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Misfit dislocations in wire composite solids

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Abstract. A theoretical model is suggested, which describes generation of misfit dislocations in film/substrate composites of wire form. In the framework of the model, the ranges of the geometric parameters (wire radius, film thickness, misfit parameter) of a wire composite are calculated at which the generation of misfit dislocations is energetically favourable. The specific features of generation of misfit dislocations in wire composites are discussed and compared with those in conventional platelike composites.

1. Introduction

Film/substrate composite solids exhibiting functional physical properties serve as key materials in many contemporary high technologies. The stability of both structure and properties of film/substrate composite solids, which is crucial for application of such solids, is strongly influenced by generation and evolution of misfit dislocations (MDs). Such MDs are generated as defects that, in part, accommodate misfit stresses occurring due to a misfit (geometric mismatch) between adjacent crystalline lattices of films and substrates. Generation and evolution of MDs in film/substrate composite solids are crucially affected by geometric parameters of such solids. The effect of the geometric parameters on behaviour of MDs is the subject of intensive experimental and theoretical studies, which commonly deal with MDs in platelike composite solids, e.g. [1–24]. However, in parallel with platelike composites, film/substrate composites of wire form are conventional functional elements used in contemporary high technologies. The cylindrical geometry of wire composites causes MDs in such composites to exhibit behaviour which is, in general, different from commonly studied behaviour of MDs in film/substrate composites. The main aims of this paper are to suggest a first approximation model of MDs in film/substrate composites of wire form and to theoretically analyse (by methods of elasticity theory of defects in solids) the effect of geometric parameters of such composites on generation of MDs.

2. Misfit dislocations in wire composite. Model

Here we model in the first approximation a wire composite (consisting of a wire substrate covered by either a thin or thick film) as a composite cylinder with radius R_2 and infinite length. The model cylinder is composed of an internal cylinder (substrate) of radius $R_1 < R_2$ and a film of thickness $H = R_2 - R_1$, which envelops the internal cylinder as shown in figure 1. In the framework of the suggested first approximation model, we will not take into account the

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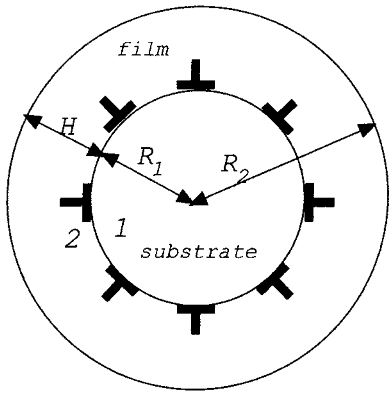


Figure 1. Misfit dislocations at the interphase boundary in a model wire composite.

crystallography of the adjacent film and substrate, in which case the interphase (film/substrate) boundary is treated as a surface of the internal cylinder (figure 1). (That is, there are no facets at the interphase boundary).

The film and substrate are assumed to be isotropic solids having the same values of the shear modulus G and the same values of Poisson ratio ν. The film/substrate boundary is characterized by the misfit parameter

$$f = \frac{2(a_2 - a_1)}{a_2 + a_1} \tag{1}$$

where a_1 and a_2 are the crystal lattice parameters of the substrate and the film, respectively.

Misfit stresses occur in film/substrate composite solids due to the geometric mismatch characterized by f at interphase boundaries between crystalline lattices of films and substrates. In most cases, a partial relaxation of the misfit stresses is realized via generation of MDs; see e.g reviews [5, 7, 21]. Let us consider MDs in the situation discussed (figure 1). Since the crystallography of the adjacent film and substrate is not taken into account, MDs, if they are formed, are supposed to be regularly distributed along the interphase boundary at thermodynamic equilibrium (figure 1) and to have Burgers vectors as shown in figure 1. In the framework of our model, MDs are of the edge type; their lines are parallel with the axis of the composite cylinder (figure 1).

Let us analyse the conditions at which the generation of MDs at the interphase boundary is energetically favourable in a wire composite solid. The same problem in the situation with two- and multi-layer platelike composites is commonly solved via both a calculation of the elastic energy density of MDs and its minimization with respect to the MD ensemble density, see e.g. [2, 4–10, 12–16, 18, 21–24]. In this paper, we will use the other calculation scheme suggested by Gutkin and Romanov [11] for an analysis of MD generation in a thin two-layer plate. This scheme is based on a comparison of energetic characteristics of two physical states realized in a composite solid, namely the coherent state with MD-free interphase boundary and the semi-coherent state with the interphase boundary containing one ('first') MD, which accommodates, in part, the misfit stresses. Thus, the wire composite in the coherent (MD-free) state is characterized by the total elastic energy (per unit length of the composite) being equal to the misfit strain energy W^f related to misfitting at the interphase boundary only. When one (first) MD is generated at the interphase boundary in the wire composite, its total energy W consists of the four terms:

$$W = W^f + W^d + W^c + W^{int} \tag{2}$$

where W^d denotes the elastic energy of the MD, W^c the energy of the MD core and W^{int} the elastic energy associated with the elastic interaction between the MD and the misfit stresses. The generation of the first MD is energetically favourable, if it leads to a decrease of the total energy, that is, if $W - W^f < 0$. With formula (2) taken into account, we come to the following criterion for the generation of the first MD to be energetically favourable:

$$W^d + W^c + W^{int} < 0. \tag{3}$$

In order to calculate the ranges of values of wire composite parameters (wire substrate radius R_1, film thickness H and misfit parameter f) at which inequality (3) is valid, in the following sections we will calculate the misfit stresses and terms W^d, W^c and W^{int}.

3. Misfit stresses in wire composite

In this section, we will calculate the misfit stresses in the model wire composite (figure 1). Let $\epsilon_{ij}^{(k)}$ be the tensor of misfit strain in the kth region, where $k = 1$ for the wire substrate and $k = 2$ for the film (figure 1). Let us suppose $\epsilon_{ij}^{(2)} = 0$. In the simple case of a dilatational misfit we assume $\epsilon_{ij}^{(1)} = f\delta_{ij}$, where $\delta_{ij} = 1$, if $i = j$, and $= 0$, if $i \neq j$. The total strain $\varepsilon_{ij}^{(k)}$ in the wire composite is the sum of the misfit strain $\epsilon_{ij}^{(k)}$ and elastic strain $e_{ij}^{(k)}$:

$$\varepsilon_{ij}^{(k)} = \epsilon_{ij}^{(k)} + e_{ij}^{(k)}. \tag{4}$$

In the cylindrical coordinate system with the z-axis being the cylinder axis, due to the axial symmetry of the model wire composite (figure 1), the total strain components are expressed via displacement as follows [25]:

$$\varepsilon_{rr}^{(k)} = \frac{\partial u_r^{(k)}}{\partial r} \qquad \varepsilon_{\varphi\varphi}^{(k)} = \frac{u_r^{(k)}}{r} \qquad \varepsilon_{zz}^{(k)} = \frac{\partial u_z^{(k)}}{\partial z} = 0. \tag{5}$$

The stress tensor can be written using Hooke's law [25] as

$$\sigma_{ij}^{(k)} = 2G\left(e_{ij}^{(k)} + \frac{\nu}{1-2\nu}e^{(k)}\right) \tag{6}$$

where $e^{(k)} = e_{ii}^{(k)}$. More precisely, in the discussed situation with the wire composite, the components of the stress tensor are as follows:

$$\sigma_{rr}^{(1)} = 2G\left(\varepsilon_{rr}^{(1)} + \frac{\nu}{1-2\nu}\varepsilon^{(1)} - \frac{1+\nu}{1-2\nu}f\right) \tag{7}$$

$$\sigma_{\varphi\varphi}^{(1)} = 2G\left(\varepsilon_{\varphi\varphi}^{(1)} + \frac{\nu}{1-2\nu}\varepsilon^{(1)} - \frac{1+\nu}{1-2\nu}f\right) \tag{8}$$

