Theoretical interpretation of the experimental electronic structure of lens-shaped self-assembled InAs/GaAs quantum dots

A. J. Williamson,* L. W. Wang, and Alex Zunger
National Renewable Energy Laboratory, Golden, Colorado 80401

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We adopt an atomistic pseudopotential description of the electronic structure of self-assembled, lens-shaped InAs quantum dots within the ''linear combination of bulk bands'' method. We present a detailed comparison with experiment, including quantites such as the single-particle electron and hole energy level spacings, the excitonic band gap, the electron-electron, hole-hole, and electron-hole Coulomb energies and the optical polarization anisotropy. We find a generally good agreement, which is improved even further for a dot composition where some Ga has diffused into the dots.

I. USING THEORY AS A BRIDGE BETWEEN THE STRUCTURE AND ELECTRONIC PROPERTIES OF QUANTUM DOTS

Self-assembled, Stranski-Krastanow grown semiconductor quantum dots have recently received considerable attention as they exhibit a rich spectrum of phenomena including quantum confinement,[1–3] exchange splittings,[4] Coulomb charging/blockade,[5–13] and multiexciton transitions.[4,14] Over the past few years a considerable number of high-quality measurements of the electronic level structure of these dot systems have been performed, using photoluminescence ~PL!,[10,12,15–20] photoluminescence luminescence excitation,[4,14] capacitance,[5–7,13] and far infrared ~FIR! spectroscopy.[7,21–26] These measurements have been able to determine the electronic level structure to relatively high precision. In parallel with these measurements, several groups have also attempted to measure the geometry and composition of these dots.[15,16,27–29] So far, however, these measurements have failed to provide details of the shape, size, inhomogeneous strain, and alloying profiles to a similar level of accuracy to that to which the electronic structure has been determined. As a result, the size of the dots were often used as adjustable parameters in models that fit experimental spectra. For example, using a single-band effective-mass model, Dekel *et al.*[14] defined an ''effective shape'' ~cuboid! and ''effective dimension'' that reproduced the measured excitonic transitions. Similar ''parabolic dot'' models have been assumed by Hawrylak *et al.*[1]

The accuracy of single-band and multiband effective-mass methods was recently examined in a series of papers.[30–34] In these papers, the shape, size, and composition of nanostructures were arbitrarily fixed, and the electronic structure was evaluated by successively improving the basis set, starting from single-band methods ~effective mass!, going to six- and eight-band methods ($k.p$), and finally, using a converged, multiband approach ~plane-wave pseudopotentials!. It was found that conventional effective-mass and $k.p$ methods can sometimes significantly misrepresent the fully converged results even when the shape, size, and composition were given. The observed discrepancies were both quantitative ~such as band-gap values, level spacings, Coulomb energies! and qualitative ~absence of polarization anisotropy in square based pyramidal dots,[34] missing energy levels.[32]! As a result of these limitations these methods may not offer a reliable bridge between the electronic and atomistic structure.

In this paper, we offer a bridge between recent measurements of the *electronic structure* and measurements of the *atomic structure* of the dots using accurate theoretical modeling. Modeling can determine if the calculated electronic structure resulting from an assumed shape, size, strain, and alloying profiles agrees with the measured electronic structure or not. A theory that can perform such a ''bridging function'' must be accurate and reliable. The pseudopotential approach to this problem qualifies, in that any discrepancy between the predicted and measured electronic properties can be attributed to incorrectly assumed shape, size, or alloying profile. We have studied a range of shapes, sizes, and alloy profiles and find that a lens-shaped InAs dot with an inhomogeneous Ga alloying profile is in closest agreement with current measurements. In the following sections we attempt to provide a consistent theoretical interpretation of numerous spectroscopic properties of InAs/GaAs dots.

