STRESS ANALYSIS OF A QUANTUM DOT REGION USING AN ELASTIC ANISOTROPIC MODEL

Eligiusz W. Postek[*], Stephen J. Hardy[*], Pawel Dluzewski[**]

[*]**School of Engineering, University of Wales Swansea**
Singleton Park, Swansea SA2 8PP, Wales, UK
e.w.postek, s.j.hardy@swansea.ac.uk
[**] **Institute of Fundamental Technological Research, Polish Academy of Sciences**
Swietokrzyska 21, 00-490 Warsaw Poland
pdluzew@ippt.gov.pl

ABSTRACT- Objects called quantum dots are formed during epitaxial growth. They have a different chemical composition than the surrounding layer and their existence creates non-uniform stress fields. The stresses can be very high in the close proximity of these islands. This paper presents a stress calculation procedure, which employs a hyperelastic anisotropic constitutive model. Results for two numerical examples are given.

INTRODUCTION: The process of manufacturing a semiconductor is based on the sequential creation of layers of different materials, for example, up to 100 alternative, separate layers of SiGe and Si. These are known as heterostructures. During the manufacture of SiGe/Si, fluctuations in the chemical composition, in the form of quantum dots of SiGe, are created. Because of the different crystallographic constants of Si and Ge, internal strains and stresses are generated (known as misfits). These strains and stresses influence, for example, the optical properties of the material. Similarly, cracking may be apparent, Einfeld *et al.* [2002]. Other examples include GaN, InGaN, InGaAs and. CdTe/ZnTe/GaAs, where similar defects can occur during their manufacture. These stress fields can be highly undesirable, for example in the composite GaN, InGaN, which is used in the production of lasers and where optical defects must be avoided.

PROCEDURE: The constitutive model is described by Dluzewski *et al.* [2000, 2005]. The kinematics of the constitutive model starts from the following decomposition, namely, $\mathbf{F} = \mathbf{F}_{lt'}\mathbf{F}_{ch}\mathbf{F}_{pl}$, where $\mathbf{F}_{lt'}$ is the lattice deformation tensor, $\mathbf{F}_{ch}$ is the chemical deformation tensor and $\mathbf{F}_{pl}$ is the dislocations gradient being a function of the continuous field of lattice distortions $\boldsymbol{\beta} = \partial\hat{\mathbf{u}}/\partial\mathbf{x}$. The field $\boldsymbol{\beta}$ is obtained by differentiating the piece-wise continuous lattice displacement field. The Cauchy stress tensor is of the form $\boldsymbol{\sigma} = \mathbf{R}\left(\hat{\mathbf{A}}:\hat{\mathbf{D}}:\hat{\boldsymbol{\varepsilon}}\right)\mathbf{R}^{\mathrm{T}}\det\left(\mathbf{F}_{lt'}^{-1}\right)$ where $\mathbf{R}$ is the rotation tensor, which is obtained from the dependencies $\mathbf{F}_{lt'} = \mathbf{VR} = \mathbf{RU}$, $\hat{\mathbf{A}}$ is a fourth-order tensor decomposed in the eigenvector basis, $\hat{\mathbf{D}}$ is a fourth order tensor of elastic stiffness and $\hat{\boldsymbol{\varepsilon}}$ is the strain tensor. The equation of equilibrium $div(\boldsymbol{\sigma}) = 0$ is discretized using the finite element method,

Zienkiewicz and Taylor [2000], taking the form $\mathbf{P}(\mathbf{a}) = \mathbf{f}$, where $\mathbf{a} = \{\mathbf{q}, \boldsymbol{\beta}\}$ The FE approximation of the displacement and the dislocation field is given by $\mathbf{q} = \sum_n N_i^u u_i$ and $\boldsymbol{\beta} = \sum_n N_i^\beta \beta_i$, where N_i^u and N_i^β are the shape functions for the displacement and dislocation fields, respectively. To solve the FE equation using the Newton Raphson method, we need the tangent stiffness

$$\mathbf{K} = \frac{\partial \mathbf{P}}{\partial \mathbf{a}}, \quad K_{ij} = \int_\Omega \nabla N_i \frac{\partial(\boldsymbol{\sigma} \det \mathbf{F})}{\partial \mathbf{a}_j} \det(\mathbf{F}^{-1}) d\Omega \tag{1}$$

The required elastic constants and the lattice constants of the alloy of SiGe are calculated by applying Vegard's law

$$c_{ij} = c_{ij(Ge)} x + c_{ij(Si)} (1-x), \quad \Delta = r_{(Si_{1-x}, Ge_x)} - [r_{Si} + (r_{Ge} - r_{Si})x] \tag{2}$$

where x denotes the amount of Ge, c_{ij} and r are the lattice constants.

NUMERICAL EXAMPLES: The first sample consists of two layers of Si (100x100x20 nm each). It contains an inclusion modelled using a 4 element patch in the centre of the sample below the surface. The inclusion consists of a 30% mixture of SiGe. The elastic constants for Si and Ge are taken from Baker and Arzt [2000] and Herzog [2000]. The lattice parameter of Si is $5.431 \cdot 10^{-10}$ m. The constants for the mixture SiGe are obtained using Vegard's law and they are presented in Table 1.

Table 1. Material constants

GPa	Si	Ge	SiGe (30%)
c11	165.8	128.5	139.69
c12	63.9	48.3	45.0
c44	79.6	66.8	75.76

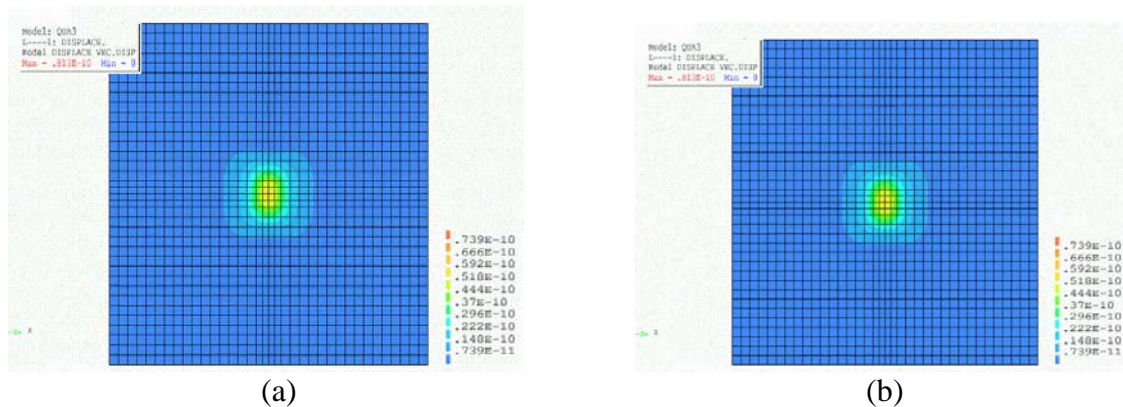(a)   (b)

Fig. 1. Effect of inclusion on (a) the vertical displacement field and (b) the stress σ_{11}

The lattice parameter for the mixture is $5.493 \cdot 10^{-10}$ m. The displacement and stress σ_{11} fields generated by the inclusion are presented in Fig. 1. The displacements are in the range $0.73 \cdot 10^{-11}$ m to $0.739 \cdot 10^{-10}$ m and σ_{11} reaches a maximum value of -200 MPa.

The second sample has dimensions 100x100x40 nm. The circular dot (SiGe) has a diameter of 20 nm and is covered by two layers of Si. The displacement and stress σ_{11} fields in the sample are shown in Fig 1. The largest displacements are concentrated around the island and the maximum value is $0.133 \cdot 10^{-10}$ m. Two regions of high absolute value of stresses can be observed. The gradients of stresses in the regions of thespots are very high since the values of stress vary from -480 MPa to 1900 MPa.
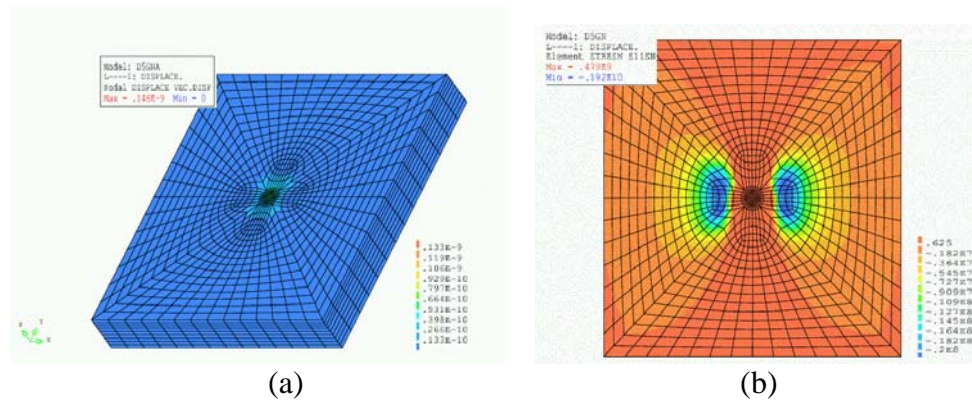

(a)   (b)

Fig. 2. Effect of a SiGe/Si dot on (a) the displacement field and (b) the stress σ_{11}

FINAL REMARKS: The results presented shows that high stresses appears in the region of quantum dot, which represent material inclusions. The results can be qualitatively compared with experimental observations.

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