$$\sigma_{zz}^{(1)} = 2G\frac{\nu\varepsilon^{(1)} - (1+\nu)f}{1-2\nu} \tag{9}$$

$$\sigma_{ij}^{(2)} = 2G\left(\varepsilon_{ij}^{(2)} + \frac{\nu}{1-2\nu}\varepsilon^{(2)}\right) \tag{10}$$

where $\varepsilon^{(k)} = \varepsilon_{ii}^{(k)}$. From the equation of mechanical equilibrium [26]

$$\frac{\partial\sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\varphi\varphi}}{r} = 0 \tag{11}$$

with the stress tensor components given by formulae (7)–(10), we find the following differential equation for displacements:

$$\frac{\mathrm{d}^2 u_r^{(k)}}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}u_r^{(k)}}{\mathrm{d}r} - \frac{u_r^{(k)}}{r^2} = 0. \tag{12}$$

Its solution is as follows:

$$u_r^{(k)} = A_k r + \frac{B_k}{r} \tag{13}$$

where the constants A_k and B_k are derived from the boundary conditions

$$u_r^{(1)}(r \to 0) \text{ has a limited value} \tag{14}$$

$$u_r^{(1)}(r = R_1) = u_r^{(2)}(r = R_1) \tag{15}$$

$$\sigma_{rr}^{(1)}(r = R_1) = \sigma_{rr}^{(2)}(r = R_1) \tag{16}$$

$$\sigma_{rr}^{(2)}(r = R_2) = 0. \tag{17}$$

As a result, we obtain these constants to be

$$A_1 = \frac{1+\nu}{1-\nu}\frac{f}{2}\frac{R_2^2 + (1-2\nu)R_1^2}{R_2^2} \qquad B_1 = 0 \qquad A_2 = A_1 - \frac{1+\nu}{1-\nu}\frac{f}{2}$$

$$B_2 = \frac{1+\nu}{1-\nu}\frac{f}{2}R_1^2. \tag{18}$$

From (5), (7)–(10), (13) and (18) we find the non-vanishing misfit stress components σ_{ij}^f (equal to $\sigma_{ij}^{(1)}$ at $r < R_1$ and to $\sigma_{ij}^{(2)}$ at $r > R_1$) as follows:

$$\sigma_{rr}^f = \sigma^* \left(\frac{R_1^2 - R_2^2}{R_2^2}\Theta[R_1 - r] + \frac{R_1^2}{R_2^2}\frac{r^2 - R_2^2}{r^2}\Theta[r - R_1] \right) \tag{19}$$

$$\sigma_{\varphi\varphi}^f = \sigma^* \left(\frac{R_1^2 - R_2^2}{R_2^2}\Theta[R_1 - r] + \frac{R_1^2}{R_2^2}\frac{r^2 + R_2^2}{r^2}\Theta[r - R_1] \right) \tag{20}$$

$$\sigma_{zz}^f = 2\sigma^* \left(\frac{\nu R_1^2 - r^2}{r^2}\Theta[R_1 - r] + \frac{\nu R_1^2}{r^2}\Theta[r - R_1] \right) \tag{21}$$

where $\sigma^* = Gf\frac{1+\nu}{1-\nu}$, and $\Theta[x]$ denotes the Heaviside function ($\Theta[x] = 1$, if $x > 0$; and $\Theta[x] = 0$, if $x < 0$). These formulae will be used in the next section to calculate energetic characteristics of MDs in wire composites.

4. Energetic characteristics of misfit dislocations in wire composites

Let us calculate the elastic energy of an MD and that of its interaction with the misfit stresses in wire composites (figure 1). In doing so, we suppose the MD line (parallel with the substrate cylinder axis) to have the Cartesian coordinates $x = x_0$ and $y = R_1$ (figure 2). The Burgers vector b of the MD is directed along the x-axis. The stress function of this dislocation can be derived from the corresponding stress function [27, 28] of a disclination of strength ω whose line is parallel to the cylinder axis but stands off it. To do so, we use the representation of a dislocation as a dipole of wedge disclinations with strengths ω and $-\omega$, distant by b/ω from each other [28]. As a result, the stress function in question is as follows [29]:

$$\chi = \frac{Db}{2}\left((y - R_1)\ln\frac{C^2 r^2}{P^2 R_2^2} + \frac{R_1(r^2 - R_2^2)(x_0^2 + R_1^2 - R_2^2)}{R_2^2 C^2} + \frac{y R_2^2 P^2}{r^2 C^2} \right) \tag{22}$$

where $P^2 = (x_0 - x)^2 + (R_1 - y)^2$, $C^2 = \left(x_0 - x\frac{R_2^2}{r^2}\right)^2 + \left(R_1 - y\frac{R_2^2}{r^2}\right)^2$, $r^2 = x^2 + y^2$ and $D = G/[2\pi(1-\nu)]$. In these circumstances, the elastic energy of the dislocation (the energy per its unit length) is expressed by the following formula [30]:

$$W^d = -\frac{b}{2}\int_{R_1+r_c}^{R_2} \sigma_{xx}^d(x = x_0, y)\,\mathrm{d}y. \tag{23}$$

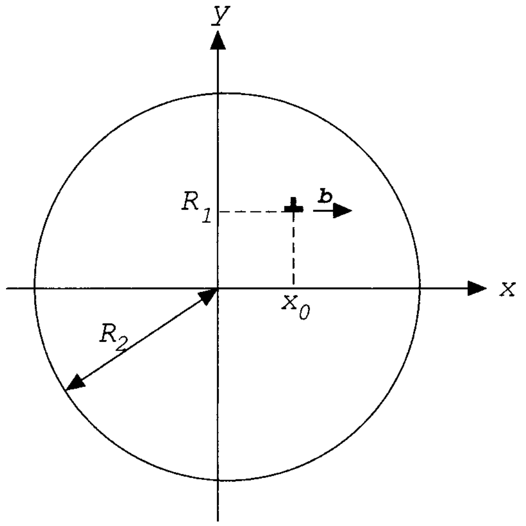


Figure 2. A dislocation in a thin cylinder.

In formula (23), r_c denotes the core cut-off radius, while the stress σ^d_{xx} is calculated with the help of formula [26]

$$\sigma^d_{xx} = \frac{\partial^2 \chi}{\partial y^2}. \tag{24}$$

Using relationship (24), equation (23) can be rewritten in the case of $x_0 = 0$ as

$$W^d = \frac{b}{2}\left(\frac{\partial \chi}{\partial y}(x = 0, x_0 = 0, y = R_1 + r_c) - \frac{\partial \chi}{\partial y}(x = 0, x_0 = 0, y = R_2)\right). \tag{25}$$

From (22) and (25) we find the following formula for the elastic energy of an MD placed at $(x = x_0 = 0,\ y = R_1)$ (figure 2):

$$W^d = \frac{Db^2}{2}\left(\frac{h(h-2)(h-r_0)(h-2-r_0)[2h(h-2-r_0)-1+2r_0]}{2[h^2-(2+r_0)h+r_0]^2} + \ln\frac{h(2-h+r_0)}{r_0}\right) \tag{26}$$

where $h = H/R_2$ is the ratio of the film thickness to the wire (cylinder) radius, and $r_0 = r_c/R_2$.

The elastic energy of the interaction between the MD and the misfit stress field is given by [30]:

$$W^{int} = -b\int_{R_1}^{R_2} \sigma^f_{xx}(x = x_0 = 0, y)\,\mathrm{d}y \tag{27}$$

where $\sigma^f_{xx}(x = x_0 = 0, y) = \sigma^f_{\varphi\varphi}(x = x_0 = 0, y)$. From (20) and (27) we obtain

$$W^{int} = \sigma^* b R_1 h(h-2). \tag{28}$$

The energy of the MD core W^c is about $Db^2/2$ [30].

