

Conduction band offset in InAs/GaAs self-organized quantum dots measured by deep level transient spectroscopy

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The heterostructure conduction band offset, ΔE_c , in InAs/GaAs self-organized quantum dots has been measured by deep level transient spectroscopy. Measurements were made with Au–Al_{0.18}Ga_{0.82}As Schottky diodes in which the multilayer dots are embedded in the ternary layer. The estimated value of the band offset $\Delta E_c = 341 \pm 30$ meV. © 2000 American Institute of Physics. [S0003-6951(00)03618-4]

Quantum dots, realized by self-organization during strained layer heteroepitaxy, have recently found applications in microelectronics and optoelectronics.^{1–4} Self-organized quantum dots in the In(Ga)As/Ga(Al)As system are approximately pyramidal in shape with a base length of about 20 nm and a height of 6–8 nm³. Typical molecular-beam epitaxial growth leads to an ordered array of 10¹⁰–10¹¹ dots/cm². However, because of the pyramidal shape and a complex strain profile within the dot, the band structure and the electronic states can only be calculated approximately. The band offsets, which are important for the design and understanding of a variety of devices, are also not known precisely. A technique that has been used with considerable success to measure heterostructure band offsets is to treat the potential of a quantum well grown with the two semiconductors analogous to that of a deep level defect and measure the temperature-dependent transient capacitance signal of a Schottky or *p-n* diode due to filling and emptying of the quantum well.⁵ The potential of a quantum dot, due to the three-dimensional confinement, is similar to that of an atom or a deep level trap. Transient capacitance measurements with InP and InAs/GaAs quantum dots have been reported.^{6–8} In this letter, we report on the determination of the band offsets in InAs/GaAs self-organized quantum dots by performing deep level transient spectroscopy (DLTS) measurements on Au–AlGaAs Schottky diodes in which the quantum dot (QD) layers are embedded in the AlGaAs layer.

The heterostructure used for the DLTS measurements, grown by molecular-beam epitaxy (MBE) on (001) *n*⁺-GaAs substrate, is schematically shown in Fig. 1. Growth is initiated with appropriate *n*⁺-GaAs and graded buffer layers. Three layers of InAs quantum dots, with 30 Å GaAs barrier layers in between, are sandwiched in a *n*-type (Si-doped) uniformly doped Al_{0.18}Ga_{0.82}As layer. This alloy composition is chosen since Al_{*x*}Ga_{1–*x*}As with *x* ≤ 0.24 does not have the dominant trap known as the *DX* center.⁹ The quantum dot region is undoped and 250 Å undoped GaAs spacer layers are also inserted on both sides of the quantum dot layer. A *n*-type 100 Å GaAs layer serves as a capping layer. It is useful to note that multiple dot layers resemble a region with a three-dimensional (3D) distribution of deep level defects in

a semiconductor. The doping and thickness of the heterostructure layers were carefully controlled so that the quantum dot layers are outside the zero bias depletion region in the Al_{0.18}Ga_{0.82}As layer under the quiescent reverse bias used in the experiments. Gold Schottky barriers with diameters ranging from 100 to 500 μm were formed on the heterostructure. Schottky diodes were also fabricated with a similar heterostructure in which the InAs dot layers were absent. These control devices were useful for identifying and eliminating DLTS signals originating from deep level traps in the heterostructure, including those in GaAs. Low-temperature (17 K) photoluminescence (PL) measurements confirmed the dominant ground state transition in the dots with the emission peak centered at 1.06 μm. DLTS measurements were performed with the sample inserted in a variable temperature cryostat and with an automated system consisting of a pulse generator, capacitance meter, and a correlator as primary components.

Capacitance–voltage measurements on the diodes at room temperature give a value of $N_D = 1.1 \times 10^{16}$ cm^{–3} in the Al_{0.18}Ga_{0.82}As layer. The first set of DLTS measurements were made with a quiescent reverse bias of –7.2 V applied to the diodes. The filling pulse height was also kept fixed at 1.01 V. The DLTS signal was recorded as temperature scans for different rate windows. The dominant DLTS signal,

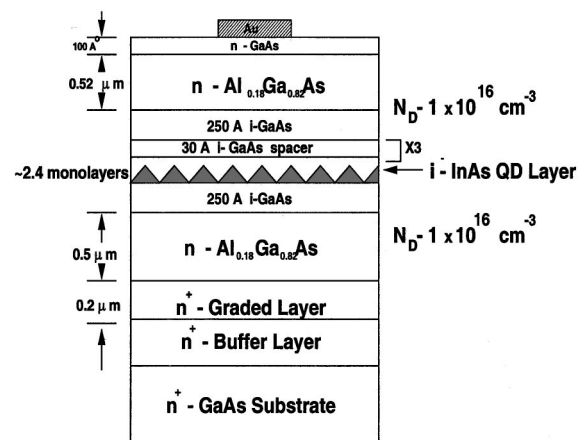


FIG. 1. InAs/GaAs/Al_{0.18}Ga_{0.82}As quantum dot heterostructure grown by molecular-beam epitaxy to form Schottky diodes.

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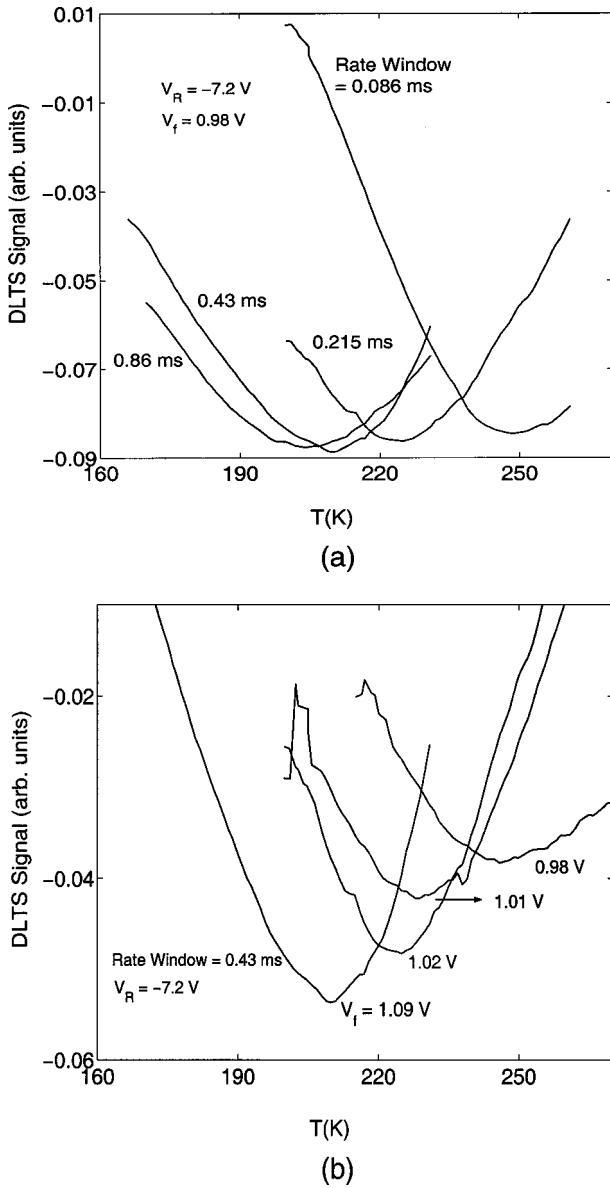


FIG. 2. DLTS signals (a) obtained with temperature scans at different rate window settings; and (b) obtained with different filling pulse amplitude at fixed values of quiescent reverse bias and rate window.

which we believe to originate from electron emission from the quantum dots, is shown in Fig. 2(a). By repeating the DLTS scan with varying rate windows, an Arrhenius plot as shown in Fig. 3 is obtained. Similar measurements, with identical parameters, made on the control samples without the dots did not produce the peaks shown in Fig. 2(a).

