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Circular dislocation loop in a three-layer nanowire

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ABSTRACT

The formation of a prismatic dislocation loop in the two interfaces of a three-layer nanowire has been theoretical studied from a static energy variation calculation, when the three layers are submitted to misfit strains. Depending on the misfits and different radii of the layers, the possibility of formation of the dislocation loop at the different layer interfaces has been characterized and a stability diagram is provided for the structure. The effect of the external radius of the nanowire is also investigated.

1. Introduction

The mechanical, electronic and optical properties of nanocomposite materials has been the topic of intensive researches from both experimental and theoretical point of view because of the numerous applications of these composite structures in engineering fields such as nanoelectronics and nanophotonics (Lauhon et al., 2002; Link and El-Sayed, 2003; Vollath and Szabó, 2004; Hu et al., 2006; Yan et al., 2011). Core–shell nanowires have been for example used in nanowire field effect transistors (Bryllert et al., 2006) or nano light emitting diodes (Hayden et al., 2005). It is now well admitted that the different properties of the nanostructures strongly depend on the stresses that may have various origins among which one can cite the mismatch between the thermal dilatation coefficients of the different phases or the misfit at the interfaces between the lattices of the different crystals composing the phases. The relaxation of the misfit stress, generated during the growth of the phases for example, can be achieved via the formation of threading or misfit dislocations which can in turn strongly modify the morphology of the nanostructures, their optical and electrical properties as well as their mechanical strength. The formation of dislocations in planar thin films on substrates or in multilayers has already been studied, based on energetic considerations (Matthews and Blakeslee, 1974; Freund, 1993). It has been found that the formation of misfit dislocations in the interfaces is energetically favorable for critical thickness depending on the misfit strain. The case of axi-symmetrical structures has also been intensively studied (Liang et al., 2005; Ertekin et al., 2005; Glas, 2006; Trammell et al., 2008). The formation of edge dislocations and prismatic dislocation loops in a two-phase composite cylinder submitted to misfit stress has been for example investigated and a critical misfit parameter has been determined as a function of the radius of the core cylinder (Gutkin et al., 2000; Ovid'ko and Sheinerman, 2004). The effect of the ratio of the shear moduli on the critical conditions for the formation of a dipole of misfit dislocations has been also investigated for a precipitate embedded in an infinite-size matrix and the equilibrium positions of the dipole have been determined (Fang et al., 2008). Likewise, the stability of a strained film grown on a nanopore has been investigated theoretically, the nanopores being considered as a new promising class of nanosensors for the identification of biomolecules for example Wanunu and Meller (2007). The critical thickness of the film associated with the formation of misfit screw dislocations in the film-substrate interface has been then determined as a function of the ratio of the shear modulii of the film and the substrate (Fang et al., 2009). Considering the plastic strains due to the misfit dislocations generated to relax the misfit strain, the critical thickness of the film in a core–shell structure has been also determined as a function of the growth direction for the formation of dislocation loops (Chu et al., 2013). In a series of papers (Fang and Liu, 2006; Fang et al., 2009; Gutkin et al., 2013; Zhao et al., 2014), the effects of interfaces have been investigated on the formation of screw and edge dislocations in core–shell nanowires and in structures composed of nanoinhomogeneities embedded in a matrix. The equilibrium positions of the dislocations have been thus determined as a function of the interface stress.

The formation of dislocations in the interfaces of a core–multishell quantum well heterostructure has been recently investigated by means of finite element simulations (Fan et al., 2014). It has been

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found that the critical thickness of the outermost barrier decreases as the well thickness increases and the core radius decreases. In the present work, the formation of a prismatic dislocation loop in the interfaces of a three-layer nanowire is investigated from an energy variation calculation. The effect of the different radii of the layers and of the misfit stress is characterized.

