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Finite element analysis of strain effects on symmetry reduction of semiconductor quantum dots

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ABSTRACT

Strain deformations and piezoelectric effects greatly modify the band edge potential profile and the symmetry of the semiconductor self-assembled quantum dot system, playing a critical role in determining the material optical and electronic properties. In this paper, based on the continuum elasticity model, we develop an easily implementable finite element method approach to calculate the material displacement, strain, stress, piezoelectric effect, and their impacts on the band edges of quantum dots. No matter the intrinsic symmetric level of the quantum dot geometric shape, we show the maximum symmetry group of the Hamiltonian for an III-V group quantum dot system is C_{2v}. Orientation changes of the quantum dot in the crystal will lead to different Hamiltonian symmetry even though the geometric symmetry groups are the same. We also notice that for a symmetric quantum dot, such as a pyramid, its smallest band gap is normally not at the geometric center, but at the base or near the top. Aspect ratio changes of quantum dots will lead to apparent bandgap variations; however, conformal size changes of the quantum dots will not result in visible bandgap modifications.

1. Introduction

Self-assembled quantum dots (QDs) have a wide range of applications in optoelectronic and quantum devices such as QD light emitting diodes (LED), laser diodes and solar cells [1–3]. Strain effects, originating from the lattice mismatch between the QD core and surrounding matrix, play an important role in QD formation and carrier confinement. Therefore, to have a clear understanding of the QD material displacement, strain, stress and their consequence to the potential deformation is of great importance to study QDs' electronic and optical properties. Currently, there are several popular approaches to study the strain related effects, including atomistic models [4–6], numerical continuum elasticity models [7–9], and analytical models [10,11]. The atomistic model provides the most accurate results. However, this approach also demands the most expensive computational resources. Additionally, a large number of atomic input parameters are required; and some of those atomic parameters are not easy to obtain. On the other hand, analytical approaches are easy to implement and efficient in computation, but this method's application range and accuracy are very limited. For example, it is almost impossible to include various complicated geometric shapes and anisotropic effects analytically. Recently, it has been reported that the analytical model can be calibrated based on accurate atomistic simulation results [13], but unfortunately, the calibrated analytical model can only predict the strain effect at the center of the dots, not the whole strain profile in the QD and matrix. As we know, the carrier bound state energies and wavefunctions are actually determined by the potential profile as a whole. The numerical continuum elasticity model, treating the QD and matrix as continuous materials, is a good compromise between the computation complexity and accuracy. Compared with atomistic models, the numerical continuum elasticity

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model is much more efficient and also accurate enough for most applications. Unlike the atomistic model, the semiconductor elasticity coefficients and band parameters, as the model inputs, are well documented and easy to obtain [14].

Because of crystal symmetry, self-assembled QDs tend to form highly symmetric shapes with the dot facet in a specific crystal plane, such as pyramids [15–17]. By certain doping techniques, QDs can also grow to other symmetric shapes, such as lenses and half-ellipsoids [17–20]. Therefore, group theory turns out to be a powerful tool to investigate the highly symmetric QDs [5,7,21,22]. However, it is noticed that the geometric symmetry of a QD is not identical to its Hamiltonian's symmetry because of strain and band-mixing effects [5,7,21]. In this paper, starting from a continuum elasticity model, using the finite element method (FEM) [23], we systematically investigate the potential symmetry reduction of a QD system due to strain and piezoelectric effects. Compared with other numerical approaches, such as finite volume methods [5,7,8], FEM is more versatile and suitable for various QD geometric shapes [9], and the boundary conditions can be naturally implemented and satisfied without any specific treatment. Additionally, our approach is presented as a set of coupled partial differential equations (PDEs) instead of searching for the minimum strain energy configuration [7,8], which makes the implementation with a FEM solver much easier. We can show for InAs/GaAs or other III-V group zinc-blende crystal quantum dots, the maximum symmetry group for the Hamiltonian is C_{2v}. This group has two symmetric reflection planes: (110) and $(1\bar{1}0)$, which pass through the central axis of the symmetric QD, and one symmetric rotation of 180° along the central axis. Any QD with these three symmetric operations will reach the maximum C_{2v} symmetry independent of the QD's original geometric symmetry group. However, if the geometric group only partially has or doesn't have these three symmetric operations, the Hamiltonian's symmetric group will be reduced to the subgroup of C_{2v} or have no symmetry at all. Besides symmetric properties, strain deformation and piezoelectric potential profiles inside a QD are not homogeneous. In this research, it is noticed that the minimum bandgap for a symmetric QD, such as a pyramid, normally is at the base or the top of the QD, not at its geometric center. We also investigate the bandgap variations with different QD shapes and sizes.

Our paper is presented as following. In Section 2, we derive a set of detailed PDEs to calculate the QD material displacement, strain, stress, piezo effect, and their effects on the band edge changes. In Section 3, we investigate the potential deformation profiles inside the QD and matrix. In this part, we explain the symmetry reduction because of strain and piezoelectric effects and discuss the bandgap variations due to QD size and shape changes. Finally, in Section 4, we give a brief conclusion.

2. Symmetric theory of strain, stress and strain induced potential energy change

For a QD embedded in the matrix, the strain tensor, which is of rank 2, can be defined as [10].

$$\bar{\bar{\varepsilon}} = \frac{1}{2}[(\nabla\vec{u}) + (\nabla\vec{u})^T] + \bar{\bar{\varepsilon}}^0_{MM}$$
or
$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \varepsilon^0_{MM}\delta_{ij} \tag{1}$$

In Eqn. (1), the superscript T denotes the transpose operation; $\vec{u} = u_x\vec{e}_x + u_y\vec{e}_y + u_z\vec{e}_z$ is the displacement vector from the originally matched position; and $\bar{\bar{\varepsilon}}_{MM}$ is the mismatch strain tensor due to the crystal lattice constant difference between the QD and the surrounding matrix. ε^0_{MM} is defined as

$$\varepsilon^0_{MM} = \begin{cases} \frac{a_M - a_Q}{a_Q} & \text{(inside QD)} \\ 0 & \text{(in the matrix)} \end{cases} \tag{2}$$

where a_M, and a_Q are the lattice constants of matrix and QD, respectively. From Eqn. (1), it is easy to show $\varepsilon_{ij} = \varepsilon_{ji}$. The stress tensor, which is also of rank 2, is calculated by the following equation

$$\bar{\bar{\sigma}} = \mathrm{C}^{(4)}\colon \bar{\bar{\varepsilon}}$$
or
$$\sigma_{ij} = C_{ijkl}\ \varepsilon_{kl} \tag{3}$$

In Eqn. (3), $\mathbf{C}^{(4)}$ is the fourth rank elasticity tensor;: denotes dyadic tensor product; and Einstein summation notation has been used. For common semiconductor materials with a cubic crystalline such as InAs and GaAs, the symmetric relations reduce the coefficients of $\mathbf{C}^{(4)}$ to three independent terms C_{11}, C_{12} and C_{44} [14,24]. Therefore, the stress tensor with $\sigma_{ij} = \sigma_{ji}$ in Eqn. (3) can be simplified as follows,

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{xz} \\ \sigma_{yz} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & 2C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2C_{44} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{xy} \\ \varepsilon_{xz} \\ \varepsilon_{yz} \end{pmatrix} \tag{4}$$

or