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Influence of scale and anisotropy on self-positioning of multi-layer nanostructures

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ABSTRACT

The paper presents results of computational modeling of multi-layer nanostructures that have curved shape due to lattice mismatch between material layers. Investigation of influence of nanostructure thickness and material anisotropy on self-positioning of bi-layer nanostructures is performed with the atomic-scale finite element method (AFEM). The AFEM computer program is applied to modeling of GaAs and InAs self-positioning nanohinges with estimation of hinge curvature radius depending on structure thickness and orientation of atomic planes. It has been found that the curvature radius follows continuum mechanics solution for thickness larger than 50 nm. For smaller thicknesses, atomic-scale effects are significant. The numerical solutions for different orientations of atomic planes revealed considerable influence of material orientation on the hinge curvature radius.

1. INTRODUCTION

Nanotechnology requires fabrication of objects having nanometer sizes. Such fabrication is a complicated task since in many cases direct machining of nano-structures is impossible. A technique for creation of multi-layer nanostructures has been proposed by Prinz (2000). Schematic of nanostructure formation is shown in Fig.1. Material nanolayers with different lattice periods a_1 and a_2 are put on a substrate using molecular epitaxial deposition. After selective etching of the sacrificial layer, the two top layers are wrapped up forming a free-standing three-dimensional nanostructure. Circular-arc shape of the nanostructure is caused by relaxation of initial stresses induced by lattice mismatch. Such self-positioning technique is employed for creation of mirrors, containers and other nanoscale structures (Vaccaro 2001, Arora 2006, Zhou 2011).

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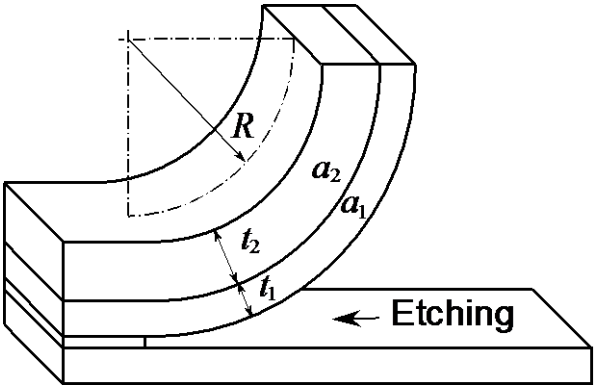

Fig. 1 Self-positioning due to lattice mismatch

In this paper, we use the atomic-scale finite element method (AFEM) for modeling of GaAs and InAs bi-layer self-positioning nanostructures. Estimation of nanohinge curvature radius dependence on structure thickness and orientation of atomic planes is performed and compared to results obtained by continuum mechanics approaches.

2. ATOMIC-SCALE FINITE ELEMENT METHOD

Traditional finite element method (FEM) is a universal numerical method for stress analysis of solids using continuum mechanics approach. Such approach produces significant results when atomic-scale effects are negligible.

To take into account such effects we use the atomic-scale finite element method (AFEM) that was introduced by Liu (2004) for multi-scale analysis of carbon nanotubes. The AFEM directly models an ensemble of atoms which interact with each other through empirical interatomic potentials. The AFEM equation system is derived from the total energy minimization, and in this regard it is similar to the traditional FEM. Total energy E consists of an energy of interatomic bonds V and a work of external forces $\mathbf{F}$ on displacements $\mathbf{u} = \mathbf{x} - \mathbf{x}_0$

$$E = V - \mathbf{u}^T \mathbf{F} \tag{1}$$

Using the Taylor expansion up to the second order terms

$$E = E_0 + d\mathbf{u}^{\mathbf{T}} \frac{\partial E}{\partial \mathbf{u}} + \frac{1}{2} d\mathbf{u}^{\mathbf{T}} \frac{\partial^2 E}{\partial \mathbf{u}^2} d\mathbf{u} \tag{2}$$

with its subsequent minimization

$$\frac{\partial E}{\partial \mathbf{u}} = 0 \tag{3}$$

it is possible to obtain the AFEM equation system in a form similar to traditional FEM

$$\mathbf{Ku} = \mathbf{f} + \boldsymbol{\psi} \tag{4}$$

Here $\mathbf{K}$ is a global stiffness matrix

$$\mathbf{K} = \frac{\partial^2 E}{\partial \mathbf{u}^2} \tag{5}$$

and $\boldsymbol{\psi}$ is the imbalance vector between the internal and external atomic loads

$$\boldsymbol{\psi} = -\frac{\partial E}{\partial \mathbf{u}} \tag{6}$$

Energy of interatomic bonds V is estimated as sum energies of atom pairs $i - j$

$$V = \frac{1}{2}\sum_i \sum_{j \neq i} V_{ij}(r_{ij}) \tag{7}$$

where r_{ij} is the distance between atoms $i - j$. We use empirical interatomic potential function proposed by Tersoff (1986) with modification of Nordlund (2000) for particular mathematical expressions of V_{ij}.