II. OUTLINE OF THE METHOD OF CALCULATION

We aim to calculate the energy associated with various electronic excitations in InAs/GaAs quantum dots. These energies can be expressed as total-energy differences and require four stages of calculation:

~i! *Assume the shape, size, and composition and compute the equilibrium displacements*: We first construct a supercell containing both the quantum dot and surrounding GaAs barrier material. The shape, size, and composition profile are taken as input and subsequently refined. Sufficient GaAs barrier is used, so that when periodic boundary conditions are applied to the system, the electronic and strain interactions between dots in neighboring cells are negligible. The atomic positions within the supercell are then relaxed by minimizing the strain energy described by an atomistic force field[35,36] including bond-bending, bond-stretching, and bond-bending/bond-stretching interactions ~see Sec. III A!. An atomic force field is similar to continuum elasticity approaches[36] in that both methods are based on the elastic constants, $C underlying bulk materials. However, atomistic approaches are superior to continuum methods in two ways, ~a! they can contain anharmonic effects, and ~b! they capture the correct point-group symmetry, e.g., the point-group symmetry of a square based, zinc-blende pyramidal dot is C_{2v}, since the @110# and @1$\overline{1}$0# directions are inequivalent while continuum methods,[36] find C_{4v}. More details of the atomistic relaxation are given in Sec. III A.

~ii! *Set up and solve the pseudopotential single-particle equation*: A single-particle Schrödinger equation is set up at the relaxed atomic positions, $\$\mathbf{R}_{na}\%$:

$$\hat{H} c_i \sim\mathbf{r}! = \left\{ -\frac{b}{2}\nabla^2 + \Bigg(_{na} \hat{v}_a \sim\mathbf{r}-\mathbf{R}_{na}! \right\} c_i\sim\mathbf{r}! = e_i c_i \sim\mathbf{r}!. \qquad \sim 1!$$

The potential for the system is written as a sum of strain-dependent, screened atomic pseudopotentials v_a, that are fit to bulk properties extracted from experiment and first-principles calculations ~see Sec. III B!. The Schrödinger equation is solved by expanding c in a linear combination of bulk states f_{nk}, from bands *n*, and *k*-points *k*,

$$c_i \sim\mathbf{r}! = \Bigg(_{n,k} c_{n,k}^{(i)} f_{nk}\sim\mathbf{r}!, \qquad \sim 2!$$

taken at a few strain values. The solution of Eqs. ~1! and ~2! provides the level structure and dipole transition matrix elements. More details on the solution of the Schrödinger equation are given in Sec. III C.

~iii! *Calculate the screened, interparticle many-body interactions*: The calculated single-particle wave functions are used to compute the electron-electron, electron-hole, and hole-hole direct, J_{ee}, J_{eh}, J_{hh}, and exchange K_{ee}, K_{eh}, K_{hh}, Coulomb energies ~see Sec. III D!.

~iv! *Calculate excitation energies as differences in total, many-particle energies*: For example, the difference between the total-energy $E_{11}@h_0^1 e_0^1\#$ of a dot with a hole in level h_0 and an electron in level e_0 and the total-energy $E_{00}@h_0^0 e_0^0\#$ of the unexcited dot is

$$E_{11}@h_0^1 e_0^1\# - E_{00}@h_0^0 e_0^0\# = \sim e_{e_0} - e_{h_0}! - J_{e_0 h_0} + 2K_{e_0 h_0} d_{S0}, \qquad \sim 3!$$

where ~in the absence of spin-orbit coupling! $d_{S0}=1$ for triplet states, and 0 for singlet states. Analagous expressions exist for electron-addition experiments ~see Sec. III D!.

The main approximations involved in our method are ~a! the fit of the pseudopotential to the experimental data for bulk materials is never perfect ~see Table I! and ~b! we neglect self-consistent iterations in that we assume that the screened pseudopotential drawn from a bulk calculation is appropriate for the dot. Our numerical convergence parameters are ~i! the size of the GaAs barrier separating periodic images of the dots, and ~ii! the number of bulk wave functions used in the linear combination of bulk bands ~LCBB! expansion of the wave functions. To examine the effects of these approximations and convergences on the ultimate level of accuracy that can be obtained with our methodology we have first applied these methods to an InGaAs/GaAs quantum well ~see Sec. III E!, where experimental measurements of the shape, size, composition, and transition energies are more established. We next describe the details of our method.

