International Journal of Mechanical Sciences 52 (2010) 212–218

Contents lists available at ScienceDirect

International Journal of Mechanical Sciences

journal homepage: www.elsevier.com/locate/ijmecsci

The influence of dislocation distribution density on curvature and interface stress in epitaxial thin films on a flexible substrate

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ARTICLE INFO

Article history:
Received 5 August 2009
Accepted 7 September 2009
Available online 12 September 2009

PACS:
68.35.Gy
68.60.Bs
81.40.Jj

MSC:
74A60
74K35
74Q05

Keywords:
Misfit dislocations
Strain relaxation
Continuous distribution of dislocations
Bimorph interface stress

ABSTRACT

We consider the problem of relaxation of coherency stresses by lattice misfit dislocations, which can be represented as edge dislocations uniformly distributed along the interface, and can be associated with the concept of dislocation density according to the mathematical theory of continuous distributions of dislocations. The orientation of dislocation line density is constrained within the plane of epitaxial layer and the Burgers vector density within the same plane is considered as a local variable of the problem. Under the external stress-free conditions the system is then enforced to satisfy the boundary conditions according to the geometry of the epitaxial film and the substrate together with the corresponding compatibility conditions. The dislocation density tensor is then connected with the deformation and rotation tensors and subsequently with the curvature of the system. The closed form solution of the problem is given for a generic one-dimensional case.

1. Introduction

In development and fabrication of electronic devices the growth of thin semiconductor layers on a bulk substrate is one of the most important and demanding parts of the process. It has been observed experimentally that particular growth mode depends on a balance between the interfacial energies of the substrate and epitaxial layer and the lattice mismatch between the layers. The stress associated with misfit strain between the thin sheet and a substrate is the main source and the driving force for formation of structural defects. The natural response of the system under such circumstances is the formation of strain relaxing mechanisms that can have adverse effects on electronic performance of semiconductor materials. In the unstrained or relaxed epitaxial film, the substrate and the film retain their bulk lattice constants and the film is not commensurate with the substrate. In this case, the mismatch is accommodated locally by the misfit dislocations where the average spacing between misfit dislocations depends on the misfit constant. To mathematically address this phenomenon we consider the problem of relaxation of coherency stresses by lattice misfit dislocations, which can be represented as edge dislocations uniformly distributed along the interface. Such distributions can be associated with the concept of dislocation density according to the mathematical theory of continuous distributions of dislocations. The orientation of dislocation density is confined to the plane of epitaxial layer, while density of the Burgers vector is considered as a local variable of the problem. Such system is then enforced to satisfy the boundary conditions according to the geometry of the epitaxial thin film and the substrate together with the corresponding compatibility conditions. In this way the dislocation density tensor can be connected with the tensor of total distortion and consequently with the deformation and rotation tensors, and at the same time with the curvature of the system, which originates from the plastic part of the distortion tensor. We show that dislocation densities in the film and the substrate have significant influence on the curvature of the system. The quantitative and qualitative behavior of the flexible bimorph element depends not only on a misfit dislocation density at the interface between both phases, but it is also strongly correlated with elastic heterogeneity of the system. Detailed analysis shows that the total curvature of a flexible epitaxial system is directly affected by elastic heterogeneity of the system, which is determined by the strength of mismatch between elastic constants in the film and in the substrate. Consequently, the problem of plastic curving of a

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doi:10.1016/j.ijmecsci.2009.09.009

flexible epitaxial system together with determination of corresponding interfacial stress can be addressed and viewed as a part of structural mechanics problem [18], continuum mechanics problem [19], phase field problem [20], or interface problem with applied special asymptotic expansion technique [3].

2. Foundations

Let $\mathcal{B}$ denote a material body in $\mathbb{R}^3$ where an arbitrary point $\boldsymbol{x} \equiv \boldsymbol{x}(x_1, x_2, x_3) \in \mathcal{B}$ is referred to a rectangular Cartesian coordinate system with fixed orthonormal basis $\{\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = \delta_{ij}, \forall (i,j) \in (1,2,3)\}$. The symbol δ_{ij} is Kronecker's delta and a summation convention on repeated indices is used throughout this paper.

2.1. Dislocations

We begin this section with an outline of the necessary parts from the theory of continuous distributions of dislocations. First, we give a brief outline of the theory. Here we predominantly follow Refs. [10,11,13,14,21]. These fundamental notions are needed in the latter development and application of the theory.

A distortion displacement gradient, or distortion in short, is defined as

$$\boldsymbol{\beta} = \nabla \boldsymbol{u} = \beta_{ij} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j, \quad \beta_{ij} = \frac{\partial u_j}{\partial x_i} = \partial_i u_j = u_{j,i}, \tag{1}$$

which is generally an asymmetric geometric object, so that by using the symmetric and skew symmetric part

$$\boldsymbol{\varepsilon} = \tfrac{1}{2}(\boldsymbol{\beta} + \boldsymbol{\beta}^T), \quad \boldsymbol{\omega} = \tfrac{1}{2}(\boldsymbol{\beta} - \boldsymbol{\beta}^T), \tag{2}$$

the total distortion can be written as

$$\boldsymbol{\beta} = \boldsymbol{\varepsilon} + \boldsymbol{\omega}. \tag{3}$$

Sometimes it is convenient to introduce a dual of the displacement curl in the form

$$\hat{\boldsymbol{\omega}} = \tfrac{1}{2} \nabla \times \boldsymbol{u} = \tfrac{1}{2} \varepsilon_{ijk} \omega_{jk} \hat{\mathbf{e}}_i = \hat{\omega}_i \hat{\mathbf{e}}_i. \tag{4}$$

