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Analysis of strain relaxation in GaAs/InGaAs/GaAs structures by spectroscopy of relaxation-induced states

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Strain relaxation in GaAs/$In_{0.2}Ga_{0.8}As$/GaAs structures is investigated by analyzing relaxation-induced traps. Strain relaxation is shown to cause carrier depletion by the induction of a 0.53 eV trap in the top GaAs layer, a 0.13 eV trap in the InGaAs layer, and a 0.33 eV trap in the neighboring lower GaAs layer. The 0.53 eV trap which exhibits a logarithmic function of transient capacitance is attributed to threading dislocations. The 0.33 eV trap exhibits an exponential transient capacitance, suggesting a GaAs point defect as its origin. Given its activation energy, it is assigned to the EL6 in GaAs, commonly considered to be As_i-V_{Ga} complexes. This trap and the 0.13 eV trap are regarded as the same, since their energy difference is comparable to the optically determined conduction-band offset. The spatial location of this trap correlates with that of misfit dislocations. Accordingly, the production of this trap is determined from the mechanism of strain relaxation. A likely mode of strain relaxation is deduced from the locations of these traps. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2433771]

I. INTRODUCTION

The InGaAs/GaAs material system is very suitable for systematically studying strain relaxation[1–4] because relaxation drastically changes the electrical[5,6] and optical properties of the system, such as photoluminescence (PL) wavelength shift,[7,8] disappearance of x-ray interference patterns,[9] a significant increase in leakage current,[10] and the generation of electrically active traps.[10–17] A relaxation-induced trap at 0.58 eV was previously observed in this system by deep-level transient spectroscopy (DLTS) and was attributed to the cores of α-type dislocations.[12] This trap has similar properties to those of the dislocation-induced trap ED1 observed by Wosinski[16] in plastically deformed GaAs. However, due to the band offset, whether the observed emission energy is related to the GaAs or InGaAs conduction band (CB) is unclear. The effect of interfacial band discontinuity on the emission properties of defect traps has not been well established. Furthermore, deep traps with their localized wave functions have been proposed to be useful as a probe of the interfacial band structure.[18,19] This work characterized the spatial locations of the relaxation-induced traps in a GaAs/InGaAs/GaAs double heterostructure (DH) using DLTS measurements. The results are compared with PL data to elucidate the effect of the interfacial band structure. The likely mechanism of strain relaxation is discussed based on the nature of the traps.

II. EXPERIMENT

The GaAs/$In_{0.2}Ga_{0.8}As$/GaAs DH samples were grown on n^+-GaAs (001) substrates by Varian Gen II molecular beam epitaxy (MBE). The details of the growth can be found elsewhere.[8] The InGaAs layer was immersed between two 0.3-μm-thick n-type GaAs layers. Both the InGaAs and the GaAs layers were doped with Si to a nominal concentration of 6×10^{16} cm^{-3}. The whole structure was grown at 550 °C. The thickness and the composition of the InGaAs layer were determined by the oscillation of reflection high-energy electron diffraction and checked with x-ray (004) double-crystal rocking curves. Metal Au with a dot diameter of 1500 μm was evaporated to fabricate Schottky diodes.

III. MEASUREMENT AND RESULTS

A. *C-V* profiling and DLTS spectra

When the thickness of the $In_{0.2}Ga_{0.8}As$ layer exceeds the critical thickness [between 200 and 300 Å (Ref. 9)], the strain is relaxed and causes carrier depletion in the InGaAs region. Figure 1 presents the apparent-carrier-concentration profiles, converted from the 300 K capacitance-voltage (*C-V*) curves (shown in the inset), measured at 1 kHz for a relaxed sample with a 1000-Å-thick InGaAs layer and a nonrelaxed sample with a 200-Å-thick InGaAs layer. Unlike the InGaAs layer of the 200 Å sample in which carriers accumulate, the InGaAs layer and neighboring GaAs layers of the 1000 Å sample exhibit significant carrier depletion, indicating that the relaxation-induced traps are electron-trapping centers. These traps were revealed by DLTS measurements. Figures 2(a)–2(c) show the DLTS spectra of the 1000 Å sample, measured by sweeping voltages from 0 to −0.5 V, from −1 to −2 V, and from −2.5 to −3.5 V to probe the upper GaAs layer, the InGaAs layer, and the neighboring lower GaAs layer, respectively. Four relaxation-induced traps are identified. The activation energies (capture cross sections) of the traps, except the high-temperature trap in Fig. 2(b), are obtained as 0.53 eV (1.1×10^{-16} cm^2), 0.13 eV (1×10^{-20} cm^2), and 0.33 eV (1.4×10^{-18} cm^2), respectively. Figure 3 shows the Arrhenius plots of the traps at 0.53 and 0.33 eV. These are probably the traps at 0.54 and 0.34 eV observed in relaxed InAs (Ref. 20) self-assembled quantum

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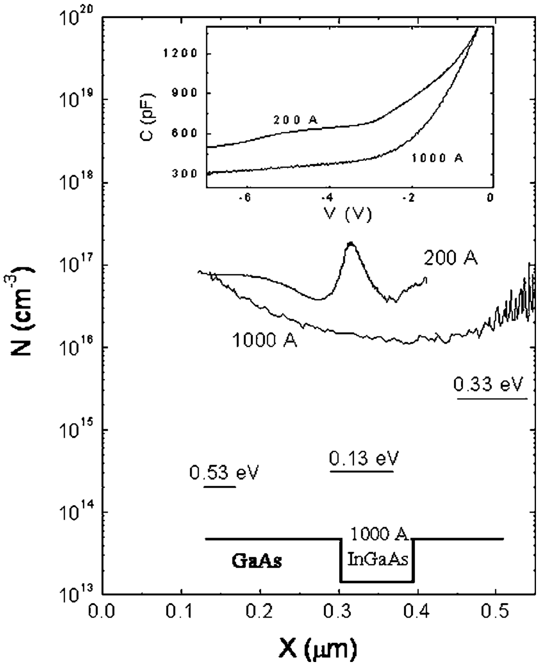

FIG. 1. Apparent-carrier-concentration profiles converted from the *C-V* curves (in the inset) of the GaAs/InGaAs/GaAs samples with 200 and 1000 Å InGaAs layers. The 1000 Å sample exhibits significant carrier depletion in the InGaAs layer and neighboring GaAs layers, due to relaxation-induced traps whose concentrations and spatial locations are as presented in Fig. 2.

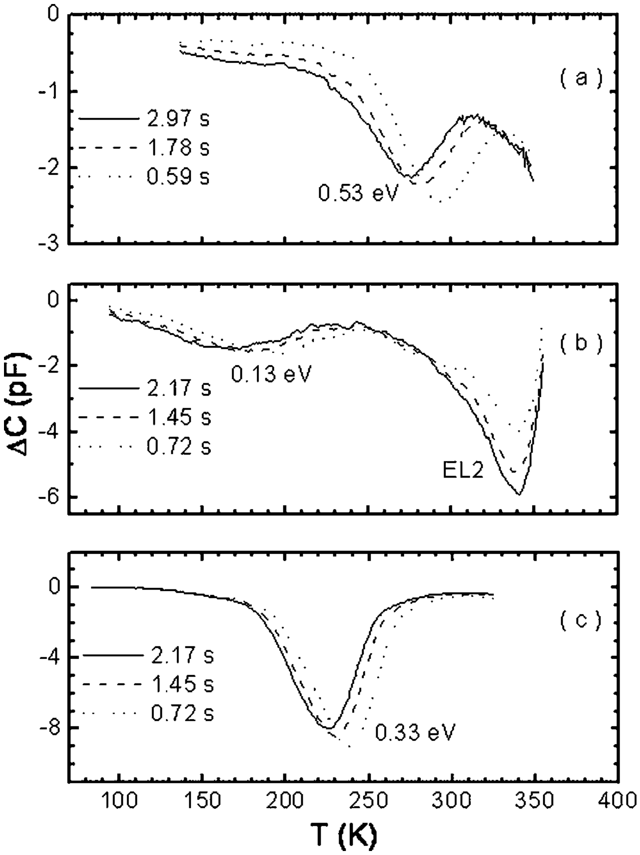

FIG. 2. DLTS spectra of the 1000 Å sample for sweeping voltages (a) from 0 to −0.5 V, (b) from −1 to −2 V, and (c) from −2.5 to −3.5 V, roughly corresponding to the upper GaAs layer, the InGaAs layer, and the lower GaAs layer, respectively. The rate windows are as indicated. The spectra show a trap at 0.53 eV in the top GaAs layer, a trap at 0.13 eV and the EL2 in the InGaAs layer, and a trap at 0.33 eV in the neighboring lower GaAs layer.

dots (QDs) and those at 0.64 and 0.35 eV observed in relaxed InAsSb (Ref. 21) QDs (E1 and E2 in Fig. 3). This result suggests that the relaxation mechanisms in the QDs and quantum-well (QW) structures are similar and that the relaxation-induced traps have distinct emission properties. Understanding the strain relaxation in QW may provide valuable information about the mechanism of strain relaxation in the QDs.

