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Equilibrium positions of misfit dislocations in a nanolayer embedded in a matrix

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ABSTRACT

The formation of two misfit edge dislocations in the interfaces of a stressed thin layer embedded in a matrix has been theoretically investigated from an energy variation calculation as a function of the lattice mismatch between the layer and matrix. The equilibrium positions of the dislocations have been determined and the two configurations where the arm orientations of the dipole are normal or inclined to the interfaces have been discussed versus the nanostructure dimensions and lattice mismatch.

1. Introduction

The mechanical stability of nanostructured materials is a long-standing problem that has been considered from both experimental and theoretical point of view (see Freund, 1993; Freund and Suresh, 2003; Gutkin et al., 2015a; Gutkin and Smirnov, 2015; Kleman and Friedel, 2008; Nix, 1989 and references therein for review). In this framework, the formation of dislocations in axi-symmetrical composite structures has been intensively studied because of the numerous applications of such nanostructures in nano-electronics and optics (Dimakis et al., 2014; Gül et al., 2014; Rieger et al., 2015). The introduction of prismatic dislocation loops in the interface between a cylindrical precipitate embedded in a finite-size matrix has been for example investigated from a static energy variation calculation and the critical thickness of the inner cylinder has been determined versus the misfit strain (Ovid'ko and Sheinerman, 2004). Likewise, the equilibrium critical thickness for the dislocation formation has been determined for pillar or fin heterostructure epitaxial film systems (Liang et al., 2005) and the effects of substrate compliance and geometry have been analysed. A methodology to produce coherent coaxial nanowire heterostructures has been then developed in Raychaudhuri and Yu (2006). The problem of formation of isolated or dipoles of edge or screw dislocations has been also considered in nanoscale cylindrical inhomogeneity due to misfit and/or interface stresses (Enzevaee et al., 2014; Fang et al., 2008; 2009a, 2009b; Shodja et al., 2015; Wang et al., 2010). For oxide-covered nanowires, a strain gradient plasticity model has been developed and the flow stress at which the interfaces are plastically deformed has been determined (Aifantis et al., 2007). Likewise, the dislocation emission from nanovoid has been studied taking into account the effect of neighbouring nanovoids and surface stress, and a model of nanovoid growth has been proposed in ductile porous materials (Zhao et al., 2014). In the case of nanowires of rectangular cross-section embedded in composites, the effects of misfit strain, nanowire size or interspacing between the nanowires have been characterized on the introduction in the nanowire interfaces of loops, semi-loops and dipoles of dislocations (Gutkin et al., 2003). For spherical precipitates embedded in a matrix, the introduction of dislocations has been also considered (Gutkin et al., 2015a; 2014a; 2015b; Gutkin and Smirnov, 2014; Gutkin et al., 2014b).

The problem of formation of misfit dislocations in planar multilayered structures has been investigated by Matthews and Blakeslee (1974) who observed that in GaAs and $GaAs_{0.5}P_{0.5}$ thin films grown on GaAs substrates, the interfaces were composed of large coherent areas separated by inclined misfit dislocations of type $\frac{a}{2}\langle 110\rangle$, with a the lattice parameter. They also determined the critical thickness of the layers as a function of the misfit strain, beyond which the formation of these dislocations is energetically favourable. Later, the formation of misfit dislocations in the interfaces of an embedded layer in a semi-infinite matrix has been then theoretically investigated and the effects of lattice mismatch and interface mixing have been characterized (Colin et al., 1997; Grilhé and Junqua, 1992). In buried or capped strained semiconductor layers such as $Si/Ge_xSi_{1-x}/Si$ and $GaA/In_xGa_{1-x}/As$, the formation of isolated and dipole misfit dislocations has been intensively studied. For layers grown in the (001) direction, the dislocations being found to be of 60° type (Gosling et al., 1993). The effect of

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predeposited interfacial dislocations in the interfaces of nanoscale multilayered structures such as Cu–Ni system has been then investigated on the propagation of threading dislocations, the effects of inclination of the Burgers vectors of the arrays of interfacial and gliding dislocations has been characterized (Akasheh et al., 2007). For strained (0001) InGaN/GaN layers, a stress relaxation mechanism has been proposed through the generation of V-shaped edge-type dislocation half-loops (Lobanova et al., 2013).

In this context, it thus appears relevant to investigate the conditions of dipole formation in the interfaces of buried and strained layers and the relative position of the dislocations. The formation of a dipole of edge dislocations in the centre of a layer embedded in a matrix has been recently analysed (Colin, 2014) when the two lateral free-surfaces are considered, this dipole configuration being either metastable or stable configuration. It is the purpose of the present paper to study from a theoretical point of view, the conditions on the layer dimensions and misfit strain required for the development of the configurations where the arm orientations of the dipole are whether normal or inclined to the interfaces, when the misfit edge dislocations are generated from the lateral free-surfaces into the layer interfaces.

2. Modelling

A thin layer of material A is embedded in a matrix of material B (see Fig. 1 for axes). The thickness of the A layer is labelled h and its length L. The width of the structure is assumed to be infinite along (Oz) axis. Due to the lattice mismatch $\delta a = a_B - a_A$ between both materials A and B along (Ox) and (Oy) axes, a misfit strain is lying in the structure which has already been calculated (Colin et al., 1997) in the framework of the plane strain hypothesis of the linear and isotropic elasticity theory, using the Airy function formalism (Hirth and Lothe, 1982; Timoshenko and Goodier, 1951), with a_A and a_B the lattice parameters of materials A and B, respectively. It is assumed for definiteness that $a_B > a_A$ such that $\delta a > 0$. For example, the shearing component of the misfit stress responsible for the dislocation formation in the interfaces has been found to be (Colin, 2014):

$$\sigma_{xy}^{0}(x,y) = \frac{\sigma_0}{2\pi}\int_{-\infty}^{+\infty}\frac{(L+x)\sinh[kx] - x\sinh[k(L+x)]}{kL+\sinh[kL]} \times (1-e^{ikh})e^{ik(y-h)}\,dk, \quad (1)$$

with $\sigma_0 = 2\mu\frac{1+\nu}{1-\nu}\frac{\delta a}{a}$ the misfit stress far from the lateral surfaces due to the lattice mismatch through the interface along the (Ox) and (Oy) axes, with $a = (a_A + a_B)/2$. It is emphasized at this point that the dislocations are assumed to pre-exist at the free-surfaces, the shearing stress in the interface being responsible for the propagation of the dislocations from the free-surfaces to a given distance in the layers. The nucleation mechanism of the dislocations at the free-surfaces, from surface steps for example, is beyond the scope of the present analysis. In particular, the nucleation of a dislocation semi-loop should be more favourable than the nucleation of the dipole composed of two parallel edge dislocations. For symmetry reason, the misfit edge dislocations of Burgers vectors $(b, 0)$ and $(-b, 0)$ considered in this work are assumed to be introduced in the interfaces at $(-L/2+d, 0)$ and $(-L/2-d, h)$ respectively, with d a positive constant characterizing the inclination of the dipole arm with respect to the vertical axis of symmetry of the structure (see Fig. 1). To determine the stress field of the dislocations, the formalism of Airy function has been used again (Timoshenko and Goodier, 1951). The well-known initial stress of the two edge dislocations in an infinite medium $\bar{\bar{\sigma}}^{d,\infty}$ is first considered (Hirth and Lothe, 1982) and the mechanical equilibrium conditions on both lateral free-surfaces located at $x=-L$ and $x=0$,

$$\sigma_{xx}^{d,\infty}(0,y) + \sigma_{xx}^{d,rel}(0,y) = 0,\ \sigma_{xy}^{d,\infty}(0,y) + \sigma_{xy}^{d,rel}(0,y) = 0, \quad (2)$$

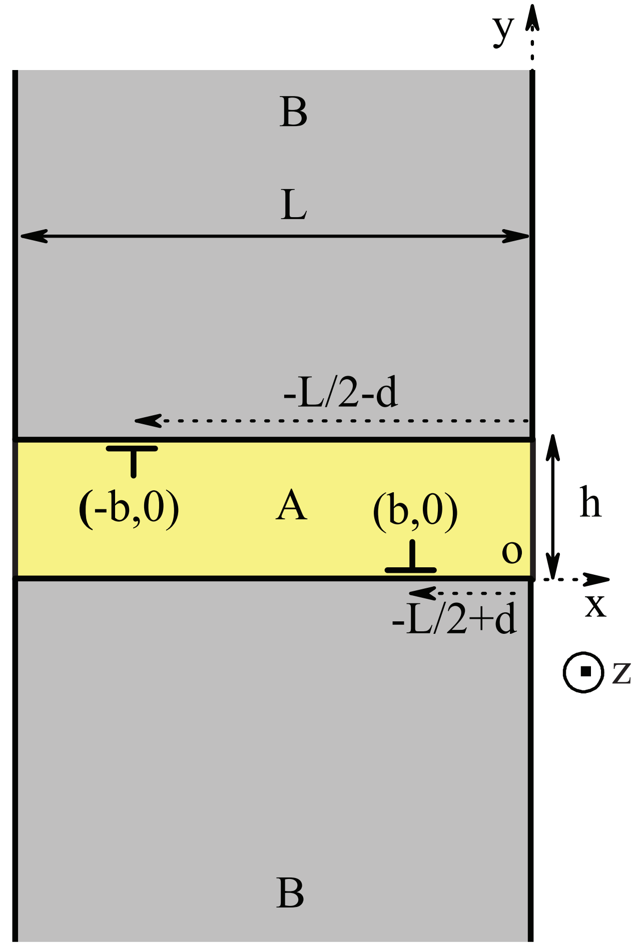

Fig. 1. A layer of material A is epitaxially strained in a matrix of material B. The thickness of the layer is labelled h and the length L. Two misfit dislocations of Burgers vectors $(b, 0)$ and $(-b, 0)$ are considered in the interfaces at $(-L/2+d, 0)$ and $(-L/2-d, h)$, respectively.

$$\sigma_{xx}^{d,\infty}(-L,y) + \sigma_{xx}^{d,rel}(-L,y) = 0,\ \sigma_{xy}^{d,\infty}(-L,y) + \sigma_{xy}^{d,rel}(-L,y) = 0, \quad (3)$$

have been then used to determine the relaxation stress $\bar{\bar{\sigma}}^{d,rel}$ due to the free-surfaces. This relaxation stress is characterized by an Airy function $\phi^{d,\,rel}$ whose general expression is (Hirth and Lothe, 1982; Timoshenko and Goodier, 1951):

$$\phi^{d,rel}(x,y) = \frac{\sigma_0}{4\pi}\int_{-\infty}^{+\infty}\Big[(A_d^{rel} + B_d^{rel}x)\cosh[kx] + (C_d^{rel} + D_d^{rel}x)\sinh[kx]\Big]e^{iky}\,dk, \quad (4)$$

with $A_d^{rel}, B_d^{rel}, C_d^{rel}$ and D_d^{rel} four constants that have been found to be with the help of Eqs. (2) and (3) (Wolfram Research, Inc., 2009):

$$A_d^{rel} = -\frac{i\mid k\mid}{4k^3}e^{-ikh-\frac{1}{2}(L+2d)|k|}(2+2d\mid k\mid + L\mid k\mid + e^{ikh+2d|k|} \times (-2+(2d-L)\mid k\mid)), \quad (5)$$

$$B_d^{rel} = -\frac{ie^{-ikh-\frac{1}{2}(L+2d)|k|}}{4\mid k\mid(1+2k^2L^2-\cosh[2kL])} \times (2kL(e^{2d|k|}(-2+(2d-L)\mid k\mid)$$