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Dislocation formation from one inclined free-surface of a buried layer in a matrix

Jérôme Colin

Institut P', Université de Poitiers, ENSMA, SP2MI-Téléport 2, Futuroscope-Chasseneuil cedex F86962, France

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ABSTRACT

The introduction of a dislocation from one lateral surface of a two-dimensional buried layer embedded in a matrix has been theoretically investigated in the interfaces between the two materials. It is found that the lower (and longer) interface is a preferential site where the dislocation can be introduced to relieve the misfit strain. For given layer thickness and lattice mismatch between the matrix and the layer phases, a critical angle has been determined beyond which the introduction of the dislocation is energetically favorable. A stability diagram associated with the dislocation formation has been then provided with respect to the misfit strain, inclination angle and layer thickness. The case of a Si_xGe_{1-x} layer embedded in a Ge matrix is finally discussed.

1. Introduction

The growth of nanostructured patterns onto the surface of solids has been the topic of intensive researches in the fields of surface physics, materials science and solid mechanics because of the paramount importance of the resulting nano-objects in the fabrication process of opto-electronic devices. For example, the extension of the emission energies into the low-loss telecom bands has been achieved for the O band at 1.3 µm by introducing a strain reducing layer for InAs/InGaAs quantum dots (Goldmann et al., 2014) or by developing dots-in-a-well structures (Liu et al., 2003). Likewise, different techniques such as the insertion of ultrathin GaAs layers (Anantathanasarn et al., 2005) or the droplet epitaxy (Skiba-Szymanska et al., 2017) have been used for the emission at the C band at 1.55 µm. The control of the mechanical properties of such nanostructures is also a challenging topic of research. In particular, the introduction of dislocations in the interface between an island epitaxially strained on its substrate has been theoretically investigated in the two-dimensional plane strain approximation of the linear and isotropic theory of elasticity (Johnson and Freund, 1997). It has been found that beyond a critical size of the island, the formation of such dislocations is energetically favorable, leading to misfit strain relaxation. In the case of $In_{0.6}Ga_{0.4}As$ islands on GaAs(001) substrates, the critical dimensions of the islands have been also determined using analytical treatment of elasticity combined with finite element simulations. Taking into account the lateral limitation of the epilayers, the phase diagram separating the coherent and incoherent regions has been found to be in agreement with the experimental observations obtained by high-resolution transmission electron microscopy (Tillmann and Förster, 2000). Later, the problem of island alloying has been considered (Spencer and Blanariu, 2005). Assuming surface diffusion is faster than deposition and bulk diffusion, it has been demonstrated that the profile of composition undergoes segregation that has been found to be maximum at intermediate compositions of the island. The interplay between morphology, composition and the optical properties of InAs/InAl/InAlGaAs/InP quantum dots developed for single-photon emission at 1.55 µm telecom wavelength has been then characterized (Carmesin et al., 2017). It has been reported that the fluctuations of composition in the dots can shift the emission energy of 200 meV.

Likewise, the introduction of dislocations in a number of structures of different geometries such as core-shell nanowires, nanovoids, spherical or decahedral particles has been studied (Gutkin et al., 2000; Liang et al., 2005; Fang et al., 2008; Lubarda, 2011; Pan and Shibutani, 2012; Ahmadzadeh-Bakhshayesh et al., 2012; Kolesnikova et al., 2013; Gutkin et al., 2014; Gutkin and Smirnov, 2015; Yu. et al., 2018) and the effects of critical parameters (size, misfit strain, etc.) have been characterized. Recently, the pileup of dislocations near a inclined free-surface has been theoretically investigated in a bimetallic interface (Lubarda, 2018) and the equilibrium positions of the dislocations as well as the back stress behind a trailing dislocation of the pileup have been determined as a function of the inclination angle of the surface with respect to the vertical axis.

E-mail address: jerome.colin@univ-poitiers.fr

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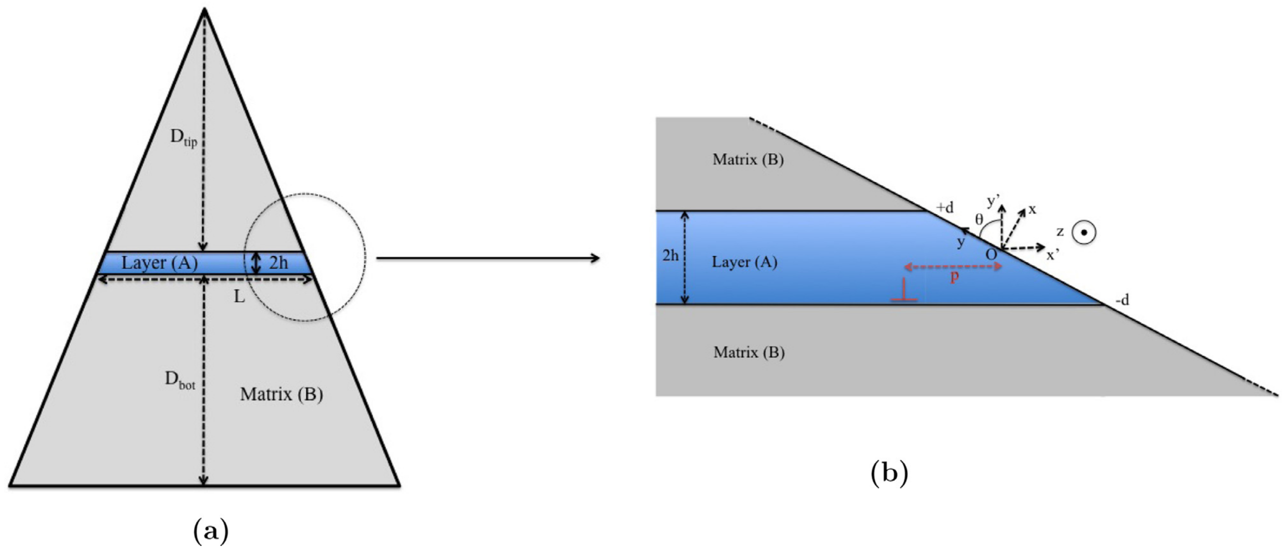

