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Strain relaxation in $In_{0.2}Ga_{0.8}As/GaAs$ quantum-well structures by x-ray diffraction and photoluminescence

J. F. Chen, P. Y. Wang, J. S. Wang, and N. C. Chen
Department of Electrophysics, National Chiao Tung University, Hsinchu, Taiwan, Republic of China

X. J. Guo
Department of Materials Science and Engineering, National Tsing-Hua University, Hsinchu, Taiwan, Republic of China

Y. F. Chen
Department of Physics, National Taiwan University, Taipei, Taiwan, Republic of China

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The onset of strain relaxation in $In_{0.2}Ga_{0.8}As/GaAs$ quantum-well structures is investigated. X-ray diffraction shows that when the InGaAs thickness increases beyond its critical thickness, another peak on the right shoulder of the GaAs peak appears, indicating that the top GaAs layer is being compressed in the growth direction by the relaxation of the InGaAs layer. Energy shifts of 44 and 49 meV are observed, respectively, from the strains of the InGaAs and GaAs top layers when increasing the InGaAs thickness from 300 and 1000 Å. These energy shifts are in agreement with theory calculated based on the relaxation process observed in x-ray diffraction, providing evidence that the relaxation occurs from near the bottom InGaAs/GaAs interface while the top interface still remains strained. This result is further corroborated by the images of cross-sectional transmission electron micrographs which show that most of the misfit dislocations are confined near the bottom interface. © *2000 American Institute of Physics.* [S0021-8979(00)07303-5]

I. INTRODUCTION

The InGaAs/GaAs material system has many important applications for electronic and optoelectronic devices. However, due to lattice mismatch between InGaAs and GaAs, there exists a critical thickness[1–4] of InGaAs. When the InGaAs increases beyond the critical thickness, strain relaxation generates misfit dislocations and degrades the device performance. Therefore, there is obvious interest in investigating the process associated with strain relaxation and results have been reported by many workers.[5–16] However, relatively little attention has been paid to the process of strain relaxation in InGaAs/GaAs quantum-well structures. We have previously studied the carrier distribution in relaxed InGaAs/GaAs (Ref. 17) quantum wells. We continue this work by using x-ray diffraction, photoluminescence, and cross-sectional transmission electron microscopy (TEM) to study the onset of strain relaxation in this material system.

II. EXPERIMENT

Five $In_{0.2}Ga_{0.8}As/GaAs$ quantum-well structures with InGaAs thicknesses of 100, 200, 300, 400, and 1000 Å were grown on n^+-GaAs(001) substrates by Varian Gen II molecular beam epitaxy. The growth conditions are described in Ref. 17. The growth begins with a 0.3-μm-thick GaAs layer, an InGaAs quantum well of different thickness, and a 0.3-μm-thick GaAs top layer. Both the InGaAs quantum well and the total 0.6-μm-thick GaAs epilayer were all Si doped with a concentration of $6\times10^{16}\,cm^{-3}$. The purpose of Si doping in the InGaAs and GaAs layers is to study the effect of relaxation on the carrier depletion.[17] This $6\times10^{16}\,cm^{-3}$ concentration allows us to penetrate the depletion region to the InGaAs layer by applying reverse voltage. The whole structure was grown at 550 °C. The thickness and composition of InGaAs were determined by oscillation of high-energy electron diffraction and confirmed by cross-sectional TEM.

III. MEASUREMENT AND RESULTS

A. X-ray diffraction

To determine the strain relaxation, the samples were examined by means of the double-crystal x-ray (004) diffraction technique, the results of which are shown in Fig. 1. The peaks at about 33° come from the GaAs layers. For the cases of 100 and 200 Å, because of its high-quality interface, the interference pattern can be observed clearly. The experimental peak positions of the interference pattern are consistent with our calculated values of θ as indicated by arrows in Fig. 1 by using $2d\sin\theta=n\lambda$ (where $\lambda=1.54\,Å$), by choosing $n=141$, 140, 139, and 138 for $d=200\,Å$ and $n=70$, and 69 for $d=100\,Å$. However, when the InGaAs thickness increases to 300 Å, the interference pattern disappears and only the InGaAs peak is visible. The InGaAs peaks are at the same angular position for 300 and 400 Å. However, when increasing to 1000 Å, the InGaAs peak moves to the right, showing a significant relaxation of the InGaAs layer. Figure 1 shows that when the InGaAs thickness increases to 300 Å, a bump on the right shoulder of the GaAs peak appears, suggesting that the top GaAs layer is being compressed in the growth direction by the relaxed InGaAs layer. This argument is supported by the movement of this bump to the right

