Misfit dislocations in multilayered films on disclinated substrates

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Abstract
A theoretical model which describes the generation of misfit dislocations
in multilayered films deposited onto plastically deformed substrates with
disclinations (defects of rotational type) is suggested. In the framework
of the model, the ranges of the parameters (disclination strength, misfit
parameters, layer thicknesses, characteristics of disclination arrangement) of
a multilayered film/substrate composite for which the generation of misfit
dislocations is energetically favourable are calculated. The specific features
of the generation of misfit dislocations in multilayered films on disclinated
substrates are discussed in relation to a technologically interesting possibility
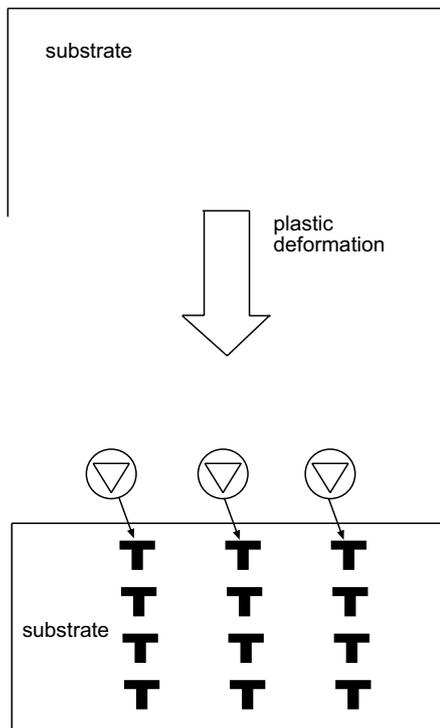for exploiting plastically deformed substrates.

1. Introduction

Multilayered films are widely exploited in high technologies. The stability of both the structure
and the properties of multilayered films, which is crucial for the application of such films,
is strongly influenced by the generation and evolution of misfit dislocations (MDs); see,
e.g., [1–5]. Such MDs are generated as defects that, in part, accommodate misfit stresses
occurring in heteroepitaxial systems due to a misfit (geometrical mismatch) between adjacent
crystalline lattices at interphase boundaries; see, e.g., [1–26]. The cores of MDs violate the
ideal (coherent) structure of interphase boundaries, as a result of which the generation of MDs
is capable of giving rise to instability and degradation of the desired—from an applications
viewpoint—properties of multilayered films.

One of the possible technological methods allowing one to affect generation of MDs is
human-controlled modification of substrates. In particular, plastic deformation of a substrate
can create defects—sources of internal stresses—in the substrate that prevent generation of
MDs in a multilayered film deposited onto the substrate. The main aims of this paper are to
suggest a first-approximation model of a plastically deformed substrate and to theoretically

analyse (by methods of the elasticity theory of defects in solids) the effect of deformation-induced dislocation walls in the substrate on generation of MDs in multilayered film/substrate systems.

2. Formation of disclinations in plastically deformed substrates

Dislocation walls (low-angle grain boundaries) which are arranged in a rather ordered manner are often formed in crystalline solids under plastic deformation [27, 28]. If such deformation-induced dislocation walls are generated in a deformed substrate, they can strongly influence the relaxation of misfit stresses in multilayered films deposited onto the substrate. In order to quantitatively examine this phenomenon, we should specify the stress fields created by the dislocation walls in the multilayered film/substrate system. The deformation-induced dislocation walls are, in general, ragged (figure 1). That is, the 'end' dislocation belonging to a dislocation wall and closest to the substrate free surface is distant by d from the free surface (figure 2). The 'end' dislocation of a ragged dislocation wall serves as a stress source of disclination type, or, in short, as a disclination [28]. The stress fields created by disclinations that terminate dislocation walls in a solid commonly dominate over any other contributions to the stress field created by dislocation walls [28]. In these circumstances, the effects of deformation-induced dislocation walls on relaxation of misfit stresses in a multilayered film, in the first approximation, can be described as those associated with stress fields of the disclinations.

Figure 1. Formation of dislocation walls terminated by stress sources of disclination type (triangles) in a plastically deformed substrate.

In the following sections of this paper, we will theoretically examine the influence of the disclinations on the generation of misfit dislocations in multilayered films deposited onto disclinated substrates under certain assumptions (that simplify our theoretical analysis). In particular, all the derivations of this paper rely on isotropic elasticity, whereas real systems are
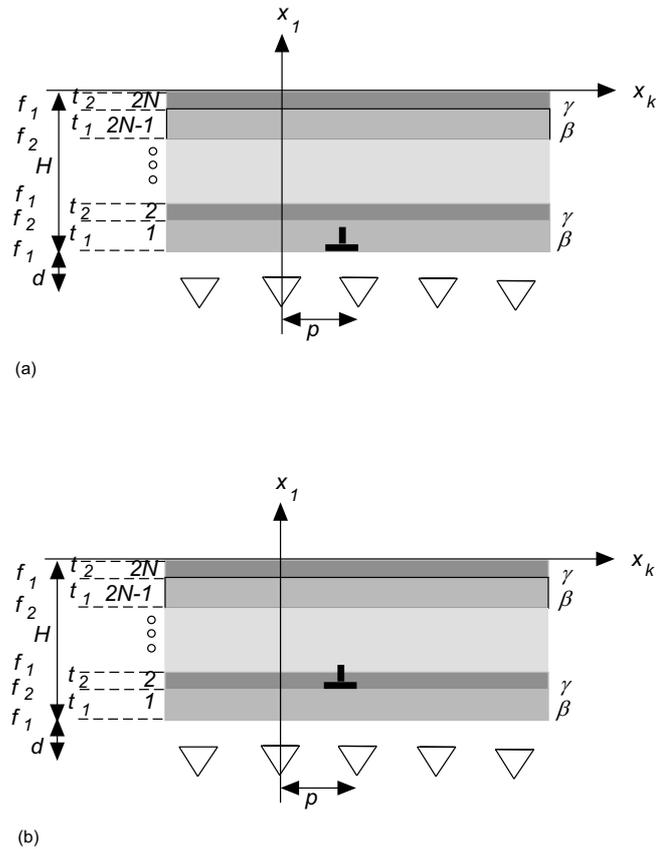
Figure 2. Misfit dislocation in a multilayered film/substrate system with a disclination network.