In a second set of measurements, the reverse bias and the rate window were kept fixed at -7.2 V and 0.43 ms, respectively, and the filling pulse height was varied with each temperature scan. Measurements were made with the Schottky diodes with and without the dot layers. Typical data for the QD samples are shown in Fig. 2(b). It is noticed that the DLTS peak position shifts in temperature with variation of filling pulse height at a fixed rate window. Such a shift is generally not observed for conventional deep level traps. The observed shift has been attributed to different degrees of coulombic charging of the dots, and filling of different levels within the bound states.¹⁰ It may be remembered that due to the vertical coupling of the dots, there is a multiplicity of levels in both the ground and excited states.

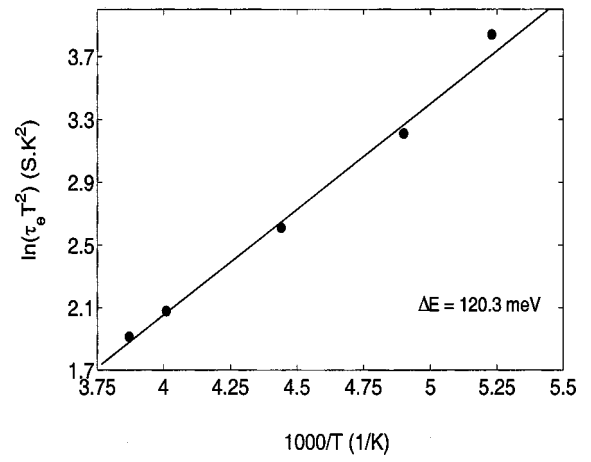


FIG. 3. Arrhenius plot of the emission time constant ($\tau_e T^2$) vs inverse temperature. The solid line is a fit to the measured data.

In order to analyze and interpret the observed data, the emission of electrons from the quantum dots has to be carefully considered. There is a thin (7 Å) InAs wetting layer below the quantum dots. The carriers can escape into the wetting layer by field-assisted tunneling with or without phonon coupling. This process is, however, not thermally activated. Electrons can be thermally emitted into the bulk GaAs spacer layer by interaction with phonons. Electrons can also be thermally emitted into the 2D wetting layer. It is assumed that emission of electrons occurs from the ground state of the dot, since the relaxation time from the excited state to the ground state is much smaller than the measured time constants.^{11,12} The thermally activated emission time constant can be expressed, from detailed balance, as

$$\tau_e = \frac{\exp(\Delta E/kT)}{\sigma_n v_{th} N_c}, \quad (1)$$

where ΔE is an activation energy, σ_n is the capture cross section, v_{th} is the thermal velocity, and N_c is the conduction band effective density of states. Assuming that electrons are emitted into the 3D (250 Å) GaAs spacer layer, Eq. (1) can be rewritten as

$$\tau_{e1} = \frac{\exp(\Delta E/kT)}{\sigma_n \gamma_n T^2}, \quad (2)$$

where $\gamma_n = (v_{th}/T^{1/2})(N_c/T^{3/2}) = 3.25 \times 10^{21} (m_n/m_0) \text{ cm}^{-2} \text{ s}^{-1} \text{ K}^{-2}$ and depend on the electron effective density-of-states mass. The fit to the data of Fig. 3 in accordance with Eq. (2) is also shown, resulting in an activation energy of 120.3 meV. On the other hand, if it is assumed that the electrons are thermally emitted from the dot to the bound state of the 2D wetting layer and then from the wetting layer to the 3D states, then

$$\tau_{e2} = \frac{\exp(\Delta E/kT)}{\sigma_n \gamma_n T^{3/2}}, \quad (3)$$

where $\gamma_n = (v_{th}/T^{1/2})(N_c/T) = 2.42 \times 10^{16} \sqrt{m_n/m_0} \text{ cm}^{-1} \text{ s}^{-1} \text{ K}^{-3/2}$. The emission time constant from the wetting layer to the 3D GaAs is assumed negligible compared to τ_{e2} due to the much smaller energy difference. In this scenario, a fit

