Strain effects on pyramidal InAs/GaAs quantum dot

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Abstract: Strain distribution in a pyramidal InAs/GaAs quantum dot is investigated. The strain field induced by mismatch of lattice constants in heterostructures is analyzed based on theories of linear elasticity and of thermal stress. The strain-induced potential is then incorporated in the steady state Schrödinger equation. Both the strain field and the solution of the steady state Schrödinger equation are found numerically with the aid of a finite element package – FEMLAB. Eigenenergy and the probability density function of conduction band of quantum dot are calculated. Results from two different models, namely anisotropic material model and isotropic material simplification, during the stage of strain analysis are also compared. Numerical results show eigenenergy and the degeneracy of low eigenenergy are affected by strains. On the other hand, the differences between anisotropic and isotropic materials are not large. Therefore, it is suitable to treat InAs/GaAs quantum dot as isotropic materials.

Key-Words: Quantum dot; Strain field; Finite element, Schrödinger equation

1 Introduction

Quantum dots (QDs), which have delta-functions distribution of density of states, discrete energy levels, and "atom-like" electronic states due to its three-dimensional quantum confinement, have recently attracted substantial attention [1-2]. The efficiency of QD is strong related to the density of dots in the quantum dot array. Self-assembled QDs (SAQDs) formed by strained epitaxy have shown promising result to have a large array of quantum dots. SAQD formation is commonly observed in large mismatch epitaxy of chemically similar materials. For example, the Stranski-Krastanow (SK) growth of InAs on GaAs first involves the growth of a ~1 to 2 monolayer thick of "wetting layer" followed by coherent island formation [1-3]. The SAQDs may be buried by a further growth of the same materials as the underlying substrate.

The strain fields inside and in the neighborhood of SAQDs strongly affect the electronic properties in vicinity of the dots, and hence the optical-electronic properties [4-5]. For the optical-electronic properties in III-V semiconductors, there are two predominated strain effects, namely changes of the the conduction and valence band levels and changes of local electric fields due to piezoelectric effect. The conduction band is only affected by the hydrostatic strain, often referred to as the dilatation or trace of the strain tensor. The valence levels can change both with hydrostatic and shear strain. In the general, for zinc blende structures, deviatoric strains give rise to piezoelectrically induced electric fields [6].

To understand the strain effects on electronic properties of QD, determination of the elastic strain field in the dots and surrounding matrix is necessary. There have been three different main methods: (i) theory of inclusions based on the analytical solution of elasticity [7-9], (ii) finite element methods (FEM) [10-13], and (iii) atomistic modeling [14-16]. The theory of inclusions provides integral expressions for elastic fields which can be integrated in closed form only for simplest inclusion shapes, e.g. cylindrical or spherical quantum dots. On the other hand, the interactions between the quantum dot and the surrounding material are not fully encountered. FEM is a very versatile and effective numerical method, which can easily accommodate various theories and model quantum dot to different levels. Atomistic models might be more reasonable, at least theoretically, to model system in nano-scale provided that accurate interatomic potentials are given. Moreover, it requires a large computing capacity to model quantum dots and the surrounding matrix.

In this article, models based on theories of linear elasticity and of thermal stress are developed to evaluate the strain distribution in the pyramidal InAs/GaAs SAQD. The mismatch of lattice constants in heterostructures induces the strain field which is then calculated with the aid of a finite element package – FEMLAB. The Schrödinger equation, including the strain-induced potential, is then solved,

again by FEMLAB. The solutions consist of eigenenergy and the probability density function of conduction band. Finally strain effects on electronic properties in pyramidal InAs/GaAs quantum dot are discussed. During the strain analysis, the materials of quantum dot are modeled by anisotropic as well as its isotropic simplification, respectively. Numerical results of two models are compared.

2 Continuum And Quantum Models

Consider a buried pyramid InAs/GaAs quantum dot structure as shown schematically in Fig. 1. The InAs island (quantum dot) is self-assembled under certain conditions during heteroepitaxy on GaAs substrates. The island is subsequently covered by additional substrate materials.

