

Comparison of two methods for describing the strain profiles in quantum dots

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The electronic structure of interfaces between lattice-mismatched semiconductors is sensitive to the strain. We compare two approaches for calculating such inhomogeneous strain—continuum elasticity @CE!, treated as a finite difference problem# and atomistic elasticity. While for *small* strain the two methods must agree, for the large strains that exist between lattice-mismatched III-V semiconductors ~e.g., 7% for InAs/GaAs outside the linearity regime of CE! there are discrepancies. We compare the strain profile obtained by both approaches ~including the approximation of the correct C_2 symmetry by the C_4 symmetry in the CE method! when applied to C_2 -symmetric InAs pyramidal dots capped by GaAs. © 1998 American Institute of Physics. @S0021-8979-98!01805-2#

I. INTRODUCTION

One of the leading methods for growing semiconductor quantum dots is via the controlled coarsening of a film of a material that is strained with respect to the substrate on which it is grown.^{1,2} This ~‘self-assembled’! coarsening/roughening is a result of lattice-mismatch-induced strains. The dots are often capped by the substrate material, thus extending the strain around the dot to all angular directions. Not surprisingly, the interpretation of the electronic structure of such dots is profoundly affected by their strain profile. Thus, in order to calculate or interpret the measured electronic structure, one has first to calculate or measure the position dependent strain tensor e_{ab} .

The three basic approaches to calculating such strains are:

(i) *Harmonic continuum elasticity*: Here, one uses classical elasticity³ within the harmonic approximation. For a cubic system, the strain energy per atom, E_{CE} , is

$$E_{CE} \approx \frac{V}{2} C_{11} (e_{xx}^2 + e_{yy}^2 + e_{zz}^2) + \frac{V}{2} C_{44} (e_{yz}^2 + e_{zx}^2 + e_{xy}^2) + \frac{1}{2} V C_{12} (e_{yy} e_{zz} + e_{zz} e_{xx} + e_{xx} e_{yy}),$$

quantum dots from experiments of Grundmann *et al.*² In a continuum representation, the strain is equal on the $\{110\}$ and $\{1\bar{1}\}$

$$D_i^2 f_{\sim \mathbf{r}}! 5^{f \sim \mathbf{r}}$$

polynomials of \mathbf{R} and \mathbf{h} . The increment Δ minimizing the elastic energy is then obtained by solving exactly

$$\frac{\partial E_{AE}(\mathbf{R}, \mathbf{h})}{\partial \Delta} = 0 \quad (17)$$

Figure 2 illustrates how the local strain is calculated. After the atomic positions are relaxed by minimizing E_{AE} , the local strain tensor $\tilde{\epsilon}$ at a cation site (for cation-mixed systems) is calculated by considering a tetrahedron formed by four nearest neighboring anions. The distorted tetrahedron edges, \mathbf{R}_{12} , \mathbf{R}_{23} and \mathbf{R}_{34} , are related to the ideal tetrahedron edges \mathbf{R}_{12}^0 , \mathbf{R}_{23}^0 and \mathbf{R}_{34}^0 via

$$\begin{pmatrix} R_{12,x} & R_{23,x} & R_{34,x} \\ R_{12,y} & R_{23,y} & R_{34,y} \\ R_{12,z} & R_{23,z} & R_{34,z} \end{pmatrix} = \begin{pmatrix} 1 & 1 & e_{xx} & e_{yx} & e_{zx} \\ e_{xy} & 1 & 1 & e_{yy} & e_{zy} \\ e_{xz} & e_{yz} & 1 & 1 & e_{zz} \end{pmatrix} \begin{pmatrix} R_{12,x}^0 & R_{23,x}^0 & R_{34,x}^0 \\ R_{12,y}^0 & R_{23,y}^0 & \end{pmatrix}$$

consistent comparisons of the two approaches. The largest differences occur around the interfaces between the dot and the cap. A significant discrepancy is also found inside the quantum dot where the InAs experiences large compressive strains: e_{xx} of the continuum elasticity is found to be more compressive than that of the atomistic elasticity, while the e_{zz} of the CE is more tensile. A similar comparison is given in Fig. 5, but this time the position vector is along the Z $5@001\#$ direction, starting from the substrate, going through the wetting layer into the pyramidal tip and then into the capping layer. Again, the discrepancy is largest around the interfaces, while the strains in the barrier \sim GaAs substrate and capping layer agree within 0.5%.

Figure 4 illustrates the extent to which the continuum elasticity description misses the correct atomic symmetry. In a pyramid made of zincblend materials on the (001) substrates, the $\$110\%$ and $\$\bar{1}10\%$ facets are symmetrically inequivalent \sim Fig. 1!. Indeed, the atomistic calculation produces different strains. The dashed lines in Fig. 4 show the difference $e_{ij}^{AE}(@110\#) \mathcal{Z} e_{ij}^{AE}(@\bar{1}10\#)$ for these two directions. We see that the anisotropy is pronounced at the interfaces. For the atomistic elasticity calculation, we construct the pyramidal structure to have an In atom at the pyramidal tip. This tip In atom has: -i! two As atoms that belong to the InAs dot and lie along the $@110\#$ direction; and -ii! the other two As atoms that belong to the GaAs capping layer and lie along the $@\bar{1}10\#$ direction. Considering only the local strain of the tip atom, one expects larger compressive e

of the quantum dot. Most notably, the real point group symmetry of the square pyramid is C_2 , but continuum elasticity spuriously produces a higher C_4 symmetry.

Regarding the quantitative effects, there are different levels of approximation for coupling the strain to the electronic structure. The most general and accurate electronic structure approach is atomistic -e.g., pseudopotentials, tight-binding!. There, the full set of atomic positions affects the electronic structure. In more approximate electronic structure approaches, such as continuum effective mass, only some aspects of the full, position-dependent-strain tensor, $e_{ij}(\mathbf{r})$ is "felt" by the electronic structure. In these approaches, one considers strain-modified potential wells as barriers. Since experiments typically measure electronic energies rather than strains, it is instructive to examine these effects.

Assuming in decoupled conduction and valence bands the strain-modified confinement potential of the conduction-band state is

$$E_c(\mathbf{r}) \approx E_c^0 + a_c \text{Tr} \mathbf{e}(\mathbf{r}), \quad (22)$$

$E_c^0(\mathbf{r})$ is the energy of the conduction-band minimum of the bulk material at \mathbf{r} and a_c is the deformation potential of the conduction band under hydrostatic deformation. The "strain" Hamiltonian of the valence states¹⁷ is

$$H_v \approx a_v \text{Tr} \mathbf{e}(\mathbf{r}) + b \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} e_{xx} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} e_{yy} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} e_{zz} + 2\sqrt{3}d \begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} e_{xy} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} e_{yz}$$

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