Our problems for self-positioning of nanostructures are characterized by absence of external forces $\mathbf{F}$ and by geometric nonlinearity due to large displacements. Geometrically nonlinear problems are modeled by step procedure with Newton-Raphson iterative search of equilibrium at each step (Nishidate 2008). Since three-dimensional nanostructures contain large number of atoms, the AFEM system (4) can contain millions of equation. This equation system is sparse because of locality of interatomic potentials (7). The preconditioned conjugate gradient (PCG) method is employed in our equation solver. The PCG is among the fastest iterative algorithms for solution of large sparse equation systems.

3. SOLUTION RESULTS

Two types of problems have been solved using atomic-scale approach of AFEM (Nishidate 2008) and continuum mechanics approach of FEM (Nikishkov 2006). In the first problem, influence of thickness on the curvature radius of self-positioning hinge two-layer nanostructure is investigated. Second problem is related to effect of anisotropy on curvature radius of same structure.

A bi-layer self-positioning nanostructure shown in Fig. 1 consists of 3c unit crystal layers of GaAs (top) and c unit crystal layers of InAs (bottom) with c being a problem size parameter in the thickness direction. The hinge length is set to $16a_0c$ where a_0 is an initial lattice period.

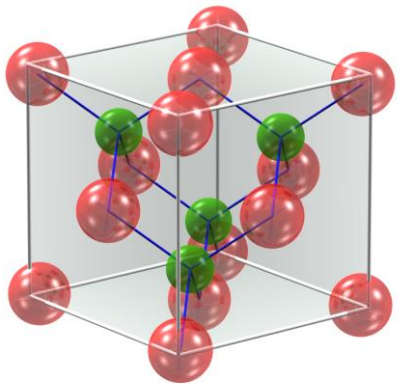

Fig. 2 Atomic configuration and bonds in zincblende unit crystal

Both GaAs and InAs have the zincblende crystalline structure shown in Fig. 2. Arsenide atoms are located at crystal corners and face centers of the unit crystal, and Gallium/Indium atoms are inside with positions (0.25, 0.25, 0.25), (0.75, 0.25, 0.75), (0.25, 0.75, 0.75) and (0.75, 0.75, 0.25) in the unit crystal. Crystals of InAs have the lattice period a_1 = 0.60584 nm and the lattice period of GaAs is a_2 = 0.56536 nm. Initial lattice period for both crystals is selected as $a_0 = (a_1 + 3a_2)/4 = 0.57546\text{nm}$.

The initial atomic structure is generated with the above initial lattice period. Then step-wise relaxation procedure with Newton-Raphson equilibrium iterations leads to the final self-positioning configuration.

3.1 Curvature radius as a function of nanostructure thickness

The GaAs and InAs bi-layer hinge structures with the problem size parameter *c* from 1 to 36 are considered that corresponds to thickness *t* from 2.56 nm to 82.9 nm with number of atoms from 1106 to 1329986. The largest atomic system requires multiple solutions of about 4 millions of equations.

Shape of GaAs and InAs bi-layer hinge structure for problem size *c*=1 after self-positioning is shown in Fig. 3. Dependence of the nanostructure curvature radius *R* determined by the AFEM (Nishidate 2007) and by the continuum mechanics approach (FEM) on the structure thickness *t* is presented in Fig. 4. Some decrease of curvature radius in continuum mechanics approach is related to artificial adjustment of thickness imitating thickness estimation in atomic structures. For larger thickness the atomic-scale and continuum mechanics solutions are practically identical. For small thickness less than 30-40 unit crystal layers their discrepancy is considerable.

3.2 Effect of material anisotropy

Atomic crystal structures possess anisotropic properties. Their mechanical parameters are different in different directions. In atomic-scale modeling, anisotropy is created by changing unit crystal orientation with respect to the hinge line. Continuum mechanics approach uses elasticity matrix for cubic crystal anisotropy with specification of material direction relative to the hinge.

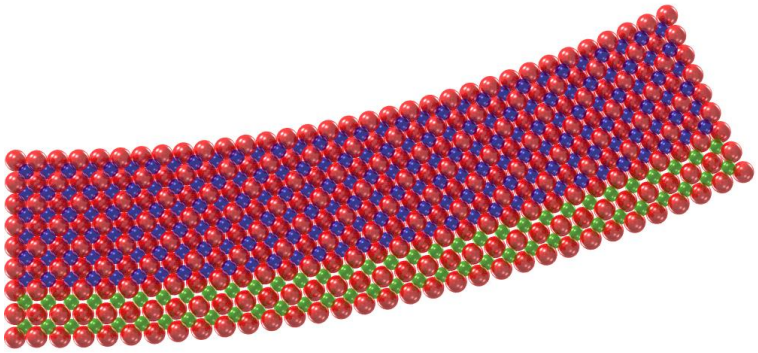

Fig. 3 Shape of GaAs–InAs bi-layer hinge structure (*c*=1) after self-positioning

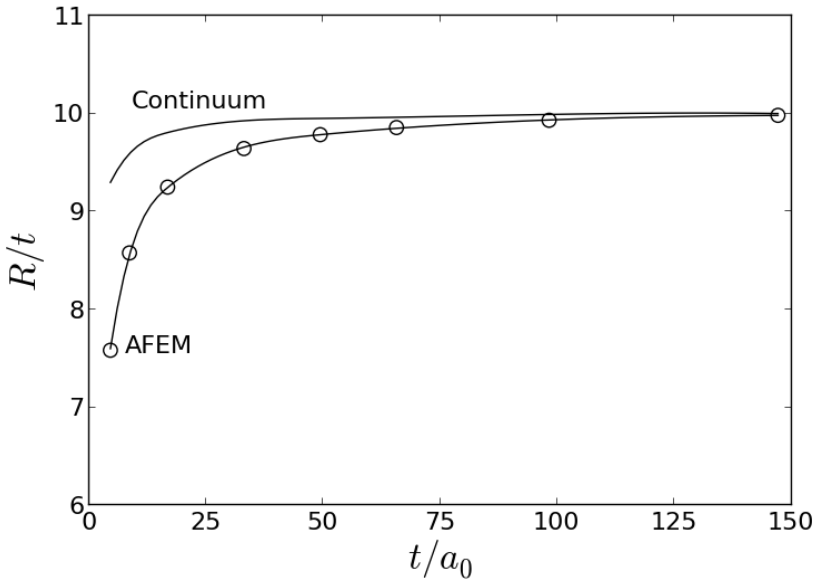

Fig. 4 Dependence of the curvature radius determined by the AFEM and the continuum mechanics solution on the nanostructure thickness

The effect of material anisotropy is investigated for GaAs-InAs bi-layer hinge structure with crystal orientation angles θ = 0, 15, 30, 45, 60, 75, and 90 degrees. Curvature radius values determined for different crystal orientation angles θ by AFEM (Nishidate 2008) and continuum mechanics solution (Nishidate 2009) are presented in Fig. 5. Results of both approaches are in reasonable agreement.

4. CONCLUSIONS

The atomic-scale finite element method (AFEM) is used for modeling self-positioning of hinge nanostructures composed of GaAs and InAs layers. Investigation of curvature radius dependence on the nanostructure thickness showed that for larger thickness atomic-scale and continuum mechanics approaches provide close results. For

thickness less than 30-40 unit crystal layers the continuum mechanics considerably overestimates the curvature radius. Modeling of anisotropic effects related to crystal orientation with respect to hinge line demonstrated that practically identical predictions are given by both atomic-scale and continuum mechanics approaches.

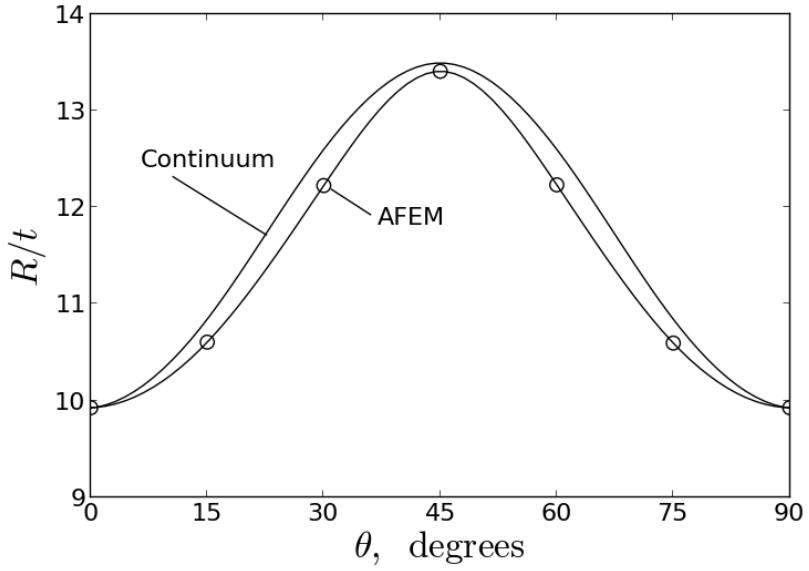

Fig. 5 Dependence of the curvature radius on the crystal orientation angle determined by AFEM and continuum mechanics approach.

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