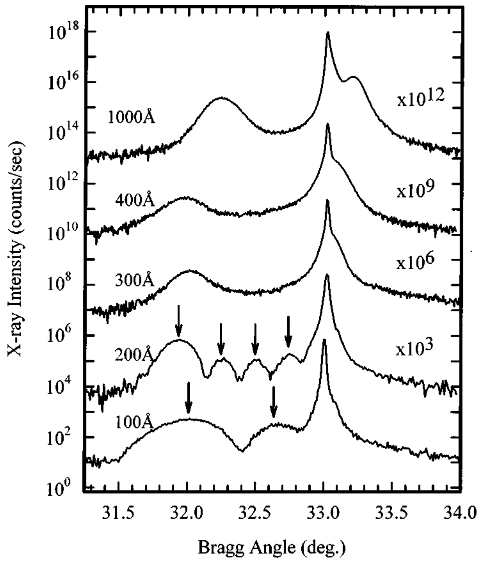

FIG. 1. Double-crystal x-ray rocking curves along the (004) diffraction for $In_{0.2}Ga_{0.8}As$/GaAs quantum-well structures with InGaAs thicknesses of 100, 200, 300, 400 and 1000 Å. The GaAs peaks are set to be about 33° on the angular scale. The peak positions of the interference pattern are calculated and are indicated by arrows.

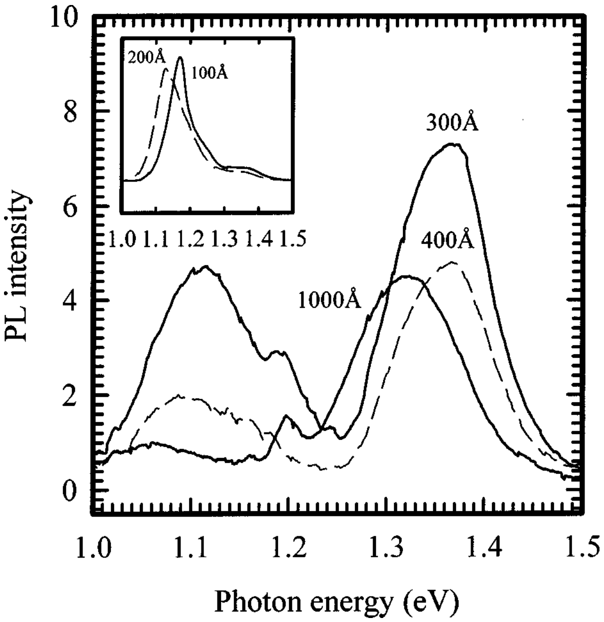

FIG. 2. Photoluminescence at 300 K for $In_{0.2}Ga_{0.8}As$/GaAs quantum-well structures with InGaAs thicknesses of 300, 400, and 1000 Å. Shown in the inset is the photoluminescence for $In_{0.2}Ga_{0.8}As$/GaAs quantum-well structures with InGaAs thicknesses of 100 and 200 Å.

with increasing InGaAs thickness. This feature suggests that when the InGaAs layer relaxes it starts presumably from the InGaAs/GaAs bottom interface while the top interface still remains strained. If the top interface remains strained, the lattice constant parallel to the interface $a_{\parallel}$ should be the same for the top GaAs and relaxed InGaAs layers. Therefore, the top GaAs layer is compressed along the growth direction, providing the bump on the shoulder of the GaAs peak.

To support this relaxation process, the peak position of the bump for the 1000 Å case is calculated here. Based on the In composition, the elastic constants for InGaAs are taken from interpolating $C_{11}=8.329\times 10^{11}$, $C_{12}=4.526\times 10^{11}\,\text{dyn/cm}^2$ for InAs, and $C_{11}=11.88\times 10^{11}$, $C_{12}=5.38\times 10^{11}\,\text{dyn/cm}^2$ for GaAs. Figure 1 shows the peak position of InGaAs is at 32.25°, which gives the lattice constant of the InGaAs perpendicular to the interface $a_{(\text{InGaAs})}$ is 5.7738 Å. According to $a=(1-\sigma_{\text{ST}}f)a$,[18] the lattice mismatch f is determined to be 7.2562×10^{-3}, where $\sigma_{\text{ST}}=2C_{12}/C_{11}$ and a is the free-standing (unstrained) lattice constant. Next, from $a_{\parallel}=(1+f)a$, $a_{\parallel(\text{InGaAs})}$ is calculated to be 5.693 988 Å. Because the top GaAs is expanded by InGaAs, from $a_{\parallel(\text{top GaAs})}=a_{\parallel(\text{InGaAs})}$ and proceeds in a similar way, $a_{(\text{top GaAs})}$ is calculated to be 5.6175 Å. Therefore, the bump should appear at 33.26°, considering the influence of the main GaAs peak, which is reasonably close to the experimental value of 33.21° as shown in Fig. 1.

The appearance of the bump for the case of 300 Å indicates that the InGaAs layer is partially relaxed, accompanied by the absence of the interference pattern, a conclusion is drawn that the critical thickness for the $In_{0.2}Ga_{0.8}As$/GaAs quantum well is between 200 and 300 Å. It should be noted that this information is difficult to obtain simply by the peak separation between GaAs and InGaAs due to a lack of sensitivity of the x-ray measurement for small relaxation. The critical thickness determined here is consistent with the transition of the carrier distribution from confinement to depletion previously observed from $C-V$ measurement.[17] The results of the x-ray diffraction show that when the InGaAs thickness exceeds the critical thickness, the top GaAs layer is being compressed in the growth direction by the relaxation of the InGaAs layer.

B. Photoluminescence

Figure 2 shows the photoluminescence PL spectra at 300 K of the samples with InGaAs thicknesses of 300, 400, and 1000 Å. The photoluminescence spectra for the samples with InGaAs thicknesses of 100 and 200 Å are shown in the inset. For the 100- and 200-Å-thick samples, strong InGaAs peaks were observed, respectively. For the 300-Å-thick samples, the InGaAs peak (at 1.114 eV) reduces in intensity and another peak at 1.367 eV can be seen, which is thought to come from the top GaAs layer. Similarly, the 400- and 1000-Å-thick samples also show two peaks originating from the InGaAs and GaAs top layers, respectively. If we compare their peaks to the 300- to 1000-Å-thick samples, we find that the InGaAs and GaAs top-layer peaks shift to the left by 44 and 49 meV, respectively. Based on the observation in the x-ray diffraction that the top GaAs layer is being compressed in the growth direction by the relaxation of the InGaAs layer, the energy peak shift due to elastic strain is calculated. Referring to the model by Asai,[19] considering only the first-order term, the energy peak shift is expressed by

$$\Delta E=\left[-2a\left(\frac{C_{11}-C_{12}}{C_{11}}\right)+b\left(\frac{C_{11}+2C_{12}}{C_{11}}\right)\right]\epsilon.$$

Here, ΔE is the energy shift due to strain, $C_{11}(=11.1698\times 10^{11}\,\text{dyn/cm}^2)$, $C_{12}(=5.2092\times 10^{11}\,\text{dyn/cm}^2)$ are elastic constants as mentioned in the section on x-ray diffraction, and a and b are the hydrostatic potential and shear deformation potential. We obtain $a = -9.016\,\mathrm{eV}$ and $b = -1.72\,\mathrm{eV}$ for $\mathrm{In_{0.2}Ga_{0.8}As}$ by interpolation from $a_{\mathrm{InAs}} = -6.0\,\mathrm{eV}$, $b_{\mathrm{InAs}} = -1.8\,\mathrm{eV}$, $a_{\mathrm{GaAs}} = -9.77\,\mathrm{eV}$, and $b_{\mathrm{GaAs}} = -1.7\,\mathrm{eV}$.

Here, we will calculate the energy peak shift based on the observation by the x-ray diffraction that the top GaAs layer is expanded by the relaxation of the $\mathrm{In_{0.2}Ga_{0.8}As}$ layer. Let us calculate the energy shift of the $\mathrm{In_{0.2}Ga_{0.8}As}$ peak from the 300 to 1000 Å case first. From the x-ray diffraction, the top GaAs layer is expanded by the relaxation of the $\mathrm{In_{0.2}Ga_{0.8}As}$ layer. Therefore, for both the 300 and 1000 Å cases, the lattice constants parallel to the growth surface are assumed to be the same for the top GaAs and $\mathrm{In_{0.2}Ga_{0.8}As}$ layer, that is, the parallel lattice constant $a_{\mathrm{InGaAs}}^{1000\,\text{Å}}$ of the $\mathrm{In_{0.2}Ga_{0.8}As}$ layer for the 1000 Å case is equal to $a_{\mathrm{GaAs}}^{\mathrm{top}} = 5.693\,988\,\text{Å}$ previously determined from the x-ray diffraction. The parallel lattice constant $a_{\mathrm{InGaAs}}^{300\,\text{Å}} (= 5.6533\,\text{Å})$ of $\mathrm{In_{0.2}Ga_{0.8}As}$ for the 300 Å case is converted from the perpendicular lattice constant from the $\mathrm{In_{0.2}Ga_{0.8}As}$ peak in the x-ray spectra as shown in Fig. 1. Because the position of the $\mathrm{In_{0.2}Ga_{0.8}As}$ peak for the 300 Å case is very close to that of a totally strained $\mathrm{In_{0.2}Ga_{0.8}As}$ layer, $a_{\mathrm{InGaAs}}^{300\,\text{Å}}$ is almost equal to the free-standing lattice constant a_{GaAs} of GaAs. Thus, the mismatch is calculated to be

$$\epsilon_{\mathrm{InGaAs}} = \frac{a_{\mathrm{InGaAs}}^{300\,\text{Å}} - a_{\mathrm{InGaAs}}^{1000\,\text{Å}}}{a_{\mathrm{InGaAs}}} = -7.0956 \times 10^{-3}.$$

Here, $a_{\mathrm{InGaAs}} = 5.7343\,\text{Å}$ is the free-standing lattice constant of InGaAs. Substituting into the energy shift equation, we obtain $\Delta E = -45\,\mathrm{meV}$ for the peak shift of the $\mathrm{In_{0.2}Ga_{0.8}As}$ layer. This calculated value based on the relaxation process observed in the x-ray diffraction is in agreement with the observed peak shift of 44 meV from the 1000 to 300 Å sample in the PL spectra.

Let us calculate the energy shift of the top GaAs layer from the 300 to 1000 Å case. Based on the x-ray diffraction, the parallel lattice constant for the top GaAs is the same as the $\mathrm{In_{0.2}Ga_{0.8}As}$ layer under it, the mismatch is

$$\epsilon_{\mathrm{GaAs}} = \frac{a_{\mathrm{GaAs}}^{300\,\text{Å}} - a_{\mathrm{GaAs}}^{1000\,\text{Å}}}{a_{\mathrm{GaAs}}} = -7.1972 \times 10^{-3}.$$

Here, $a_{\mathrm{GaAs}}^{300\,\text{Å}} = a_{\mathrm{InGaAs}}^{300\,\text{Å}} = 5.6533\,\text{Å}$ and $a_{\mathrm{GaAs}}^{1000\,\text{Å}} = a_{\mathrm{GaAs}}^{\mathrm{top}} = 5.693\,988\,\text{Å}$ from the x-ray diffraction. We obtain $\Delta E = -53\,\mathrm{meV}$ for the peak shift of the GaAs top layer from the 300 to 1000 Å sample. This value is close to the peak shift of 49 meV observed from the PL spectra. The agreement for both the InGaAs and GaAs peak shifts confirms the basic assumption for the calculation that the top GaAs layer is totally expanded by the relaxed InGaAs layer. This result provides another evidence for the relaxation process observed in x-ray diffraction that the relaxation occurs near the bottom InGaAs/GaAs interface while the top interface still remains strained.

C. Cross-sectional transmission electron microscopy (TEM)

In order to see the structural properties, cross-sectional transmission electron microscopy images were taken for all samples. The TEM images for the 300 and 1000 Å cases are shown in Figs. 3(a) and 3(b), respectively. For the 200 Å case (below the critical thickness), the interface between InGaAs and GaAs is smooth with very few dislocations, which are about 2–3 μm apart, scattered around. For the 300 Å case, as shown in Fig. 3(a), many more dislocations can be seen around the bottom interface, which are about 300–500 Å apart. Some dislocations are found to penetrate into the bottom GaAs layer and bent along the interface direction, forming dislocation networks.[14,15] For the 1000 Å case, many more dislocations including dislocation networks, threading dislocations, and stacking faults, can be seen with dislocations being bent much deeper into the GaAs bottom layer. Some of the threading dislocations and stacking faults are seen to propagate toward the top GaAs cap layer.

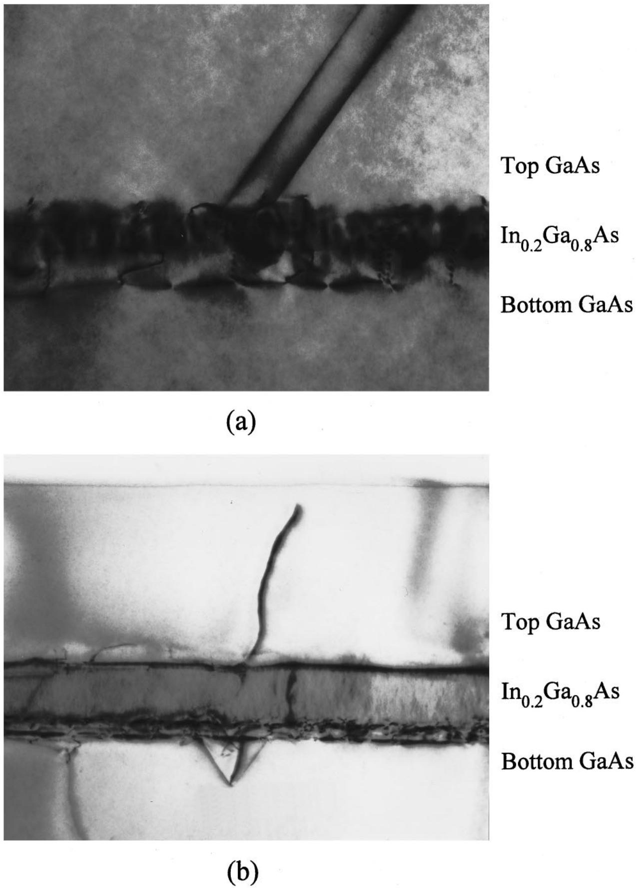

FIG. 3. Cross-sectional transmission electron micrographs for $\mathrm{In_{0.2}Ga_{0.8}As}$/GaAs quantum-well structures with InGaAs thicknesses of (a) 300 and (b) 1000 Å.

As can be clearly seen in Fig. 3(b), TEM images show that most of the misfit dislocations are confined near the bottom interface of InGaAs and GaAs. Elastic strain created by lattice mismatch between GaAs and InGaAs is believed to confine the dislocations by bending.[10] This dislocation confinement is consistent with the observations by the x-ray diffraction and PL energy shifts that the strain relaxation occurs near the bottom InGaAs/GaAs interface while the top interface still remains strained.

IV. CONCLUSIONS

The onset of the relaxation process in $In_{0.2}Ga_{0.8}As$/GaAs quantum-well structures is investigated by x-ray diffraction. We found that when the InGaAs thickness increases beyond its critical thickness, the top GaAs layer is being compressed in the growth direction by the relaxation of the InGaAs layer. This relaxation process is supported by the peak shifts in photoluminescence. The experimental peak shifts due to the elastic strains in the InGaAs and the top GaAs layers are in agreement with the theoretical calculation based on this proposed relaxation process. This result is further supported by the cross-sectional TEM images, which show that most of the misfit dislocations are confined near the bottom interface, leading us to conclude that the relaxation occurs near the bottom InGaAs/GaAs interface while the top interface still remains strained.

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