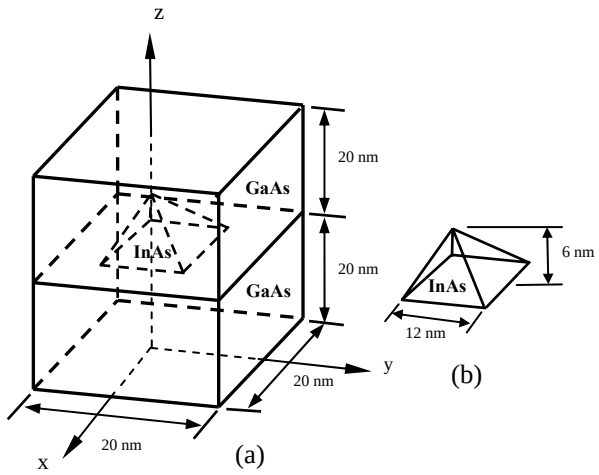


Fig.1. Schematics of (a) the buried InAs/GaAs quantum dot structure and (b) the island (InAs quantum dot).

In this article, the analysis of a quantum dot is divided into two parts. First, a linear elastic finite element calculation is performed to determine the strain field in the quantum dot structure. Second, a time-independent Schrödinger equation, with a strain-induced potential calculated using deformation potential theory, is solved numerically to obtain the spectrum of energies and probability density functions of available states.

2.1 Continuum model

Epitaxially grown semiconductor heterostructures, such as SAQDs, often consist of several materials with lattice parameters that are mismatched. The mismatch of lattice parameters gives rise to strain field in a quantum dot structure, which will then affect the electric properties of the quantum dots. Lattice mismatch parameter is usually defined as [17]

$$\varepsilon_0 = \frac{a_s - a_d}{a_d}, \tag{1}$$

where a_s and a_d are the lattice parameter of the substrate and quantum dot materials, respectively. The lattice mismatch parameter is a system parameter of the quantum dot. In this article, the parameter ε_0 is simulated as an initial strain in the island/substrate interface. This initial strain will induce further strain in the system.

In order to analyze the effect caused by initial strain ε_0 in the island/substrate interface, theory of elasticity together with thermal stress theory [18] are utilized. The initial strain in the quantum dot is then treated as thermal strain under the thermal stress theory. Since mismatch lattice parameters is only along the island/substrate interface (i.e., 1-2 plane or x-y plane as depicted in Fig. 1), the thermal strains in the island/substrate interface are specified as

$$\beta_{11} = \beta_{22} = \varepsilon_0 \ ; \quad \text{orther} \quad \beta_{ij} = 0. \tag{2}$$

By linear elasticity and thermal stress theory, the relationship between the stresses and the strains in a quantum dot structure is expressed as

$$\tau_{ij} = C_{ijkl}\left(\varepsilon_{kl} - \beta_{kl}\right), \quad i,j,k,l = 1,2,3, \tag{3}$$

where τ_{ij} and ε_{kl} are the stress and strain tensors, respectively, C_{ijkl} is the elastic stiffness tensors, and β_{kl} is the thermal strain tensors.

The linear elasticity boundary value problem, arising from the mismatch in lattice parameters between the island and substrate materials, is solved using the finite element package – FEMLAB. We consider that all outer boundaries are traction free surfaces, and the substrate bottom is fixed. The displacement compatibility across the interface of island/substrate is satisfied automatically in the finite element formulation with displacement field as unknowns.

2.2 Quantum model

The strain components will induce an extra potential field which may affect the probability density functions and energies of the electrons in the quantum dot structure. Pikus-Bir Hamiltonian [4-5] together with the computed strain field from

above-mentioned continuum model are used to analyze strain-induced effects in quantum dots.

The behavior of individual electron in an undeformed crystal is governed by the steady state Schrödinger equation:

$$\left[\frac{\mathbf{p}^2}{2m_0} + V_0(\mathbf{r}) \right] \psi_n(\mathbf{r}) = E_n \psi_n(\mathbf{r}), \quad (4)$$

where $\mathbf{p} = -i\hbar\nabla$ is the momentum operator, $V_0(\mathbf{r})$ the potential field, m_0 the electron rest mass, $\hbar$ the Planck's constant, and E_n and $\psi_n(\mathbf{r})$ the nth eigenenergy and the corresponding probability density function, respectively. The $\mathbf{r}$ and ∇ are the position vector and the Laplacian operator, respectively, in the undeformed crystal coordinate. Once there being strains, the steady state Schrödinger equation (4) is modified according to Pikus-Bir Hamiltonian [4] as

$$\left[H_0 + H_\varepsilon\right] \psi_n\left[(\mathbf{I}+\boldsymbol{\varepsilon})\mathbf{r}\right] = E_n \psi_n\left[(\mathbf{I}+\boldsymbol{\varepsilon})\mathbf{r}\right], \quad (5)$$

where

$$H_0 = \frac{\mathbf{p}^2}{2m_0} + V_0(\mathbf{r}), \quad (6)$$

$$H_\varepsilon = \sum_{\alpha,\beta} \left(-\frac{p_\alpha p_\beta}{m_0} + \frac{\partial V}{\partial \varepsilon_{\alpha\beta}}\bigg|_{\varepsilon_{\alpha\beta}\to\mathbf{0}} \right) \varepsilon_{\alpha\beta} . \quad (7)$$