As a result of our calculations, from (3), (26) and (28) we find the following criterion for the generation of MDs in a wire composite to be energetically favourable:

$$f > f_c(R_1, H) \tag{29}$$

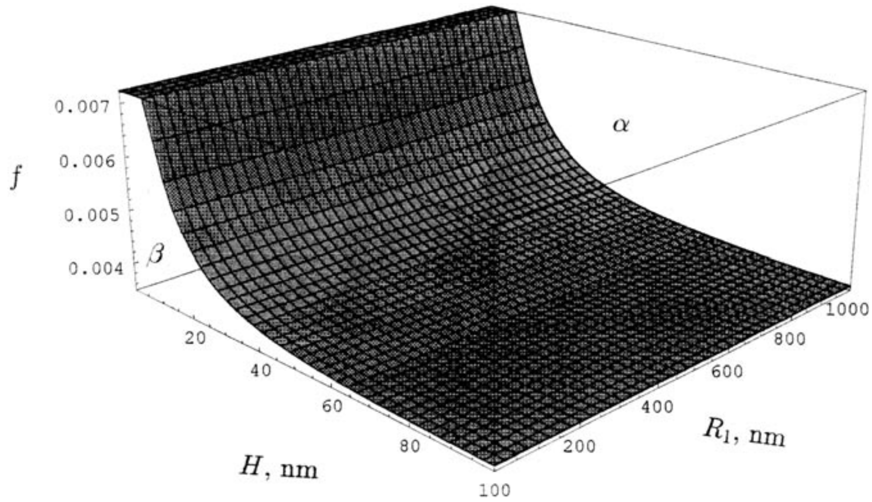


Figure 3. The surface $f_c(R_1, H) = f$ separates regions α (interphase with MDs) and β (interphase without MDs) in the space of geometric parameters of a wire composite.

where

$$f_c(R_1, H) = \left(1 + \frac{h(h-2)(h-r_0)(h-2-r_0)[2h(h-2-r_0) - 1 + 2r_0]}{2[h^2 - (2+r_0)h + r_0]^2} + \ln\frac{h(2-h+r_0)}{r_0}\right)\frac{b}{4\pi(1+\nu)R_1 h(2-h)}. \tag{30}$$

In equation 30, $f_c(R_1, H)$ denotes the critical misfit above which an MD is favoured to nucleate.

The surface $f_c(R_1, H) = f$ in the space of parameters (R_1, H, f) is shown in figure 3, for $\nu = 0.3$ and $r_c = b = 0.4$ nm. This surface separates the two regions α and β, in which case the combinations of parameters R_1, H and f corresponding to points in the region α (β, respectively) are such that the generation of MDs is energetically favourable (unfavourable, respectively).

In general, the following three situations can occur depending on the relationship between the substrate radius R_1 and film thickness H:

(i) *Thin film* ($H \ll R_1$). In this situation, the energetic criterion for the generation of MDs entails from both equation (29) and the relationship $R_1/H \gg 1$. The generation of MDs is energetically favourable at interphase boundaries if the film thickness is higher than the critical thickness H_c derived from the equation

$$1 - \frac{2H_c(H_c - r_c)}{(2H_c - r_c)^2} + \ln\frac{2H_c - b}{r_c} = 8\pi(1+\nu)f\frac{H_c}{b}. \tag{31}$$

This equation for the critical thickness of a thin wire film coincides with that for the critical thickness of a thin platelike film [2]. The dependence of H_c on the misfit parameter f is shown in figure 4.

(ii) *Small cylindrical substrate* ($H \gg R_1$). In this situation, the energetic criterion for the generation of MDs is caused by both equation (29) and the relationship $R_1/H \ll 1$. So, the generation of MDs is energetically favourable, if

