

Effect of interfacial states on the binding energies of electrons and holes in InAs/GaAs quantum dots

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The interface between an InAs quantum dot and its GaAs cap in “self-assembled” nanostructures is non-homogeneously strained. We show that this strain can lead to localization of a GaAs-derived X_{1c} -type interfacial electron state. As hydrostatic pressure is applied, this state in the GaAs barrier turns into the conduction-band minimum of the InAs/GaAs dot system. Strain splits the degeneracy of this X_{1c} state and is predicted to cause electrons to localize in the GaAs barrier above the pyramidal tip. Calculation -present work! or measurement -Itskevich *et al.*! of the emission energy from this state to the hole state can provide the hole binding energy, $D_{\text{dot}}^{(h)}$. Combining this with the zero-pressure electron-hole recombination energy gives the electron binding energy, $D_{\text{dot}}^{(e)}$.

Since Eq. ~3! gives the hole confinement energy at P . P

The method of Itskevich *et al.* assumes that above the critical pressure P_c , the emission takes place from the X_{1c} level in the GaAs barrier, to the confined hole state, h^{InAs} , with an emission energy, $E_{\text{dot}}(X_{1c}^{\text{GaAs}} \rightarrow h^{\text{InAs}}; P)$. Combining this value with the bulk GaAs indirect transition energy at this pressure, $E_{\text{bulk}}(X_{1c}^{\text{GaAs}} \rightarrow G_{15v}^{\text{GaAs}}; P)$ the hole binding energy within the dot, $D_{\text{dot}}^{(h)}(P)$, can be obtained from Fig. 1-a!

$$D_{\text{dot}}^{(h)}(P) \approx E_{\text{bulk}}(X_{1c}^{\text{GaAs}} \rightarrow G_{15v}^{\text{GaAs}}; P) - E_{\text{dot}}(X_{1c}^{\text{dot}} \rightarrow h^{\text{InAs}}; P) + d_{\text{loc}}(P). \quad \sim 3!$$

This approach assumes that the emitting state X_{1c}^{dot} has precisely the energy of the threefold degenerate X_{1c} level in bulk GaAs under pressure P , i.e., that it is an extended Bloch state. This neglects the Eshelby strain that could exist at the GaAs-InAs interface, and the ensuing wave-function localization at the interface. This localization could shift the emitting state @Fig. 1-a!#. An extra correction term $d_{\text{loc}}(P)$, is therefore included in Eq. ~3! to allow for emission from the ‘‘split X_{1c} state,’’ called X_{1c}^{dot} , rather than from bulk X_{1c}

$$d_{\text{loc}}(P) \approx E(X_{1c}^{\text{GaAs}} \rightarrow X_{1c}^{\text{dot}}; P). \quad \sim 4!$$

The electron binding energy $D_{\text{dot}}^{(e)}(P)$, can then be determined @Fig. 1-b!# by subtracting from the zero-pressure direct gap of GaAs the measured zero-pressure electron-hole recombination energy $E_{\text{dot}}(e^{\text{InAs}} \rightarrow h^{\text{InAs}}; P \approx 0)$, and the zero-pressure hole confinement energy:

$$D_{\text{dot}}^{(e)}(P) \approx E_{\text{bulk}}(G_{1c}^{\text{GaAs}} \rightarrow G_{15v}^{\text{GaAs}}; P \approx 0) - E_{\text{dot}}(e^{\text{InAs}} \rightarrow h^{\text{InAs}}; P \approx 0) - D_{\text{dot}}^{(h)}(P \approx 0). \quad \sim 5!$$

$P \approx 0$ the ground electron state is confined *within* the InAs dot (Fig. 2-a), while at the pressure where the GaAs barrier undergoes a $G_{1c} \rightarrow X_{1c}$ transition, the GaAs/InAs interfacial strain produces a strain-split, *localized* X_{1c} state (Fig. 2-b) localized *outside* the dot, above its tip. The energy of this state differs in energy by 0.024 eV from a Bloch-extended bulk GaAs X_{1c} state obtained in our calculation at a position far away from the dot, where the Eshelby strain (Eqs. 1-2) has decreased to zero. The *hole* states do not significantly change their character with pressure and are always localized within the dot. Our directly calculated values at 60 kbar (see Table I) for Eq. 3 are

$$D_{\text{dot}}^{(h)}(P \approx 60) \approx 1.850 \pm 1.528 \pm 0.021 \pm 0.301 \text{ eV} \quad (8)$$

and for Eq. 5

$$D_{\text{dot}}^{(e)}(P \approx 0) \approx 1.548 \pm 1.180 \pm 0.271 \pm 0.097 \text{ eV}. \quad (9)$$

For a larger dot (base $\approx 150 \text{ \AA}$, height $\approx 15 \text{ \AA}$) we obtain $D_{\text{dot}}^{(h)}(P \approx 60) \approx 0.338$ and

GaAs/InAs nanostructure into “cells” with position vector \mathbf{R} and then performing 60 bulk band-structure calculations of InAs and GaAs, thus obtaining the bulk eigenvalues $E_{nk}(\mathbf{R})$ for band n at wave vector k within each cell, using the strained In-As or Ga-As bond geometry in that cell.¹⁴ These solid lines in Fig. 3-a! show that far from the dot where the strain is small, the offsets approach the unstrained value, however the compressive strain within the InAs dot, increases the valence-band offset from 0.11 to 0.41 eV ~allowing more confined hole states! and decreases the conduction-band offset from 1.01 to 0.55 eV ~reducing the number of confined electron states!.

Figure 3-b! shows the band offsets under 60 kbar of pressure. The GaAs barrier material has already undergone a conduction band $G_{1c} \rightarrow X_{1c}$ crossing, while the InAs remains direct. We observe that the strained band offset for X_{1c} electrons has developed *local minima* ~indicated by arrows! just above the tip and below the base of the InAs dot. The development of these minima is principally due to the splitting of the triply degenerate X_{1c} -derived states by the epitaxial strain at the interface between the dot and the barrier as predicted by Yang *et al.*² It is within these minima that the lowest energy conduction state localizes. This leads to trapping of the electron wave function at the interface, and to a lowering of the energy level relative to the bulk GaAs X_{1c} level.

In conclusion, our pseudopotential calculations show that the InAs/GaAs interfacial strain leads to the development of a trough in the X

earlier. In Fig. 3, we use atomistic calculations to illustrate the effects on the band offsets of applying hydrostatic pressure to a GaAs embedded, strained InAs *pyramidal* quantum dot. The *unstrained* band offsets between GaAs and InAs are shown as dashed lines at zero pressure in Fig. 3-a!. They show that at $P=0$ the natural GaAs/InAs offsets allow InAs to act as a “well” for both the conduction-band G_{1c} electrons and the valence-band G_{15v} holes ~a “type I” offset!. The solid lines in Fig. 3-a! show the offsets subject to the local strain $\epsilon(\mathbf{R})$, plotted along a $[001]$ direction down through the tip of the InAs pyramid ~see inset!. We obtain the position-dependent strained offsets by discretizing the