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A geometrically nonlinear finite element model of nanomaterials with consideration of surface effects

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ABSTRACT

In conventional continuum mechanics, the surface energy is usually small and negligible. But at nano-length scale, it becomes a significant part of the total elastic energy due to the high specific surface area of nanomaterials. A geometrically nonlinear finite element (FE) model of nanomaterials with considering surface effects is developed in this paper. The aim is to extend the conventional finite element method (FEM) to analyze the size-dependent mechanical properties of nanomaterials. A numerical example, analysis of InAs quantum dot (QD) on GaAs (0 0 1) substrate, is given in this paper to verify the validity of the method and demonstrate surface effects on the stress fields of QDs.

1. Introduction

The numerical simulation models of materials in mechanics mainly include the continuum models and the atomic-scale models. The latter ones, such as molecular dynamics, Monte Carlo methods, lattice dynamics and etc., have aroused general interest in nanomechanics research. However, these computation methods are rather expensive and time-consuming due to the limited computational power of current available devices, which hinders the application of atomic-scale simulation to some complex problems, such as analysis of nano-electromechanical system (NEMS). On the other hand, the conventional finite element method (FEM) is not applicable to nano-scale problems. Although some works [1–3] have been done to extend FEM to nanomaterials research recently, the theory studies are far from enough and they are all built in small deformation context. Surface deformation of nanomaterials is a geometrically nonlinear problem by nature, so the theory framework shall be built in the context of finite deformation. In this work, a geometrically finite element (FE) model of nanomaterials with considering surface effects is developed. Analysis of InAs quantum dot (QD) on GaAs (0 0 1) substrate is given in this paper to verify the validity of the method and demonstrate the surface effects on the stress fields of QDs.

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The quantum effects, surface effects and size effects of nanomaterials have become very hot topics nowadays [4–9]. Nanomaterials show up interesting size-dependent elastic properties because of the intrinsic surface effects, or alternatively, the surface energy. Due to undercoordination, the atoms at the surface have extra energy, i.e. the source of surface energy, than those in the bulk. Because nanomaterials have high specific surface area, the surface energy becomes a significant part of the total elastic potential energy, which is the sum of the volume elastic strain energy and the surface energy.

In 1928, Gibbs defined the Eulerian form of surface free energy density γ as the reversible work involved in creating a unit area of new surface at constant temperature, volume and chemical potential. In terms of the current configuration, the Eulerian form of surface stress $\sigma^S_{\alpha\beta}$ is related to γ via [10]

$$\sigma_{\alpha\beta} = \frac{1}{A}\frac{\partial(A\gamma)}{\partial\varepsilon^S_{\alpha\beta}} = \gamma\delta_{\alpha\beta} + \frac{\partial\gamma}{\partial\varepsilon^S_{\alpha\beta}}, \quad (\alpha,\ \beta = 1,\ 2), \tag{1}$$

where A is the deformed surface area, $\varepsilon^S_{\alpha\beta}$ is the Lagrange surface strain, and $\delta_{\alpha\beta}$ is the kronecker delta symbol. Similar to Eq. (1), $\sigma^S_{\alpha\beta}$ may also be written as [11]

$$\sigma^S_{\alpha\beta} = \sigma^0_{\alpha\beta} + S_{\alpha\beta\gamma\delta}\varepsilon^S_{\gamma\delta}, \quad (\alpha,\ \beta,\ \gamma,\ \delta = 1,\ 2), \tag{2}$$

where $\sigma^0_{\alpha\beta}$ denotes the surface stress at zero strain, and $S_{\alpha\beta\gamma\delta}$ is the fourth order surface elastic tensor which determines the change in the surface stress with strain. The value can be determined from atomistic calculations [12,13].

