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Interface Stress at InGaPAs/GaAs Heterojunction

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Interface stress at InGaPAs/GaAs heterostructure has been investigated using the energy shift and splitting of the Cr-related zero-phonon photoluminescence line at 0.839 eV in the GaAs:Cr substrate. It has been found that both the compressive uniaxial stress and the tensile hydrostatic pressure act on the substrate side of the heterostructure, on the basis of the results about the shift and splitting of the luminescence line.

§1. Introduction

Much attention has been paid to effects of the interface stress at a heterojunction. The interface stress induced by a lattice mismatch in a heteroepitaxy plays an important role in the interfacial electrical properties as well as the physical properties of the epi-layer. For example, especially in a semiconductor laser, a degradation occurs accompanied with a dark-line-defect (DLD) due to the misfit stress at the heterojunctuon. In general, such interface stress has been estimated by the strain-stress relationship in connection with of the lattice mismatch by X-ray diffraction measurements[1]. However, such a method cannot enable us to obtain a net magnitude of the stress at the hetero-interface, since the stress can be easily relaxed by the formation of misfit dislocation, and the analyzed region is too large compared with the interface region in problem. In recent years, Raman scattering has come to be used to estimate the stress at the heterostructures such as silicon-on-sapphire (SOS)[2] and InGaAs/GaAs[3]. Raman spectra are, however, insensitive to the stress. The detection limit is about 100 MPa (10^9 dyn/cm^2) and therefore the Raman measurement is restricted to the heterostructure with extremely large stress.

From these points of view, a new powerful technique for the characterization of the interface stress is strongly desired. We have previously demonstrated that the Cr-related photoluminescence (PL) zero-phonon line at 0.839 eV is very sensitive to the residual stress, and that the residual stress in a plastically-bent semi-insulating GaAs:Cr wafer can be characterized with respect to its magnitude and direction[4].

In this work, we have applied this PL method to the characterization of the stress at the interface of the $In_{1-x}Ga_xP_{1-y}As_y$ ($y \sim 0.04$)/GaAs heterostructure, which is very important for the fabrication of a visible-light semiconductor laser. The systematic measurements on the Cr-related zero-phonon line at 0.839 eV have been done for a series of (100) or (111) oriented InGaPAs/GaAs:Cr heterostructure with different lattice mismatch and the results are discussed in connection with the stress-strain analysis.

§2 Experimental

Samples used in this work were a series of InGaPAs/GaAs:Cr heterostructures with different lattice mismatches. The InGaPAs layers of 3 μm in thickness were grown on the (100) or (111) oriented GaAs:Cr substrate of 350 μm in thickness by liquid phase epitaxy (LPE) at 785°C or 795°C using the two-phase melt method with excess GaP sources as described elsewhere[5]. The InGaPAs LPE layer has the energy gap of 1.9 eV since the InGaPAs LPE layer was grown from the In-rich melt containing very small As (0.05 at.%).

PL measurements were carried out with specimens directly immersed in the liquid He at 4.2K. The InGaPAs/GaAs:Cr heterostructure was photo-excited from the InGaPAs LPE-layer side by the 514.5 nm CW radiation of an Ar^+ laser. The other part of measurement system was the same as we have reported previously[4].

§3. Results and discussion

With the photo-excitation of InGaPAs epi-layer ($E_g \sim 1.9$ eV) by the 514.5 nm (2.41 eV) Ar^+ laser, the PL emission from the GaAs substrate can be observed as well as that of the InGaPAs epi-layer. The emission intensity from the GaAs substrate was comparable with that from the InGaPAs epi-layer. Since the photon energy of the excitation radiation is $\sim$0.5eV larger than the energy gap of the epi-layer, and since the thickness of the epi-layer ($\sim 3\mu m$) is large enough to absorb the excitation radiation completely, the PL emission obtained from the GaAs side is probably due to the photo-excitation by the near-band-edge emission of the InGaPAs epi-layer or due to the diffusion of the photo-excited carrier from the InGaPAs surface region to the interface region. Therefore, it is tought that the main emission from GaAs comes from the interface region between InGaPAs and GaAs.