Fig. 1. A strained layer of material A and thickness $2h$ is embedded in a matrix of material B. (a) General view. (b) When $D_{tip} >> 2h$, $D_{bot} >> 2h$ and $L >> 2h$, the problem reduces to the study of the introduction of a dislocation in the interface of a buried layer in a semi-infinite matrix, from an inclined free-surface of an angle θ with respect to the vertical axis.

In this work, the introduction of a dislocation in the interfaces of a strained two-dimensional layer embedded in a matrix has been studied from one free-surface of the system, in the hypothesis where the surface is inclined with respect to the interface plane. From an energy variation calculation, the combined effects of the misfit strain in the layer and of the inclination angle of the free-surface have been characterized, assuming the other dimensions of the system are greater than the layer thickness. The dislocation formation from a {105} surface of a Si_xGe_{1-x} layer embedded in the Ge matrix is finally analyzed.

2. Modeling and discussion

A two-dimensional nanostructure composed of a layer of material A and thickness $2h$ lying in a matrix of material B is displayed in Fig. 1a. The elastic constants of the two materials are assumed to be equal, the shear modulus and Poisson ratio being labeled μ and ν, respectively. Assuming the layer width L and the distances D_{tip} and D_{bot} between the layer and the other matrix surfaces are much greater than the layer thickness, i.e. $L >> 2h$, $D_{tip} >> 2h$ and $D_{bot} >> 2h$, the problem of the dislocation introduction in the layer interfaces from one free-surface has been simplified as follows. A buried layer in a semi-infinite matrix is considered near an inclined free-surface making an angle θ with the vertical axis (see Fig. 1b). The lattice mismatch at the interfaces $\delta a > 0$ between both materials A and B generates misfit stress. In the framework of the linear and isotropic elasticity theory (Timoshenko and Goodier, 1951; Landau and Lifshitz, 1970), this misfit stress tensor has been first calculated within the plane strain hypothesis. Far from the free-surface, the initial stress tensor in the layer A in the $(Ox'y')$ coordinate system is given by:

$$\bar{\bar{\sigma}}_0' = \begin{pmatrix} \sigma_0 & 0 \\ 0 & 0 \end{pmatrix}, \tag{1}$$

with $\sigma_0 = 2\mu/(1-2\nu)\delta a/a$ and a the reference lattice parameter. In the following, the elasticity calculation has been performed in the $(0xy)$ coordinate system. Introducing the rotation matrix,

$$R = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \tag{2}$$

the initial stress tensor due to the misfit writes:

$$\bar{\bar{\sigma}}_0 = R^{-1}\bar{\bar{\sigma}}_0' R = \begin{pmatrix} \sigma_0\cos^2\theta & -\sigma_0\sin\theta\cos\theta \\ -\sigma_0\sin\theta\cos\theta & \sigma_0\sin^2\theta \end{pmatrix}. \tag{3}$$

The first step of this work has been to determine the elastic relaxation near the free-surface. To do so, the biharmonic Airy function φ_r has been considered (Timoshenko and Goodier, 1951) such that $\Delta^2\varphi_r(x,y) = 0$, with $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$ the Laplacian operator. Taking for $x < 0$,

$$\varphi_r(x,y) = \int_0^\infty (a_1 + b_1 x)\, e^{kx}\cos ky\, dk + \int_0^\infty (a_2 + b_2 x)\, e^{kx}\sin ky\, dk, \tag{4}$$

the components of the relaxation stress tensor $\bar{\bar{\sigma}}_r$ are defined as:

$$\sigma^r_{xx}(x,y) = \frac{\partial^2\varphi_r(x,y)}{\partial y^2},\ \sigma^r_{yy}(x,y) = \frac{\partial^2\varphi_r(x,y)}{\partial x^2}, \quad \sigma^r_{xy}(x,y) = -\frac{\partial^2\varphi_r(x,y)}{\partial x\partial y}, \tag{5}$$

with a_1, a_2, b_1 and b_2 four constants to be determined writing the mechanical equilibrium condition onto the free surface at $y = 0$ as:

$$\left(\bar{\bar{\sigma}}_0 + \bar{\bar{\sigma}}_r\right)\mathbf{n} = 0, \tag{6}$$

with $\mathbf{n}^t = (1,0)$ the unit normal to the surface. From Eq. (6), it yields:

$$\sigma^r_{xx}(0,y) + \sigma_0\cos^2\theta\,\Pi_{2d}(y) = 0, \tag{7}$$

$$\sigma^r_{xy}(0,y) - \sigma_0\sin\theta\cos\theta\,\Pi_{2d}(y) = 0, \tag{8}$$

where the rectangular function Π_{2d} of half-width d:

$$\Pi_{2d}(y) = \frac{1}{2\pi}\int_0^\infty \frac{4}{k}\sin kd\cos ky\, dk, \tag{9}$$

has been introduced to express onto the free-surface and in a compact form, the misfit stress located in the interval $-d \le y \le d$, with $d = h/\cos\theta$. From Eqs. (7) and (8), the constants a_i and b_i have been determined, but not shown in this Paper, with $i = 1, 2$. The Airy function φ_r has been thus found to be: