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Transition of carrier distribution from a strained to relaxed state in InGaAs/GaAs quantum well

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This work investigates the transition of carrier distribution from the strained to the relaxed state in InGaAs/GaAs quantum well by measuring capacitance voltage and analyzing x-ray diffraction. According to these results, there is carrier confinement in the InGaAs quantum well with well thickness less than the critical thickness. Increasing the well thickness beyond the critical thickness leads to a significant carrier depletion around the quantum well. Double-crystal x-ray rocking curves reveal that when InGaAs well thickness increases beyond the critical thickness, the interference pattern disappears and relaxation begins to occur from near the bottom InGaAs/GaAs interface while the top interface still remains strained. Results obtained from the critical thickness determined from x-ray diffraction correspond to the transition of carrier distribution, illustrating that the capacitance–voltage measurement is a rather effective means of determining the critical thickness.

The InGaAs/GaAs material system has been extensively applied in electronic and optoelectronic devices. However, due to lattice mismatch between InGaAs and GaAs, there exists a critical thickness of InGaAs, beyond which strain relaxes, accompanied by the generation of misfit dislocations, subsequently degrading device performance. Therefore, precisely determining the critical thickness is essential for fabricating high quality optoelectronic devices. Many problems in this system such as strain relaxation, misfit dislocations, and deep traps have been studied by Hall effect, double-crystal x-ray diffraction, photoluminescence, deep-level transient spectroscopy, capacitance–voltage (C–V) method and cross-sectional transmission electron microscopy. However, some of these measurement results are not consistent with each other. For example, the critical thickness reported by Laidig et al. from x-ray diffraction is more than a factor of 2, i.e., larger than that determined from the efficiency of stimulated emission. In addition, the critical thicknesses determined from different theoretical models, such as the energy balance model of People and Bean and the mechanical equilibrium model of Matthews and Blakeslee, significantly differ from each other. Therefore, the critical thickness and the nature of lattice strain and relaxation must be more thoroughly elucidated.

Although C–V measurement has been used to examine the carrier distribution, the correlation between the carrier distribution and the critical thickness has not been studied in detail. Therefore, in this investigation, we use C–V measurement to investigate the transition of carrier distribution in InGaAs/GaAs quantum well from the strained to the relaxed state by varying the InGaAs well width. To correlate these results with strain relaxation, the double-crystal x-ray diffraction is performed to characterize the samples.

Five InGaAs/GaAs quantum well structures with the well width varying from 100 to 1000 Å were grown on n+–GaAs(001) substrates by Varian Gen II molecular beam epitaxy. The InGaAs quantum well, which is located 0.3 μm from the surface, was immersed in a GaAs Schottky diode to provide the C–V measurement. Both the InGaAs quantum well and the total 0.6-μm-thick GaAs epilayer were all Si doped with a nominal concentration of 6×10^16 cm^-3. The entire structure was grown at 550 °C to avert any unnecessary interruptions in growth which might incorporate some undesired impurities into the interfaces of the quantum well. The thickness and composition of InGaAs were then determined by oscillation of reflection high energy electron diffraction. Finally, Schottky diodes were fabricated by evaporating Al on samples with a dot diameter of 1500 μm.

Figure 1 summarizes the C–V measurement results for the five samples at reverse bias. These curves can be separated into two groups. One group consists of samples with small well widths of 100 and 200 Å. The capacitance of these samples falls initially in a well-behaved manner and then levels off at −3 to −5 V and again falls thereafter. Another group consists of samples with large well widths of 300, 400, and 1000 Å. The capacitance of these three samples falls sharply and then levels off at approximately −2 V, implying that the depletion region reaches down to the substrate when the applied voltage surpasses −2 V.

Figure 2 presents the corresponding carrier depth profiles from C–V measurement. A concentration peak obviously appears for samples with small well widths of 100 and 200 Å, implying the existence of carrier confinement in the quantum well. The broader peak for 200 Å reflects its larger...
Herein, a numerical simulation resembling that used by Missous and Rhoderick is undertaken on the C-V and carrier depth profile by solving the Poisson equation. The inset of Fig. 2 displays the simulated (solid dots) and experimental (curve) carrier profiles for the well width of 100 Å. Simulation results can correlate well with the carrier profiles for well widths of 100 and 200 Å with a good accuracy, indicating that the quantum structures are of high quality for both cases.

Figure 2 also reveals markedly different carrier distributions for well widths of 300, 400, and 1000 Å. Instead of containing peaks, their curves illustrate that the carriers in the quantum well are depleted. This carrier depletion is so pervasive that it goes beyond the quantum well region and spreads to GaAs layers on both sides. This carrier depletion is possibly attributed to the fact that when the InGaAs thickness increases to 300 Å, misfit dislocations occur from strain relaxation. These misfit dislocations act like traps which deplete carriers both in the quantum well and the GaAs layers around it. If this assumption is valid, the critical thickness for In0.2Ga0.8As quantum well should range between 200 and 300 Å. To verify this assumption, double-crystal x-ray rocking curves along (004) diffraction are taken for all samples, thereby allowing us to directly measure the lattice spacing in the growth direction.

