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Elastic fields in quantum dots arrays: A three-dimensional finite element study

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Abstract

In this paper, a three-dimensional finite element analysis is used to study the strain, stress and stain energy density distributions in quantum dots (QDs) arrays. Two different QD geometries are simulated: truncated-pyramidal and lens-shaped. The effect of the material anisotropy and the cap layer thickness on the elastic fields is studied. The simulation results show that the material anisotropy has significant influence on the strain distribution. The average compressive strain ε_{xx} in the QDs increases as the anisotropy ratio A increases from 1.0 to 4.0, while it decreases as A is reduced from 1.0 to 0.25. When the anisotropy ratio $A>1$, [1 0 0] and [$\bar{1}$ 0 0] are the "elastic soft" directions with the strain ε_{xx} decaying rapidly in these directions. However, these lattice directions become "elastic hard" when $A<1$. Due to the elastic interaction among the QDs, various distributions of strain energy density can be obtained by changing the material anisotropy and the cap layer thickness, possibly resulting in different vertically ordered QD structures. The distribution of the strain energy minima at the cap layer surface is not sensitive to the two different QD shapes studied, though the strain and stress distributions in the QDs and the matrix are.

Keywords: Quantum dot; Finite element analysis; Strain; Elastic field; Vertical alignment

1. Introduction

Quantum dots (QDs) are nanometer-sized semiconductor structures, usually made from semiconductor materials like silicon, germanium, cadmium selenide, gallium arsenide and so on. In recent years, QDs have drawn immense attention due to its potential application in a wide variety of novel optoelectronic and microelectronic devices, such as light emitting diodes, photovoltaic cells, and quantum semiconductor lasers [1,2]. An effective method of fabricating QDs is to grow the dots directly by depositing a thin layer of material on a substrate under appropriate growth conditions. QDs can then evolve via the Stranski–Krastanow (SK) growth mode that consists of three-dimensional (3D) inlands growth on a two-dimensional (2D) wetting layer. The driving force behind this SK growth mode is the elastic fields induced by the lattice misfit between the thin layer and the substrate [3,4]. Due to the misfit strain, the thin layer deposited on the substrate roughens to form the QD islands.

QDs are often grown in multiple layers to form QD superlattice. It is found that the elastic fields induced from the buried QDs have a strong influence on QDs formation in the subsequent layer [5]. The QDs tend to align directly on top of the buried QDs and form a vertical aligned structure. It is well accepted that this vertical correlation is a direct result of the strain or stress induced by the buried islands. Experiments have also showed that the QDs can exhibit vertical anti-correlation [6]. This misalignment was explained by the elastic anisotropy and the crystallographic orientation of the materials, which resulted in the shift of the locations of the strain energy minima [7].

Besides having strong influence on the QDs formation, the strain and stress distributions also have a significant effect on the electronic and optical properties of the QD microstructure [8–12]. The strain and stress fields in the QDs will (i) change the conduction and valence band levels of the QD structure [8–10]; (ii) induce local electric fields due to piezoelectric effect [11]; and (iii) modify the photon

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frequencies in the QDs [12]. Therefore, the elastic fields in and around the QDs strongly affects the performance of QD based microelectronic devices. For the above reasons, it is often the goal to obtain highly ordered and regularly sized QD superlattices.

QDs can exist in a wide variety of shapes, including cuboidal, pyramidal, truncated-pyramidal, and lens-shaped. The stress and strain fields in QDs structure can be analyzed with many different modeling techniques, which are generally classified into three main categories: atomistic approach, analytical continuum approach, and finite element approach. In the atomistic approach [13,14], the ab-inito atomic simulations or classical molecular dynamics simulations with empirical potentials are used to calculate the strain fields. Because a large number of atoms is required in the analysis (especially for a QD superlattice array), this approach is computationally intensive and usually pose a very low maximum limit to the length and time scales of the model. In the analytical continuum approach [15–18], the QDs are treated as inclusions in an infinite matrix. The elastic fields due to the lattice mismatch between the QDs and the matrix are obtained by integrating the Green's function over the volume of the inclusions. However, the integration can only be done for some simple inclusion shapes, such as cuboid, pyramid and truncated pyramid. In the finite element approach [19–21], the finite element method (FEM) is employed to determine the strain and stress distributions in the QD microstructure. Comparing to the above two approaches, the FEM technique is more efficient and can be used for structures of any geometrical shape.

