The InGaAs/GaAs Quantum Dots under Effective and *Ab Initio* Treatments: Comparison and Results

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ABSTRACT

The 3D model for InGaAs/GaAs quantum dots (QD), based on a single sub-band approach taking into account the effect of non-parabolicity of the conduction band is presented. We apply an effective approach in which the combined effect of strain, piezoelectricity and interband interactions are simulated by an effective potential. The strength of the effective potential V_s is determined by analysis of capacitance-gate-voltage (CV) data and photoluminescence spectra for QDs and quantum rings (QR). The model is compared with one based on the 8-band ***kp***-theory, which takes into account interband interactions, strain and piezoelectric effects in an *ab initio* manner. The atomistic pseudopotential approach is also taken for comparison. It is found that disagreements between predictions obtained in the framework of our model and of these models are related to strength of the electron confinement. It is shown that our approach accurately reproduces photoluminescence measurements for excitons when there is a significant Ga fraction in the QDs

Keywords: quantum dots and rings, single carrier levels, optical properties, excitons, Coulomb shifts,

1 INTRODUCTION

The theoretical modeling for semiconductor InGaAs/GaAs quantum dots (QDs) must take into account such effects as strain, piezoelectric and interband interactions [1]. In addition, the effect of non-parabolicity of the conduction band also has to be taken into account for QDs having base size of few nanometers [2]. As an example of a realistic model one can consider the 3D model [1,3] based on the 8-band ***kp***-theory, which takes into account the interband interactions and in which strain and piezoelectric effects are treated in an *ab initio* manner. In another realistic model [4] the atomistic pseudopotential approach was considered. Until now there is no direct comparison of these two models. Here we present an effective approach in which the combined effect of strains, piezoelectricity and interband interactions are simulated by an effective potential. Additionally, in the model, an analog of the Kane formula is implemented to take into account the effect of non-parabolicity of the conduction band. Based on our model, we performed an analysis of capacitance-gate-voltage (CV) data [5] and photoluminescence spectra for QDs, QRs, and double concentric QRs. We show that our approach reproduces both the few electron energy level spectra and the increase of the electron effective mass relative its bulk value due to non-parabolicity. We compare our model with the 8-band ***kp***-theory [1,3], which takes into account interband interactions, strain and piezoelectric effects in an *ab initio* manner. It is shown that our effective approach allows us to reproduce results calculated with the realistic ***kp***-model for pure InGaAs/GaAs QDs. It accurately reproduces the CV experimental data when there are significant Ga fractions in the QDs. The calculations for the QDs with 22% -25% Ga fractions match both the CV data and the photoluminescence measurements [5-6] for Coulomb shifts of exciton complexes (X^-,X^+,XX). We compared our results with those obtained within the framework of the atomistic pseudopotential approach [4, 7]. It was found that the considerable disagreements between predictions obtained in the framework of our model and predictions of the pseudopotential model are related to strength of the electron confinement. Our calculations allow us to formulate a conclusion about the strength of confinements of the realistic models. These confinements are quite different; the atomistic pseudopotential approach produces a stronger confinement for electrons and heavy holes.

2 EFFECTIVE APROACH

A 3D heterostructure is modeled utilizing a ***kp***-perturbation single subband approach with an energy dependent quasi-particle effective mass [2,8,9]. The energies and wave functions of a single carrier in a semiconductor structure are solutions of the nonlinear Schrödinger equation:

$$\left(-(\nabla\frac{\hbar^2}{2m^*(r,E)}\nabla)+V_c(r)+V_s(r)\right)\psi=E\psi \qquad (1)$$

where $V_c(r)$ is the band gap potential, proportional to the energy misalignment of the conduction (valence) band edges of the InAs QD (index 1) and the GaAs substrate (index 2). Inside the substrate $V(r)=V_c$ and inside the quantum dot $V(r)=0$. The electron effective mass

$m^* = m^*(x, y, z, E)$ is linearly dependent on energy for $0 < E < V_c$ and varies within the limits of the QD/substrate bulk effective mass values. Bulk effective masses of InAs and GaAs are $m^*_{0,1}$=0.024 m_0 and $m^*_{0,2}$=0.067 m_0, respectively, where m_0 is the free electron mass. The value of m*=0.4 m_0 is used for the effective mass of the heavy hole for both the QDs and the substrate. The band structure model presented is noted as "unstrained" in Figure 1. A model for QDs must take into account the band-gap deformation potential, the strain-induced potential, and the piezoelectric potential in addition to the band-gap potential. Realistic (*ab initio*) models treat these effects by applying corresponding classical theories [1]. Alternatively, one can take these potentials into account by an effective manner. In [8] we introduced the potential V_s, which simulates the integrated effect of all aforementioned potentials. The effective potential V_s has an attractive character and acts inside the volume of the QD. The magnitude of the potential must be chosen to reproduce experimental data.

