Strain effects on the Electronic and Optical Properties of InAs/GaAs Quantum Dots: Tight-binding Study

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Abstract. We present an atomistic investigation of strain effects on the electronic and optical properties of capped pyramidal InAs/GaAs quantum dots (QD's) within an empirical sp^3s^* tight-binding model with interactions up to 2nd nearest neighbors and spin-orbit coupling. The strain is incorporated through the atomistic valence-force field model. We demonstrate that the strain: (i) significantly increases the QD gap, (ii) induces a macroscopic spatial asymmetry in the ground state wave functions, (iii) strongly enhances the oscillator strength of the fundamental optical transition and (iv) introduces a spatial anisotropy of the optical absorption coefficient of this transition.

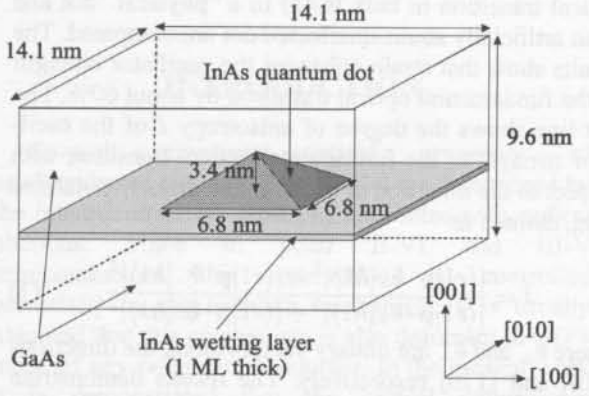

FIGURE 1. Schematic view of the pyramidal InAs QD buried in the GaAs matrix. The supercell contains 85000 atoms.

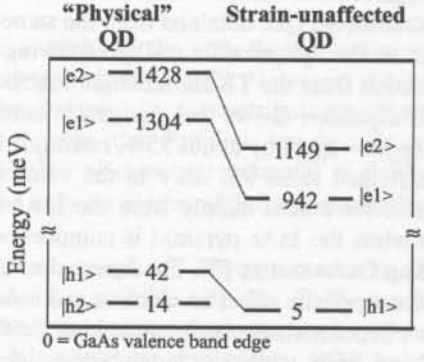

FIGURE 2. QD bound state energies calculated by our TB approach. Values here differ slightly from those given in Ref. [5] due to corrected atomic relaxation algoritm adopted here.

We present a study of the influence of strain on the electronic and optical properties of pyramidal InAs quantum dots (QD's) buried in GaAs matrices. The system is characterized by a significant strain field inside and around the InAs pyramid. Despite the many theoretical studies addressing the electronic and optical properties of such system (in the framework of the $\mathbf{k}\cdot\mathbf{p}$ model [1], the empirical pseudopotential model [2] or the tight-binding (TB) model [3]), no systematic investigations of the influence of the strain on the electronic spectrum and the related optical transitions have been carried out. We employ an empirical sp^3s^* TB model with interactions up to 2nd nearest neighbors and spin-orbit coupling [4], that we generalized to include the effects of bond length and bond angle deviations from the ideal InAs and GaAs zinc-blende structure [5]. This approach allows for these effects to be selectively removed from the electronic-structure calculation, giving quantitative information on the importance of the strain effects on the electronic and optical properties of QDs. Piezoelectric effects are not included here.

Fig. 1 shows our model system. It consists in a pyramidal InAs QD buried in a GaAs matrix. The equilibrium atomic positions, employed for the electronic calculation, were obtained by minimizing the total elastic energy within the Keating's valence-force field model [6].

Fig. 2 shows, on the left side (QD), the QD bound state energies calculated by our TB model by including all strain effects in the TB Hamiltonian. We found two bound electron states ($|e1\rangle$ and $|e2\rangle$) and two bound hole states ($|h1\rangle$ and $|h2\rangle$). In order to have a direct quanti-

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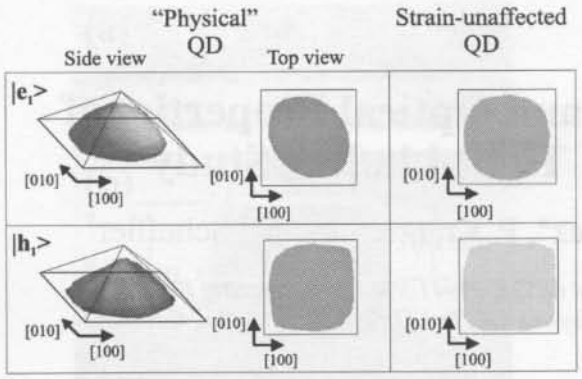

FIGURE 3. Isosurface plots of the charge densities $e|\varphi(\mathbf{r})|^2$ relative to the states $|e1\rangle$ (top) and $|h1\rangle$ (bottom). Each surface corresponds to the 50% of the maximum charge-density value.

tative measure of the strain contribution, we compare, in the same figure, these results with those of an artificially strain-unaffected QD, obtained from the same atomic positions as the "physical" case by removing any strain contribution from the TB Hamiltonian matrix elements. The comparison shows that the strain increases the QD gap ($\varepsilon_{|e1\rangle} - \varepsilon_{|h1\rangle}$) by about 35%, raising it from the strain-unaffected value 937 meV to the value 1262 meV. This behavior comes mainly from the InAs band gap increase when the InAs pyramid is compressed by the surrounding GaAs matrix [5]. The figure shows that the strain has an opposite effect on electron and hole states: the former become shallower, approaching the GaAs conduction-band edge, while the latter become deeper, moving away from the valence-band edge.

Fig. 3 shows the strain effects on the charge density $e|\varphi(\mathbf{r})|^2$ relative to the ground electron ($|e1\rangle$) and hole ($|h1\rangle$) bound states. Results for the "physical" QD and for the strain-unaffected QD are compared. The figure shows that the strain introduces a macroscopic spatial asymmetry between the directions [110] and [1$\bar{1}$0], which is a consequence of the different strain profiles along these two directions, obtained from our atomistic treatment [2].

Table 1 gives, on the first two lines, the effect of the strain on the charge fraction ΔQ within the QD, calculated as $\Delta Q = \int_{QD} |\psi(\mathbf{r})|^2 d^3r$, for the electron state $|e1\rangle$ and the hole state $|h1\rangle$. For the "physical" dot, ΔQ for $|e1\rangle$ and $|h1\rangle$ are comparable, while removing strain effects causes a strong difference in the ΔQ values for $|e1\rangle$ and $|h1\rangle$. In particular, we notice that removing the strain, the electron state becomes more spatially confined (and deeper, see Fig. 2), while the hole state becomes less spatially confined (and shallower). This results in a stronger overlap between these two states in the presence of strain, suggesting a larger oscillator strength of the corresponding optical transition. This is confirmed in the third line of the table, where the oscillator strength f_{QD} of the fundamental optical transition $|h1\rangle \rightarrow |e1\rangle$ (normalized with respect to the oscillator strength f_{InAs} of the fundamental optical transition in bulk InAs) in a "physical" dot and in an artificially strain-unaffected dot are compared. The results show that strain enhances the oscillator strength of the fundamental optical transition by about 60%. The last line shows the degree of anisotropy I of the oscillator strength of the fundamental optical transition with respect to the direction of the in-plane linearly polarized light, defined as

$$I = \frac{|\langle e1|\mathbf{p}\cdot\hat{\mathbf{e}}_+|h1\rangle|^2 - |\langle e1|\mathbf{p}\cdot\hat{\mathbf{e}}_-|h1\rangle|^2}{|\langle e1|\mathbf{p}\cdot\hat{\mathbf{e}}_+|h1\rangle|^2 + |\langle e1|\mathbf{p}\cdot\hat{\mathbf{e}}_-|h1\rangle|^2}, \qquad (1)$$

where $\hat{\mathbf{e}}_+$ and $\hat{\mathbf{e}}_-$ are unitary vectors along the directions [110] and [1$\bar{1}$0] respectively. The results demonstrate that the strain introduces an anisotropy in the optical absorption coefficient, as a result of the macroscopic spatial asymmetry shown in Fig. 3.

TABLE 1. Charge fraction within the QD (first two lines), InAs-normalized oscillator strength f_{QD}/f_{InAs} and degree of anisotropy I (eq. (1)) of the $|h1\rangle \rightarrow |e1\rangle$ optical transition transition.

	"Physical" QD	Strain-unaffected QD
$\|e1\rangle$	64%	75%
$\|h1\rangle$	54%	11%
f_{QD}/f_{InAs}	0.19	0.12
I	2.5%	$\sim 0^*$

* within the numerical precision

In conclusion, we showed that the strain plays an important role in the electronic and optical properties of InAs/GaAs pyramidal QD's. It significantly increases the QD gap, it enhances the oscillator strength of the fundamental optical transition, and it introduces a macroscopic in-plane asymmetry of the ground state wave functions, which leads to an in-plane anisotropy of the optical absorption coefficient of the fundamental transition.

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