The gradient of the dual of antisymmetric part of the distortion tensor defines the contortion tensor

$$\varkappa = \hat{\boldsymbol{\omega}} \nabla = \varkappa_{mn} \hat{\mathbf{e}}_m \otimes \hat{\mathbf{e}}_n, \quad \varkappa_{mn} = \frac{\partial \hat{\omega}_m}{\partial x_n} = \hat{\omega}_{m,n} \tag{5}$$

and is also important in the latter development since it defines torsion or curvature of the system. A mathematical definition of conditions of compatibility is given as

$$\nabla \times \boldsymbol{\varepsilon} \times \nabla = \mathbf{0}. \tag{6}$$

The equation which defines the Burgers vector $\boldsymbol{b}$ of the dislocation line as a result of complete encirclement of the singularity of displacement field $\boldsymbol{u}$ reads

$$\oint_{\mathcal{L}} d\boldsymbol{u} = \oint_{\mathcal{L}} d\boldsymbol{x} \cdot \boldsymbol{\beta} = -\boldsymbol{b}. \tag{7}$$

However, since we are dealing with the theory of continuous distributions of dislocations, the Burgers vector $\boldsymbol{b}$ should be understood as a resulting vector of all dislocations which intersect the transversal surface $\mathcal{S}$

$$\boldsymbol{b} = \int_{\mathcal{S}} \boldsymbol{n} \cdot \boldsymbol{\alpha}\, dS = \left(\int_{\mathcal{S}} n_i \alpha_{ik}\, dS \right) \hat{\mathbf{e}}_k, \tag{8}$$

where $\boldsymbol{\alpha}$ represents a dislocation density tensor. With the help of Eq. (1) and Stokes' theorem we obtain

$$\oint_{\mathcal{L}} d\boldsymbol{x} \cdot \boldsymbol{\beta} = \int_{\mathcal{S}} \boldsymbol{n} \cdot (\nabla \times \boldsymbol{\beta})\, dS. \tag{9}$$

By comparison among Eqs. (7)–(9) and by considering Eqs. (3), (5) and (4), after some calculations we observe that the dislocation density tensor can be written as

$$\boldsymbol{\alpha} = -\nabla \times \boldsymbol{\beta} = -\nabla \times \boldsymbol{\varepsilon} + \varkappa - \mathrm{Tr}\, \varkappa \boldsymbol{I}, \tag{10}$$

which represents a fundamental field equation in continuum theory of dislocations. If a total distortion due to internal stresses is split into elastic and plastic part, henceforth designated with the superscripts E and P, respectively, then the symmetric part of the total distortion represents the tensor of total deformation, and we can write

$$\boldsymbol{\beta} = \boldsymbol{\beta}^E + \boldsymbol{\beta}^P, \quad \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^E + \boldsymbol{\varepsilon}^P. \tag{11}$$

The reason for such decomposition is twofold. The elastic reversible part induces stress according to standard assumptions of elasticity theory, while plastic irreversible part, as a main cause of permanent deformation, can be understood in a sense of eigenstrain theory as a source of internal stress generated by continuously distributed defects. This leads to self-equilibrated internal stress distributions in systems under traction-free boundary conditions without imposed external stresses. Since the total strain satisfies the conditions of compatibility in contrast to elastic and plastic part which in general may not fulfill compatibility conditions individually, from Eq. (6) it follows that

$$\nabla \times (\boldsymbol{\varepsilon}^E + \boldsymbol{\varepsilon}^P) \times \nabla = \mathbf{0}. \tag{12}$$

If we consider Eqs. (6), (10) and (11) we can deduce that plastic distortion can be connected with the dislocation density tensor as

$$\boldsymbol{\alpha} = \nabla \times \boldsymbol{\beta}^P. \tag{13}$$

Details of such a derivation can be found in cited literature, [10,11] in particular.

2.2. Field equations

Momentum balance is given in the form of a divergence free stress field

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0} \tag{14}$$

with associated traction free boundary conditions

$$\boldsymbol{n} \cdot \boldsymbol{\sigma}_{\mathcal{S}} = \mathbf{0}. \tag{15}$$

The elastic part of constitutive relation is governed by Hooke's law

$$\boldsymbol{\sigma} = \mathcal{C} : \boldsymbol{\varepsilon}^E = \mathcal{C}_{ijkl} \varepsilon^E_{kl} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j, \tag{16}$$

where $\mathcal{C}$ in general represents a tensor of spatially heterogeneous elastic moduli. The stress divergence free and boundary traction free conditions have an important implication in spatial averaging, namely the stress average over the whole body $\mathcal{B}$ of volume $\mathcal{V}$ vanishes

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{\mathcal{V}} \int_{\mathcal{B}} \boldsymbol{\sigma}\, d\mathcal{B} = \mathbf{0}. \tag{17}$$

This result is valid regardless of the origin of internal stresses and constitutive relations.

3. Strained epitaxial layer

Due to their large importance in technological applications especially in semiconductor industry, various epitaxial systems have been investigated in the past. For exhaustive reviews see [2,4]. In this work, we try to generalize and extend already known results by establishing a general framework and methodology for analysis of different types of effects induced by dislocation distributions in the film, at the interface, and in the substrate, on overall behavior of the flexible epitaxial system. We consider a