Figure 3 summarizes the results of the double-crystal x-ray diffraction. The GaAs peaks are set to approximately 33° on the angular scale. For the cases of 100 and 200 Å, the interference pattern can be clearly observed where peak positions correlate with our calculation as denoted by the arrows in Fig. 3, showing a good interface flatness of the quantum well. The interference peak positions are calculated as follows. For the case of 200 Å, while considering a slight variation of well width during the growth, we substitute a fitted well width of 200.63 Å into \( d \sin \theta = n \lambda \), where \( \lambda = 1.54 \text{ Å} \), \( \theta \) is calculated to be 32.76°, 32.50°, 32.24°, and 31.98° for \( n = 141, 140, 139, \) and 138, respectively. These values closely resemble the experimental values of 32.75°, 32.50°, 32.26°, and 31.94° in Fig. 3. For the case of 100 Å, using \( d = 100 \text{ Å} \), the calculated \( \theta \) are 32.62° and 32.09° for \( n = 70 \) and 69, which closely resemble the experimental values of 32.68° and 32.04°. However, when InGaAs thickness increases to 300 Å, the interference pattern disappears and only the InGaAs peak is visible. The InGaAs peaks are at nearly the same angular position for 300 and 400 Å. However, when the well width increases to 1000 Å, the InGaAs peak moves to the right, showing the relaxation of the InGaAs layer.

Figure 3 also reveals that when InGaAs thickness increases to 300 Å, a bump on the right shoulder of the GaAs peak appears. The appearance of this bump suggests that a strained GaAs layer exists whose lattice is compressed in the growth direction. Figure 3 reveals that this bump moves to the right with an increasing InGaAs thickness. This observation implies that the compression of this strained GaAs layer in the growth direction is attributed to the relaxation of the

FIG. 1. The C-V measurement of In0.2Ga0.8As/GaAs strain quantum well structures with well thickness 100, 200, 300, 400, and 1000 Å.

FIG. 2. The corresponding carrier concentration depth profiles for In0.2Ga0.8As/GaAs quantum well structures with well width 100, 200, 300, 400, and 1000 Å. Shown in the inset are the simulated (solid dots) and experimental (curve) carrier profiles for the well width of 100 Å.

FIG. 3. Double-crystal x-ray rocking curves along (004) diffraction for In0.2Ga0.8As/GaAs quantum well structures with well width 100, 200, 300, 400, and 1000 Å. The GaAs peaks are set to be about 33° on the angular scale.
InGaAs layer. 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. A previous investigation using photoluminescence measurement observed a similar phenomenon. If this is valid, the lattice constant parallel to the interface \(a_{\parallel}\) should be the same for the top GaAs and the relaxed InGaAs layer. Therefore, the top GaAs layer is compressed along the growth direction, providing the bump on the shoulder of GaAs peak. To prove this assumption, this study also calculates the peak position of the bump for the 1000 Å case. The elastic constants for InGaAs are calculated from the In composition using \(C_{11} = 8.329 \times 10^{11}\), \(C_{12} = 4.526 \times 10^{11}\) dyn/cm\(^2\) for InAs and \(C_{11} = 11.88 \times 10^{11}\), \(C_{12} = 5.38 \times 10^{11}\) dyn/cm\(^2\) for GaAs. From the peak position (32.25°) of InGaAs in Fig. 3, the lattice constant of the InGaAs perpendicular to the interface \(a_{\perp \text{(InGaAs)}}\) is 5.7738 Å. According to \(a_{\perp} = (1 - \sigma_{ST} f)a_{\parallel}\), the lattice mismatch \(f\) is determined to be \(7.2562 \times 10^{-3}\), where \(\sigma_{ST} = 2C_{12}/C_{11}\) and \(a\) denotes the natural (unstrained) lattice constant. Next, from \(a_{\parallel} = (1 + f)a_{\parallel}\), \(a_{\parallel \text{(InGaAs)}}\) is calculated to be 5.6926 Å. Because the fact that the top GaAs is expanded by InGaAs, from \(a_{\parallel \text{(top GaAs)}} = a_{\parallel \text{(InGaAs)}}\) and proceeds in a similar manner, \(a_{\perp \text{(top GaAs)}}\) 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. 3.

The appearance of the bump for the case of 300 Å indicates that the InGaAs layer is partially relaxed. This relaxation is accompanied by the generation of misfit dislocations which degrade the structure quality, as evidenced by the absence of an interference pattern. From these results, we can infer that the critical thickness for InGaAs quantum well ranges between 200 and 300 Å. Notably, this information is difficult to obtain merely by the peak separation between GaAs and InGaAs. Our results further indicate that the calculated perpendicular lattice constant of a strained InGaAs (without relaxation) is in close proximity to the InGaAs peaks for the cases of 300 and 400 Å. This is likely attributed to a lack of sensitivity of x-ray measurement for samples with small relaxation. Figure 3 depicts a slight variation in the InGaAs peaks for 300 and 400 Å, which is likely attributed to a variation of In composition during the sample growth. The critical thickness (between 200 and 300 Å) determined herein corresponds to the transition of carrier distribution from confinement to depletion, as indicated from \(C-V\) measurement.

In summary, this work investigates the correlation between the carrier distribution and critical thickness in InGaAs/GaAs quantum well. According to those results, a transition from carrier confinement to depletion occurs when InGaAs thickness increases beyond the critical thickness. This finding suggests that the capacitance–voltage measurement is a very sensitive technique for determining the critical thickness. X-ray diffraction results indicate that a clear interference pattern can be observed when the InGaAs thickness is below the critical thickness. When the InGaAs layer exceeds the critical thickness, relaxation begins to occur from near the bottom InGaAs/GaAs interface while the top interface still remains strained. The critical thickness determined herein is consistent with the critical thickness reported by Fritz et al. from low temperature Hall-effect measurement and photoluminescence microscopy.

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