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Misfit dislocations in an annular strained film grown on a cylindrical nanopore surface

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The critical thickness of a film for the formation of a misfit dislocation in the system of a strained film grown on a nanopore is studied. The influence of the ratio of the shear modulus between the film and the substrate, the misfit strain and the radius of the nanopore on the critical thickness of the film is discussed. New phenomena concerning the critical thickness of the film are obtained due to the difference in elastic constants of the film and the substrate.

Keywords: Misfit dislocations; Nanopores; Critical film thickness

Nanopores have emerged in recent years as an exciting new class of nanosensors that can be used for rapid electrical detection and characterization of biomolecules [1,2]. Control of the nanoscale surface properties of nanopores can govern their interactions with various analytes, resulting in "smart" nanopore sensors. Various approaches for nanopore functionalization have been reported, from deposition of metals [3] and oxides [4] to various organic modifications [5]. As a result, the nanopore structure often gains significant thickness (coating) [2]. In general, when the thickness of the coating is beyond a critical value, the stability of both the structure and the performance of the nanopores, which is crucial for applications of such structures, may be influenced by the generation and evolution of misfit dislocations (MDs) [6,7].

On the other hand, nanochannel-array materials have been extensively used in nanotechnology. They can be used not only as filters and catalysts, but also as templates for nanosized structures, such as magnetic, electronic and optoelectronic devices [8]. It has been shown that, by increasing the surface coating of the cylindrical nanopores, nanochannel-array materials can be made stiffer than their non-porous counterparts [9]. Similarly, both the structure and properties of these nanoporous materials are strongly affected by misfit stresses arising due to a misfit between the crystal lattices of adjacent component phases. A partial relaxation of misfit stresses often occurs by the generation and evolution of MDs at the interphase boundaries [10]. In addition, the control of the MDs at the interfaces can enhance the coherency-strain strengthening effect in nanostructured materials [11].

In this paper, the critical thickness of a film for the formation of MDs in the system of a strained annular film grown on a cylindrical nanopore embedded in an infinite substrate is investigated theoretically. The film and the substrate have different elastic constants. This system can potentially be fabricated through the implantation of a material into the cylindrical pores of a porous solid or by the synthesis of nanotubes and their embedding into a solid matrix. The problem of MD generation has been extensively studied for plate-like composites because planar heterostructures are widely used in contemporary nano- and optoelectronic devices where MDs may cause the degradation of their functional properties [12–16]. In addition, investigations have also been carried out to study the critical conditions required for the formation of MDs in strained nanowires or quantum dots [17–23]. The critical thickness of a film for the formation of MDs in the system of a strained annular film grown on a cylindrical hole embedded in an infinite substrate with same elastic properties has also been investigated by Sheinerman and Gutkin [24]. It should

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be mentioned that most work [12–24] involving the critical thickness of thin films for MD formation in various systems is based purely on an elastic continuum approach. The work of Vellinga et al. [25] and Hosson et al. [26] indicates that the structure of the MDs depends on both the misfit strain and the bond strength across the interface, and the elastic continuum approach cannot account for the possible configurations at the interface. According to Vellinga et al. and Hosson et al.'s results, it should be realized that, if the effect of the bond strength of the interface is considered, a modification of the critical thickness condition of thin film is required, because the relaxation of the interface at various values of interaction parameter (i.e. bond strength) leads to different values of the interface energy. This needs further study in the future.

Let us consider a model of a two-phase misfitting film/substrate structure, as shown in Figure 1. The substrate is treated as an infinite medium with a cylindrical hole of radius R_2 and infinite length. The film is assumed to be a hollow cylinder, coaxial with the hole, with an internal radius R_1. The thickness of the film is $h = R_2 - R_1$. The film and the substrate are assumed to be elastically isotropic solids with different shear moduli, μ_1 and μ_2, respectively. Because of the mismatch of the lattices of the two materials, significant mismatch strains may exist in the film. In general, the misfit strains can be relaxed via the generation of various defect configurations, such as isolated MDs, MD dipoles, MD loops and semi-loops [6]. Here, we analyze mainly the conditions at which the generation of an isolated MD at the interphase (film/substrate) boundary is energetically favorable in this structure. In considering extensions of this analysis to include the effects of the elastic modulus difference between the film and the substrate, the analysis becomes complicated. For the purposes of illustrating important ideas in strain relaxation without this encumbrance, we consider the case of strain relaxation by screw MDs. All physical conclusions obtained for screw dislocations remain valid for the general case, namely MDs with both screw and edge components [6]. Screw MDs have their Burgers vector b in the interphase (film/substrate) boundary and their lines are parallel with the axis of the nanohole (Fig. 1). The lattice mismatch strain can be treated as eigenstrain ε_m [27].