in many cases elastically anisotropic. The assumption of isotropic elasticity is conventional in the theory of MDs in heteroepitaxial systems; see, e.g., the reviews [7, 9, 21]. A theoretical description of defects in heteroepitaxial systems which accounts for anisotropic effects (e.g., [18]) gives rise to inessential (about 10%) corrections of isotropic-theory-based estimates of the critical thickness. At the same time, calculations that deal with elastic anisotropy are very complicated and labour-intensive. In view of these factors, here we will restrict our theoretical analysis to the model situation with elastic isotropy. Also, in the framework of our consideration, disclinations in plastically deformed substrates are assumed to be identical and form a regular network consisting of orthogonal rows equally distant from the free surface. The consideration under simplifying assumptions will allow us to reveal the key specific features of the formation of misfit dislocations in multilayered films on disclinated substrates and will serve as a basis for further, more detailed examinations of the behaviour exhibited by multilayered films deposited onto plastically deformed substrates.

## 3. Multilayered films on disclinated substrates; the model

Let us consider a multilayered film of thickness H deposited on a model semi-infinite substrate (phase α) (figure 2). Let $2N$ be the number of alternate layers, β and γ, that compose the film. For simplicity, the thickness t_1 (t_2) is assumed to be the same for all the layers β (γ). The film

layers and the substrate are assumed to be isotropic solids having the same values of the shear modulus G and the same values of Poisson ratio ν. In the first approximation, disclinations in the substrate are supposed to be of wedge type and to form a regular square network with a distance p between neighbouring parallel disclinations (figure 2). All the disclinations are assumed to be characterized by the same value ω of the disclination strength and to be distant by d from the film/substrate interphase boundary (figure 2).

Interphase boundaries between cubic crystal lattices α and β as well as β and γ are characterized by two-dimensional dilatation misfits f_1 and f_2, respectively. They are given as follows: $f_1 = 2(a_1 - a_2)/(a_1 + a_2)$ and $f_2 = 2(a_1 - a_3)/(a_1 + a_3)$, where a_1, a_2, and a_3 are the crystal lattice parameters of the phases α, β, and γ, respectively.

In the situation with coherent (defect-free) interphase boundaries, dilatation misfits between the adjacent crystalline phases and the disclination network cause the multilayered film to be elastically strained. The interphase boundaries in the layered composite can transform into the semi-coherent state (with misfit dislocations) at some critical values of the characteristic parameters f_1, f_2, h, t_1, t_2, p, and ω. In these circumstances, the misfit dislocations accommodate, in part, the misfit stresses and, at the same time, their cores violate the pre-existent coherency of the interphase boundaries. The coherent-to-semicoherent transformations of the interphase boundaries give rise to a modification (often suppression) of the functional properties of multilayered films, in which case knowledge of the critical parameters is of crucial importance for applications of such films. In this paper we will focus our examination on the critical conditions at which the generation of misfit dislocations (the coherent-to-semicoherent transformation) occurs at the α/β boundary or at the β/γ boundary closest to the substrate/film (α/β) boundary. The generation of misfit dislocation is most favourable at the interphase boundaries discussed. Therefore, our consideration of the generation of misfit dislocations at these boundaries will reveal the conditions at which the generation of misfit dislocations occurs in the multilayered film/substrate composite as a whole.

To determine the critical conditions in question, we will calculate the difference in energy density (energy per unit length of misfit dislocation) between the coherent interphase boundary and the boundary with one (the 'first') misfit dislocation. In doing so, we assume that the spatial positions of the disclinations in the substrate are not affected by the generation of the misfit dislocation. In the framework of the suggested model description, the misfit dislocation is of edge type and has the Burgers vector $\boldsymbol{b} = b_l \boldsymbol{e}_l$, where $\boldsymbol{e}_l$ denotes the unit vector parallel to the plane Ox_2x_3 and rotated by φ around the axis Ox_2 (figure 3). The dislocation line is located along the m-axis ($x_2 = x_2^0 - m\sin\varphi$, $x_3 = x_3^0 + m\cos\varphi$), where x_2^0 and x_3^0 are constants.
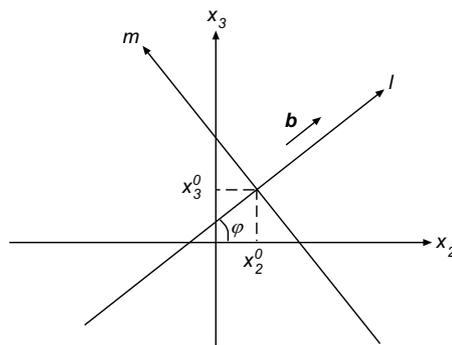
Figure 3. Two coordinate systems in a plane. The Burgers vector of the misfit dislocation is oriented along the l-axis. The dislocation line coincides with the m-axis.

In the situation with coherent interphase boundaries, the energy density W_0 is given as

$$W_0 = W^f + W^{ar} + W^{ar-f} \tag{1}$$

where W^f denotes the misfit strain energy density of the film, W^{ar} the proper energy density of the disclination network, and W^{ar-f} the energy density that characterizes the interaction between the disclinations and the misfit stresses. The energy density W_i of the multilayered film/substrate system with the misfit dislocation is as follows:

$$W_i = W^f + W^{ar} + W^{ar-f} + W_i^d + W_i^{f-d} + W_i^{ar-d} + W^c \tag{2}$$

where $i = 1$ ($i = 2$) corresponds to the case with the misfit dislocation at the substrate α/layer β boundary (layer β/layer γ boundary), W_i^d denotes the proper energy density of the misfit dislocation, W_i^{f-d} the energy density that characterizes the interaction of the misfit dislocation and the misfit stresses, W_i^{ar-d} the energy density that characterizes the interaction of the misfit dislocation and the disclination network, and W^c the energy density of the misfit dislocation core.