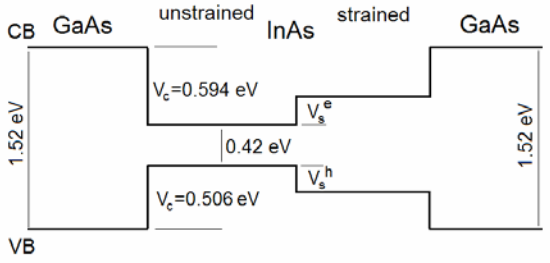

Figure 1. Band structure model for InAs/GaAs QDs.

3 STRENGTH PARAMETER OF THE EFFCTIVE POTENTIAL

The effective potential V_s=0.31 eV reproduces the capacitance-gate-voltage experiments [5] in which the spectra of few electrons tunneling into QDs were observed. There are two *s* and four *p*-shell electron levels below the GaAs conduction band edge [5]. The first level of the *d*-shell is located above this threshold, but it can be observed by the Zeeman effect in a magnetic field. With the above effective potential, the electron spectra calculation results in localization of the *s*-shell electron level with respect to the conduction band edge of the GaAs substrate, similar to that derived from the CV measurements (~180 meV). First order perturbation theory calculations [9] give a spectral picture that is in agreement with the CV data. This situation is shown in Fig. 2. The effect of non-parabolicity, taken into account in our model by means of the energy dependent effective mass approximation, leads to a change in the electron effective mass of the QDs with respect to the bulk value. For the QDs considered, the effective mass in InAs increases from the initial bulk value of 0.024 m_0 to 0.057 m_0 (for the *p*-wave electron), which agrees with the experimental value of 0.057 m_0 ± 0.007 m_0 obtained from CV measurements by the Zeeman splitting of *p*-shell levels [5]. One can see that the agreement between our results and the experimental data is acceptable taking into account uncertainties of QD geometry and material mixing between the QDs and the substrate. Effective potential strength for valence band can be chosen from experimental data for heavy holes [6]. We assume that the effective model with the magnitude of the effective potential V_s^e=0.21 eV for the conduction band and V_s^h=0.28 eV for the valence band describes pure InAs/GaAs QDs. This is supported by comparison of our results with *ab initio* calculations [1] for electrons and [3] for heavy holes. Difference between the effective potential strengths, obtained from the CV experimental data ($V_s = V_s^e$=0.31 eV, V_s^h is not defined) in [8, 9] and from the *ab initio* calculation [1] ($V_s^e = V_s^h$=0.21 eV) and [3] (V_s^e=0.21, V_s^h=0.28 eV), may be related to the existence of a significant Ga fraction in the experimentally fabricated QDs [10].