TABLE I. Fitted bulk electronic properties for GaAs and InAs using the screened atomic pseudopotentials, in Eq. ~7!. The hydrostatic deformation potential of the band gap and G_{15v} levels are denoted by a_{gap} and $a_{G_{15v}}$. The biaxial deformation potential is denoted by b and the spin-orbit splittings at the G_{15v} and L_{1v} points are denoted by D_0 and D_1.

Property	GaAs		InAs	
	EPM	Expt.[a]	EPM	Expt.[a]
E_{gap}	1.527	1.52	0.424	0.42
$E_{X_{5v}}$	−2.697	−2.96	−2.330	−2.40
$E_{X_{1c}}$	1.981	1.98	2.205	2.34
$E_{X_{3c}}$	2.52	2.50	2.719	2.54
$E_{L_{3v}}$	−1.01	−1.30	−5.76	−6.30
$E_{L_{1c}}$	2.36	1.81	1.668	1.71
m_e^*	0.066	0.067	0.024	0.023
$m_{hh}^*@100\#$	0.342	0.40	0.385	0.35
$m_{hh}^*@111\#$	0.866	0.57	0.994	0.85
$m_{lh}^*@100\#$	0.093	0.082	0.030	0.026
a_{gap}	−7.88	−8.33	−6.79	−5.7
$a_{G_{15v}}$	−1.11	−1.0	−0.826	−1.0
b	−1.559	−1.7	−1.62	−1.7
D_0	0.34	0.34	0.36	0.38
D_1	0.177	0.22	0.26	0.27

[a] Reference 41.

III. DETAILS OF THE METHOD OF CALCULATION

A. Calculation of equilibrium atomic positions for a given shape

To calculate the relaxed atomic positions within the supercell, we use a generalization of the original valence force field ~G-VFF![35] model. Our implementation of the VFF includes bond-stretching, bond-angle bending, and bond-length/bond-angle interaction terms in the VFF Hamiltonian. This enables us to accurately reproduce the C_{11}, C_{12}, and C_{44} elastic constants in a zinc-blende bulk material. We have also included higher-order bond-stretching terms, which lead to the correct dependence of the Young's modulus with pressure. The G-VFF total energy can be expressed as

$$\begin{aligned} E_{VFF} = {} & \Bigg(_i \Bigg(_j^{nn_i} \frac{3}{8} @ a_{ij}^{(1)} D d_{ij}^2 + a_{ij}^{(2)} D d_{ij}^3 \# \\ & + \Bigg(_i \Bigg(_{k>j}^{nn_i} \frac{3 b_{jik}}{8 d_{ij}^0 d_{ik}^0} @\sim\mathbf{R}_j - \mathbf{R}_i! \cdot \sim\mathbf{R}_k - \mathbf{R}_i! \\ & - \cos u_{jik}^0 d_{ij}^0 d_{ik}^0 \#^2 + \Bigg(_i \Bigg(_{k>j}^{nn_i} \frac{3 s_{ijk}}{d_{ik}^0} D d_{ij} \\ & \times @\sim\mathbf{R}_j - \mathbf{R}_i! \cdot \sim\mathbf{R}_k - \mathbf{R}_i! - \cos u_{jik}^0 d_{ij}^0 d_{ik}^0 \#, \qquad \sim 4! \end{aligned}$$

where $D d_{ij} = @(R_i - R_j)^2 - d_{ij}^{0^2}\# / d_{ij}^0$. Here $\mathbf{R}_i$ is the coordinate of atom *i* and d_{ij}^0 and the ideal ~unrelaxed! bond distance between atom types of *i* and *j*. Also, u_{jik}^0 is the ideal

~unrelaxed! angle of the bond angle $j-i-k$. The $(^{nn_i}$ denotes summation over the nearest neighbors of atom i. The bond stretching, bond-angle bending, and bond-length/bond-angle interaction coefficients $a_{ij}^{(1)}(\,[\,a)$, b_{jik}, and s_{jik} are related to the elastic constants in a pure zinc-blende structure in the following way:

$$C_{11}+2C_{12}=\sqrt{\frac{3}{4d_0}}\sim 3a+b-6s!,$$

$$C_{11}-C_{12}=\sqrt{\frac{3}{d_0}}b,$$

$$C_{44}=\sqrt{\frac{3}{d_0}}\frac{@\sim a+b!\sim ab-s^2!-2s^3+2abs\#}{\sim a+b+2s!^2}. \qquad \sim 5!$$