Previous studies are mainly on the elastic field of a single QD, which prove to be insufficient as recent experiments [22] showed that the elastic interaction (interference) between QDs has a strong influence on the vertical alignment. In this paper, we have used three-dimensional FEM simulations to study the elastic fields of a QD array. We studied how the elastic anisotropy and the thickness of the cap layer both contribute to the vertical ordering of the QD layers. We also studied two different QD shapes (truncated-pyramidal and lens-shaped) and analyze the sensitivity of island geometry to the elastic fields.

2. Finite element modeling

In the FEM, the displacement vector $\mathbf{D}(x,y,z)$ is interpolated using shape functions

$$\mathbf{D} = \mathbf{N}\mathbf{d}_e \tag{1}$$

where the nodal displacement vector $\mathbf{d}_e$ (for a three-dimensional hexahedral element) is given by

$$\mathbf{d}_e^{\mathrm{T}} = \{\mathbf{d}_{e1} \quad \mathbf{d}_{e2} \quad \mathbf{d}_{e3} \quad \mathbf{d}_{e4} \quad \mathbf{d}_{e5} \quad \mathbf{d}_{e6} \quad \mathbf{d}_{e7} \quad \mathbf{d}_{e8}\} \tag{2}$$

in which the displacement at node i is given as

$$\mathbf{d}_{ei}^{\mathrm{T}} = \{u_i \quad v_i \quad w_i\} \quad i = 1,2,\ldots,8 \tag{3}$$

The shape function matrix is given by

$$\mathbf{N} = [\mathbf{N}_1 \quad \mathbf{N}_2 \quad \mathbf{N}_3 \quad \mathbf{N}_4 \quad \mathbf{N}_5 \quad \mathbf{N}_6 \quad \mathbf{N}_7 \quad \mathbf{N}_8] \tag{4}$$

in which each sub-matrix $\mathbf{N}_i$ ($i = 1,2,\ldots,8$) is

$$\mathbf{N}_i = \begin{bmatrix} N_i & 0 & 0 \\ 0 & N_i & 0 \\ 0 & 0 & N_i \end{bmatrix} \quad i = 1,2,\ldots,8 \tag{5}$$

The shape function for a linear, hexahedral element can be described as

$$N_i = \tfrac{1}{8}(1+\xi\xi_i)(1+\eta\eta_i)(1+\zeta\zeta_i) \quad i = 1,2,\ldots,8 \tag{6}$$

where ξ, η and ζ are the natural coordinates of a unit cube that each hexahedron element is being mapped to. The general equation of motion can be obtained by using Lagrange's equation, which takes on the general form of

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{q}_j}\right) + \frac{\partial D}{\partial \dot{q}_j} + \frac{\partial U}{\partial q_j} = Q_j \quad j = 1,2,\ldots,n \tag{7}$$

where T is the kinetic energy of the system, U is the strain energy of the system, D is a dissipation function, q_j is the generalized displacements, and Q_j are the generalized forces. However, since the problem here is a static problem, the terms involving the kinetic energy can be omitted. There is also no need for a dissipation function since we are assuming that the structural damping of the material used can be neglected. Eq. (1) can then be substituted into the constitutive equation

$$\sigma = \mathbf{c}(\varepsilon + \varepsilon_{\mathrm{T}}) \tag{8}$$

where $\mathbf{c}$ is the elasticity matrix and ε_{T} is the thermal strain. The constitutive equation can then be substituted into the Lagrange's equation in Eq. (7) to obtain the form of the equilibrium equation for each element

$$\mathbf{k}_e\mathbf{d}_e = \mathbf{f}_e \tag{9}$$

where $\mathbf{k}_e$ is the element stiffness matrix and $\mathbf{f}_e$ is the element force vector. The matrix equations for all the elements are assembled to give

$$\mathbf{K}\mathbf{d} = \mathbf{f} \tag{10}$$

where $\mathbf{K}$ is now the global stiffness matrix, $\mathbf{d}$ is the global displacement vector, and $\mathbf{f}$ is the global force vector. Eq. (10) can then be solved to obtain the global displacements and hence the strain and stress in the model. Detailed formulation of the finite element equations can be obtained in most finite element literature.

Fig. 1 is an illustration of an array of truncated-pyramidal QDs on a wetting layer deposited on a substrate and the array is subsequently encapsulated by a cap layer. The QDs are assumed to distribute uniformly in the array. Due to periodicity of the structure, we only model the central square area bounded by the heavy dotted lines, which includes one complete QD and four quarter QDs.