In terms of the referential configuration, the Lagrange form of surface stress $\Sigma^S_{\alpha\beta}$ is related to Γ via

$$\Sigma^S_{\alpha\beta} = \frac{1}{A_0}\frac{d(A_0\Gamma)}{d\varepsilon^S_{\alpha\beta}} = \frac{d\Gamma}{d\varepsilon^S_{\alpha\beta}}, \quad (\alpha,\ \beta = 1,\ 2), \tag{3}$$

where Γ is the Lagrange form of the surface free energy density, $\Sigma^S_{\alpha\beta}$ the second Piola–Kirchhoff surface stress tensor which decides the dependence of Γ on surface strain, A_0 the undeformed surface area, and $A = A_0(1+\varepsilon^S_{\eta\eta})$. According to Dingreville et al. [14], the surface free energy density Γ may be written as a Taylor series expansion about the Lagrange surface strain. In this paper, Γ is assumed to be linear in $\varepsilon^S_{\alpha\beta}$, i.e. $\Gamma = \Gamma_0 + \Sigma^0_{\alpha\beta}\varepsilon^S_{\alpha\beta}$. For two-dimensional (2D) problem, it is reduced into $\Gamma = \Gamma_0 + \mathbf{\Sigma}_0\boldsymbol{\epsilon}$.

Need to mention, in the above the surface energy and the surface effect are defined as macroscopic thermodynamic quantities. That is valid on the assumption: the bulk volume is much larger than several atomic sizes. At the early stage of our study, 2D models are reported in this paper and 2D axi-symmetric model is used to model QD island shape in reality. It is feasible because former FEM results show 2D model gives satisfactory results [15,16]. Further insight into 3D model shall be performed in future.

2. A FE model of nanomaterials built on the basis of nonlinear kinematics

2.1. Overview of finite deformation theory

According to finite deformation theory, we introduce Lagrange frame and Eulerian frame to describe, respectively, the fixed reference configuration and the current configuration.

Describe a typical material point position by vector $\mathbf{X}$ and $\mathbf{x}$, respectively, in Lagrange frame and Eulerian frame. The relationship between $\mathbf{X}$ and $\mathbf{x}$ is given as $\mathbf{x} = \mathbf{X} + \mathbf{U}$, where $\mathbf{U}$ is the Lagrange displacement; or alternatively, $\mathbf{X} = \mathbf{x} - \mathbf{u}$, where $\mathbf{u}$ is the Eulerian displacement.

Vector $\mathbf{X}$ is mapped to $\mathbf{x}$ by the deformation gradient $\mathbf{F}$, i.e. $\mathbf{F} = \partial\mathbf{x}/\partial\mathbf{X}$. The determinant of the deformation gradient is $J = \det\mathbf{F}$; the left-deformation tensor is $\mathbf{B} = \mathbf{F}\mathbf{F}^{\mathrm{T}}$; and the right-deformation tensor is $\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}$.

The components of the Green strain $\mathbf{E}$ defined in reference configuration are related to the deformation gradient tensor through $E_{IJ} = \frac{1}{2}(C_{IJ} - \delta_{IJ})$; the components of the Almansi strain $\mathbf{e}$ are $e_{ij} = \frac{1}{2}(\delta_{ij} - B^{-1}_{ij})$.

The second Kirchhoff stress $\mathbf{S}$ and the Cauchy stress $\boldsymbol{\sigma}$ are stress measures defined with respect to the reference configuration and the current configuration, respectively. The Cauchy stress $\boldsymbol{\sigma}$ is the true stress in the current configuration, defined as $\boldsymbol{\sigma} = d\mathbf{T}/d\mathbf{s}$, where $\mathrm{d}\mathbf{T}$ is the force acting on the deformed area $\mathrm{d}\mathbf{s}$. The second Kirchhoff stress $\mathbf{S}$ is defined as $\mathbf{S} = d\mathbf{T}^K/d\mathbf{S}_0$, where $d\mathbf{T}^K = \mathbf{F}^{-1}\,d\mathbf{T}$, and $d\mathbf{S}_0 = (1/J)\mathbf{F}^{\mathrm{T}}\,d\mathbf{s}$. In component form, $\mathbf{S}$ is related to $\boldsymbol{\sigma}$ through $S_{IJ} = JF^{-1}_{Im}F^{-1}_{Jn}\sigma_{mn}$.

2.2. FE formulation

2.2.1. 2D plane problem

Consider 2D plane problems of an elastic body which occupies referential configuration B and surface area $\hat{B}_i$. After deformation, B is mapped into b, and surface $\hat{B}_i$ is mapped into $\hat{b}_i$. The surface deformation can be described by surface stretch ratio Λ [6], defined by

$\Lambda = dl/dL$, where L and l are the arc lengths along $\hat{B}_i$ and $\hat{b}_i$, respectively.