Since the conduction band is only affected by the hydrostatic strain [6], the diagonal term of Eq. (7) leads to

$$\left[H_\varepsilon \right]_{nn} = a_c \left(\boldsymbol{\varepsilon}_{xx} + \boldsymbol{\varepsilon}_{yy} + \boldsymbol{\varepsilon}_{zz} \right), \quad (8)$$

where a_c is deformation potential constant shown in Table 1.

Equation (5) is then solved numerically again by means of the finite element method in order to obtain eigenenergy and the probability density function of conduction band in a quantum dot structure. The boundary conditions on the quantum dot/substrate interface are

$$\begin{cases} \psi_d = \psi_s \\ \left(\mathrm{d}\psi_d/\mathrm{d}i\right)/m_{d_i} = \left(\mathrm{d}\psi_s/\mathrm{d}i\right)/m_{s_i}, \ i = x, y, z \end{cases} \quad (9)$$

where subscripts d and s correspond to the quantum dot and substrate regions, respectively, index i corresponds to one of the three possible coordinaes x, y, z and electron effective mass is taken along one of three coordinate axes.

Table 1 Material property [6]

Material		InAs	GaAs
electron effective mass (m^*/m_0)		0.023	0.067
lattice parameter a (nm)		0.605	0.565
Yang's modulus (Gpa)		51.3	85.5
Poisson's ratio		0.354	0.316
C_{ij}	C_{11}	8.329	11.879
	C_{12}	4.526	5.376
	C_{44}	3.96	5.94
deformation potential a_c (eV)		-5.08	-7.17
energy gap E_g (eV)		0.354	1.424

Note: 1. C_{ij} is elastic constants (Unit : 10^{10} N/m^2).

3 Numerical Results

The materials are modeled by anisotropic and its isotropic simplification, respectively, during the strain analysis to investigate the strain field in the pyramidal InAs/GaAs quantum dot structure. The geometry and material properties of the quantum dot structure are shown in Fig. 1 and Table 1, respectively.

Figures 2–3 show the strain components along $(x = 0,\ z = 25)\,\mathrm{nm}$. Fig. 2 are ε_{xx} and ε_{yy}, while ε_{zz} for Fig. 3. It is easily to see that these components have significant variation with position throughout the structure. Moreover, strains are more nonuniform at InAs/GaAs interface due to the pervasive effect of relaxation.

The eigenenergies of the quantum dot structure are shown in Table 2. The strain effects shift all energy states, as one would expect, especially the first energy state increased about 0.2 eV. Furthermore, degeneracy of energy states is also shifted by strain effect.

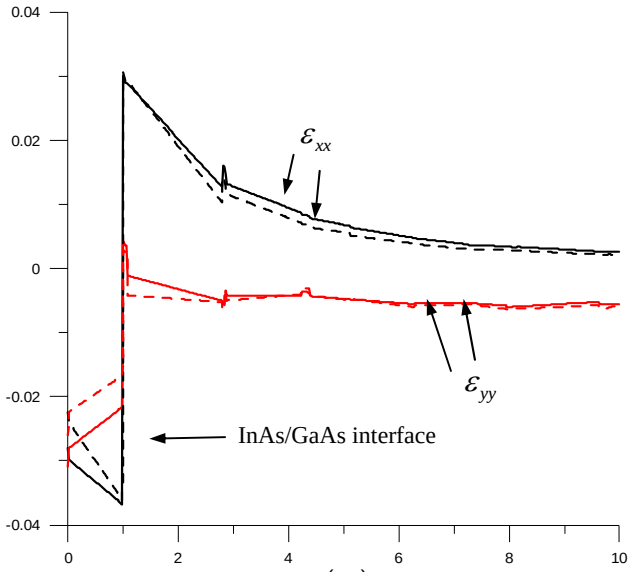


Fig. 2. Plot of Strain components ε_{xx} and ε_{yy} at $(x = 0, z = 25)$ nm ; a solid line is for anisotropic analysis, a dashed line is for isotropic analysis.