2. Modeling

A nanowire of length L and external radius r_3 is composed of three layers with r_1 the interface radius between the layers 1 and 2 and r_2 the interface radius between the layers 2 and 3, with $L \gg r_3$ (see Fig. 1). The elastic coefficients of the three layers are assumed to be identical, the shear modulus is labeled μ and the Poisson's ratio ν. Due to the lattice mismatches at both interfaces, a misfit strain $\epsilon_{rr}^{*,i} = \epsilon_{\theta\theta}^{*,i} = \epsilon_{zz}^{*,i} = \epsilon_i^*$ is considered in the layer i, with $i = 1$ for the inner layer, $i = 2$ for the annular layer and (r, θ, z) the cylindrical coordinate system. The elastic state of the structure is first determined in the framework of the isotropic linear elasticity theory taking the general form of the displacement field as (Timoshenko and Goodier, 1951):

$$u_r^i(r) = A_i r + \frac{B_i}{r}, \tag{1}$$

$$u_z^i(z) = C_i z, \tag{2}$$

in the layer i, with $i = 1, 2, 3$. Assuming the elastic displacement field should be finite as $r \to 0$, it yields $B_1 = 0$. The other constants are determined from the following set of equations derived from the mechanical equilibrium conditions of the structure (Liang et al., 2005):

$$\sigma_{rr}^1(r_1) = \sigma_{rr}^2(r_1), \tag{3}$$

$$\epsilon_1^* r_1 + u_r^1(r_1) = \epsilon_2^* r_1 + u_r^2(r_1), \tag{4}$$

$$\epsilon_1^* z + u_z^1(z) = \epsilon_2^* z + u_z^2(z), \tag{5}$$

$$\sigma_{rr}^2(r_2) = \sigma_{rr}^3(r_2), \tag{6}$$

$$\epsilon_2^* r_2 + u_r^2(r_2) = u_r^3(r_2), \tag{7}$$

$$\epsilon_2^* z + u_z^2(z) = u_z^3(z), \tag{8}$$

$$\sigma_{rr}^3(r_3) = 0, \tag{9}$$

$$(r_3^2 - r_2^2)\sigma_{zz}^3 + (r_2^2 - r_1^2)\sigma_{zz}^2 + r_1^2 \sigma_{zz}^1 = 0, \tag{10}$$

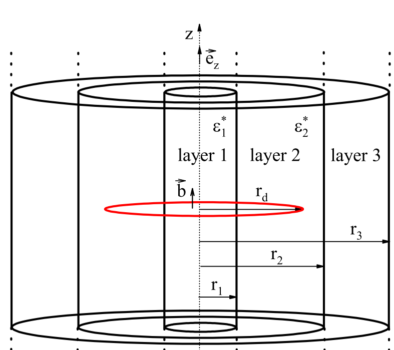

Fig. 1. Schematic representation of an axi-symmetrical structure of length L and external radius r_3, with $L \gg r_3$. The nanowire is composed of three layers 1, 2 and 3. Misfit strains ϵ_1^* and ϵ_2^* are considered in the layer 1 of radius r_1 and in the annular layer 2 of thickness $r_2 - r_1$, respectively. A prismatic dislocation loop of radius r_d and Burgers vector $\vec{b} = b\vec{e}_z$ is lying in the layer 2.

where σ_{kl}^i and ϵ_{kl}^i correspond to the components of the stress and elastic strain tensors of the layer i, respectively. To the first order in ϵ_1^* and ϵ_2^*, the constants A_i, B_i and C_i have been determined to be:

$$A_1 = \frac{1-3\nu}{1-\nu}\,\frac{\epsilon_2^*(r_2^2 - r_1^2) - \epsilon_1^*(r_3^2 - r_1^2)}{2r_3^2}, \quad B_1 = 0, \tag{11}$$

$$C_1 = -\epsilon_1^* + \frac{(\epsilon_1^* - \epsilon_2^*)r_1^2 + \epsilon_2^* r_2^2}{r_3^2}, \tag{12}$$

$$A_2 = \frac{1-3\nu}{1-\nu}\,\frac{\epsilon_1^* r_1^2 - \epsilon_2^*(r_3^2 + r_1^2 - r_2^2)}{2r_3^2}, \quad B_2 = \frac{1+\nu}{1-\nu}\,\frac{(\epsilon_1^* - \epsilon_2^*)r_1^2}{2}, \tag{13}$$

$$C_2 = \frac{\epsilon_1^* r_1^2 - \epsilon_2^*(r_3^2 + r_1^2 - r_2^2)}{r_3^2}, \tag{14}$$

$$A_3 = \frac{1-3\nu}{1-\nu}\,\frac{(\epsilon_1^* - \epsilon_2^*)r_1^2 + \epsilon_2^* r_2^2}{2r_3^2}, \quad B_3 = \frac{1+\nu}{1-\nu}\,\frac{(\epsilon_1^* - \epsilon_2^*)r_1^2 + \epsilon_2^* r_2^2}{2}, \tag{15}$$

$$C_3 = \frac{(\epsilon_1^* - \epsilon_2^*)r_1^2 + \epsilon_2^* r_2^2}{r_3^2}. \tag{16}$$

It can be stated at this point that the present calculation of the misfit stress in a three-layer nanowire is a generalization of the equivalent calculation performed in the case of a two-layer nanostructure (Aifantis et al., 2007).

The problem of the determination of the stress and strain fields of a circular prismatic dislocation loop lying in the plane $z = 0$ is now considered where r_d is the radius of the dislocation and $\vec{b} = b\vec{e}_z$ its Burger vector, with b a positive constant and $\vec{e}_z$ the unit vector along (Oz) axis (see Fig. 1). It is emphasized that the present study is restricted to the case where $\epsilon_1^* > 0$ and $\epsilon_2^* > 0$ such that the formation of the present dislocation loop is assumed to be favorable. The formation of a dislocation loop of Burgers vector $\vec{b} = -b\vec{e}_z$ when $\epsilon_1^* < 0$ and $\epsilon_2^* < 0$ can be derived from the present analysis. Following Kroupa (1960), the stress field in the case of an infinite-size solid is fully determined from a biharmonic function ϕ^0, whose Hankel's transform defined by Sneddon (1951):

$$G^0(k, z) = \int_0^\infty r\phi^0(r, z) J_0(kr)\, dr, \tag{17}$$

is given by:

$$G^0(k, z) = \frac{1-2\nu}{4(1-\nu)} b r_d \frac{J_1(kr_d)}{k^3}(2\nu + kz)e^{-kz}, \tag{18}$$

with J_0 and J_1 the Bessel's functions of the first kind of zero and first order, respectively. The different stress components σ_{ij}^0 can be deduced from this function ϕ^0. When the nanostructure is limited by an axi-symmetrical free surface at $r = r_3$, a relaxation stress σ_{ij}^{rel} should be considered such that the following boundary conditions are satisfied at $r = r_3$ (Ovid'ko and Sheinerman, 2004; Cai and Weinberger, 2009):

$$\sigma_{rr}^0(r_3, z) + \sigma_{rr}^{rel}(r_3, z) = 0, \tag{19}$$

$$\sigma_{rz}^0(r_3, z) + \sigma_{rz}^{rel}(r_3, z) = 0. \tag{20}$$

The solution to the problem provided by Ovid'ko and Sheinerman (2004) is used in this work and the relaxation stress σ_{ij}^{rel} has been characterized by a new bi-harmonic function ϕ^{rel} defined as (Timoshenko and Goodier, 1951):

$$\phi^{rel}(\tilde{r}, \tilde{z}) = \frac{\mu b^3}{2(1-\nu)} \tilde{r}_d^2 \int_0^\infty [\rho_1 I_0(\tilde{r}k) - \tilde{r}k\rho_2 I_1(\tilde{r}k)] \sin(k\tilde{z})\, dk, \tag{21}$$