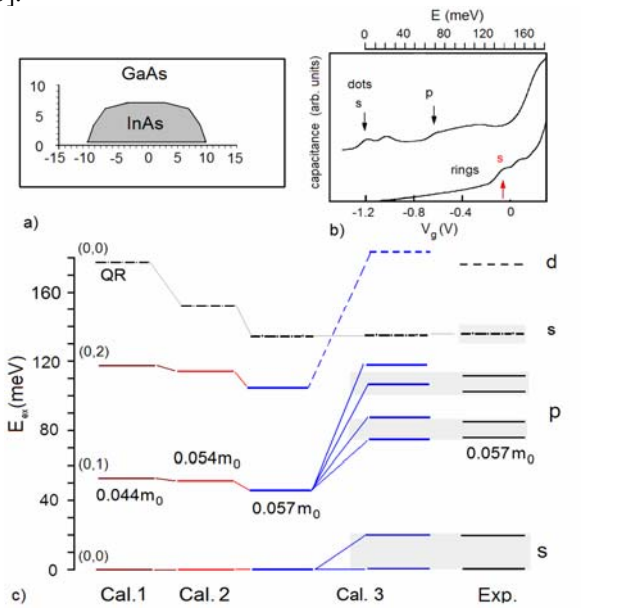

Figure 2. a) Cross section of InAs QDs having a semi-ellipsoidal shape embedded into the GaAs substrate. Geometrical parameters are given in [5].
b) Electron CV traces obtained in the capacitance-gate-voltage experiments [5] for QDs and QRs.
c) First order perturbation theory calculations [9] (Cal. 3) and energy levels given by the CV data. The Cal.1 and Cal. 2 correspond to the Model 1 and Model 2 single electron calculations.

4 COMPARISONS

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In this section a comparison of our model and "ab initio model" is presented. The results of 8-band kp-model [3] and the atomistic pseudopotential approach [4,7] are given in Table 1 along with results of our calculations. In these calculations two band structure models are used.

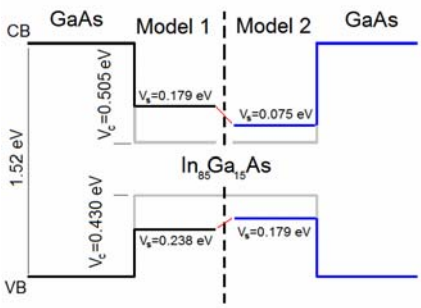

Figure 3. Band structure model used for comparison with ***kp*** [1, 3] and atomistic pseudopotential calculations [4,7]. Model 1 corresponds to choosing the strength of the effective potential to reproduce the ***kp*** calculation. Model 2 corresponds to results of the pseudopotential atomistic calculations.

	Ref. 14	Effective Model	
		Model 1	Model 2
m^*_{QD}/m_0	--	0.061	0.056
$\Delta E(e)$	209	136	208
$\Delta E(h)$	199	143	198
e_1-e_0	58	48	54
e_2-e_1	60	50	60
h_0-h_1	13	12	14
h_1-h_2	13	14	14
E^c_{e0e0}	29	23.0	24.2
E^c_{e0e1}	24	18.9	19.9
E^c_{e1e1}	25	17.4	18.4
E^c_{h0h0}	32	30.8	31.9
E^c_{e0h0}	31	26.1	27.2
E_{ex}	1080	1216	1088
d_{00}	0.05	0.08	0.07

Table 1. Calculated results for lens-shaped InGaAs QDs with Ga fractions of 15%. Single electron (hole) energy-level spacing $e\,(h)$, electron (hole) binding energy $\Delta E(e)\,(\Delta E(h))$, electron-electron, electron-hole and hole-hole Coulomb energies $E^c_{\alpha\beta}$ (α,β=e,h), excitonic band gap E_{ex} (in meV), exciton dipole moment d_{00} (in nm) and effective mass of the QD material for semi-ellipsoidally shaped InGaAs QDs (Ga fraction in %) embedded in GaAs. Electron (hole) energy of the ground state is measured from the GaAs conduction (valence) band. The value of the effective mass is given for the p-wave electron level. The QD has a height H =3.5 nm. The QD base size is 25.2 nm.

The first (Model 1) corresponds to choosing the strength parameters for effective potential which reproduce results of the ***kp*** calculation [1,3]. For the second, the strength parameters are chosen to reproduce results calculated in framework of the pseudopotential atomistic approach from [4,7]. Difference between Model1 and Model 2 is illustrated by Fig. 3. One can see from the Table 1 that Model 2 reproduces the results of the pseudopotential calculation from [4] with good accuracy. In the same time the results obtained for Model 1 and Model 2 are quite different. One can conclude the same from Fig. 2c) where the results of calculations with Model 1 and Model 2 are shown as Cal. 2 and Cal. 1. In particular, from Fig. 2c) it is clear that the Model 2 cannot reproduce CV QD (QR) experimental data.

We have to note that the good agreement of the results obtained in our Model 2 and the pseudopotential atomistic approach in Table 1 does not guarantee coincidence of the results for the Coulomb energy vs. QD height [7] for single carriers. This situation is illustrated by Fig. 4.