Assume the surface energy density is linear in Λ, i.e.

$$\Gamma(\Lambda) = \sigma_0 + \Sigma_0\Lambda = \Gamma_0 + \Sigma_0\varepsilon, \tag{4}$$

where ε is the surface strain, $\varepsilon = \Lambda - 1$, and $\Gamma_0 = \sigma_0 + \Sigma_0$.

The total potential energy Π may be written as

$$\Pi = U_e + U_s - V, \tag{5}$$

where U_e is the volume elastic strain energy, U_s the surface free energy, V the work done by all external forces acting on the body and its stress boundary $\hat{B}_0$. They are given as follows:

$$U_e = \int_B W\,dA = \int_B \tfrac{1}{2}E_{IJ}S_{IJ}\,dA, \tag{6a}$$

$$U_s = \int_{\hat{B}_i} \Gamma\,dL, \tag{6b}$$

$$V = \int_B \mathbf{U}^{\mathrm{T}}\mathbf{P}\,dA + \int_{\hat{B}_0} \mathbf{U}^{\mathrm{T}}\mathbf{T}\,dL. \tag{6c}$$

According to the minimum potential energy theory, the variation of functional Π vanishes, i.e.

$$\delta\Pi = \int_B \delta E_{IJ}S_{IJ}\,dA + \int_{\hat{B}_i}\Sigma_0\delta\Lambda\,dL - \int_B \delta U_I P_I\,dA - \int_{\hat{B}_0}\delta U_I T_I\,dL = 0. \tag{7}$$

Based on the definition of surface stretch ratio, we have $\Lambda^2 = \mathrm{d}x_i\cdot\mathrm{d}x_i/(\mathrm{d}L)^2$. The variation of Λ^2 may be written as

$$\Lambda\delta\Lambda = \frac{dx_i}{dL}\frac{\delta dx_i}{dL} = \frac{dx_i}{dL}\frac{d}{dL}\delta U_i. \tag{8}$$

In view of $\delta\mathbf{x} = \delta\mathbf{u} = \delta\mathbf{U}$, it yields

$$\delta\Lambda = \frac{1}{\Lambda}\frac{dx_i}{dL}\frac{d}{dL}\delta U_i = \frac{1}{\Lambda}\frac{d}{dL}\delta\mathbf{u}^{\mathrm{T}}\frac{dx}{dL}. \tag{9}$$

Eq. (7) is a nonlinear equation, so it needs to be linearized in the reference configuration. Assume that $\varphi = \delta\Pi$, and an incremental displacement vector $\Delta\mathbf{u}$ is given. Using $\Delta\delta\mathbf{u} = 0$, the incremental form of φ may be written as

$$\Delta\varphi = \int_B \Delta(\delta E_{IJ})S_{IJ}\,dA + \int_B \delta E_{IJ}\Delta S_{IJ}\,dA + \int_{\widehat{B_i}}\Sigma_0\Delta(\delta\Lambda), \tag{10}$$

where

$$\delta E_{IJ} = \delta\left(\frac{1}{2}F_{kI}F_{kJ}\right) = \frac{\partial x_k}{\partial X_I}\frac{\partial\delta u_k}{\partial X_J}.$$

In view of $S_{IJ} = JF^{-1}_{Im}F^{-1}_{Jn}\sigma_{mn}$ and $J\,\mathrm{d}A = \mathrm{d}a$, the first term in Eq. (10) may be written as

$$\int_B \Delta(\delta E_{IJ})S_{IJ}\,dA = \int_B \frac{\partial\Delta u_k}{\partial X_I}\frac{\partial\delta u_k}{\partial X_J}S_{IJ}\,\mathrm{d}A = \int_b \frac{\partial\Delta u_k\partial\delta u_k}{\partial x_m\partial x_n}\sigma_{mn}\,\mathrm{d}a. \tag{11}$$