Figure 1 also plots the concentrations of the traps at 0.53, 0.13, and 0.33 eV versus spatial locations. The concentrations were estimated from the expression $(2\Delta C/C)N$, where ΔC is the maximum of the transience in the DLTS spectra and N was the background concentration of 6×10^{16} cm^{-3}. The spatial locations were obtained from their corresponding capacitance C (neglecting the λ effect) of the sweeping voltages used in the DLTS measurements. Since a trap is observed when the Fermi level crosses the trap level, the estimated spatial locations of the traps are shifted to a slightly greater depth. As shown in Fig. 1, the traps at 0.53 and 0.33 eV are clearly located in the upper GaAs layer and the lower GaAs layer, respectively. The trap at 0.13 eV is approximately located in the InGaAs layer. Strain relaxation induces the trap at 0.53 eV with an estimated concentration of about 2×10^{14} cm^{-3} in the top GaAs layer. The intensity of this trap increases with the duration of the filling pulse. The transient-capacitance–time plot of this trap is a logarithmic function,[21] which is a characteristic of the Coulombic repulsion of the carriers captured at the traps along with the linearly arrayed dislocation lines.[16] This trap is therefore attributed to the threading dislocations that were observed by transmission electron microscopy (TEM) images in the top GaAs layer.[8] This trap has similar emission properties to the dislocation-induced trap ED1 observed by Wosinski[16] in plastically deformed GaAs (E1 in Fig. 3) and is probably to be the trap at 0.58 eV that was observed in InGaAs/GaAs by

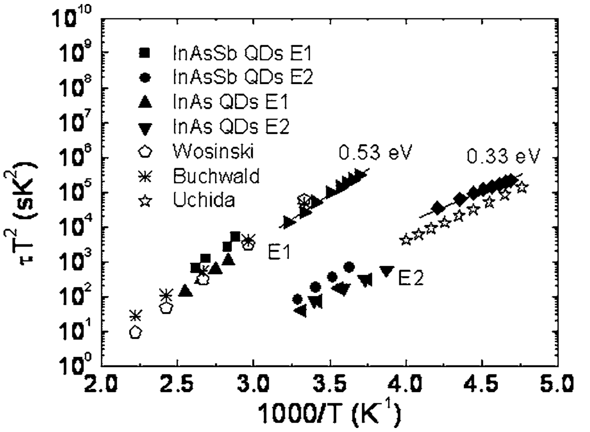

FIG. 3. Arrhenius plots for the traps at 0.53 and 0.33 eV in Fig. 2. Also included are the traps that were previously observed in relaxed InAs (Ref. 20) (E1: 0.63 eV, E2: 0.37 eV) and InAsSb (Ref. 21) (E1: 0.64 eV, E2: 0.35 eV quantum dots, plastically deformed GaAs by Wosinski (Ref. 16), a relaxed $In_{0.083}Ga_{0.917}As$/GaAs sample used by Buchwald *et al.* (Ref. 15), and a relaxed GaAs/$In_{0.2}Ga_{0.8}As$/GaAs sample used by Uchida *et al.* (Ref. 11).

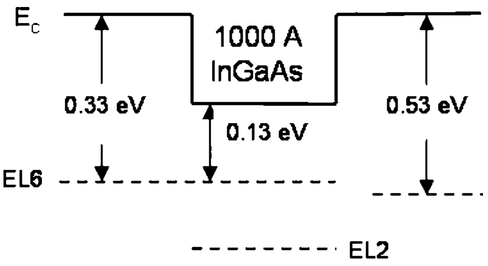

FIG. 4. Simplified conduction-band diagram of energy and spatial locations of the observed traps.

Watson *et al.*[12] who attributed it to the cores of α-type dislocations. Buchwald *et al.*[15] observed a similar trap at 0.58 eV in relaxed $\mathrm{In}_{0.083}\mathrm{Ga}_{0.917}\mathrm{As}$/GaAs sample (E1 in Fig. 3).

Figure 2(b) shows that the InGaAs layer contains the trap at 0.13 eV, with a concentration of 3.1×10^{14} cm^{-3}, and a trap at around 350 K. This high-temperature trap is not well behaved; therefore, its activation energy cannot be determined. However, the temperature range suggests that this trap may be the well-known EL2.[22,23] This assignment was supported by the data of Irvine and Palmer[24] who observed EL2 in a relaxed InGaAs layer grown on GaAs by MBE and attributed it to an interaction between Ga vacancies and misfit dislocations. Figure 2(c) shows that the lower GaAs layer contains the trap at 0.33 eV with a concentration of 2.4×10^{15} cm^{-3}. The magnitude of this trap initially increases and finally saturates as the filling pulse duration time increases. The transient-capacitance–time plot of this trap is an exponential function,[21] suggesting that its origin is an isolated point defect, rather than a dislocation. Since this trap is detected in the GaAs layer, its activation energy is unambiguously related to the GaAs CB edge. By comparison, it is tentatively assigned to the EL6 ($E_c - 0.35$ eV) in GaAs, which is considered to be a $\mathrm{As}_i - V_{\mathrm{Ga}}$ complex.[25] This trap is probably the one at 0.395 eV previously observed by Uchida *et al.*[11] in a relaxed $\mathrm{GaAs/In}_{0.2}\mathrm{Ga}_{0.8}\mathrm{As/GaAs}$ sample (E2 in Fig. 3). Although conclusive evidence is lacking, this trap is considered to be the trap at 0.13 eV observed in the InGaAs layer. The difference between their energies may arise from the fact that this trap is located across the lower interface with a CB offset. The band offset is such that whether its 0.13 eV activation energy is related to the InGaAs or GaAs CB edge is unclear. However, as shown in Fig. 1, the carriers are depleted in the InGaAs layer, and thus the Fermi level falls well below the InGaAs CB edge in the InGaAs layer. If the trap was at 0.13 eV below the GaAs CB edge, due to a CB band offset of 0.2 eV, it would be above the InGaAs CB edge and the carriers therein would be depleted, contradicting the observation that this trap is present with a considerable concentration. Hence, the trap is considered to lie 0.13 eV below the InGaAs CB edge. For a CB band offset of 0.2 eV, this energy happens to align with the trap at 0.33 eV, observed in the lower GaAs layer, suggesting that they are the same. Any energy perturbation at the interface is neglected, and the traps are then presented in the simplified CB diagram in Fig. 4. Upon modulation, the electrons in the 013 eV traps are thermally activated to the InGaAs CB and subsequently to the GaAs bottom electrode. This latter process was not resolved because of its short emission time (which was less than 10^{-6} s at 10 K, estimated from the nonrelaxed samples in which the electron accumulation peak exhibits no frequency-dependent attenuation up to 10^6 Hz at 10 K).

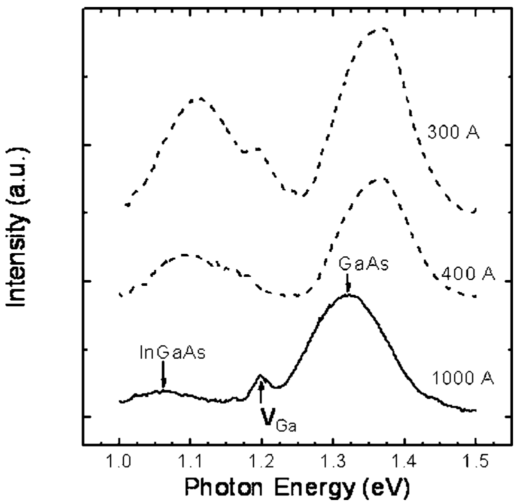

FIG. 5. 300 K PL spectra of relaxed 300, 400, and 1000 Å samples. In each case, the energy separation between the GaAs and InGaAs peaks is about 0.26 eV. The emission at around 1.2 eV is speculated to be a defect emission that is related to Ga vacancies.

