Numerical Simulations of Residual Stresses and Their Effects on Electronic Properties in Quantum Dots

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ABSTRACT

Numerical modeling methods have been applied to study the residual stresses and their effects on the electronic properties in quantum dots. A finite element method is used in the residual stress simulations. Both thermal expansion differences and lattice mismatch between quantum dots and substrate materials are included in the residual stress modeling. The time-independent Schrödinger equation, which includes the strain-induced potential and the potential caused by the heterostructures, has been solved with a finite difference method. The wave functions and the energies of the confined states have been calculated. These allow us to compute the electronic and transport properties of the devices.

Keywords: Quantum dots, residual stress, Schrödinger equation, finite element method, finite difference method

1. INTRODUCTION

Quantum dots have been proposed as one of the promising nano devices that have many applications, such as high efficiency solar cells, information storage etc. They are usually fabricated by growing nanometer sized semiconductor materials on various substrates. Due to the differences in thermoelastic properties, between the quantum dots and the substrate materials, residual stresses will be generated in the quantum dots. It can cause defects and micro-structural changes in the nano devices. The electrical, optical, photovoltaic properties, and device lifetime can be detrimentally affected. For example, dislocations formed at the interface will affect the material transport properties. Band gap variation with pressure (for materials such as CuInTe2, \( \delta E / \delta P = 53 \text{meV/GPa} \)) has been widely observed for semiconductor materials. The electron mobility also changes with the residual lattice strain, which is influenced by the residual stresses.

We have applied the finite element method to simulate the residual stress distributions in the quantum dots. Figure 1 provides the distribution of residual stress in radial direction within a gold quantum dot grown on silicon substrate. The growth temperature is 1000 Kelvin. Both lattice mismatch and thermal expansion effects are included. Our calculation indicates that the residual stresses concentrate at the edge and the interface of the sample. The dominant effect, which causes the residual stress, is the lattice mismatch between quantum dot material and the substrate.

![Figure 1. Residual stress \( \sigma_{rr} \) in a Au quantum dot grown on Si substrate](image)

The effects of residual stresses on the electronic and optical properties are also studied. The additional potential field induced by the residual strain has been included in the time-independent Schrödinger equation to calculate the energies and wave functions.

2. Quantum mechanical model

The energies and wave functions of a single carrier in the semiconductor structure are solutions of the time-independent Schrödinger equation

\[
\sum_{\beta=1}^{4} \left( H_{k,p}^{\alpha\beta} \Psi^{\beta} + V^{\alpha\beta} \Psi^{\beta} \right) = E \Psi^{\alpha}
\]
where $\Psi^\alpha$ is the wave function in subband $\alpha$, $E$ is the energy, $H_{\mathbf{k}\mathbf{p}}^{\alpha\beta}$ is the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian operator, and $V^{\alpha\beta}$ is a position dependent potential. The $\mathbf{k}\cdot\mathbf{p}$ perturbation method is used to model the medium. In this case the Hamiltonian is

$$H_{\mathbf{k}\mathbf{p}}^{\alpha\beta}(\mathbf{r}) = \begin{bmatrix} L_{ij}^{11}\nabla_{ij}^2 & L_{ij}^{12}\nabla_{ij}^2 & L_{ij}^{13}\nabla_{ij}^2 & L_{ij}^{14}\nabla_{ij}^2 \\ L_{ij}^{21}\nabla_{ij}^2 & L_{ij}^{22}\nabla_{ij}^2 & L_{ij}^{23}\nabla_{ij}^2 & L_{ij}^{24}\nabla_{ij}^2 \\ L_{ij}^{31}\nabla_{ij}^2 & L_{ij}^{32}\nabla_{ij}^2 & L_{ij}^{33}\nabla_{ij}^2 & L_{ij}^{34}\nabla_{ij}^2 \\ L_{ij}^{41}\nabla_{ij}^2 & L_{ij}^{42}\nabla_{ij}^2 & L_{ij}^{43}\nabla_{ij}^2 & L_{ij}^{44}\nabla_{ij}^2 \end{bmatrix}$$

(2)

where the $L_{ij}^{\alpha\beta}$ tensors on the diagonal of the matrix are the effective-mass tensors for each subband, and the off-diagonal ones introduce $\mathbf{k}\cdot\mathbf{p}$ coupling of subbands. These tensors come from the Luttinger-Kohn Hamiltonian that contains material constants, and vary spatially throughout the device.