The second-order bond-stretching coefficient $a^{(2)}$ is related to the pressure derivative of the Young's modulus by dB/dP, where $B=(C_{11}+2C_{12})/3$ is the Young's modulus. Note that in the standard[35] VFF, which we have used previously,[37–39] the last terms of Eq. ~4! are missing, so $s=0$ in Eq. ~5!. Thus there were only *two* free parameters (a,b) and therefore three elastic constants could not, in general, be fit exactly. The G-VFF parameters and the resulting elastic constants are shown in Table II for GaAs and InAs crystals. For an InGaAs alloy system, the bond-angle and bond-length/bond-angle interaction parameters b, s for the mixed cation Ga-As-In bond angle are taken as the algebraic average of the In-As-In and Ga-As-Ga values. The ideal bond angle u_{jik}^{0} is 109° for the pure zinc-blende crystal. However, to satisfy Vegas's law for the alloy volume, we find that it is necessary to use $u^{0}_{\text{Ga-As-In}}=110.5°$ for the cation mixed bond angle.

As a simple test of this G-VFF for alloy systems, we compared the relaxed atomic positions from G-VFF with pseudopotential LDA results for a ~100! $(\text{GaAs})_1/(\text{InAs})_1$ superlattice where the c/a ratio is fixed to 1, but we allow energy minimizing changes in the overall lattice constant (a_{eq}) and the atomic internal degrees of freedom (u_{eq}). We find $a_{eq}^{LDA}=5.8612$ Å and $u_{eq}^{LDA}=0.2305$, while the G-VFF

$$\langle k_1|\hat{H}_{SO}|k_2\rangle = \sum_l \frac{4i\pi}{\Omega}(2l+1)\left[\frac{dP_l(\cos\theta_{k_1k_2})}{d\cos\theta_{k_1k_2}}\right](\hat{k}_1\times\hat{k}_2)\cdot\hat{S} \times\int_0^{\infty} V_l^{SO}(r)\,j_l(|k_1|r)\,j_l(|k_2|r)\,r^2dr. \qquad (10)$$

Here, $\theta_{k_1k_2}$ is the angle between k_1 and k_2, Ω is the volume of the unit cell, and j_l is a spherical bessel function. In our calculations, we have only included the effects of $l=1$ (p states), and have used a Gaussian model for V_l^{SO}

resulting effect on single-particle energy *differences* is therefore a fraction of an meV and so we choose to neglect this

$E = 1520$ meV. All energy levels can be referenced with rewell-established ‘‘lens-shaped’’ dot geometry from Refs. 5–12. The shape of this dot is shown in Fig. 3. The profile is obtained by selecting the section of a pure InAs sphere that yields a circular base with diameter 252 Å and a height of 35 Å. The main experimental uncertainty about this dot is the composition profile. It is not known if the dots are pure InAs or if Ga has diffused into the dots. For comparison, we also calculate the electronic structure of a square based InAs pyramid with a base of 113 Å and a height of 56 Å. This is not believed to be a realistic geometry, however, it has been used as a benchmark for many previous theoretical calculations[34,37,38,52,53] and we include it here for comparison purposes. In the following sections these two geometries will be referred to as the ‘‘lens’’ and the ‘‘pyramid.’’ The results of our calculations are shown in Table IV and Fig. 4.

