

Anisotropy of the electron energy levels in $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ quantum dots with non uniform composition

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Abstract

Atomistic simulations that use the Tersoff empirical potential accurately reproduce the effects of the presence of compositional disorder in strained semiconductor alloys. This method is applied to InGaAs quantum dot islands, for which gradients in the In composition distribution have been observed and accurately measured, and we demonstrate that the internal piezoelectric fields contribute strongly to the nature of the electron wavefunctions. The theoretical predictions are supported by experimental evidence: intersubband absorption measurements confirm that the p-states degeneracy for the electron first excited state is lifted and a minimum splitting of at least 5 meV is to be generally expected.

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1. Introduction

Atomistic simulations that use the Tersoff empirical potential applied to semiconductor nanostructures is a rapidly growing field [1–3]. This is in part because of the capability of correctly treating compositional disorder, which in InGaAs

quantum dots (QDs) is of particular importance: non uniform compositions and the presence of an In rich dot apex have been measured both directly [4] and indirectly [5]. The consequence of the presence of compositional gradients on the energy levels has also been investigated [6–8], but with methods that often underestimate the influence of compositional disorder. The importance of the local fluctuations has been recognized by Bester and Zunger [9], who however have not included

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the effect of the piezoelectric field in their theoretical model.

The piezoelectric (PE) effect originates from the lack of inversion symmetry of III–V semiconductors which makes the crystal respond to shear strain by producing a dipole charge. Prior to this work the effect was theoretically investigated in pure InAs QDs, and in this limiting case the conclusion has been that for pyramidal dots the PE potential influence is relegated to the corners of the pyramid and depends strongly on the size of the islands, though in most cases its magnitude is not large enough to affect the electron and hole wavefunctions [10,11].

In the case of gradients of composition where alloy fluctuations become important, it is found that the PE field increases in magnitude [12]. This is because the expression for the PE charges originating from the presence of shear strain is given by

$$\rho(\mathbf{r}) = -\nabla \cdot (2e_{14}(\mathbf{r}) \cdot [\varepsilon_{yz}(\mathbf{r})\mathbf{i} + \varepsilon_{xz}(\mathbf{r})\mathbf{j} + \varepsilon_{xy}(\mathbf{r})\mathbf{k}]), \quad (1)$$

where e_{14} is the composition dependant PE constant and ε_{yz} , ε_{xz} and ε_{xy} are the position dependant non diagonal components of the strain tensor. The PE potential is then obtained upon solving Poisson's equation in the case of a variable dielectric constant ε_s :

$$\nabla(\varepsilon_s(\mathbf{r})) \cdot \nabla\phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon_0}, \quad (2)$$

where $\phi(\mathbf{r})$ is the potential and ε_0 is the permittivity of free space. From Eqs. (1) and (2) it is obvious that there are three distinct contributions to the magnitude of the PE potential: the magnitude variation of the strain components (increased by the presence of alloy fluctuations), the variation of e_{14} and variations in the local dielectric constant. An accurate calculation of the PE effect must include all three contributions. It is also obvious that the presence of compositional gradients increases the need for taking into account the contribution from ε_s : in fact in this case gradients in the composition create diffused interfaces the effect of which would not be correctly reproduced by solving Poisson's equation with a constant ε_s in both the QD island and the GaAs barrier.

2. Theoretical predictions

In order to accurately evaluate the effect of the presence of the PE field on the electron energy levels of InGaAs and InAs QDs we implemented a Tersoff potential atomistic simulation (TPAS) in which atomistic models are built and then relaxed using the OXON code [13]. From the relaxed structures the atomic displacements that minimize the total energy are found and successively used to evaluate the six components of the strain tensor which are then used to evaluate the PE charges and potential. The conduction band energy levels are calculated with a singleband approximation in which the bandstructure is obtained in terms of material dependent parameters, including the effect of the strain through the use of deformation potentials. To improve the singleband approximation accurate effective masses are calculated using 8 band $\mathbf{k} \cdot \mathbf{p}$ theory [8,14,15].

For these particular simulations the QD model consists of a capped pyramidal island with smoothed edges: it is worth stressing that the particular choice of square base with smoothed corners, inspired by evidence of faceting in uncapped islands [16], does not alter the general role of the PE field compared to having a lens shape [17]. The sizes of the pyramid were obtained from typical TEM micrographs of QDs grown by molecular beam epitaxy with the deposition of 7ML of InGaAs at 500 °C. The characteristic dimensions are: base length 21 nm, height 4 nm and facet angle 35°.

We then created four models with identical dimensions and different compositions: a pure InAs (A), a uniformly distributed $\text{In}_{1-x}\text{Ga}_x\text{As}$ alloy with $x = 0.5$ (B), one trumpet shaped [1,4] ranging from 50% In at the base and 80% at the top (C), and another trumpet shaped with 30% In at the bottom and 80% In at the top (D). In order to reveal the effect of the PE field on the conduction band energy levels, the TPAS for all four models was performed with and without the inclusion of the PE potential for the electronic calculations.

Results for the calculated separation between the electron ground and first excited states (ΔE) and the splitting of the doubly degenerate p type

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