

Thus, the results described above indicate that the Ge_4Si_{12} SLS sample has the direct band gap. The observation of direct transition means that the band structure is converted from indirect to direct on account of the zone-folding effect of the Ge_nSi_m SLS structure, considering that the conduction band minima of Si are located along [001] direction in k-space.

In conclusion, the Ge_4Si_{12} SLS sample grown by PLE method showed the direct band gap transition. This result is thought to be the first verification of the band structure conversion from indirect to direct band gap type due to superlattice structure.

References

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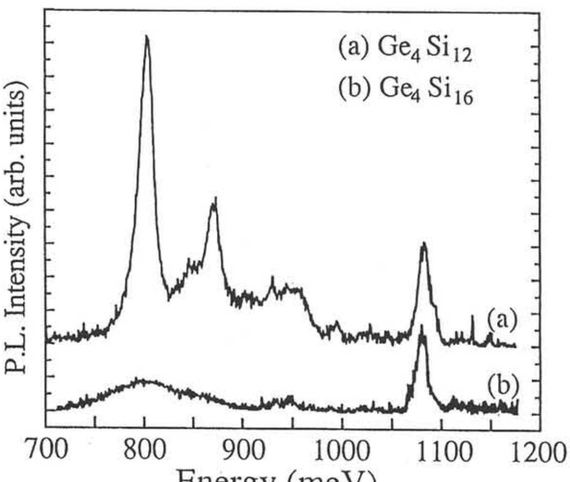

Fig.1. Photoluminescence spectra of (a) $(Ge_4Si_{12})_{69}$ and (b) $(Ge_4Si_{16})_{60}$ SLS's measured at 4.2K. The peaks at about 1100meV are due to the emission from Si substrates.

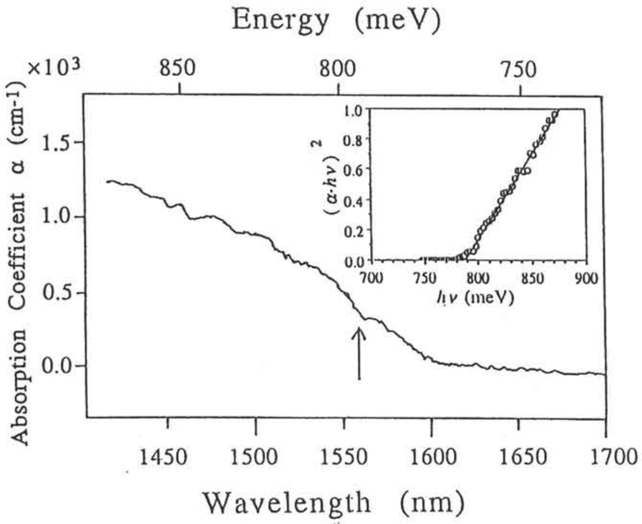

Fig.2. Optical absorption spectrum of $(Ge_4Si_{12})_{69}$ SLS measured at 2.8K. The arrow indicates the energy position of the strongest photoluminescence emission line shown in Fig.1. Relation of $(h\nu\,\alpha)^2$ vs. hν is shown in the inset.