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Edge misfit dislocations in core–shell nanowire with surface/interface effects and different elastic constants

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ABSTRACT

A model of the generation for an edge misfit dislocation in the system of a nanowire surrounded by a co-axial film with surface/interface effects is investigated. The critical conditions of an edge misfit dislocation formation at the interface are analyzed, under considering the influence of the material elastic dissimilarity, misfit strains, the radius of the nanowire, core radius of the misfit dislocation and the surface/interface effects. The results show that the critical film thickness reduces with increment of the misfit strains, nanowire radius and core radius of the edge misfit dislocation, below the critical values of which, the misfit dislocation is energetically unfavorable whatever the film thickness. Critical film thickness first decreases and then increases with increasing the ratio of the shear modulus. There exists a critical film thickness below which no interfacial misfit dislocation could be introduced whatever the ratio of the shear modulus. There also exists a critical value of the ratio of the shear modulus, above which edge misfit dislocation does not form at any film thickness. The negative (positive) surface/interface stress can decrease (increase) the formation energy of the edge misfit dislocation. The positive (negative) surface/interface stress would increase (decrease) the critical film thickness, critical misfit strains and critical nanowire radius. The positive (negative) surface/interface stress would decrease (increase) the range of the film thickness and the critical ratio of the shear modulus. The larger the values of the surface/interface stress qualities, the greater the influence of the surface/interface stress on critical parameters.

1. Introduction

In general, the stability of both the structures and properties of crystalline nanocomposites are strongly influenced by misfit stresses arising due to a misfit between the crystal lattices of the adjacent component phases at interface boundaries. A partial relaxation of misfit stresses often occurs by nucleation and evolution of misfit dislocations (MDs) at interface boundaries in thin-film and bulk nanocomposites [1–5]. Dislocation generation mechanism is also considered to be an effective way in plastic deformation of composite materials [6,7]. Additionally, experiments studied the critical conditions of the generation for the misfit defects at the interface boundary [8].

During recent years, great effort has focused on the synthesis, fabrication and characterization of so-called core/shell nanostructures [9,10]. The investigation of MD in composite cylinder (core–shell nanowire) was motivated by the synthesis of these solid nanowires. The lattice mismatch between adjacent materials results in internal strains during the syntheses of the core–shell nanowires, which could be partially/fully relaxed via the formation of misfit/threading dislocations. These defects can negatively affect the physical behavior, e.g., mechanical strength, features of the electric and optical spectra [1]. A first approximation model of MDs in film/substrate composites of wire form was suggested Gutkin et al. [11], and the effects of geometric parameters of such composites on generation of MDs were theoretically analyzed by methods of elasticity theory of defects in solids. The results showed that in considering misfit composite structure of cylindrical (wire) form, the set of geometric parameters crucially affecting the generation of MDs contains the wire composite radius, film thickness and misfit strain. In order to simplify the analysis, the most studies on the critical condition for the formation of MDs or dislocation loops in the strained core–shell structures [12,13], the cylinder (core) and surface film (shell) have the same values of elastic

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constants, which cannot reflect the real properties of the elastic mismatch between the substrate and the surrounding film. Fang et al. [14–16] examined the influence of the difference of elastic constants on the critical thickness of the film and critical radius of the strained inhomogeneity for screw misfit dislocation formation. Yi et al. [17] have extended the 3D Eshelby formalism to multi-shell nano-onions and applied to quantum dots of uniform and non-uniform compositions. Duan et al. [18,19] have considered quantum dots with incompatible strain fields and given conditions when misfit dislocations (MD) are emitted. Zhao et al. [20] investigated the model of an edge misfit dislocation at the interface of the hollow nanopore and the infinite substrate with surface/interface stress. The influence of the ratio of the shear modulus between the film and the infinite substrate, the misfit strain, the radius of the nanopore and the surface/interface stress on the critical thickness of the film was discussed.

Additionally, interfacial bonding condition is one of the important factors that control the local elastic fields and the overall properties of composites. When the size of the inclusion is of the order of nanometer, the inclusion–matrix interface energy cannot be neglected because of the increased contribution to the total energy from the surface/interface [21,22]. In recent decade, the theory of the surface/interface elasticity has been used to analyze many size-dependent elastic problems on the nanoscale. The dependence of the effective elastic or thermoelastic properties on the size of the particulate composite materials highlights the importance of the surface/interface in analyzing the deformation of nano-scale structures [23,24]. The influences of particle size and interface energy on the void nucleation and evolution mechanism were investigated [25,26]. One-dimensional coherent nanowires with tilted internal twins exhibit anisotropic size effect: their strengths show no apparent change if only their thicknesses reduce, but become stronger as the sample sizes are reduced proportionally, which could help to develop straightforward understanding on the origin of size effect in strength [27,28]. A classical continuum model for elastic solids incorporating surface/interface energy (surface/interface stress) was first formulated by Gurtin and Murdoch [29]. This model (namely, surface/interface stress model) has been adopted by some authors in studying nanoscale structures, thin films, nanocomposites and quantum dots [30–40]. As will be seen, the surface/interface effects are a critical factor in the physical behavior of the materials containing nanowire of a sufficiently small size.

In this paper, we consider a two-phase misfit nanowire system which consists of a cylindrical nanowire and a co-axial cylindrical film, and suppose the misfit strain is accommodated through the generation of edge MD at the interface boundary. Critical film thickness for the generation of the first edge MD at the interface (film/nanowire) boundary to be energetically favorable is calculated, especially considering the influence of the surface/interface effects and the material elastic dissimilarity. The presence of MDs has a detrimental effect on the performance of the strained material systems. Therefore, understanding and controlling the generation of MDs are very important. Such control is necessary in manufacturing (e.g., microelectronics) where defects must be minimized [1,41]. Due to these factors, the investigation of the critical conditions for the generation of MDs becomes significant.

2. Critical condition for generation of edge MD

Here the model considered is that the cylinder consists of a nanowire of radius R_1 and film of thickness $h=R_2-R_1$, as shown in Fig. 1. The elastic constants of the nanowire and film indicate μ_1,υ_1 and μ_2, υ_2, where μ_i is shear modulus of the material and υ_i is Poisson's ratio. In the following analysis, we will use the subscripts 1 and 2 to identify the corresponding physical quantities in the region of the nanowire and the film, respectively. The edge MD with Burgers vector $(0,\ b_y)$ at the interphase (film/nanowire) boundary and its lines are parallel with the axis of the nanowire. The lattice mismatch strains would be expressed as uniform strains ε_x^0, ε_y^0 and ε_{xy}^0.

In view of the works of Gutkin et al. [2,11], and Freund and Suresh [1], the criterion for the generation of the first edge MD at the interface (film/nanowire) boundary to be energetically favorable is as follows:

$$\Delta W = W_d + W_m + W_c \le 0 \tag{1}$$

Where W_d denotes the elastic energy of the edge MD in the nanowire and film system, W_m is the elastic energy associated with the elastic interaction between the edge MD and the misfit stress and W_c is the energy of the MD core. Hereon, in order to fully and accurately analyze the influence of various parameters on the edge MD formation and the critical geometries, the energy of the MD core is considered. According to the Hirth and Lothe [42], the energy of the MD core W_c is about $\mu_2 {b_y}^2/[4\pi(1-\upsilon_2)]$.

The elastic energy of an edge dislocation (the energy per its unit length) under consideration can be expressed as follows [42]:

$$W_d = \frac{b_y}{2}\int_{R_1+r_0}^{R_2} \sigma_{\theta\theta d}(x,0)dx \tag{2}$$

Where $\sigma_{\theta\theta d}(x,0)$ is the stress component of the edge MD in the nanowire and film system and r_0 is the core radius of the edge dislocation.

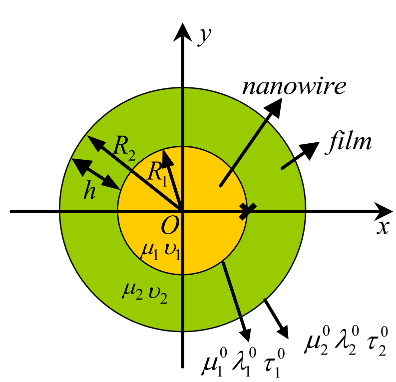

Fig. 1. Edge MD at the interface boundary in a nanowire composite with surface/interface effects.