The generation of the misfit dislocation is energetically favourable if

$$W_i - W_0 = W_i^d + W_i^{f-d} + W_i^{ar-d} + W^c < 0. \tag{3}$$

To reveal the ranges of parameters at which the generation of the misfit dislocation is energetically favourable, in the next section we will calculate the terms W_i^d, W_i^{f-d}, W_i^{ar-d}, and W^c appearing in formula (3).

4. Energy of the misfit dislocation in a multilayered film/substrate composite with disclinations

First, let us consider the generation of the misfit dislocation at the substrate α/layer β boundary (figure 2(a)). In this situation the proper energy density of the misfit dislocation is given as [29]

$$W_1^d = \frac{Db^2}{2}\left(\ln\frac{2h - b}{b} - \frac{1}{2}\right) \tag{4}$$

where b is the Burgers vector magnitude and $D = G/[2\pi(1 - \nu)]$.

The energy density W_1^{f-d} that characterizes the interaction of the dislocation and the misfit stresses is given by the following formula [30]:

$$W_1^{f-d} = -b_l \int_{-h}^{0} \sigma^f(x_1)\,\mathrm{d}x_1 \tag{5}$$

with

$$\sigma^f(x_1) = 4\pi(1 + \nu)D \sum_{k=0}^{N-1}\{f_1[\Theta(x_1 - x_1^{(2k)}) - \Theta(x_1 - x_1^{(2k+1)})]$$
$$+ f_2[\Theta(x_1 - x_1^{(2k+1)}) - \Theta(x_1 - x_1^{(2k+2)})]\} \tag{6}$$

where $\Theta(t)$ is the Heaviside function, equal to 1 for $t \geqslant 0$ and equal to 0 for $t < 0$; $x_1^{(2i+1)} = -h + t_1 + (t_1 + t_2)i$, $x_1^{(2i)} = -h + (t_1 + t_2)i$, $i = 0, \ldots, N$.

With (6) substituted into formula (5), we find

$$W_1^{f-d} = -4\pi(1 + \nu)Db_l h f_e \tag{7}$$

where $f_e = (f_1 t_1 + f_2 t_2)/(t_1 + t_2)$.

The mean energy density that characterizes the interaction of the misfit dislocation and the disclination network is given as

$$W_1^{ar-d} = -b_l \left\langle \int_{-h}^{0} \sigma_{ll}^{ar}(x_1, x_2 = x_2^0 - m\sin\varphi, x_3 = x_3^0 + m\cos\varphi)\,\mathrm{d}x_1 \right\rangle_m \tag{8}$$

where $\langle \ldots \rangle_m$ means averaging over the coordinate m associated with the misfit dislocation line, $\sigma_{ll}^{ar}(x_1, x_2, x_3) = \sigma_{22}^{ar}(x_1, x_2) \cos^2 \varphi + \sigma_{33}^{ar}(x_1, x_3) \sin^2 \varphi$ is the tensor component of the stress created by the disclination network in the substrate (figure 2) with $\sigma_{22}^{ar}(x_1, x_2)$ and $\sigma_{22}^{ar}(x_1, x_2)$ being the stresses of two disclination rows parallel to the axes x_2 and x_3, respectively. In order to calculate W_1^{ar-d}, let us write the stresses $\sigma_{22}^{ar}(x_1, x_2)$ and $\sigma_{33}^{ar}(x_1, x_3)$ in the following form:

$$\sigma_{kk}^{ar}(x_1, x_k) = \sum_{n=-\infty}^{\infty} \sigma_{kk}^{\triangle}(x_1, x_k - np) \qquad k = 2, 3 \tag{9}$$

where $\sigma_{kk}^{\triangle}(x_1, x_k)$ is the tensor component of the stress created by a disclination having the strength ω and the disclination line ($x_1 = -h - d$, $x_k = 0$) (see figure 4). The stress $\sigma_{kk}^{\triangle}(x_1, x_k)$ is expressed via the stress function $\chi(x_1, x_k)$ of the disclination under consideration as follows [31]:

$$\sigma_{kk}^{\triangle}(x_1, x_k) = \frac{\partial^2 \chi(x_1, x_k)}{\partial x_1^2} \qquad k = 2, 3. \tag{10}$$

From (8)–(10) we find

$$W_1^{ar-d} = b_l \left\langle \sum_{n=-\infty}^{\infty} \left(\frac{\partial \chi(x_1, x_2)}{\partial x_1} \cos^2 \varphi + \frac{\partial \chi(x_1, x_3)}{\partial x_1} \sin^2 \varphi \right) \Big|_{x_1=h}^{x_1=0} \right\rangle_m. \tag{11}$$

Then, with the formula [28]

$$\chi(x_1, x_k) = \frac{D\omega}{4}[(x_1 + h + d)^2 + x_k^2] \ln \frac{(x_1 + h + d)^2 + x_k^2}{(x_1 - h - d)^2 + x_k^2} \qquad (k = 2, 3) \tag{12}$$

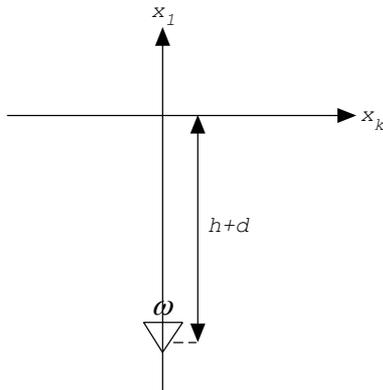for the stress functions, $\chi(x_1, x_2)$ and $\chi(x_1, x_3)$, substituted into formula (11), we get

$$W_1^{ar-d} = -\frac{D\omega b_l d}{2}(\langle g((x_2^0 - m \sin \varphi)/p)\rangle_m \cos^2 \varphi + \langle g((x_3^0 + m \cos \varphi)/p)\rangle_m \sin^2 \varphi) \tag{13}$$

where

$$g(t) = \sum_{n=-\infty}^{\infty} \left[\ln \frac{d^2 + p^2(t-n)^2}{(2h+d)^2 + p^2(t-n)^2} - \frac{4h(h+d)(2h+d)/d}{(2h+d)^2 + p^2(t-n)^2} \right]. \tag{14}$$

After summing in formula (14), we find

$$g(t) = \ln \frac{\cosh(2\pi d/p) - \cos(2\pi t)}{\cosh(2\pi(2h+d)/p) - \cos(2\pi t)}$$
$$- \frac{4\pi h(h+d)}{pd} \frac{\sinh(2\pi(2h+d)/p)}{\cosh(2\pi(2h+d)/p) - \cos(2\pi t)}. \tag{15}$$

Figure 4. A wedge disclination near the free surface of a semi-infinite solid.

The energy density of the misfit dislocation core is $W^c \approx Db^2/2$ [27]. With this taken into account, from formulae (3), (4), (7), and (13) we find the following criterion for the misfit dislocation generation to be energetically favourable:

$$\frac{b}{h}\left\{\ln\frac{2h-b}{b} + \frac{1}{2} - \frac{\omega d}{b}\operatorname{sgn}(b_l)[\langle g((x_2^0 - m\sin\varphi)/p)\rangle_m \cos^2\varphi\right.$$
$$\left. + \langle g((x_3^0 + m\cos\varphi)/p)\rangle_m \sin^2\varphi]\right\} < 8\pi(1+\nu)\operatorname{sgn}(b_l)f_e. \qquad (16)$$

5. Critical parameters of multilayered films deposited onto disclinated substrates

In order to reveal the ranges of parameters (appearing in formula (16)) at which the generation of the misfit dislocation at the substrate α/layer β boundary is energetically favourable, first let us consider the situation where the projection of the dislocation line on the disclination network plane is parallel to one of the disclination rows that form the network—that is, the situation with $\varphi = s\pi/2$, where $s = -1, 0, 1, 2$. In the situation discussed, $\langle g((x_2^0 - m\sin\varphi)/p)\rangle_m \cos^2\varphi = 0$, $\langle g((x_3^0 + m\cos\varphi)/p)\rangle_m \sin^2\varphi = g(x_3^0/p)$ for $\varphi = \pm\pi/2$; and $\langle g((x_2^0 - m\sin\varphi)/p)\rangle_m \cos^2\varphi = g(x_2^0/p)$, $\langle g((x_3^0 + m\cos\varphi)/p)\rangle_m \sin^2\varphi = 0$ for $\varphi = 0$ or π. In these circumstances, the ranges of the parameters f_e and h which correspond to the generation of the misfit dislocation are dependent on the displacement x_2^0 (or x_3^0) of the dislocation line relative to the disclination network. The displacements x_2^0 and x_3^0 will be calculated below from the condition that the energy density W_1^{ar-d} is minimum.

The dependences $g(x_k^0/p)$ ($k = 2$ or 3) are presented in figure 5 for various values of d/p and h/p. From figure 5 it follows that the maxima of the function $g(x_k^0/p)$ are located at the points $x_k^0 = (j + 1/2)p$ while their minima are located at the points $x_k^0 = \tilde{j}p$, where j and $\tilde{j}$ are integers, and[1] $k = 2$, for $\varphi = 0$ or $\varphi = \pi$, or $k = 3$, for $\varphi = \pm\pi/2$. As a corollary, the energy density W_1^{ar-d} has a minimum at $x_k^0 = (j + 1/2)p$, for $b_l = b$, and at $x_k^0 = \tilde{j}p$, for $b_l = -b$. With the two different sets of equations, $\{x_k^0 = p/2, b_l = b\}$ and $\{x_k^0 = 0, b_l = -b\}$ (where $k = 2$, if $\varphi = 0$ or $\varphi = \pi$, or $k = 3$, if $\varphi = \pm\pi/2$), substituted into formula (16), we find the two following formulae for the critical values of the misfit parameter:

$$8\pi(1+\nu)f_e^+ = \frac{b}{h}\left\{\ln\frac{2h-b}{b} + \frac{1}{2} + \frac{2\omega d}{b}\left[\ln\frac{\cosh\pi(2h+d)/p}{\cosh\pi d/p}\right.\right.$$
$$\left.\left. + \frac{2\pi h(h+d)}{pd}\tanh\pi(2h+d)/p\right]\right\} \qquad (17)$$

[1] The same result can be obtained from differentiation of formula (15)).
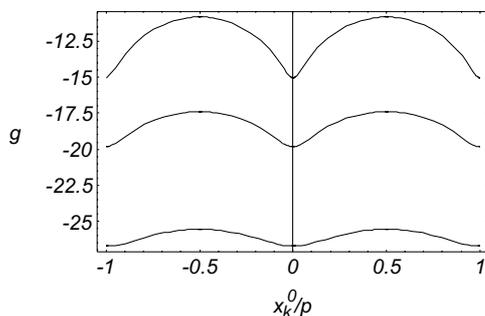
Figure 5. Dependences of g on x_k^0/p, for the following values of parameters: $d/p = 0.05$ and $h/p = 0.3$; $d/p = 0.1$ and $h/p = 0.5$; $d/p = 0.2$ and $h/p = 0.8$ (from top to bottom).

$$8\pi(1+\nu)f_e^- = \frac{b}{h}\left\{ -\ln\frac{2h-b}{b} - \frac{1}{2} + \frac{2\omega d}{b}\left[\ln\frac{\sinh\pi(2h+d)/p}{\sinh\pi d/p} \right.\right.$$

$$\left.\left. + \frac{2\pi h(h+d)}{pd}\coth\pi(2h+d)/p \right]\right\}. \tag{18}$$

Here f_e^+ is the critical (minimum) effective misfit parameter, such that the generation of the misfit dislocation with $b_l = b$ and $\varphi = s\pi/2$ is energetically favourable if $f_e > f_e^+$. f_e^- is the critical (maximum) effective misfit parameter, such that the generation of the misfit dislocation with $b_l = -b$ and $\varphi = s\pi/2$ is energetically favourable if $f_e < f_e^-$.