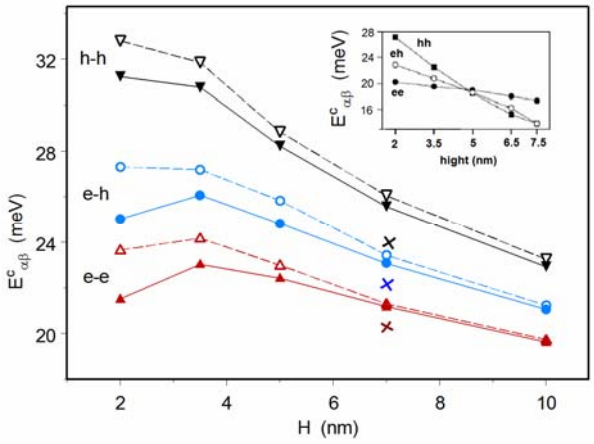

Figure 4: The height dependence of electron-electron, electron-hole and hole-hole Coulomb energies $E^c_{\alpha\beta}$ (α,β=e,h). The QD has a Ga fraction of 15%. The solid (open) symbols correspond to Model 1 (Model 2) calculations. For comparison results of pseudopotential calculations [7] are presented by the inset. The colored crosses mean the CV data from [5]. The QD has a height H =3.5 nm and base size is 25.2 nm.

One can see that in our calculation there is no value of the QD height for which the Coulomb energies $E^c_{\alpha\beta}$ are crossing. In the pseudopotential calculations [7] the

Coulomb energies $E^c_{\alpha\beta}$ as functions of QD height are crossed at value of 5 nm, approximately.

5 COULOMB SHIFTS OF EXCITONS

Our model is tested by comparison with available experimental data [6] for the Coulomb shifts of the transition energies for positively (X^+) and negatively (X^-) charged trions and biexcitons (XX) as a function of the neutral exciton (X) recombination energy. Results of our calculations for various base size parameters (b=9 nm; 10 nm; 11 nm) of QDs are depicted in Fig. 5, along with experimental data (the QD height is 3.5 nm).

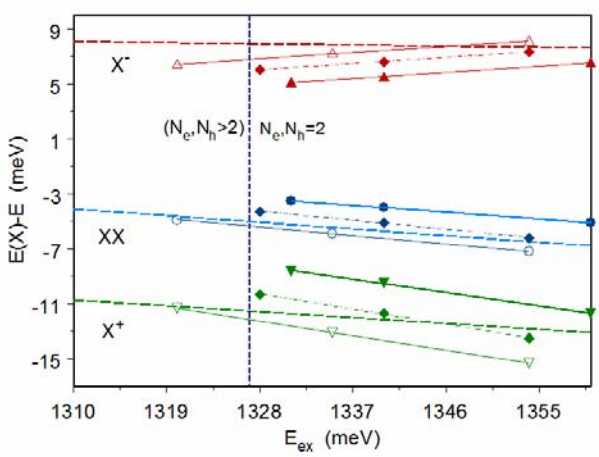

Figure 5. Coulomb shifts of transition energies for positively (X^+) and negatively (X^-) charged trions and biexcitons (XX) as a function of neutral exciton (X) recombination energy. Results of the calculations for various base size parameters of QDs are depicted by solid triangles (X^+, X^-) and dots (XX). The dashed lines correspond to root mean square fits to experimental data from Ref. [6]. The solid lines (and dot-dashed lines) correspond to root mean square fits to the calculated results. The vertical line shows the transition energy, which corresponds to the limit of the QD sizes for which there are only two electrons and two heavy holes levels. The amount of the Ga fraction in our calculations was chosen to be 20% (triangles down), 25% (diamonds) and 30% (triangles up).

From Fig. 5 we conclude that better matching of the experimental data is obtained with a value of 25% for Ga fraction in QD. In Model 2 one has to increase the Ga fraction in the QDs to 40% to reproduce the data with the same accuracy. Taking into account that the experimental data correspond to pure InAs/GaAs QDs [6], such a large Ga fraction appears unrealistic.

6 SUMMARY

In the framework of an effective model one can obtain satisfactory description of CV and PL experimental data for InGaAs/GaAs QDs. It was found that the amount of the Ga-fraction cannot exceed the value of 25% to reproduce experimental data. Comparison between theoretical models demonstrates stronger QD confinement of carriers produced by the atomistic approach than one obtained by our effective approach and in ***kp***-model of [1,3].

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