A. Confined electron states

Figure 4 shows the calculated square of the envelope function for the electron states in the pyramidal- and lens-shaped InAs/GaAs quantum dots. For the lens-shaped dot, the electron states can be approximately interpreted as eigenstates of the $\hat{L}_z$ operator.[1] Here we plot only the first six bound states corresponding to $l_z=0, \pm 1$, and ± 2. The first state e_0, has $l_z=0$ and is commonly described as *s*-like as it has no nodes. The e_1 and e_2 states have $l_z=\pm 1$, and are *p*-like with nodal planes ~110! and $(\bar{1}10)$. The e_3, e_4, and e_5 states have $l_z=\pm 2$ and 0, respectively, and are commonly described as $d_{x^2-y^2}$, d_{xy}, and $2s$, respectively. Due to the underlying zinc-blende atomistic structure, the $C_‹$ symmetry is reduced to C_{2v}. Hence, the e_0 to e_5 states correspond to the a_1, b_1, b_2, a_1, a_2, and a_1 irreducable representations of the C_{2v} group, rather than eigenstates of $\hat{L}_z$. This allows states e_0, e_3, and e_5 to couple. This coupling is evident, for example, in the larger charge density along @110# compared to @$1\bar{1}0$# in the e_3 state, due to its coupling with e_1. The observable effect of this C_{2v}The 418.199 141.928 Tm (2)Tj 9.4

fects of the spin-orbit interaction, which reduces the C_{2v} group to a double group with the same single representation for all the states. In our calculations the spin-orbit interaction is included, but is produces no significant effects for the electron states.

The electron states in the pyramidal dot also belong to the C_{2v} group and show a one-to-one correspondence with those in the lens-shaped dot. However, there are only five bound states in the pyramidal dot due to its smaller size. Here we define an electron state as bound if its energy is below that of the unstrained, bulk GaAs conduction-band edge.

The calculated values of the s-p and p-d energy spacings, δ_{sp}, and, δ_{pd}, for the lens- and pyramidal-shaped dots, are 65 and 68 meV and 108 and 64 meV, respectively. The splitting of the two p states, $\delta_{pp}=e_2-e_1$ are 2 and 26 meV, respectively. The calculated values of the electron binding energy, $\Delta E(e)$, are 271 and 171 meV, respectively. The electron-electron direct Coulomb energies, $J^{ee}_{e_0e_0}$, $J^{ee}_{e_1e_1}$, and $J^{ee}_{e_0e_1}$ in the lens and pyramidal dots are calculated as 32, 25, and 25 meV and 40, 35, and 36 meV respectively. On applying a magnetic field in the growth direction, we calculate an increase in the splitting of the two p states (e_2-e_1) in the

B. Confined hole states

Figure 4 shows calculated wave functions squared for the hole states in pyramidal- and lens-shaped InAs/GaAs quantum dots. Unlike the electron states, the hole states cannot be approximated by the solutions of a single band Hamiltonian. Instead there is a strong mixing between the original bulk Bloch states with G_{8v} and G_{7v} symmetry. The larger effective mass for holes results in a reduced quantum confinement of the hole states and consequently many more bound hole states. Only the six bound hole states with the highest energy are shown in Fig. 4.

The calculated values of the h_0-h_1, h_1-h_2, and h_2-h_3 hole level spacings for the pyramidal- and lens- shaped dots are 8, 7, and 6 meV and 15, 20, and 1 meV respectively. The calculated hole binding energies, $\mathsf{D}E(e)$, are 194 and 198 meV. We calculate the highest-energy hole level in pure InAs wetting layers, $\mathsf{D}E_{WL}^{(h)}$, with thicknesses of 1 and 2 ML to reside 30 and 50 meV above the VBM of unstrained bulk GaAs. The hole-hole Coulomb energies, $J_{h_0 h_0}^{hh}$, are 25 and 31 meV.