The dependences of $8\pi(1+\nu)f_e^+$ and $8\pi(1+\nu)f_e^-$ on h/b are shown in figure 6, for various values of the disclination strength ω. The generation of the misfit dislocation is energetically unfavourable in both the cases $b_l = b$ and $b_l = -b$ if $f_e^- < f_e^+$ and f_e lies in the range $f_e^- < f_e < f_e^+$. If $\omega > 0$, f_e^+ decreases and then increases with increase of the film thickness h. In this case, the misfit dislocation with $b_l = b$ is generated, if the film thickness h ranges from h_{c1} to h_{c2}, for $f_e > f_0$ (where f_0 is the minimum value of the function $f_e^+(h/b)$), and is not generated at any value of the film thickness for $f_e < f_0$. The dependences $f_e^+(h/b)$ are qualitatively similar to the dependences of the critical misfit parameter on the film thickness in the case with film/substrate composites of wire form [26]. This similarity can be related to the curvature of the composites that exists due to disclinations in the case considered in this paper and due to cylindrical geometry in the case of wire composites.

Now let us examine the conditions of the misfit dislocation generation at the layer β/layer γ boundary closest to the substrate α/layer β boundary (figure 2(b)). In doing so, first let us consider the situation where the projection of the misfit dislocation on the disclination network plane is parallel to one of the disclination rows that form the network. In the situation discussed, the energy densities W_2^d, W_2^{f-d}, and W_2^{ar-d} (appearing in inequality (3)) are calculated in the same way as the energy densities W_1^d, W_1^{f-d}, and W_1^{ar-d} (see above). With this taken into account, after some algebra we find the following formulae for the critical values of the effective misfit parameter:

$$8\pi(1+\nu)\tilde{f}_e^+ = 8\pi(1+\nu)f_1\frac{t_1}{h} + \frac{b}{h}\left\{ \ln\frac{2(h-t_1)-b}{b} + \frac{1}{2} \right.$$

$$+ \frac{2\omega d}{b}\left[\frac{t_1+d}{d}\ln\frac{\cosh\pi(2h+d-t_1)/p}{\cosh\pi(t_1+d)/p} \right.$$

$$\left.\left. + \frac{2\pi(h-t_1)(h+d)}{pd}\tanh\pi(2h+d-t_1)/p \right]\right\} \tag{19}$$

$$8\pi(1+\nu)\tilde{f}_e^- = 8\pi(1+\nu)f_1\frac{t_1}{h} + \frac{b}{h}\left\{ -\ln\frac{2(h-t_1)-b}{b} - \frac{1}{2} \right.$$

$$+ \frac{2\omega d}{b}\left[\frac{t_1+d}{d}\ln\frac{\sinh\pi(2h+d-t_1)/p}{\sinh\pi(t_1+d)/p} \right.$$

$$\left.\left. + \frac{2\pi(h-t_1)(h+d)}{pd}\coth\pi(2h+d-t_1)/p \right]\right\}. \tag{20}$$

Here $\tilde{f}_e^+$ and $\tilde{f}_e^-$ are defined as the critical misfit parameters that characterize the misfit dislocation generation at the layer β/layer γ boundary in the same way as f_e^+ and f_e^-, respectively (see above).

In figure 6 the states of the composite are shown using the coordinates $(h/b, 8\pi(1+\nu)f_e)$ for various values of the disclination strength ω. Generation of the misfit dislocation is energetically unfavourable at the layer β/layer γ boundary in both the cases $b_l = b$ and $b_l = -b$ if $\tilde{f}_e^-(h/b) < \tilde{f}_e^+(h/b)$ and $\tilde{f}_e^-(h/b) < f_e < \tilde{f}_e^+(h/b)$. The misfit dislocation

(a)

(b)

(c)
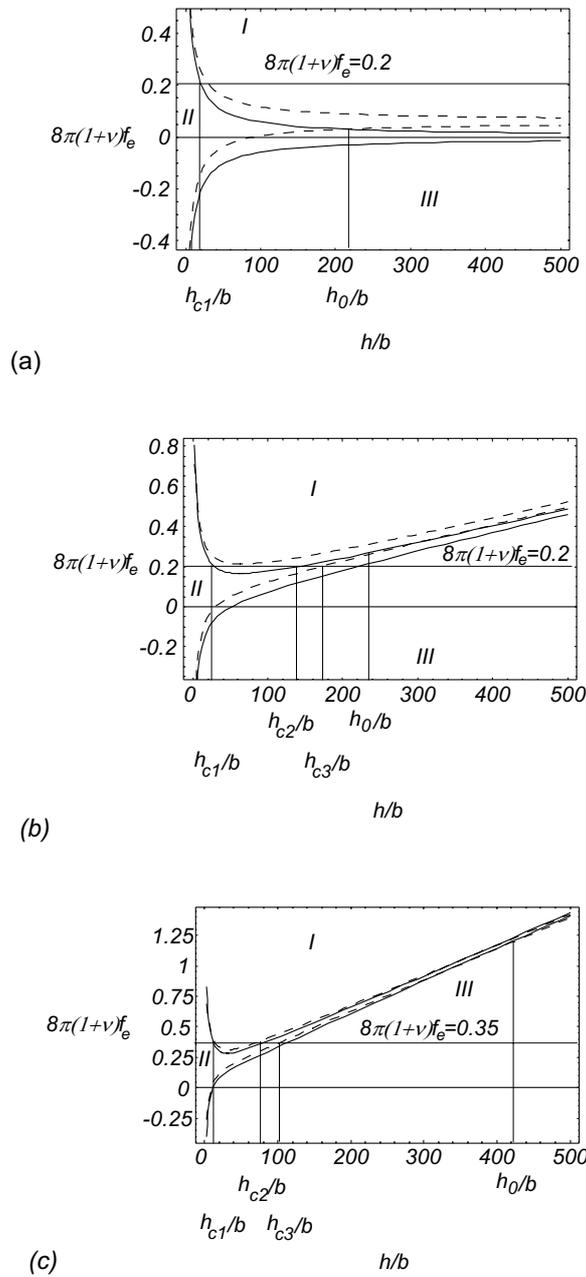
Figure 6. Diagrams of states of a composite with coordinates $(h/b, 8\pi(1+\nu)f_e)$ in the situation where the Burgers vector of the misfit dislocation is parallel to a disclination row, for $d = 20b$, $p = 250b$, $8\pi(1+\nu)f_1 = 0.3$, $t_1 = h/5$; with disclination strength (a) $\omega = 0$, (b) $\omega = 1°$, and (c) $\omega = 3°$. The upper and lower solid curves correspond to f_e^+ and f_e^-, respectively. The upper and lower dashed curves correspond to $\tilde{f}_e^+$ and $\tilde{f}_e^-$, respectively.