The nonuniform potential $V^{\alpha\beta}$ consists of contributions from two sources and is given by

$$V^{\alpha\beta}(\mathbf{r}) = V_C^{\alpha\beta}(\mathbf{r}) + V_\epsilon^{\alpha\beta}(\mathbf{r})$$

(3)

where $V_C^{\alpha\beta}(\mathbf{r})$ is due to the valence-band alignment of material at a given position in the device, and $V_\epsilon^{\alpha\beta}(\mathbf{r})$ is the strain-induced potential. The solution of the problem depends on boundary conditions; free surfaces impose the physical requirement that $\Psi^\alpha(\mathbf{r}) = 0$ for all $\alpha$. Conditions on boundaries that are remote from the regions of interest in the device do not significantly affect energies or wave functions in the regions of interest.

3. Modeling and Simulation

The Schrödinger equation (1) is solved using the finite-difference approximation for the variable $z$ and spline-decomposition for the variable $r$, formulated to include three spatial dimensions and one quantum mechanical dimension that in this case is taken to be the heavy hole valence subband for Si$_x$Ge$_{1-x}$ structure. Since the quantum dot system has axial symmetry, a cylindrical coordinate system ($z$, $\rho$, $\phi$) is used. The wave function can then be written as:

$$\Psi(\mathbf{r}) = \Phi(z, \rho) \exp(il\phi)$$

(4)

where $l = 0, \pm 1, \pm 2, \ldots$ is the electron orbital quantum number. Eq. (1) has the form

$$\left\{ -\frac{\hbar^2}{2m_0}(\gamma_1 + \gamma_2) \left( \frac{\partial^2}{\partial z^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} - \frac{l^2}{\rho^2} \right) + \frac{\hbar^2}{2m_0}(\gamma_1 - 2\gamma_2) \frac{\partial^2}{\partial \rho^2} + V_C(z) + V_\epsilon(z, \rho) \right\} \Phi = E\Phi$$

(5)

where $\gamma_1$ and $\gamma_2$ are Luttinger-Kohn parameters, $m_0$ is the electron mass. At this stage we do not take into account the strain-induced potential. The band structure potential contribution $V_C^{\alpha\beta}(\mathbf{r})$ is due to the energy misalignment of the valence band maximum in adjacent layers of material, which is proportional to the Si concentration in a Si$_x$Ge$_{1-x}$ structure. For a valence band model in this system, the value of the valence-band contribution is given by

$$V_C(z) = f(z)V_0,$$

(6)

where $f(z)$ is the Si concentration as a function of position, and $V_0$ was chosen 0.56eV.

The finite-difference approximation for the variable $z$ and spline-decomposition for the variable $\rho$ lead to algebraic eigenvalue problem, which can be written in a matrix form as

$$A_{ij}\Phi_j = E\Phi_i$$

(7)

The matrix $A$ is of dimension $N_zN_\rho \times N_zN_\rho$ and has a tri-block-diagonal structure. Here, $N_z$ is the number of points in the variable $z$ and $N_\rho$ is the number of points in the variable $\rho$. Similar approach was successfully applied to calculate the bound states of $\mu$pp, $\mu$dd, $\mu$t mesic molecules. To solve the eigenvalue problem (7), we use the method of inverse iterations with the Rayleigh identity

$$(A - Ip)\Phi^{k+1} = \Phi^k,$$

$$E^{k+1} = p + \frac{\left< \Phi^{k+1}, \Phi^k \right>}{\left< \Phi^{k+1}, \Phi^{k+1} \right>} \left< \Phi^j, \Phi^j \right> = \sum_{j=1}^{N} \Phi_j^* \Phi_j$$

(8)

where $p$ is the initial approximation for the eigenvalue. To obtain the stable eigenvalues and wave functions, about 20 iterations are required. In Figs. 2 and 3 the wave functions for the bound
and excited states are provided. It is shown that the finite-difference method allows us to calculate the physical characteristics of different quantum dot systems simply and accurately. This approach can be easily extended to more complex quantum dot systems where many subbands and strain-induced potential are taken into account.

Figure 2. The bound state wave function

Figure 3. The wave function for excited state.
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REFERENCES