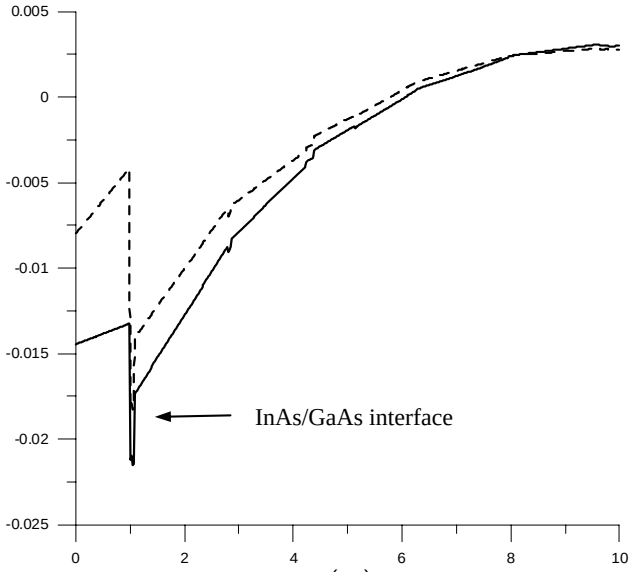


Fig. 3. Plot of Strain ε_{zz} at $(x = 0, z = 25)$ nm ; a solid line is for anisotropic analysis, a dashed line is for isotropic analysis.

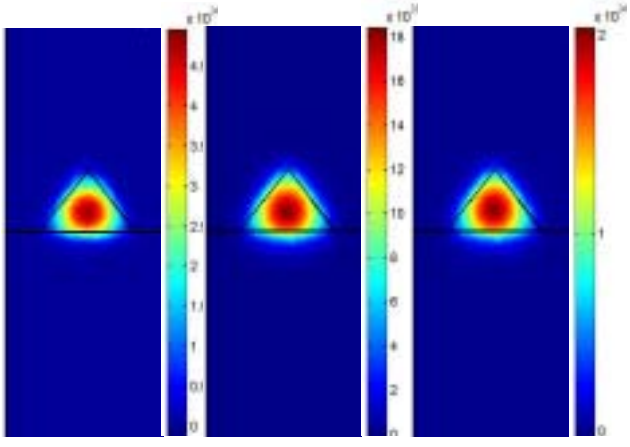
Probability density profiles, given by square of probability density functions, namely $|\psi_1|^2$ and $|\psi_2|^2$, for the two lowest energy states in a quantum dot structure, are shown Fig. 4–5, respectively. Subfigure 4(a) is the result for an unstrained quantum dot structure. The states are almost entirely confined to the island region. Subfigures 4(b)–4(c) are results of the anisotropic analysis and the isotropic analysis, respectively, for a strained quantum dot structure. The distribution of confined states is enlarged due to strain effect. In the subfigure 5(a), the states are confined to two regions in a unstrained island. In strained cases, subfigures 5(b)–5(c) show the results of isotropic analysis are similar to the results of anisotropic analysis

Three-dimensional view of the isosurface of the squared probability density functions in QD structure is shown in Fig. 6. Subfigures 6(a)-6(b) are the results for the 2nd energy state and 3rd energy state, respectively, without stain effect. The states are confined to two regions in y axis (for the 2nd energy state) and two regions in x axis (for the 3rd energy state), respectively. Subfigures 6(c)-6(d) are the results of the anisotropic analysis, for the 2th energy