generation is energetically unfavourable at both the substrate/layer β and layer β/layer γ boundaries if $\tilde{f}_e^-(h/b) < f_e < f_e^+(h/b)$ (region II in figure 6). Generation of the misfit

dislocation with $b_l = b$ is energetically favourable at $f_e > f_e^+(h/b)$ (region I in figure 6), while generation of the misfit dislocation with $b_l = -b$ occurs as an energetically favourable process at $f_e < \tilde{f}_e^-(h/b)$ (region III in figure 6).

From figure 6 it follows that misfit dislocations can be generated at any value of the effective misfit parameter f_e if the film thickness h exceeds some critical value h_0 ($h > h_0$). For $\omega = 0$ (disclinations are absent in the substrate) (figure 6(a)), the generation of misfit dislocations at interphase boundaries of both types (α/β and β/γ) is energetically unfavourable if $h > h_{c1}(f_e)$. Here h_{c1} is the critical film thickness which can be found (at $\omega = 0$) from one of the following conditions: $f_e^+(h_{c1}/b) = f_e$ or $f_e^-(h+c1/b) = f_e$. For $\omega = 0$, h_{c1} decreases as $|f_e|$ increases. In the situation with $\omega > 0$ (figures 6(b) and 6(c)) generation of misfit dislocations is energetically favourable (i) within the interval $h < h_{c1}(f_e)$ only if $f_e < f_0$ or $f_e > f_e^+(h_0/b)$; and (ii) within the intervals $h < h_{c1}$ and $h_{c2} < h < h_{c3}$ if $f_0 < f_e < f_e^+(h_0/b)$ (see figures 6(b) and 6(c)). The critical thickness h_{c1} increases, then (at $f_e = f_0$) abruptly decreases, and then slowly decreases with growth of the effective misfit parameter f_e. The region II of parameters at which misfit dislocation generation is energetically unfavourable shifts to large values of f_e as the disclination strength ω increases (figures 6(b) and 6(c)). That means that formation of disclinations in plastically deformed substrates hampers generation of MDs in multilayered films characterized by large values of the effective misfit parameter. This is interesting in view of the growing technological needs for film/substrate composites with large misfits.

In figure 7 the states of the system are shown with the coordinates $(h/b, 8\pi(1+\nu)f_e)$, for various values of the parameters d and p. Generation of MDs with $b_l = +b$ is energetically favourable provided that $f_e > f_e^+(h/b)$ (region I in figure 7). Generation of MDs with $b_l = -b$ is energetically favourable at $f_e < \tilde{f}_e^-(h/b)$ (region III in figure 7). Generation of MDs is energetically unfavourable at $\tilde{f}_e^-(h/b) < f_e < f_e^+(h/b)$ (region II in figure 7). As the spacing p between disclinations decreases and/or distance d between disclinations and the substrate free surface increases, region II in the state diagram (figure 7) shifts to large values of the effective misfit parameter f_e.

Now let us consider the situation where the projection of the MD line on the plane of the disclination network is not parallel to either of the two disclination rows—that is, $\varphi \neq n\pi/2$, with n being integer. In order to analyse this situation, we need to calculate the quantities $\langle g(x_2^0 - m\sin\varphi)\rangle_m$ and $\langle g(x_3^0 + m\cos\varphi)\rangle_m$ appearing in formula (16). With periodicity of the function $g(t)$ as well as the conditions $\sin\varphi \neq 0$ and $\cos\varphi \neq 0$ taken into account, we find

$$\langle g(x_2^0 - m\sin\varphi)\rangle_m = \langle g(x_3^0 + m\cos\varphi)\rangle_m = \langle g(t)\rangle_t = \frac{1}{2\pi}\int_{-\pi}^{\pi} g(t)\,dt. \quad (21)$$

After integration in (21), we get

$$\langle g(x_2^0 - m\sin\varphi)\rangle_m = \langle g(x_3^0 + m\cos\varphi)\rangle_m = -\frac{4\pi h(h+2d)}{pd}. \quad (22)$$

With (22) substituted into (16), we have two equations: the first one is for the minimum value $f_e'^+$ of the effective misfit parameter f_e, that corresponds to energetically favourable generation of the MD with $b_l = +b$ and $\varphi \neq n\pi/2$; and the second one is for the maximum value $f_e'^-$ of the effective misfit parameter, that corresponds to energetically favourable generation of the MD with $b_l = -b$ and $\varphi \neq n\pi/2$:

$$8\pi(1+\nu)f_e'^+ = \frac{b}{h}\left(\ln\frac{2h-b}{b} + \frac{1}{2} + \frac{4\pi\omega h(h+2d)}{bp}\right) \quad (23)$$