Note that $\delta F_{iJ} = \partial\delta u_i/\partial x_k\,\partial x_k/\partial X_J$, thus we have $\delta\mathbf{F} = \nabla(\delta\mathbf{u})\mathbf{F}$. It follows that

$$\delta\mathbf{E} = \delta(\tfrac{1}{2}\mathbf{F}^{\mathrm{T}}\mathbf{F}) = \tfrac{1}{2}[\mathbf{F}^{\mathrm{T}}\nabla(\delta\mathbf{u}^{\mathbf{T}})\mathbf{F} + \mathbf{F}^{\mathbf{T}}\nabla(\delta\mathbf{u})\mathbf{F}] = \mathbf{F}^{\mathbf{T}}\boldsymbol{\delta\zeta}\mathbf{F}, \tag{12}$$

where $\zeta = \frac{1}{2}[\nabla(\mathbf{u})^{\mathrm{T}} + \nabla(\mathbf{u})]$.

For the purpose of linearization, $\Delta\mathbf{S} = J\mathbf{F}^{-1}\Delta\boldsymbol{\sigma}\mathbf{F}^{-\mathbf{T}}$ is approximately given. Using $\Delta\mathbf{S} = \mathbf{D}_0\Delta\mathbf{E}$, we have $\Delta\boldsymbol{\sigma} = \mathbf{D}\Delta\zeta$, where $\mathbf{D}_0$ and $\mathbf{D}$ denote the material moduli in the reference configuration and the current configuration, respectively, and $J\mathbf{D} = \mathbf{F}\mathbf{F}\mathbf{D}_0\mathbf{F}^{\mathbf{T}}\mathbf{F}^{\mathbf{T}}$.

Consequently, the second term in Eq. (10) may be written as

$$\int_B \delta E_{IJ}\Delta S_{IJ}\,dA = \int_B \tfrac{1}{2}F_{kI}(\delta u_{k,l}+\delta u_{l,k})F_{lJ}JF^{-1}_{Ik}\Delta\sigma_{kl}F^{-1}_{Jl}\,dA$$
$$= \int_b \delta\zeta_{kl}\Delta\sigma_{kl}\,\mathrm{d}a. \tag{13}$$

Using FEM theory [17], divide the region into elements in current configuration. According to the isoparametric concept, the FE approximations for displacements and coordinates in an element are given by

$$\mathbf{u} = \sum_{I=1}^{n} N_I(\xi)\mathbf{u_I^e}, \tag{14a}$$

$$\mathbf{x} = \sum_{I=1}^{n} N_I(\xi)\mathbf{x_I^e}, \tag{14b}$$

where N_I is the shape function at node I, ξ natural coordinates for the element, $\mathbf{u_I}^\mathbf{e}$ the displacement vector at node I , and $\mathbf{x_I}^\mathbf{e}$ the coordinate vector at node I.

Using the Vigot notation, $\boldsymbol{\sigma}$ and $\delta\boldsymbol{\zeta}$ in 2D plane problem are given by

$$\boldsymbol{\sigma} = [\sigma_{11}\ \ \sigma_{22}\ \ \sigma_{12}]^{\mathrm{T}}, \tag{15}$$

$$\delta\boldsymbol{\zeta} = [\delta\zeta_{11}\ \ \delta\zeta_{22}\ \ \delta\zeta_{12}]^{\mathrm{T}}. \tag{16}$$

So it follows that

$$\delta\boldsymbol{\zeta} = \mathbf{B_I}\delta\mathbf{u_I}, \tag{17}$$

where

$$\mathbf{B_I} = \begin{bmatrix} N_{I,1} & 0 \\ 0 & N_{I,2} \\ N_{I,2} & N_{I,1}\end{bmatrix}, \quad N_{I,1} = \frac{\partial N_I}{\partial x_1}.$$