Figure 1 shows the Cr-related PL spectra of GaAs in the 0.839 eV region for (100) InGaPAs/GaAs:Cr heterostructures with different lattice mismatches together with that of a GaAs:Cr semi-insulating wafer. It can be seen in the figure that the peak at 0.8396 eV in GaAs:Cr shifts to lower energy and the half-width (FWHM) becomes larger as the lattice mismatch perpendicular to the interface ($\Delta a/a$) increases. This shift and the FWHM increase of the 0.8396 eV peak are considered to be due to the stress existing at the InGaPAs/GaAs:Cr hetero-interface, not due to other effects such as thermal damage, based on the following results. For one reason, the negative peak shift increases as $\Delta a/a$ increases, as can be seen in Figs.1 and 2. Moreover, the thickness of the InGaPAs epi-layer (d_e) is changed by the successive etching of the epi-layer and the peak shift has been measured as a function of d_e. The result is, as indicated in Fig.3, that the negative peak sift becomes smaller linearly as d_e decreases and becomes zero when d_e is zero. In the same manner, it was found that the negative peak shift is inversely proportional to the substrate thickness (d_s). Therefore the peak shift is proportional to the thickness ratio d_e/d_s, which satisfies the following stress-strain formulation indicated in eq.(1) with the assumption $d_e/d_s \ll 1$. In the InGaPAs/GaAs heterostructure, the lattice mismatch is positive, i.e. the unstrained lattice constant of the InGaPAs epi-layer is larger than that of the GaAs

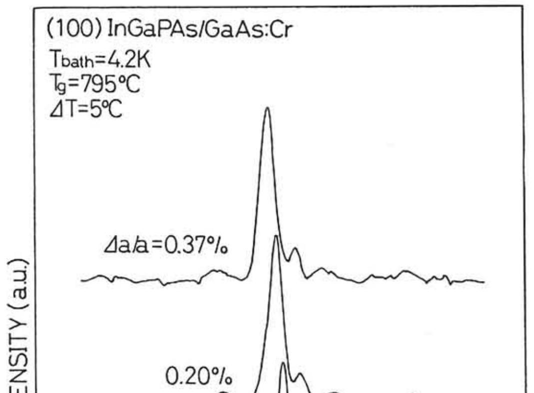

Fig.1 Cr-related PL spectra of GaAs emitted from (100) InGaPAs/GaAs:Cr heterostructure with various lattice mismatches.

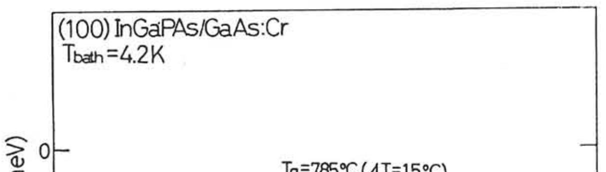

Fig.2 Peak shift of Cr-related PL line at 0.8396 eV plotted as a function of lattice mismatch perpendicular to the interface.

substrate. If the lattice mismatch is not so large, the InGaPAs epi-layer is tetragonally deformed due to a biaxial compressive stress parallel to the [100] or [111] axis, T^e_{xx} and T^e_{yy}. Therefore the GaAs substrate suffers a biaxial tensile stress, T^s_{xx} and T^s_{yy}, to satisfy the balance of the total forces. In this case $T^s_{xx}=T^s_{yy}$ and T^s_{xx} for the (100) orientation is expressed as

$$T^s_{xx}=\frac{-C^e(d^e/d^s)(\Delta a/a)}{\frac{C^e_{11}+2C^e_{12}}{2C^e_{12}}+\frac{C^s_{11}+2C^s_{12}}{2C^s_{12}}\,\frac{C^e d^e}{C^s d^s}} \quad (1)$$

where

$$C^k=(2C^k_{12}-(C^k_{11}+C^k_{12})/2C^k_{12})),\ k=e,s \quad (2)$$

and C^e_{ij} and C^s_{ij} are the elastic stiffness of the epi-layer and the substrate, respectively. These tensile biaxial stress acting on the substrate can be decomposed into a compressive uniaxial stress component, T^s_z, and a tensile hydrostatic pressure component, P^s. T_z and P^s are expressed as

$$T^s_z=-T^s_{xx}\left(1+\frac{T^s_{xx}}{C^s_{11}+2C^s_{12}}\right)^{-1} \quad (3)$$

$$P=(C^s_{11}+2C^s_{12})(K^3-1)/3 \quad (4)$$

where

$$K=(C^s+C^s_{11}T^s_{xx})/(C^s-C^s_{12}T^s_z) \quad (5)$$

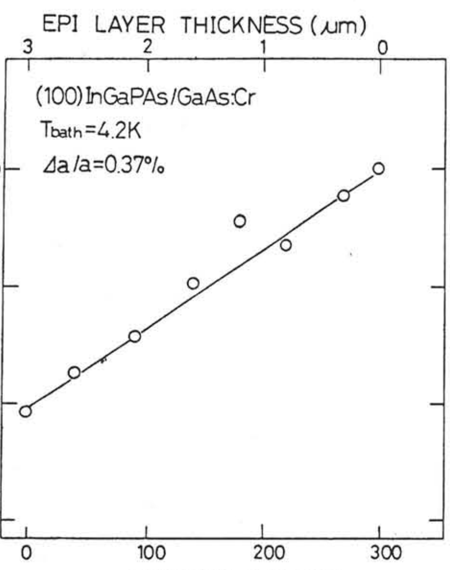

Fig.3 Peak shift of Cr-related PL line at 0.8396 eV plotted as a function of the thickness ratio of epi-layer and substrate for (100)InGaPAs/GaAs with $\Delta a/a$ of 0.37 %.

$$C^s=C^s_{11}(C^s_{11}+C^s_{12})-2C^s_{12} \quad (6).$$

If T^s_{xx} is small compared with the elastic stiffness, T^s_z and P^s are proportional to T^s_{xx}. For typical values of $\Delta a/a$ of 0.2 % and d_e/d_s of 0.01, we obtain T^s_{xx}= 1.2 x 10^7 dyn/cm^2, T^s_z= 1.2 x 10^7 dyn/cm^2 and P^s= 1.2 x 10^7 dyn/cm^2. According to the uniaxial stress data, the uniaxial stress along [100] crystallographic axis does not cause the main peak shift but splits it off[4,6]. In this case, T^s_z of 1.2 x 10^7 is not enough to split the line. However, the increasing FWHM of the PL line indicates the unresolved splitting of the PL line. Therefore, the T^s_z estimated in this experiment is the order of 10^7 dyn/cm^2 and agrees with the calculated value.

Let us consider the hydrostatic pressure component. Since the uniaxial stress does not cause the main peak shift, the negative peak shift observed in Figs.1 and 2 is considered to be due to the hydrostatic component. From the stress analysis, it is thought that the tensile hydrostatic pressure acts on the GaAs substrate. The tensile hydrostatic pressure component

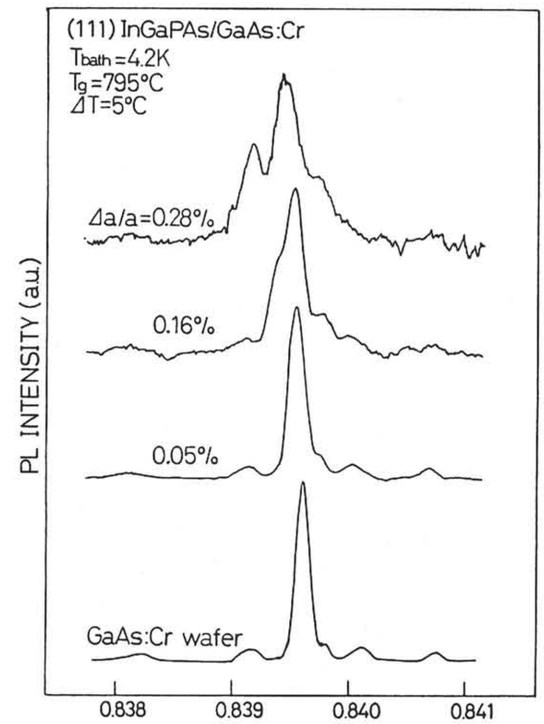

Fig.4 Cr-related PL spectra of GaAs emitted from (111) InGaPAs/GaAs:Cr heterostructure with various lattice mismatches.

increases the lattice constant and therefore decreases the crystal field around the Cr ion at the Ga site in GaAs. This decrease of the crystal field decrease the transition energy between $^5E-^5T_2$, responsible for the 0.839 eV PL line. Therefore the negative shift of the Cr-related PL line is interpreted in terms of the hydroststic pressure component. Unfortunately, the hydrostatic pressure coefficient of the Cr-related PL line at 0.8396 eV has not yet been measured and we can not obtain the magnitude of the pressure component at the interface from this shift of the PL line.

In Fig.2, the peak shift of the PL line at 0.8396 eV in (100) InGaPAs/GaAs:Cr is plotted as a function of $\Delta a/a$. The results of the two series of samples grown with the different supercooling (ΔT) are shown. Though the PL line of both series shifts to lower energy as $\Delta a/a$ increases, the series with ΔT of 15°C shows smaller shift than that with ΔT of 5°C. This fact suggests that the relaxation of stress occurs in the LPE growth with ΔT of 15°C. This may be due to the formation of the transition layer or misfit dislocation due to the large ΔT.

It is also observed that the negative peak shift of $\sim$0.04 meV is observed even in the sample with $\Delta a/a$ of 0%. This may be due to the stress caused by the positive $\Delta a/a$ at 4.2K caused by the difference of in thermal expansion between InGaPAs and GaAs during the cooling process from room temperature to 4.2K.

In Fig.4, the Cr-related PL spectra in (111) InGaPAs/GaAs hetero-structures with different lattice mismatches are shown. As can be seen in the figure, a new line appears in the low energy side of the main peak and the main peak shifts to lower energy as $\Delta a/a$ increases. The line shape of these spectra is in good agreement with that of plastically bent GaAs samples with uniaxial compressive stress along the [111] direction[4]. In the uniaxial compressive stress, the main peak shifts to higher energy with the stress. Therefore, the negative peak shift shown in Fig.4 is due to the tensile hydrostatic pressure component. The uniaxial stress component present at this heterostructure can be obtained from the splitting of the line using the results of the uniaxial stress experiment previously reported[4,6]. The value obtained for the sample with $\Delta a/a$ of 0.28 % shown in Fig.4 is 2.5×10^8 dyn/cm^2, which is five times as large as the calculated value of 4.4×10^7 dyn/cm^2 using the similar relation for (111) orientation to eqs.(1) and (3). Compared with the measurements of (100) oriented samples, the interface stress at (111) InGaPAs/GaAs is larger than that at the (100) case.

In the present study, we have characterized the interface stress from the substrate side. The stress acting on the epi-layer can be easily estimated with a simple multiplication of the interface stress acting on the substrate by a factor of $-(d_s/d_e)$.

§4. Conclusion

The interface stress at the InGaPAs/GaAs heterostructure has been characterized using the energy shift and splitting of the Cr-related zero-phonon photoluminescence line at 0.839 eV of the GaAs:Cr substrate at 4.2K. We have illustrated the existence of both compressive uniaxial stress and the tensile hydrostatic pressure components acting on the GaAs substrate side of the InGaPAs/GaAs heterostructure.

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