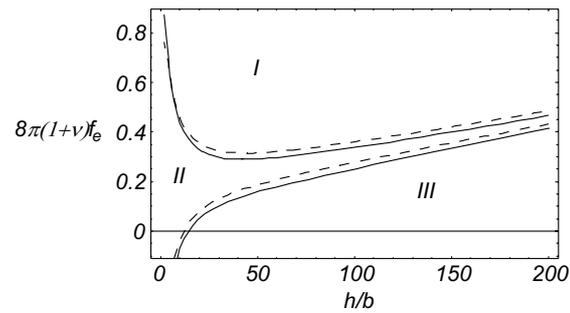$$8\pi(1+\nu)f_e'^- = \frac{b}{h}\left(-\ln\frac{2h-b}{b} - \frac{1}{2} + \frac{4\pi\omega h(h+2d)}{bp}\right). \quad (24)$$
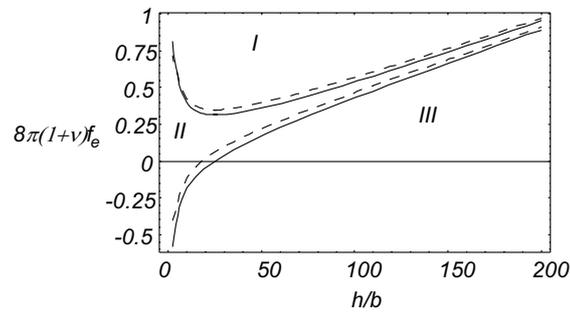
(a)
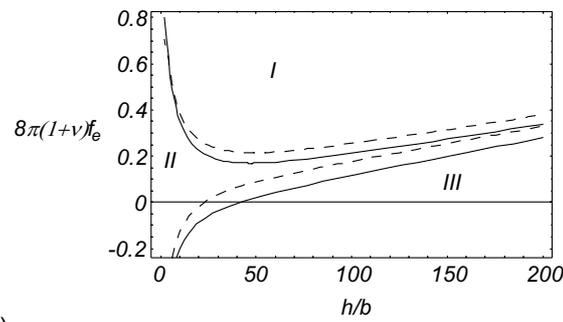
(b)

(c)

Figure 7. Diagrams of states of a composite with coordinates $(h/b, 8\pi(1 + \nu)f_e)$ in the situation where the Burgers vector of the misfit dislocation is parallel to a disclination row, for the following values of parameters: $\omega = 2°$, $8\pi(1+\nu)f_1 = 0.3$, $t_1 = h/5$, and (a) $d = 5b$, $p = 100b$; (b) $d = 5b$, $p = 300b$; (c) $d = 50b$, $p = 300b$. The upper and lower dashed curves correspond to $\tilde{f}_e^+$ and $\tilde{f}_e^-$, respectively.

The formulae for the critical (maximum and minimum) misfit parameters $\tilde{f}_e'^{+}$ and $\tilde{f}_e'^{-}$ that characterize energetically favourable generation of the MD at the layer β/layer γ boundary

are derived in the same way as formulae (23) and (24). These formulae are as follows:

$$8\pi(1+\nu)\tilde{f}_e'^{+} = 8\pi(1+\nu)f_1\frac{t_1}{h} + \frac{b}{h}\left(\ln\frac{2(h-t_1)-b}{b} + \frac{1}{2} + \frac{4\pi\omega(h-t_1)(h+2d+t_1)}{bp}\right)$$
(25)

$$8\pi(1+\nu)\tilde{f}_e'^{-} = 8\pi(1+\nu)f_1\frac{t_1}{h} + \frac{b}{h}\left(-\ln\frac{2(h-t_1)-b}{b} - \frac{1}{2} + \frac{4\pi\omega(h-t_1)(h+2d+t_1)}{bp}\right).$$
(26)

From formulae (25) and (26) it follows that the curves for $f_e'^{+}$, $f_e'^{-}$, $\tilde{f}_e'^{+}$, and $\tilde{f}_e'^{-}$ shift to large values of f_e if ω or d increases and/or p decreases.

In figure 8 the states of the composite are shown in the situation where the crystallography of the composite admits generation of MDs with Burgers vectors that can be either parallel or not parallel to disclination rows in the substrate. As follows from figure 8, the parameter regions of MD generation do not significantly depend on the orientation of MD Burgers vectors relative to the disclination rows. As ω grows, the region $\tilde{f}_e^{-} < f_e < \max\{f_e^{+}, f_e'^{+}\}$ (where generation of the MD with an arbitrarily oriented line is energetically unfavourable) shrinks and shifts to large values of f_e.

6. Discussion and concluding remarks

Here we have suggested a first-approximation model of plastically deformed substrates such as those containing disclination defects that terminate deformation-induced dislocation walls (figure 1). In the framework of the model suggested, we have theoretically examined the generation of MDs (defects that, in part, accommodate the misfit stresses) in multilayered films on disclinated substrates. The results of our quantitative examinations are in short as follows:

(i) Generation of MDs is energetically favourable in multilayered films on disclinated substrates when their parameters are in certain ranges (calculated above; see figures 6 to 8) that are different from the parameter ranges in the commonly studied situation with disclination-free substrates. In particular, as the disclination strength ω grows, the range of parameters at which generation of MDs is energetically unfavourable shrinks and shifts to large values of the effective misfit parameter $f_e = (f_1t_1 + f_2t_2)/(t_1 + t_2)$. This means that formation of disclinations in plastically deformed substrates hampers generation of MDs in multilayered film/substrate composites characterized by large values of the effective misfit parameter.

(ii) The set of parameters crucially affecting the generation of MDs in multilayered composite films on disclinated substrates contains the disclination strength ω, the spacing p between disclinations, the distance d between disclinations and the film/substrate boundary, the layer thicknesses t_1 and t_2, and the misfit parameters f_1 and f_2.