Apply Eqs. (15) and (16) into Eq. (10), and use Eqs. (14a) and (14b) for discretization. Leaving out $\delta\mathbf{d}$ ($\mathbf{d}$ is the displacement vector of all the body nodes, i.e. $\mathbf{d} = \sum_\mathbf{e}\mathbf{u^e}$), we have $\Delta\varphi = \mathbf{K_T}\Delta\mathbf{d}$. Define $\mathbf{K_T}$ as the stiffness matrix, written as

$$K_T = \sum_e\left[\int_{b^e}\frac{d\mathbf{N^T}}{d\mathbf{x}}\boldsymbol{\sigma}\frac{d\mathbf{N}}{d\mathbf{x}}\,da + \int_{b^e}\mathbf{B^TDB}\,da + \int_{\hat{b}_i^e}\Sigma_0\frac{d\mathbf{N^T}}{dl}\frac{d\mathbf{N}}{dl}\,dl\right.$$
$$\left. - \int_{\hat{b}_i^e}\Sigma_0\frac{d\mathbf{N^T}}{dl}\frac{d\mathbf{x}}{dl}\frac{d\mathbf{x^T}}{dl}\frac{d\mathbf{N}}{dl}\,dl\right], \tag{18}$$

where $\mathbf{B} = [\mathbf{B_1}\ \cdots\ \mathbf{B_I}\ \cdots\ \mathbf{B_n}]$, $\mathbf{N} = [\mathbf{N_1}\ \cdots\ \mathbf{N_I}\ \cdots\ \mathbf{N_n}]$, and $\mathbf{N_I} = \begin{bmatrix} N_I & 0 \\ 0 & N_I\end{bmatrix}$.

Accordingly, Eq. (18) may also be expressed as

$$\mathbf{K_T} = \mathbf{K^m} + \mathbf{K^g} + \mathbf{K^s}, \tag{19}$$

where $\mathbf{K^m}$, $\mathbf{K^g}$ and $\mathbf{K^s}$ are the material tangent matrix, the geometric stiffness matrix and the surface stiffness matrix, respectively. They are given as follows:

$$(K^m)_{IJ} = \sum_e\left[\int_{b^e}\mathbf{B_I^T}\mathbf{D}\mathbf{B}_J\,\mathrm{d}a\right], \tag{20a}$$

$$(K^g_{ij})_{IJ} = \sum_e\left[\int_{b^e}\frac{\partial N_I}{\partial x_m}\sigma_{mn}\frac{\partial N_J}{\partial x_n}\,\mathrm{d}a\delta_{ij}\right], \tag{20b}$$

$$(K^s_{ij})_{IJ} = \sum_e\left[\int_{\hat{b}_i^e}\Sigma_0\frac{dN_I}{dl}\frac{dN_J}{dl}\,dl\delta_{ij} - \int_{\hat{b}_i^e}\Sigma_0\frac{dN_I}{dl}\frac{dx_i}{dl}\frac{dx_j}{dl}\frac{dN_J}{dl}\,dl\right]. \tag{20c}$$

Leaving out $\delta\mathbf{d}$, we can get the Eulerian form of φ as

$$\sum_e\left[\int_{b^e}\mathbf{B}^{\mathrm{T}}\boldsymbol{\sigma}\,\mathrm{d}a + \int_{\hat{b}_i^e}\Sigma_0\frac{d\mathbf{N}^{\mathrm{T}}}{dl}\frac{d\mathbf{x}}{dl}\,dl - \int_{b^e}\mathbf{N}^{\mathrm{T}}\mathbf{p}\,da - \int_{\hat{b}_0^e}\mathbf{N}^{\mathrm{T}}\mathbf{t}\,dl\right] = 0, \tag{21}$$

where $\mathbf{p}$ and $\mathbf{t}$ is Eulerian form of $\mathbf{P}$ and $\mathbf{T}$.

Define the resultant force $\mathbf{R}$ as

$$\mathbf{R} = \sum_e\left[\int_{b^e}\mathbf{N}^{\mathrm{T}}\mathbf{p}\,da + \int_{\hat{b}_0^e}\mathbf{N}^{\mathrm{T}}\mathbf{t}\,dl - \int_{b^e}\mathbf{B}^{\mathrm{T}}\boldsymbol{\sigma}\,da - \int_{\hat{b}_i^e}\Sigma_0\frac{d\mathbf{N^T}}{dl}\frac{d\mathbf{x}}{dl}\,dl\right]. \tag{22}$$

Finally, the Newton algorithm for nonlinear equations is given by

(1) Initialize $\mathbf{d}^0 = \mathbf{0}$.
(2) Loop over steps, k

$$\mathbf{K_T}(\mathbf{d^k})\Delta\mathbf{d^k} = \mathbf{R}(\mathbf{d^k}), \tag{23a}$$

$$\mathbf{d^{k+1}} = \mathbf{d^k} + \Delta\mathbf{d^k}. \tag{23b}$$

(3) Repeat step 2 until $\mathbf{R}$ is small enough to be almost zero.