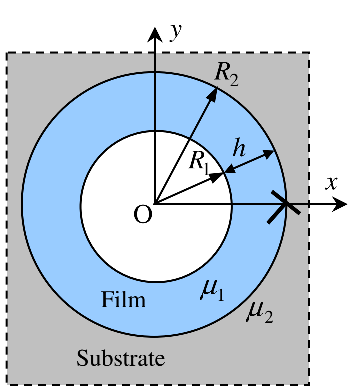

Figure 1. MD formation at the interphase boundary in the system of a strained film grown on a nanopore surface.

According to the work of Freund and Suresh [6], the criterion for the generation of the first MD to be energetically favorable is:

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

where W_d denotes the elastic energy of the MD in the solid and W_m is the elastic energy associated with the elastic interaction between the MD and the misfit stress. The elastic strain energy of the screw dislocation (the energy per its unit length) in the interface between the film and the substrate can be expressed by the following formula [28]:

$$W_d = -\frac{b}{2}\int_{R_1}^{R_2-r_0} \sigma_{zy2}(x,0)dx \tag{2}$$

where r_0 is the core radius of the dislocation and σ_{yz2} is the stress component in the film. By using the complex potential method, the stress component σ_{yz2} can be derived [29]. Substituting of the obtained the stress component σ_{yz2} into Eq. (2), the elastic strain energy of the MD in the interface can be derived:

$$\begin{aligned} W_d = {} & \frac{\mu_1 b^2}{4\pi}\ln\frac{h}{r_0} + \frac{\mu_1 b^2}{2\pi}\sum_{k=0}^{\infty}\frac{1}{k+1}\frac{\mu_2}{\Gamma_1} \\ & \times\left[\frac{(R_2-h)^{k+1}}{R_2^{k+1}} - \frac{(R_2-h)^{2(k+1)}}{R_2^{k+1}(R_2-r_0)^{k+1}}\right] \\ & + \frac{\mu_1 b^2}{4\pi}\sum_{k=0}^{\infty}\frac{1}{k+1}\frac{\mu_2-\mu_1}{\Gamma_1} \\ & \times\left[\frac{(R_2-h)^{3(k+1)} - (R_2-h)^{2(k+1)}(R_2-r_0)^{k+1}}{R_2^{3(k+1)}}\right. \\ & \left. - \frac{(R_2-r_0)^{k+1} - (R_2-h)^{2(k+1)}}{R_2^{k+1}}\right] \end{aligned} \tag{3}$$

where $\Gamma_1 = (\mu_2 + \mu_1) + (\mu_2 - \mu_1)[(R_2 - h)/R_2]^{2(k+1)}$ and $h = R_2 - R_1$.

The elastic energy of the interaction between the MD and the misfit stress field is given by

$$W_m = -b\int_{R_1}^{R_2-r_0} \sigma_{yzm}(x,0)dx \tag{4}$$

where $\sigma_{yzm}(x,0) = \tau_m$ denotes the misfit stress. Considering that the mismatch strain can be treated as eigenstrain ε_m, the misfit stress $\sigma_{yzm}(x,0)$ can be calculated using the following complex potential method [18]:

$$\sigma_{yzm}(x,0) = -\frac{2\mu_1\mu_2\varepsilon_m}{\Gamma_2} - \frac{2\mu_1\mu_2\varepsilon_m}{\Gamma_2}\left(\frac{R_2-h}{x}\right)^2 \tag{5}$$

where $\Gamma_2 = (\mu_1 + \mu_2) + (\mu_2 - \mu_1)[(R_2 - h)/R_2]^2$. Substitution of Eq. (5) into Eq. (4) yields

$$W_m = -\frac{2b\mu_1\mu_2\varepsilon_m}{\Gamma_2}\left[R_2 - r_0 - \frac{(R_2-h)^2}{(R_2+r_0)}\right] \tag{6}$$

As a result of our calculations, from Eqs. (1), (3), and (6) we find the following criterion is necessary for the generation of MD to be energetically favorable: