Numerical Simulation of electronic properties in quantum dot heterostructures

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ABSTRACT

A confined structure in all three dimensions leads to carrier's discrete energy level spectrum in quantum dots. This property has profound impact on many applications, such as single electron transistors, quantum dot laser, high efficiency photovoltaic cells, information storage etc. A finite element method is utilized to model the residual stress distribution. The effect of residual stress on the electronic and optical properties is studied. This is accomplished by incorporating both the valence subbands and the strain-induced potential field into Schr dinger equation. A finite-difference method was applied to solve the equation system. The density of states is obtained from the spectrum of the eigenstates. The discrete eigenstate distributions for both with and without residual stress are compared. The effect of the quantum dot size and geometry to the energy state distribution is discussed.

Keywords: Numerical Modeling, Quantum Dots, Residual Stress, Electronic State

INTRODUCTION AND METHODS

Quantum dots have been the research topics of many publications because of their unique electronic properties. Many research papers involving both experiments and theoretical modeling have been published since the early 1990s. Publications on quantum dots prior to 1998 have been reviewed by Bimberg et al. [1].

Quantum dots are usually fabricated by growing nanometer sized materials on various substrates. The differences in material's properties between the quantum dots and the substrate material, such as lattice parameters and thermal expansion coefficients, will generate residual stress in the quantum dots. The residual stress affects the electrical, optical properties, and device lifetime. The theoretical simulations in quantum dots can help to understand various effects that will have impacts on the electronic properties. Many approaches have been applied in the quantum dot simulations. Besides the dependence on the material properties, the electronic properties of quantum dots also strongly depend on the quantum dot size and geometry. The complex geometry of quantum dots and the anisotropy of materials often cause simulation challenges. Numerical methods, such as finite element and finite difference method, are avenues to model the distribution of the lattice mismatch and thermal residual stress, their effects on the electronic, transport, and photovoltaic properties in quantum dots. Johnson et al. [2,3,4] have applied finite element modeling to simulate the residual stress distribution and its effects on electrical and optical properties of quantum dots.

Due to the strong dependence of energy levels on the geometry and sizes, the quantum dots are perfect candidates for high efficiency photovoltaic cells. Solar cells with 63% efficiency have been predicted by theoretical work [5,6]. Recently, we have developed numerical computer programs for simulation of residual stress distributions and its effects on the electrical, transport, and optical properties in the quantum dots [7,8]. A finite element method has been utilized to model the residual stress distribution. The effects of lattice mismatch, thermal expansion, and geometry of the sample have been systematically studied.

A finite difference method was applied to model the electronic properties. The effects of residual stresses on the electronic and optical properties are also studied. This was accomplished by incorporating both the valence subbands and the strain-induced potential field into the time-independent Schr dinger equation

$$\sum_{\beta=1}^{4} H_{k.p}^{\alpha\beta} \quad \beta \quad V^{\alpha\beta} \quad \beta \quad E \quad \alpha \qquad (1)$$

where ? ^{a} is the wave function in subband a, E is the energy, $H_{k.p}^{\alpha,\beta}$ is the **k**.**p** Hamiltonian operator, and V$^{a\beta}$ is a potential.

$$V^{\alpha\beta} \quad V_C^{\alpha\beta} \quad V_\varepsilon^{\alpha\beta} \qquad (2)$$

where V $_C$ is due to the valence-band alignment of material at a given position in device and V is strain-induced potential. Finite-difference method was then applied to solve the equation system[8]. Description of the algorithm can be found in our earlier paper[8]. The density of states are obtained from the spectrum of the eigenstates in the numerical solutions.

RESULTS

Calculations have been performed on a series of quantum dots with different size and geometry. Figure 1 provides an example of the strain distribution in a stand alone Ge quantum dot grown on a Si substrate. Growth temperature is assumed to be 1000K. The diameter of the quantum dot is 20 nm. For the system with axial symmetry, only three components of the strain tensor are needed. As it is shown,

the residual strain is mainly concentrated at the interface and the edge of the quantum dot.