$$H < b\exp\left(4\pi(1+\nu)f\frac{R_1}{b} + \frac{1}{2}\right) \tag{32}$$

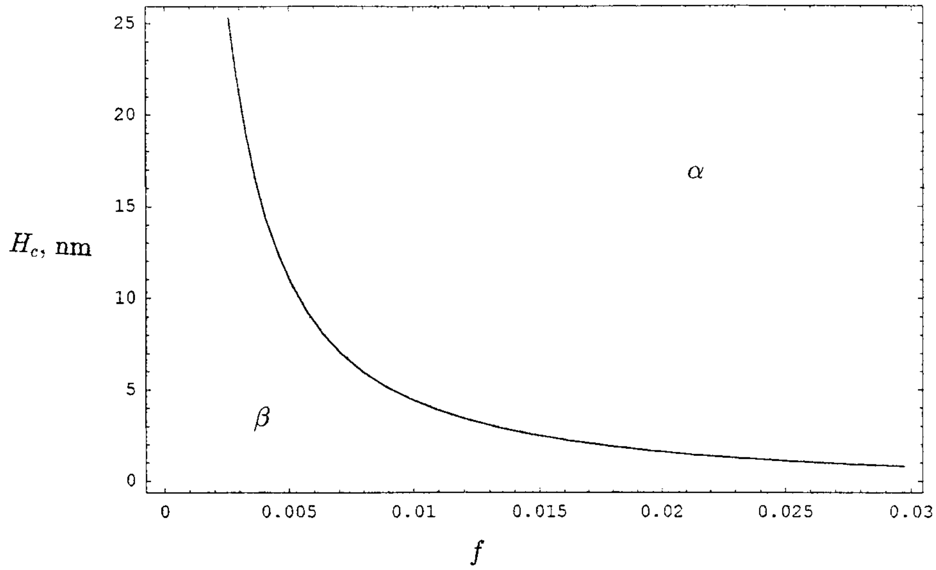


Figure 4. Critical thickness H_c of a thin wire film against misfit parameter f.

that is, if the film thickness is lower than some critical thickness. Inequality (32) can be rewritten as follows:

$$R_1 > \frac{(\ln \frac{H}{b} - \frac{1}{2})b}{4\pi(1+\nu)f}. \tag{33}$$

Formula (33) is indicative of the fact that the generation of MDs is energetically favourable, if the substrate radius R_1 is higher than some critical radius.

(iii) *Substrate radius and film thickness are of the same order* ($R_1 \approx H$). In this situation, the following cases can be realized depending on the parameters of a wire composite (figure 5):

(a) Generation of MDs is energetically unfavourable at any value of the film thickness. This is illustrated in figure 5(a), by the horizontal line $f = 0.003$, which does not intersect the plot of the function $f_c(R_1, H)$.

(b) Generation of MDs is energetically favourable, if the film thickness H is in some range, that is, if $H_{c1} < H < H_{c2}$. This situation is illustrated in figure 5(b), see the horizontal line $f = 0.004$, which intersects the plot of the dependence $f_c(R_1, H)$ at the two points, $H = H_{c1}$ and $H = H_{c2}$.

Figure 5 illustrates also the fact that the formation of MDs is energetically unfavourable in wire composites with misfit parameter f lower than some misfit parameter f_0 depending on the substrate radius R_1 ($f < f_0(R_1)$). In order to reveal the character of dependences of H_{c1}, H_{c2} and f_0 on R_1, the functions $f_c(R_1, H)$ are calculated and shown in figure 6. From figure 6 it follows that f_0 increases, and the interval $[H_{c1}, H_{c2}]$ decreases when R_1 decreases. As a corollary, wire composites tend to be free from MDs when the substrate radius R_1 decreases. In contrast, f_0 decreases, H_{c1} decreases and H_{c2} increases with growth of R_1 (see figure 6). In the limiting case with $R_1 \to \infty$, we find that $f_0 \to 0$ and $H_{c2} \to \infty$.

Finally, let us briefly discuss possible mechanisms for generation of MDs in wire composites. One of the most effective mechanisms in questions, as with the situation with conventional platelike composites, is nucleation of edge dislocations at a free surface of a wire

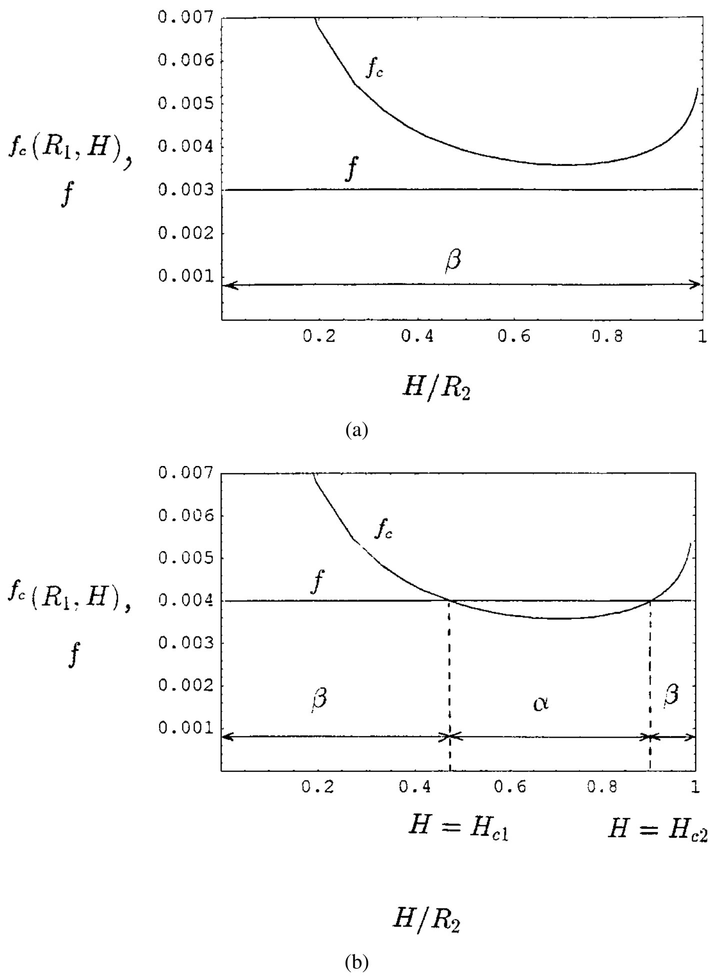


Figure 5. The dependence $f_c(R_1, H)$ shown for the case $R_1 = 100$ b. Horizontal lines correspond to different values of misfit parameter f; (a) $f = 0.003$, interphase without MDs, (b) $f = 0.004$, interphase without MDs when $H < H_{c1}$ or $H > H_{c2}$, and interphase with MDs when $H_{c1} < H < H_{c2}$.

composite and their consequent motion (gliding plus climbing) to the interphase boundary. In this situation, orientation of Burgers vectors of MDs at the interphase boundary relative to cylindrical surface of the boundary is rather arbitrary, because glide planes of the film intersect the interphase boundary surface at widely varied angles. (This is in contrast to MDs in conventional platelike composites where glide planes of the film intersect a plane interphase boundary at fixed angles.) Other possible mechanisms for generation of MDs in a wire composite, that are analogies of such mechanisms in conventional platelike composites, are as follows: gliding of dislocations from internal dislocation sources to the interphase boundary; nucleation of dislocation semi-loops at a free surface and their consequent expansion and motion to the interphase boundary; and formation of partial MDs and their consequent merging into perfect MDs. Action of the mechanisms for generation of MDs is sensitive to geometry of a wire composite and, in general, is different from that in conventional platelike composites. More than that, there are mechanisms which are realized in only wire composites.

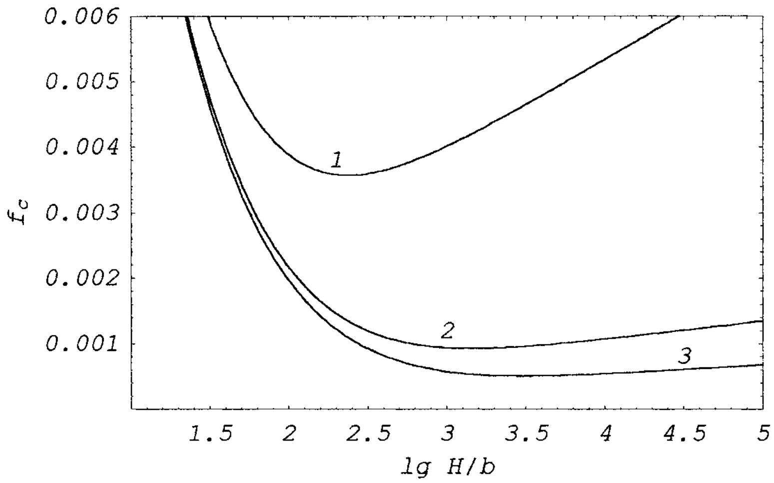
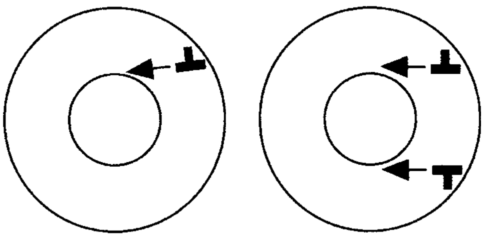