Table 2 Numerical results for eigenenergy

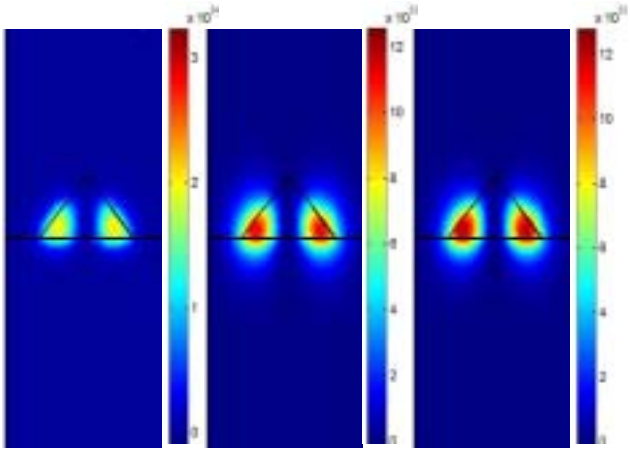
Eigenenergy	Unstrained	Strained	
		Isotropic	Anisotropic
1	0.429	0.649	0.677
2	0.7	0.849	0.858
3	0.7	0.849	0.858
4	0.865	0.879	0.877
5	0.865	0.885	0.883
6	0.885	0.915	0.916
7	0.891	0.924	0.923
8	0.924	0.924	0.923
9	0.924	0.930	0.929
10	0.928	0.930	0.929

Unit : eV



(a) (b) (c)

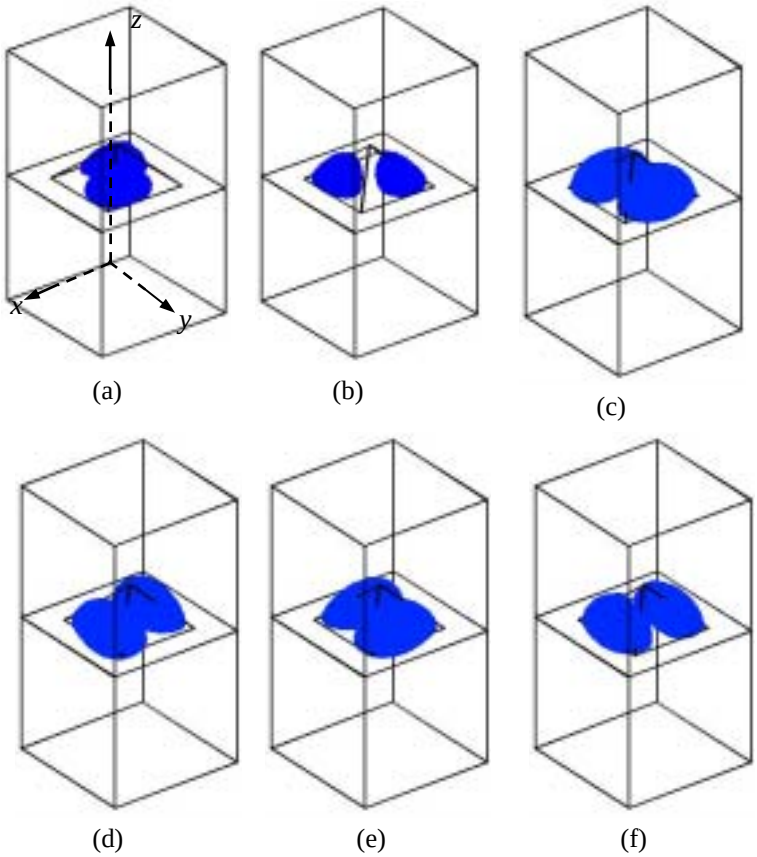
Fig. 4. Probability density fields for the 1st energy state, by (a) unstrained analysis; (b) anisotropic analysis for strained QD; (c) isotropic analysis for strained QD. The cross section is the $y-z$ plane through the dot center.



(a) (b) (c)

Fig. 5. Probability density fields for the 2nd energy state, by (a) unstrained analysis; (b) anisotropic analysis for strained QD; (c) isotropic analysis for strained QD. The cross section is the $y-z$ plane through the dot center.

state and 3th energy state, respectively. Due to strain effect, the distribution of confined states is enlarged to the island region and substrate region. Further, the states are confined to two regions in x axis (for the 2th energy state) and two regions in y axis (for the 3th energy state), respectively. Subfigures 6(e)-6(f) are the results of the isotropic analysis, for the 2th energy state and 3th energy state, respectively. However, the results of isotropic analysis are similar to the results of anisotropic analysis.



(a) (b) (c)

(d) (e) (f)

Fig. 6. The isosurface of the squared probability density functions in QD structure, (a) for the 2nd eigenenergy state without strain; (b) for the 3rd eigenenergy state without strain; (c) for the 2th eigenenergy state by anisotropic analysis with strain; (d) for the 3th eigenenergy state by anisotropic analysis with strain; (e) for the 2th eigenenergy state by isotropic analysis with strain; (f) for the 3th eigenenergy state by isotropic analysis with strain.

4 Conclusion

In this article, we have analyzed both the continuum mechanics and conduction band quantum mechanics of a strained pyramidal InAs/GaAs quantum dot, using the finite element package – FEMLAB. The strain fields in and around quantum dot induced by the lattice mismatch of the quantum dot structure have been calculated. Moreover, the steady state Schrödinger equation has been analyzed, and the eigenenergy and the probability density function of conduction band in a quantum dot structure have been found.

Numerical results have shown that strain effects will shift the eigenenergy and the degeneracy of low eigenenergy. The first eigenenerergy increased about 0.2 eV. Moreover, during the strain analysis, the quantum materials have been modeled by both anisotropic and its isotropic simplification, respectively. According to the numerical results of eigenenergy and the corresponding probability density function, the differences between two material models are small. Therefore, it is suitable to simplify InAs and GaAs as equivalent isotropic materials

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References:

[1] D. Bimberg, M. Grundmann & N. N. Ledentsov, *Quantum Dot Heterostructures*, John Wiley & Sons, New York, 1999.

[2] P. Harrison, *Quantum Wells, Wires and Dots: theoretical and computational physics*, John Wiley & Sons, New York, 2000.

[3] T. Chakraborty, *Quantum Dots: a survey of the properties of artificial atoms*, Elsevier, Amsterdam, 1999.

[4] G. E. Pikus & G. L. Bir, Effects of deformation on the hole energy spectrum of gernasium and silicon, *Sov. Phys. Solid State*, Vol.1, 1960, pp. 1502-1517.

[5] G. E. Pikus & G. L. Bir, *Symmetry and Strain-Induced Effects in Semiconductors*, Wiley New York, 1974.

[6] Shun Lien Chuang, *Physics of optoelectronic devices*, John Wiley & Sons, New York, 1995.

[7] V. A. Shchukin, D. Bimberg, V. G. Malyshkin & N. N. Ledentsov, Vertical correlations and anticorrelations in multisheet arrays of two dimensional islands, *Phys. Rev. B*, Vol.57, 1998, pp. 12262.

[8] D. Andreev, J. R. Downes, D. A. Faux & E. P. O'Reilly, Strain distributions in quantum dots of arbitrary shape, *J. Appl. Phys.*, Vol.86, 1999, pp. 297.

[9] G. S. Pearson & D. A. Faux, Analytical solutions for strain in pyramidal quantum dots, *J. Appl. Phys.*, Vol.88, 2000, pp.730.

[10] T. Benabbas, Y. Androussi & A. Lefebvre, A finite element study of strain fields in vertically aligned InAs islands in GaAs, *J. Appl. Phys.*, Vol.86, 1999, pp. 1945.

[11] G. Muralidharan, Strains in InAs quantum dots embedded in GaAs: A finite element study, *Jpn. J. Appl. Phys.*, Vol.39, 2000, L 658.

[12] H. T. Johnson, L. B. Freund, C. D. Akyüz & A. Zaslavsky, Finite element analysis of strain effects on electronic and transport properties in quantum dots and wires, *J. Appl. Phys.*, Vol.84, 1998, pp. 3714.

[13] L.B. Freund & H.T. Johnson, The influence of strain on confined electronic states in semi-conductor quantum structures, *J. Mech. Phys. Solids*, Vol.38, 2001, pp. 1045.

[14] M. Tadic, F. M. Peeters, K. L. Janssens, M. Korkusinski & P. Hawrylak, Strain and band edges in single and coupled cylindrical InAs/GaAs and InP/InGaP self-assembled quantum dots, *J. Appl. Phys.*, Vol.92, 2002, pp. 5819.

[15] C. Pryor, J. Kim, L. W. Wang, A. J. Williamson & A. Zunger, Comparison of two methods for describing the strain profiles in quantum dots, *J. Appl. Phys.*, Vol.83, 1998, pp.2548.

[16] M. E. Bachlechner, A. Omeltchenko, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjö, A. Madhukar & P. Messina, Multimillion-atom molecular dynamics simulation of atomic level stresses in Si(111)/Si3N4(0001) nanopixels, *Appl. Phys. Lett.*, Vol.72, 1998, pp. 1969.

[17] L. B. Freund, The mechanics of electronic materials, *J. Mech. Phys. Solids*, Vol.37, 2000, pp. 185.

[18] J. Aboudi, *Mechanics of Composite Materials*, Elsevier, Amsterdam, 1999.