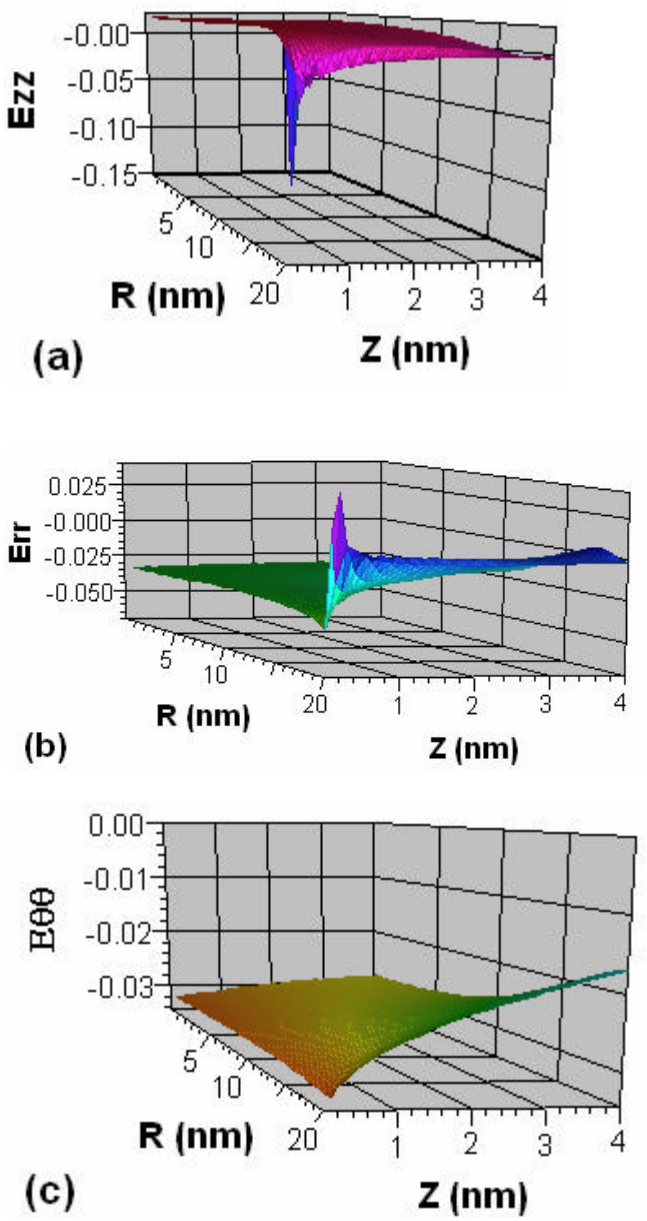

Figure 1. Distribution of residual strain in Ge Quantum Dot

Figure 2 provides the distribution of energy levels for cone shape quantum dots with different diameters. The discrete distributions of the energy levels and the effects of quantum dot size can be clearly observed

We have also studied the effects of different geometries. The energy level distributions for two quantum dots with different shape are provided. Figure 3(a) is for a conical quantum dot with a diameter of 40 nm and a height of 4 nm. Figure 3(b) is for a pyramidal shape studied by Johnson et al. [3]. Their results are redrawn here for comparison. The impact of residual stress can be clearly observed. The geometry of the quantum dot has shifted the energy distribution significantly.

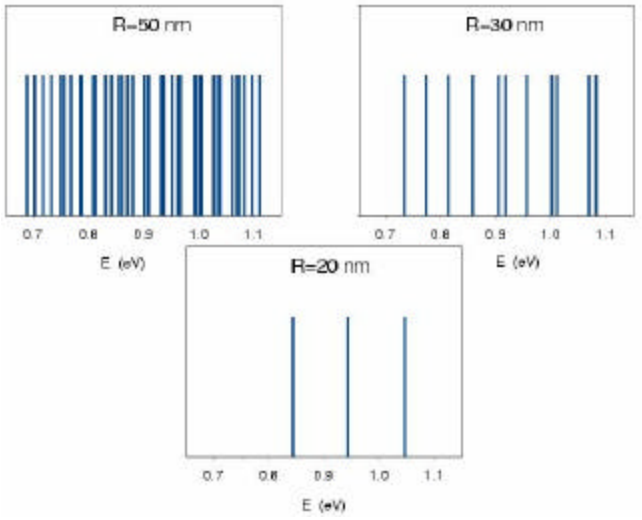

Figure 2. Distribution of energy levels for cone shape quantum dots with diameters of 40nm, 60nmand 100nm

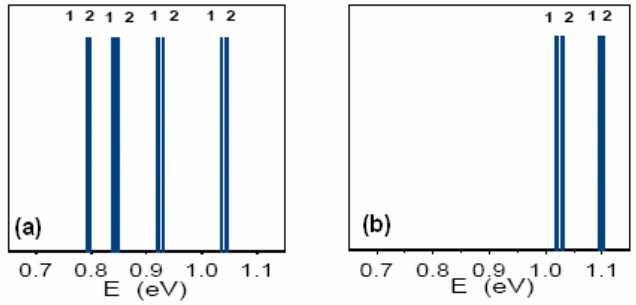

Figure 3. Effects of strain on the confined energies for cylindrical and pyramidal quantum dots. (a) is for cylindrical geometry and (b) is for pyramidal geometry. 1s indicate the energy level without the effects of strain and 2s when the strain potential is taken into account.