These results are important for technological applications of multilayered film/substrate composites. In particular, point (i) is worth noting in relation to a technologically interesting possibility for exploiting plastically deformed substrates in fabrication of multilayered film/substrate composites. Indeed, the coherency of interphase boundaries is often desired from an applications viewpoint. In these circumstances, in order to exploit highly functional properties of multilayered film/substrate composites with coherent interphase boundaries, predeformation of substrates that creates dislocation walls in substrates can be effective.

The model of multilayered films on plastically deformed substrates, elaborated in this paper, uses assumptions that simplify our analysis of the generation of MDs in such films. In
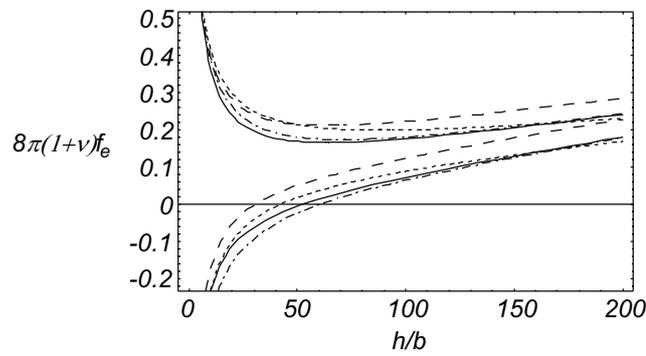
(a)
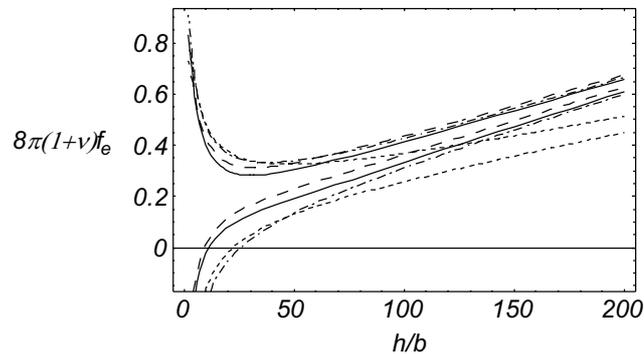
(b)

Figure 8. Diagrams of states of a composite with coordinates $(h/b, 8\pi(1 + \nu) f_e)$ in the situation where the misfit dislocation line is arbitrarily oriented relative to the disclination rows in the substrate, for $d = 20b$, $p = 250b$, $8\pi(1 + \nu) f_1 = 0.3$, $t_1 = h/5$, and (a) $\omega = 1°$, (b) $\omega = 3°$. The upper and lower solid curves correspond to f_e^+ and f_e^-, respectively. The upper and lower long-dashed curves correspond to $\tilde{f}_e^+$ and $\tilde{f}_e^-$, respectively. The upper and lower dotted curves correspond to $f_e'^+$ and $f_e'^-$, respectively. The upper and lower short-dashed curves correspond to $\tilde{f}_e'^+$ and $\tilde{f}_e'^-$, respectively.

particular, deformation-induced sub-boundary patterns in substrates have been assumed to be regular, whereas sub-boundary patterns with disorder are formed in real materials under plastic deformation [28, 32]. The disorder in spatial arrangement of sub-boundaries and, therefore, disclinations modifies slightly the conditions for the energetically favourable generation of MDs in local regions of multilayered films which have been found in this paper. That is, there are local regions in a real multilayered film where the generation of MDs is slightly facilitated or hampered, compared to the model situation (figure 1) with regular distribution of dislocations. The difference discussed here between real and model systems is standard in the theory of defects in heteroepitaxial systems. For example, the formation of MDs at film/substrate boundaries in conventional heteroepitaxial systems depends on many factors

(relief of the film free surface, distribution of pre-existent dislocations in a substrate, etc) which are not taken into account in theoretical models that commonly deal with the averaged and technologically controlled characteristics (the mean film thickness and misfit parameter) of heteroepitaxial systems; see, e.g., the reviews [7, 9, 21]. Although the theoretical model suggested in this paper does not take into consideration the disorder in spatial arrangement of deformation-induced sub-boundaries, its results allow one to estimate in the first approximation the influence of pre-deformation of substrates on the formation of MDs in multilayered films deposited onto the deformed substrates. These results could be used in further, more detailed theoretical and experimental examinations of multilayered films.

Of particular interest for further investigations are the specific structural and behavioural features of MDs in composite films with alternating nanoscale layers deposited onto plastically deformed substrates, because such nanoscale layered films exhibit outstanding properties widely used in applications. In order to effectively model the behaviour of MDs in nanoscale films on deformed substrates, one should take into account the effects of dislocation cores (see, e.g., [33–35]), their possible splitting (see, e.g., [22, 36–38]), and amorphization at interphase boundaries (see, e.g., [39, 40]). Such effects play an important role in the films and layered composites with vanishingly small film/layer thickness, where the dislocation core diameter and the interphase boundary thickness are close to the film/layer thickness. A theoretical description of the peculiarities of MDs in nanoscale layered films on plastically deformed substrates will be a subject of our future investigations.

In this paper the theoretical analysis has been focused on multilayered composite films consisting of alternating single-crystalline layers. However, the results of our consideration can also be used for a first-approximation description of multilayered films with nanocrystalline (nanograined) layers of alternating composition deposited onto plastically deformed substrates. In particular, plastic deformation of substrates is intrinsic in thermal spray synthesis of nanocrystalline films, which consists in heating and accelerating solid particles by injecting them into a hot gas stream, then impacting them onto a substrate to form a coating [41–43].

The quantitative results obtained in this paper are approximate. However, they can be used, on the one hand, in estimating the structural stability and stability of functional properties of real multilayered film/substrate composites and, on the other hand, as a basis for further investigations of such composites.

Acknowledgments

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