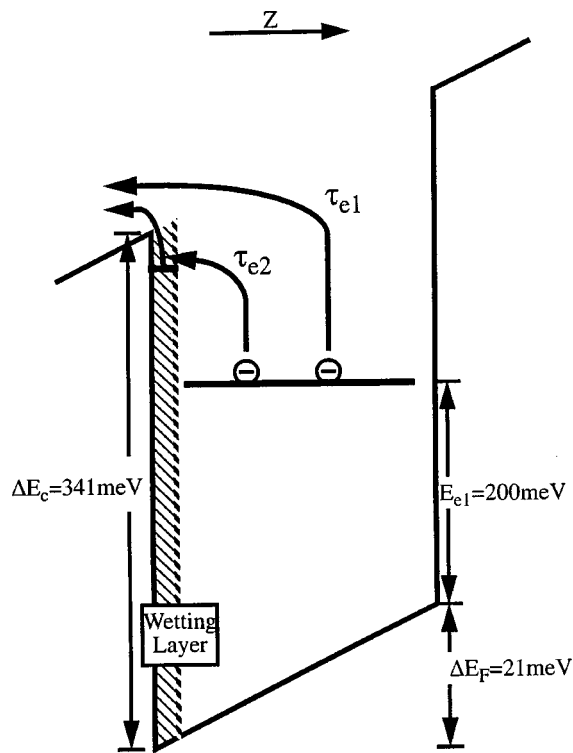


FIG. 4. Schematic of conduction band profile of self-organized InAs/GaAs quantum dot with wetting layer along the grown (z) direction under reverse bias conditions. The different emission mechanisms that have been considered are shown. Note that emission of the electrons from the dot occurs towards the wetting layer. The theoretically calculated ground state binding energies in the dot and wetting layer are also shown.

cannot be obtained with the data in Fig. 3. Hence, thermal emission into the wetting layer can be excluded in the context of the present experiment.

In order to estimate the conduction band offset ΔE_c , this quantity is expressed in terms of the measured activation energy ΔE as

$$\Delta E_c = \Delta E + E_{e1} + \Delta E_F, \quad (4)$$

where E_{e1} is the ground state energy in the dot and ΔE_F is the band bending due to the applied bias (Fig. 4). We calculate the ground state energy, E_{e1} , as follows. The strain distribution is first calculated using the valence force field (VFF) model.^{13,14} Then, to determine the energy levels in the dot we use a full 3D eight-band $\mathbf{k} \cdot \mathbf{p}$ model, incorporating the strain effect on the Hamiltonian using deformation potential theory. Details of the calculation formalism can be found in Ref. 15. We use a eight-band model, as opposed to the more

common conduction-band effective-mass model, because the effective-mass model has been found to be inadequate.¹⁶ Because strain in the dot is nonuniform, the conduction band edge energy varies in the dot. Therefore, defining a conduction band offset between the dot and the GaAs matrix is somewhat arbitrary. We choose to use the conduction band energy in the center of the dot which gives a calculated ground state energy of 200 meV. Adding the electric field contribution, ΔE_F , of 21 meV, gives a conduction band offset of 341 meV. Due to the inhomogeneity in the dot size and shape, however, the actual conduction band offset for a given dot will be 341 ± 30 meV, where broadening effects are approximated from typically observed PL emission linewidths.

In summary, we have used transient capacitance measurement in the DLTS mode, to determine the heterostructure band offset in InAs/GaAs self-organized quantum dots embedded in the depletion region of $\text{Al}_{0.18}\text{Ga}_{0.82}\text{As}-\text{Au}$ Schottky diodes. The estimated value of the band offset $\Delta E_c = 341 \pm 30$ meV. The technique can be extended to other dot compositions.

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