C. Electron-hole excitonic recombination

Figure 5 shows our calculated single exciton absorption spectrum for a pure InAs, lens-shaped dot with a base of 252 Å and a height of 35 Å. The energies of each of the absorption peaks are calculated from Eq. ~15!. The ratios of the dipole matrix elements for light polarized along @110# and @1$\bar{1}$0# are calculated from Eq. ~17!. Figure 5 illustrates that, for a lens-shaped dot, both the conventional $e_i \rightarrow h_i$ transitions and additional e_1-h_2, e_2-h_1, e_3-h_4, and e_4-h_3 transitions are strongly allowed. The ratio of the polarization anisotropies l are shown in Table V. As a result of the circular symmetry of the lens-shaped dot, we calculate a polarization ratio of $\mathsf{l}=1.03$ for the e_0-h_0 transition. This value is in contrast to that calculated value for a pyramidal dot of $\mathsf{l}=1.2$.[45] For the higher-angular momentum transitions we find larger deviations from unity. The magnitude of the ratios pyramidal dots. The calculated ground-state electron-hole exchange energies, $K^{eh}_{e_0h_0}$ are an order of magnitude smaller, with values of 3 and 0.2 meV. These yield excitonic band gaps of 1.03 and 1.12, respectively. The calculated excitonic dipoles @Eq. ~18!# are 3.1 and 0.16 Å, respectively. A positive dipole is defined as the center of the hole wave function being located above the center of the electron wave function.

VI. ANALYSIS OF PERTINENT EXPERIMENTAL MEASUREMENTS

A. The intraband *s*-*p* and *p*-*d* electron energy spacings

Measurements of the spacing between the e_0- and e_1-like electron levels (s-like and p-like! are based on infrared absorption. For the lens-shaped dots, Fricke *et al.*[7] load electrons into the dots by growing a sample consisting of an *n*-type doped layer, a tunneling barrier, a layer of InAs/GaAs lens-shaped dots, a GaAs spacer, and a GaAs/AlAs short period superlattice. By applying a voltage between the *n*-doped layer at the bottom of the sample and a Cr contact grown on top of the SPS, electrons are attracted from the *n*-doped layer into the InAs dots. Infrared photons were used to excite electrons from the occupied e_0 level into the e_1 level. Neglecting the small exchange energy, the energy differences for the e_1-e_0 excitations when one and two electrons are present in the dot are

$$E_{01}@e_1^1\#-E_{01}@e_0^1\#=\sim e_{e_1}-e_{e_0}!,$$

$$E_{02}@e_0^1e_1^1\#-E_{02}@e_0^2\#=\sim e_{e_1}-e_{e_0}!+@J^{ee}_{e_1,e_0}-J^{ee}_{e_0,e_0}\#. \qquad \sim 19!$$

The first of these energy differences yields a direct measurement of the s-p energy spacing, d_{sp}, of 49.1 meV. The second energy difference was measured at 50.1 meV. Drexler *et al.*[5] also used infrared transmission spectroscopy to measure an energy spacing, $d_{sp}=41$ meV. Pan *et al.*[21,26,22] have also performed infrared-absorption measurements on

$$E_{02}@e_0^1 e_2^1\# - E_{02}@e_0^2\# = \sim e_{e_2} - e_{e_0}! +$$

25, and 37, respectively, compared to measured values of 23, 24, 18, and 33.3 meV.

The calculated polarization anisotropies, l, for the e_0-h_0 recombination in lens and pyramidal shaped, pure InAs dots are l =

As increasing ~decreasing! the dimensions of the dot acts to decrease ~increase! both the level spacings and the gap, it is clear that changing the dot geometry alone will not significantly improve the agreement with experiment as this requires a simultaneous *decrease* in the energy-level splittings and *increase* in the band gap. However, Ga in-diffusion into the dots acts to *increase* the band gap of the dot while decreasing the energy-level spacings.

Table IV shows that adopting a geometry with a base of 275 Å and a height of 35 Å and a uniform Ga composition of $Ga_{0.15}In_{0.85}As$ produces the best fit to the measurements in Refs. 7 and 11.

In conclusion, our results strongly suggest that to obtain very accurate agreement between theoretical models and experimental measurements for lens-shaped quantum dots, one needs to adopt a model of the quantum dot that includes some Ga in-diffusion within the quantum dot. When Ga in-diffusion is included, we obtain an excellent agreement between state of the art multiband pseudopotential calculations and experiments for a wide range of electronic properties. We are able to predict most observable properties to an accuracy of ± 5 meV, which is sufficient to make predictions of both the geometry and composition of the dot samples.

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*Present address: Lawrence Livermore National Laboratory, Livermore, California 94550.

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