B. PL spectra

Figure 5 shows the 300 K PL spectra of the relaxed 300, 400, and 1000 Å samples to evaluate the CB offset. Relaxation causes their PL spectra to be markedly inferior to that of the nonrelaxed samples. Therefore, a relatively high excitation power was used for the measurements, probably causing the sample temperature to exceed 300 K. Each sample clearly shows two emissions from the GaAs and InGaAs layers with an energy separation of about 0.26 eV. If the ratio of the CB and valence-band (VB) offsets is taken as 7.7:2.3 (which is close to the 7:3 reported by Marzin *et al.*[26]), then the CB offset would be 0.2 eV, which is the activation energy difference between the traps at 0.13 and 0.33 eV. Thus, this energy difference is attributed to an effect of band offset. This result suggests the possibility of using this defect trap as a local probe for the interfacial band structure. Figure 5 reveals that, besides the GaAs and InGaAs peaks, the spectra display an additional peak at around 1.2 eV. The origin of this peak is not clear. However, it is suspected to be a defect emission that is related to Ga vacancies. A similar emission around this wavelength was observed in the back-side illumination of the studied samples. This emission is often present in liquid encapsulated Czochralski (LEC) GaAs substrates.[25] Chiang and Pearson[27] and Ohbu *et al.*[28] observed a similar emission (at 1.24 eV) in low-temperature-grown GaAs films and attributed it to a Ga vacancy (V_{Ga}) state. Yu *et al.*[25] observed a broad emission centered on ~1.1 eV in low-temperature-grown GaAs films and also attributed it to a V_{Ga}-related emission. This assignment is supported by the observation of the EL6 ($\mathrm{As}_i - V_{\mathrm{Ga}}$ complexes), since the presence of V_{Ga} favors the formation of the EL6.

C. Mode of strain relaxation

A likely mode of strain relaxation is deduced from the spatial locations of these traps. In a previous work, strain relaxation in the GaAs/InGaAs system occurred at the lower interface, whereas the upper interface remains coherently strained,[14] according to x-ray (004) double-crystal diffraction spectra, which showed an emergent peak on the right-side shoulder of the GaAs peak, suggesting the lateral expansion of the top GaAs layer[8] by the expanded InGaAs layer. This relaxation mode was confirmed by TEM images, which show misfit dislocations in the vicinity of the lower interface.[8] In a similar work,[17] the electron-beam induced current technique revealed a network of misfit dislocations along two orthogonal $\langle 110 \rangle$ directions. The spatial location of the EL6 (As_i-V_{Ga}) correlates with that of the misfit dislocations. Hence, the production of the EL6 is deduced from the strain relaxation. As the InGaAs layer grown on GaAs is laterally compressed, at the critical point, the associated stress can be relieved by removing As atoms from their lattice sites,[24] leading to excess As, probably in the form of As_i. When misfit dislocations are available, As_i may interact with the misfit dislocations and produce Ga vacancies (V_{Ga}) by the reaction[24] $As_i + \text{dislocation} \rightarrow \text{dislocation climb} + V_{Ga}$. The nonzero V_{Ga} is consistent with the 1.2 eV emission in Fig. 5. The induced V_{Ga} can interact with As_i and form As_i-V_{Ga} complexes, leading to the observation of the EL6. With continued InGaAs growth, we suggest a transformation of the EL6 to the EL2 (As_{Ga}) by dissociation of the As_i-V_{Ga} complexes and the subsequent reaction, $As_i + V_{Ga} \rightarrow As_{Ga}$. This transformation can increase the EL2 concentration and reduce the EL6 concentration near the outer surface of the InGaAs layer. This result may explain the data of Irvine and Palmer[24] who observed only the EL2 in a relaxed 1.5-μm-thick InGaAs layer grown on GaAs by MBE. Significant relaxation is associated with a large leakage current that might prevent them from probing the interfacial region for detecting the EL6. In fact, they mentioned that electrical breakdown in one of their samples prevented DLTS measurements at over 0.8 μm from the front surface. Since the strain is relaxed at the lower interface and the upper interface still remains coherently strained, the top GaAs layer is expanded laterally. In this case, no driving force for removing As from their lattice sites to relieve stress exists. Without excess As, the production of the EL6 and in turn the EL2 is suppressed, which, in fact, may explain the observation of only the 0.53 eV trap, related to the cores of α-type threading dislocations, in the top GaAs layer.

IV. CONCLUSIONS

Strain relaxation is shown to cause significant carrier depletion by the generation of a trap at 0.53 eV in the top GaAs layer (associated with threading dislocations), a trap at 0.13 eV and the EL2 in the InGaAs layer, and a trap at 0.33 eV in the neighboring lower GaAs layer. The traps at 0.13 and 0.33 eV are considered to be the same trap because the difference between their energies is comparable to the optically determined conduction-band offset. This result suggests a method for probing interfacial band discontinuity. Given its activation energy, the 0.33 eV trap is assigned to the EL6 in GaAs, which is often considered to be As_i-V_{Ga} complexes. A likely mode of strain relaxation is deduced from the spatial locations of these traps.

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