Figure 6. The dependences of critical misfit parameter f_c on log H/b. Curves 1, 2 and 3 correspond to substrate radius $R_1 = 100b$, $500b$, $1000b$, respectively.



(a) (b)

Figure 7. Mechanisms for generation of misfit dislocations in a wire composite. (*a*) Nucleation of a dislocation at a free surface and its consequent motion to the interphase boundary. (*b*) Nucleation of a dislocation dipole at a free surface and its consequent motion to the interphase boundary.

For instance, nucleation of a dislocation dipole at a free surface and its consequent motion to the interphase boundary (figure 7(b)) is effective in only wire composites. In doing so, stress fields of the dislocations composing the dipole (figure 7(b)) screen each other. As a corollary, the energetic barrier for nucleation of the dipole and its motion near the free surface is lower than that in the situation with an isolated dislocation (figure 7(a)). A detailed quantitative (cumbersome and labour intensive) examination of the mechanisms discussed is beyond the scope of this paper. This will be the objective of further studies based on the results of the present work.

5. Concluding remarks

Here we have suggested a first approximation model of film/substrate composite solids of wire form that are often used in contemporary high technologies. In the framework of the model, composites are represented as elastically isotropic solid cylinders, each consisting of an internal cylinder (a substrate) covered by a film (figure 1). The elastic constants (the shear modulus, Poisson ratio) are assumed to be the same for the substrate and the film composing a wire solid, while an interphase boundary is characterized by non-zero misfit parameter f and serves as a source of misfit stresses. In the framework of the suggested model, we have theoretically examined the generation of MDs (defects that, in part, accommodate the misfit stresses) at interphase boundaries in wire composites. The results of our quantitative examinations are in short as follows:

(i) As with the commonly studied situation with platelike film/substrate composites, generation of MDs is energetically favourable in wire composites when their geometric parameters are in certain ranges (calculated above; see figures 3–6).
(ii) The set of geometric parameters crucially affecting the generation of MDs in wire composites contains the wire composite radius R_2, the film thickness H and the misfit parameter f.
(iii) The cylindrical geometry of film/substrate wire composites and finiteness of their substrate radii cause the generation of MDs (as an energetically favourable process) to be limited in such composites as compared with platelike film/substrate composites having semi-infinite substrates. More precisely, in wire composites, at sufficiently small values of their misfit parameter f and internal radius R_1, MDs are not generated at any film thickness, whereas in composites with platelike semi-infinite substrates, there always exists a critical thickness above which MDs may be formed.

These results are important for technological applications of wire composites. In particular, point (iii) is worth noting in context of a technologically interesting possibility of exploiting wire composites with thin films instead of platelike composites (if it is admissible). Actually, both a large value of the thin film thickness and the coherency of interphase boundaries are often highly desired from an application viewpoint. In these circumstances, in order to exploit high functional properties of film/substrate composites with comparatively large values of H and coherent interphase boundaries, one can use wire composites instead of platelike ones (if it is admissible).

The quantitative results obtained in this paper are approximate. However, they can be used, on the one hand, to estimate the structural stability and stability of functional properties of real wire composites and, on the other hand, as a basis for further investigations of film/substrate composites with wire geometry as well as composites with an alternative non-trivial geometry.

Acknowledgments

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