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Effect of Substrate Orientation on the Photoluminescence of GaAs on Si

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The photoluminescence (PL) of undoped GaAs on Si grown by MOCVD has been investigated. Three peaks in low-temperature (4 K) PL spectra are attributed to defect-induced bound excitons, carbon acceptors and defect complexes, respectively. The relative peak intensity of excitons against carbon acceptors increases and that of defect complexes decreases for GaAs on Si substrates with orientations exact (100), several degrees off (100) tilted around <011> axis and exact (211), in that order. The band-to-band emission at 77 K from the surface of GaAs on (211) Si is strongly polarized parallel to [$\bar{1}$11]. This suggests the anisotropy of strain relaxation between [0$\bar{1}$1] and [$\bar{1}$11] derections on the (211) substrate.

1. Introduction

Recently, many GaAs devices such as solar cells, LEDs, laser diodes, FETs, HEMTs and HBTs have been fabricated on Si substrates. However, the performance of these GaAs devices on Si substrates, especially that of optical devices, is somewhat inferior to that of these devices on GaAs substrates. It seems that the large differences in both lattice constants and thermal-expansion coefficients cause a high density of defects and degrade the optical property of the epitaxially grown GaAs. To characterize the optical property, photoluminescence (PL) measurements have been often used. Some unusual peaks have been observed in the PL spectra of GaAs on Si.[1-6] However, the assignments of the PL peaks have been heretofore uncertain for GaAs on Si. The definitive assignments of the PL peaks are required for the characterization of GaAs on Si.

On the other hand, it was shown in our previous paper[7] that the off orientation from (100) around <011> axis is essential for the growth of high quality GaAs on Ge. Fischer et al.[8] reported that the surface morphology of GaAs on Si is improved by the use of an orientation tilted several degrees off (100). Uppal et al.[6] reported that (211)-oriented growth is free from antiphase domain disorder. These results suggest that the optical properties of GaAs on Si are strongly affected by the surface orientation of the substrates.

The main purpose of the present paper is to investigate the effect of substrate orientation for GaAs on Si by the low temperature PL measurements. In order to assign PL peaks, (1) the temperature dependence of PL and (2) the relation between the energy shift of PL peaks and biaxial strain are studied. Then, PL spectra of GaAs on Si substrates with different orientations are examined. The polarization properties of PL are also discussed.

2. Experiment

Undoped GaAs epitaxial layers were simultaneously grown on Si, Ge and GaAs substrates with various orientations by LPMOCVD with a barrel type reactor.[1] The Si substrates used for the experiments have orientations exact (100), 2-8 degrees off (100) tilted around <011> or <010> axes and exact (211). Before the growth, the surfaces of substrates were cleaned by the heat treatment at 900^{o}C. Thin GaAs layers of less than 200 Å were deposited at 450^{o}C. Subsequently, typically 3 μm thick GaAs layers were grown at 750^{o}C. The GaAs layers obtained were n-type with carrier concentration of ~10^{16} cm^{-3}.

PL from front surface were measured using the 488 nm line from an Ar^{+} laser for excitation and a one meter monochromator with 0.5 nm resolution. The excitation power was about 5 W/cm^2. A cooled photo-multiplier with S1 response was used to measure the luminescence. The measurements were carried out at both 4 K and 77 K for all the samples. The PL spectra at various temperatures were measured for GaAs on Si tilted 3°off (100) around <011> axis to correlate 4-K spectra with 77-K spectra and to identify the emission peaks. Additional informations about polarization of the luminescence were provided using a linear polarizer.

3. Results and Discussion

Figure 1 shows the PL spectra of GaAs on Si tilted 3°off (100) around <011> axis taken at various temperatures. The highest energy peak A is prove to be band-edge emission since it dominates the spectra at high temperatures. The peak B is approximately 17 meV lower in energy than the peak A. The peak B is attributed to carbon acceptors, which is in agreement with earlier studies.[1-5]

The peak C is about 37 meV lower in energy than the peak A and is attributed to germanium acceptors in some of earlier studies.[3,9] However, the peak due to germanium acceptors is not observed for either GaAs on GaAs or GaAs on Ge[7] which were grown simultaneously with GaAs on Si. Therefore, it is unlikely that the peak C is due to germanium acceptors.

On the other hand, Soga et al.[2] supposed that an acceptor level splits into two levels by the biaxial strain in GaAs on Si and results in two peaks, B and C, in the PL spectra. According to this model, the splitting between B and C should become larger with increasing biaxial strain. The strain in GaAs on (100)- and near-(100)-oriented Si was determined from the X-ray diffraction determination of the perpendicular lattice constant $a_\perp$. Figure 2 shows the PL peak energies of GaAs on (100)- and near-(100)-oriented Si at

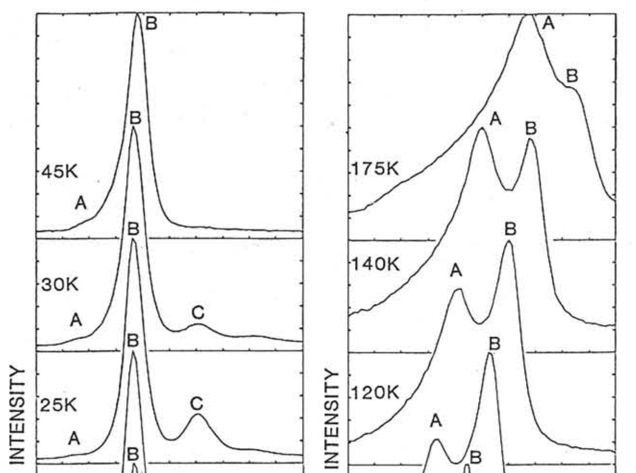

Fig. 1. PL spectra of GaAs on Si tilted 3°off (100) around <011> axis taken at various temperatures between 10 K and 175 K. The spectra are normarized by each maximum peak intensity.

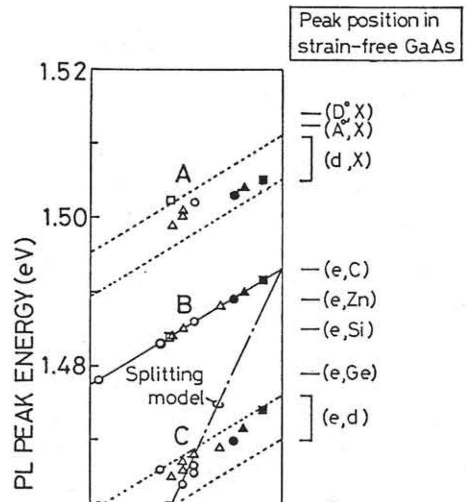

Fig. 2. PL peak energy of GaAs on (100)- and near-(100)-oriented Si at low temperature (2-10 K) as a function of biaxial strain. ○-present study, △-Masselink et al.,[1] □-Soga et al.,[2] ●-Duncan et al.,[3] ▲-Wang,[4] ■-Sheldon et al.[5] The solid line indicates the relation between the energy shift of the carbon acceptor peak B and biaxial strain: $\Delta E(\mathrm{meV}) = 6\times10^{-3}\ (\Delta a_\perp/a_0)$. The dot dashed line indicates the peak splitting model proposed by Soga et al.[2]

4 K as a function of the strain perpendicular to (100) surface, $\Delta a_{\perp}/a_0$ ($\Delta a_{\perp} = a_{\perp} - a_0$, a_0 is the lattice constant for strain-free GaAs). Linear relationship between the energy shift of the carbon acceptor peak B, ΔE, and the strain can be seen from Fig. 2: $\Delta E(\mathrm{meV}) = 6\times10^{-3}\ (\Delta a_{\perp}/a_0)$. This relation is indicated by solid line in Fig. 2. The PL peak energies of GaAs on (100)- and near-(100)-oriented Si at low temperatures (2-10 K) obtained in earlier studies[1-5] are also plotted in Fig. 2. The strains for them are estimated from the energy shift of their carbon acceptor peak using above relation. The difference in biaxial strain among these studies is probably due to the difference in eptaxial layer thickness or growth temperature. Peak splitting model proposed by Soga et al.[2] is also indicated in Fig. 2 by dot dashed line. It is clear from Fig.2 that the peak C does not split from the peak B but all the peaks including the peak C shift parallel to the peak B as is indicated by dotted lines. Furthermore, the extrapolation to strain-free situation indicates that the peaks A and C are due to defect-induced bound excitons and defect complexes, respectively.

We now compare the PL spectra of GaAs on Si substrates with different orientations.

Figures 3(a) and 3(b) show the PL spectra of GaAs on exact (100) Si at 4 K and 77 K, respectively. At 4 K, the defect complex peak C is larger than the carbon acceptor peak B and the exciton peak A does not appear. In the 77-K spectrum, which is similar to that of Ref.10, the peak A appears as a shoulder of the peak B. This is in contrast to the 77-K PL spectra of homoepitaxial GaAs[11] grown simultaneously with GaAs on Si where the band-edge emission is the dominant peak and the carbon acceptor peak is very small.

The spectra of GaAs on Si tilted 2^{o}off, 3^{o}off, 4^{o}off, 6^{o}off and 8^{o}off (100) around <011> axis are almost the same. Figures 4(a) and 4(b) show the spectra of GaAs on Si tilted 8^{o}off (100) around <011> axis at 4 K and 77 K, respectively. At 4 K, the peak B is larger than the peak C and the peak A appears as a small peak. At 77 K, the peak A becomes to be clearly observed. This indicates that the cristalline quality of GaAs on Si is improved by tilting the substrate orientation from

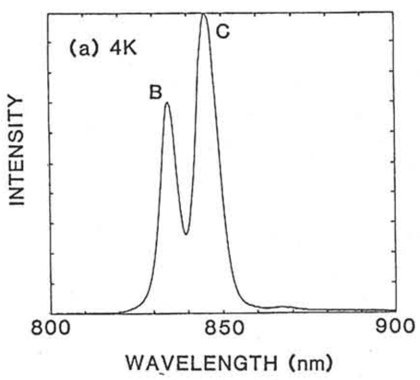

Fig. 3. PL spectra of GaAs on exact (100) Si at 4 K (a) and at 77 K (b). The luminescence is unpolarized.

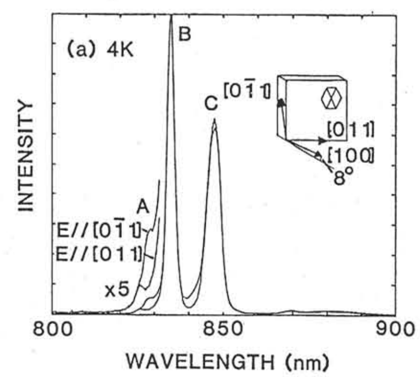

Fig. 4. Polarized PL spectra of GaAs on Si tilted 8^{o}off (100) around <011> axis at 4 K (a) and at 77 K (b). The inset is a schematic of the sample with crystallographic directions and a etch pit shape.

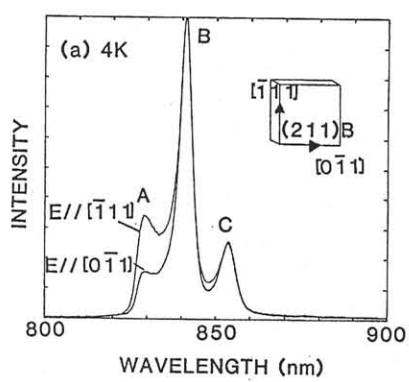

Fig. 5. Polarized PL spectra of GaAs on (211) Si at 4 K (a) and at 77 K (b). The inset is a schematic of the sample with crystallographic directions.

(100) around <011> axis. On the other hand, when an orientation tilted around <010> axis is used, the PL properties are not improved.

Polarization measurements revealed that the lower part of the exciton emission band A at 4 K is polarized parallel to [0$\bar{1}$1] for GaAs on Si tilted several degrees off (100) around <011> axis, as is seen from Fig. 4(a). The [0$\bar{1}$1] direction in GaAs is identified from the etch pit shape etched by molten KOH (see inset of Fig. 4(a)) and is proved to coincide with one of <011> directions in Si which is selected to be the off direction. Skolnick et al.[12] and Beye et al.[13] reported that some of the peaks due to defect-induced bound excitons are polarized parallel to [0$\bar{1}$1]. The present results agree with their observations.

Figures 5(a) and 5(b) show polarized PL spectra of GaAs on (211) Si at 4 K and 77 K, respectively. The energy shift of PL peaks is extremely larger[6] than that for GaAs on (100)- or near-(100)-oriented Si. At 4 K, the peak A is larger than the peak C and smaller than the peak B. At 77 K, the peak A becomes larger than the peak B. This indicates that the crystalline quality of GaAs on Si is much improved by the use of (211) substrates.

Polarization measurements revealed that the peak A is strongly polarized parallel to [$\bar{1}$11] for GaAs on (211) Si, not only at 4 K but also at 77 K. The polarization of peak A at 77 K cannot be attributed to the polarization property of defect-induced bound excitons, since exciton emission becomes weaker drastically with increasing temperature and will not appear at 77 K. The peak A at 77 K is dominated by band-to-band emission. Bert et al.[14] reported that band-to-band emission from cleaved surface perpendicular to (100) surface of lattice mismatched InGaAsP epitaxial layer on (100) InP at 77 K is polarized. This is due to the anisotropy in strain between [100] direction and (100) plane. The polarization of emission A from (211) GaAs surface on Si at 77 K indicates that the anisotropy in strain exists not only between [211] direction and (211) plane but also between [$\bar{1}$11] and [0$\bar{1}$1] directions in (211) plane. This may be understood in terms of the anisotropic strain relaxation in GaAs on (211) Si by the generation of dislocations which are along {111} slip plane, while the strain relaxation is isotropic in GaAs on (100) Si.

4. Conclusions

The PL of GaAs on Si grown by MOCVD has been studied. The peaks in low-temperature PL spectra are attributed to defect-induced bound excitons, carbon acceptors and defect complexes. The relative intensity of exciton peak increases and that of defect compex peak decreases in the spectra of GaAs on Si substrates with orientations exact (100), several degrees off (100) tilted around <011> axis and exact (211), in that order. The polarization properties of PL suggest the anisotropy of strain in the growth plane of GaAs on (211) Si.

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