2.2.2. 2D axi-symmetric problem

For 2D axi-symmetric problem, the displacements depend only on the r and z coordinates, so the displacement and the coordinate fields are given as

$$\mathbf{u} = [u_r\ \ u_z]^{\mathrm{T}}, \quad \mathbf{x} = [r\ \ z]^{\mathrm{T}}. \tag{24}$$

Using the Vigot notation, $\boldsymbol{\sigma}$ and $\delta\boldsymbol{\zeta}$ are written as

$$\boldsymbol{\sigma} = [\sigma_{rr}\ \ \sigma_{zz}\ \ \sigma_{\theta\theta}\ \ \sigma_{rz}]^{\mathrm{T}}, \tag{25}$$

$$\delta\boldsymbol{\zeta} = [\delta\zeta_{rr}\ \ \delta\zeta_{zz}\ \ \delta\zeta_{\theta\theta}\ \ \delta\zeta_{rz}]^{\mathrm{T}}. \tag{26}$$

It follows that

$$\delta\boldsymbol{\zeta} = \mathbf{B_I}\delta\mathbf{u_I}, \tag{27}$$

where

$$\mathbf{B_I} = \begin{bmatrix} \frac{\partial N_I}{\partial r} & 0 & \frac{N_I}{r} & \frac{\partial N_I}{\partial z} \\ 0 & \frac{\partial N_I}{\partial z} & 0 & \frac{\partial N_I}{\partial r}\end{bmatrix}^{\mathrm{T}}.$$

So we have

$$\mathbf{K_T} = \mathbf{K^m} + \mathbf{K^g} + \mathbf{K^s} \tag{28}$$

where

$$(K^m)_{IJ} = \sum_e\left[\int_{b^e}\mathbf{B_I^T}\mathbf{D}\mathbf{B_J}r\,\mathrm{d}r\,\mathrm{d}z\right], \tag{29a}$$

$$(K^g_{ij})_{IJ} = \sum_e\left[\int_{b^e}\frac{\partial N_I}{\partial x_k}\sigma_{kl}\frac{\partial N_J}{\partial x_l}r\,\mathrm{d}r\,\mathrm{d}z\delta_{ij}\right], \tag{29b}$$

$$(K^s_{ij})_{IJ} = \sum_e\left[\int_{\hat{b}_i^e}\Sigma_0\frac{dN_I}{dl}\frac{dN_J}{dl}r\,\mathrm{d}l\delta_{ij}\right.$$
$$\left. - \int_{\hat{b}_i^e}\Sigma_0\frac{dN_I}{dl}\frac{dx_i}{dl}\frac{dx_j}{dl}\frac{dN_J}{dl}r\,\mathrm{d}l\right]. \tag{29c}$$

The resultant force $\mathbf{R}$ is

$$\mathbf{R} = \sum_e\left[\int_{b^e}\mathbf{N}^{\mathrm{T}}\mathbf{p}r\,dr\,dz + \int_{\hat{b}_0^e}\mathbf{N}^{\mathrm{T}}\mathbf{t}r\,dl - \int_{b^e}\mathbf{B}^{\mathrm{T}}\boldsymbol{\sigma}r\,dr\,dz\right.$$
$$\left. - \int_{\hat{b}_i^e}\Sigma_0\frac{d\mathbf{N^T}}{dl}\frac{d\mathbf{x}}{dl}r\,dl\right]. \tag{30}$$

3. Analysis of InAs QD grown on GaAs (0 0 1) substrate

QDs have attracted much interest due to their special electronic and optical properties these years [16–21]. Because of the difference in the lattice parameters of the two materials, self-organized InAs QD islands are grown epitaxially on GaAs (0 0 1) substrate. This is the called Stranski–Krastanow (SK) growth mode, which consists of two kinds of growth: firstly, layer-by-layer growth mode (i.e. FvdM growth), and afterwards, 3D island growth (i.e. VW growth). The phenomena happen because of the gain of the strain energy during islanding, but at the cost of increased surface energy. Previous FEM studies of QDs [15] didn't consider surface effects.

As shown in Fig. 1, a typical InAs QD shape can be modeled as a 2D conical axi-symmetric island. Four nodal, 2D solid, quadrilateral elements are employed for the meshing. The nodes along the $x=0$ and 30 lines are constrained in the x-direction. The system is assumed isotropic because 2D strain calculations, taking into account anisotropic behavior, show no significant effect. The isotropic material properties and lattice parameters of GaAs and InAs are given in Table 1. From Table 1, the lattice mismatch can be calculated as $\varepsilon_0 = (a_{\mathrm{GaAs}} - a_{\mathrm{InAs}})/a_{\mathrm{InAs}} = -0.067$.

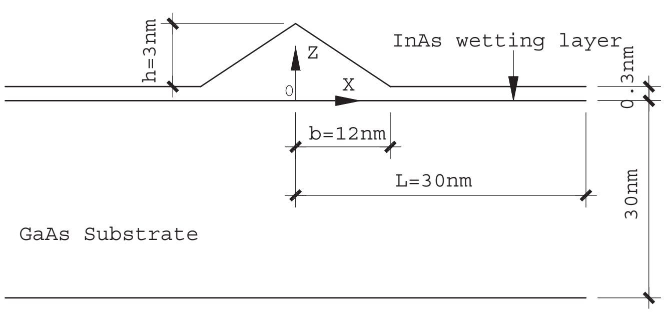

Fig. 1. 2D axi-symmetric conical QD model.

Table 1
Isotropic material properties and lattice parameters.

Material	E (GPa)	ν	Lattice parameter (Å)
GaAs	86.92	0.31	5.64325
InAs	51.42	0.35	6.05830

The island is bigger than 1000 atoms, so it can be well described by continuum elasticity theory. In order to simulate the system's intrinsic residual stress induced by the lattice mismatch, we introduce the framework of thermo elasticity. Set the thermal expansion coefficient α_{T} of InAs and GaAs as 0.067 and zero, respectively, and raise the temperature of the system by 1 K. So the thermal strain of InAs island is $\varepsilon_{\mathrm{T}} = \alpha_{\mathrm{T}}\Delta T = 0.067$. Consider the surface energy of the InAs island and set the surface stress constant as $\Sigma_0 = 47\,\mathrm{meV/Å^2} = 0.752\,\mathrm{N/m}$ [16]. A 'tied contact' condition is specified on the interface edges between the QD island and the GaAs (0 0 1) substrate. The stress (σ_{xx}, σ_{zz}) fields of QD island with and without considering surface effects are shown in Figs. 2 and 3, respectively.

4. Result and discussion

Taking note of the right color index value in Fig. 2, the QD island is subjected to compressive stress σ_{xx}, and the minimum absolute value of σ_{xx} is found at the apex of the island. That verifies that islanding happens to release strain elastic energy. With considering surface effects, the minimum absolute value is increased from 1.13 to 1.43 (GPa) and the relative difference is about 27%. According to the minimum potential energy theory, surface effects always trend to contract surface area, and hinder the formation of island to reduce surface free energy. So, surface effects are contrary to the effects of islanding, and that leads to the increase of σ_{xx}. From Fig. 3, we can also see the stress distributions of σ_{zz} are greatly affected with considering surface effects, especially for the top area of island. Comparing Figs. 3a and b, intensive compressive σ_{zz} is induced by surface effects at the apex of island. That explains the formation of truncated QD island which is frequently observed during QD growth.

In this paper, we incorporate surface effects into conventional FEM, and develop a geometrically nonlinear FE model of nanomaterials. Analysis of InAs QD grown on GaAs (0 0 1) substrate is given to demonstrate the surface effects on the stress fields of QD which explains the formation of truncated QD during QD growth.

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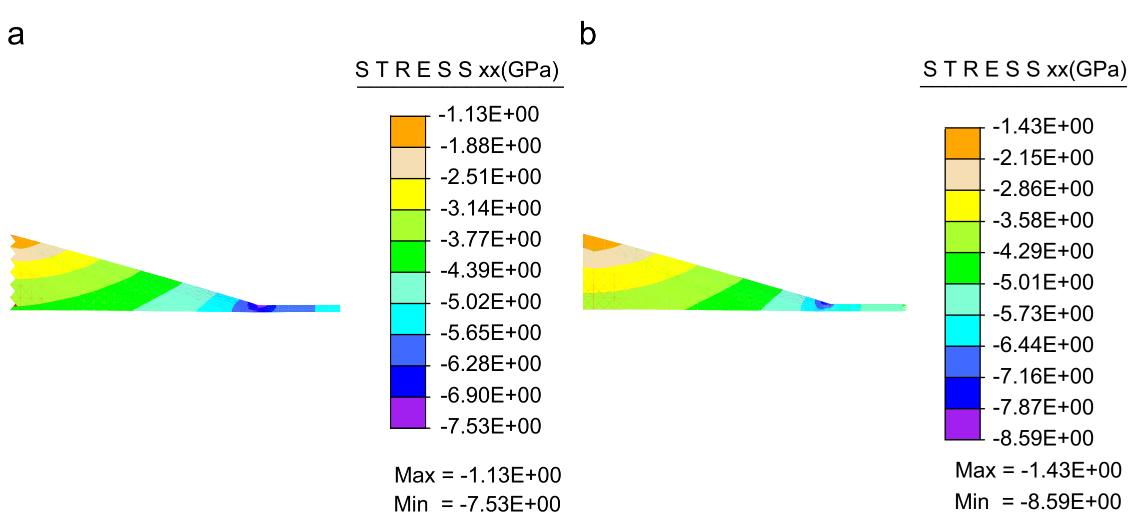

Fig. 2. The stress σ_{xx} distribution of QD island: (a) without considering surface effects and (b) with considering surface effects.

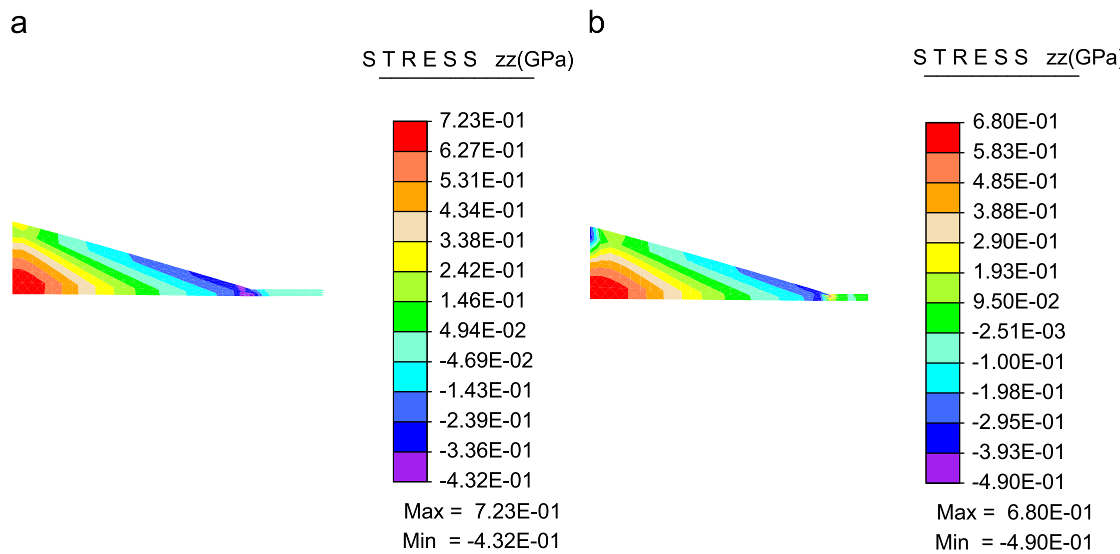

Fig. 3. The stress σ_{zz} distribution of QD island: (a) without considering surface effects and (b) with considering surface effects.

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