Figure 4 illustrates the effects of residual strain on the wave function for energy level E_{13} of a cylindrical Ge quantum dot with a radius of 20 nm. Where the first index "1" in E_{13} would indicate the first energy level or ground state in z direction and the second index "3" would indicate the third energy level or the second excited state in r direction, if z and r variables would be possible to be separated. In our case they are not separable because of the residual strain potential. However, the strain potential is a

perturbation of our problem defined by equation (1) - (2) and in this approach the nomenclature is appropriate. The wave function displayed in Figure 4(c) is for the quantum dot with strain field included in the calculation. Figure 4(a) and 4(b) are the wave function distribution viewed from the angle along the radius direction inside the quantum dots. Figure 4(a) is the wave function without the effect of the strain and figure 4(b) is the one with strain effects. The differences can be clearly observed in figure 4.

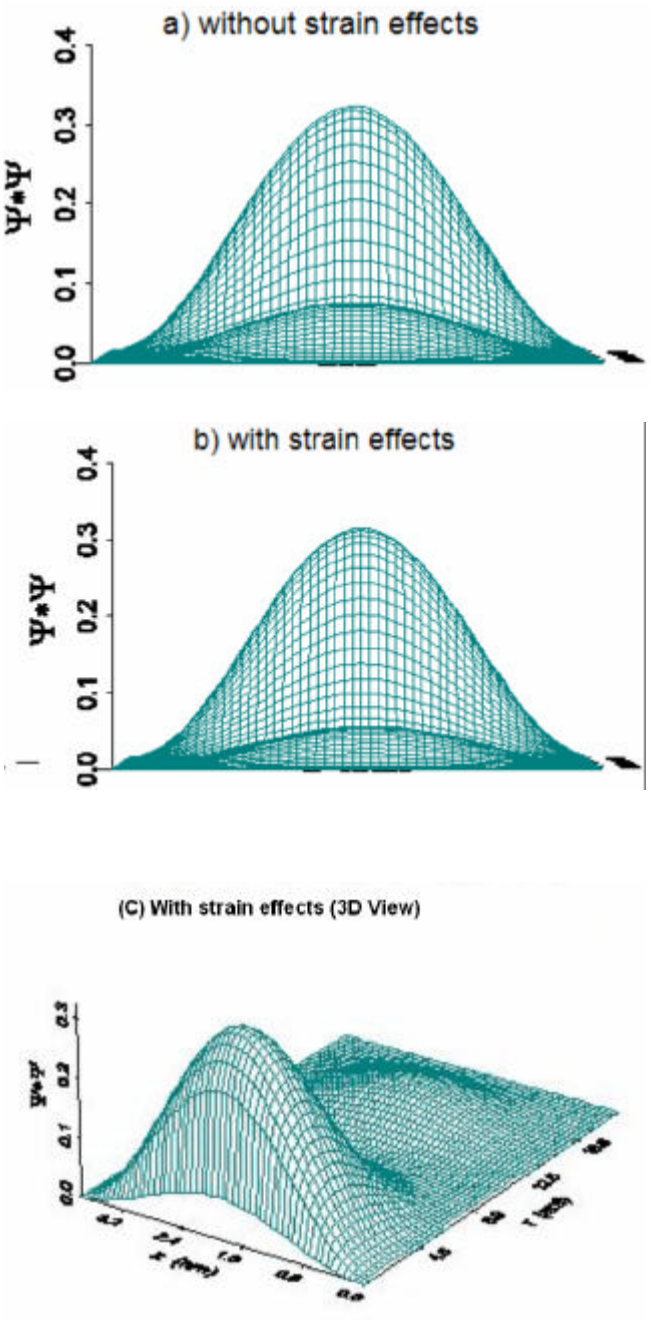

Figure 4. Square wave functions for a cylindrical quantum dot.

CONCLUSIONS

The time independent 3D Schr dinger equation is solved using finite element method. The effects of the shape and quantum dot size on the electron wave function and electron energy level distribution inside quantum dots are demonstrated for conical, pyramidal and cylindrical quantum dots structures. The comparison of wave functions and eigenstates for calculations with and without the strain potential demonstrate the significance of the residual stress impact. The effects of size, confinement, and thermal stress which is related to the material composition can be seen directly from the energy level distribution. Since the density of the states can be obtained from the spectrum of the eigenstates, the effect on the optical properties and charge transport can be estimated. The impact of the considered parameters is significant, consequently the accurate calculations should be made when specific device is to be considered for potential application.

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