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Misfit Disclination Structures in Nanocrystalline and Polycrystalline Films

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Abstract A new physical mechanism for relaxation of misfit stresses in nanocrystalline and polycrystalline films is theoretically examined. The mechanism deals with the formation of misfit disclinations at interphase (film/substrate) and intergrain (between nanograins) boundaries. Characteristics (stored elastic energy, equilibrium residual strain, and critical thickness) of films with misfit disclinations are investigated. It is shown that the formation of misfit disclinations is energetically favorable, in the film thickness ranges from 0 to some optimum value h_0.

1. Introduction

Solid films exhibit the functional properties widely exploited in contemporary high technologies; see, *e.g.*, [1-3]. The properties of films are strongly influenced by misfit stresses generated due to geometric mismatch between crystalline lattices of films and substrates.

The most effective channel for relaxation of misfit stresses in conventional single crystalline films is the generation of misfit dislocations that form dislocation rows at interphase (film/substrate) boundaries; see, *e.g.*, [4-23]. Stress fields of misfit dislocations partly compensate misfit stresses; this often improves functional characteristics of films. However, in the situation discussed misfit dislocation cores are located at interphase boundaries, violating the ideal structure of interphase boundaries and causing degradation of their functional properties.

Recently, a new micromechanism for relaxation of misfit stresses, namely the formation of misfit disclinations (defects of the rotational type) has been suggested [24-29] as an alternative to the conventional formation of misfit dislocation rows. This micromechanism is theoretically revealed as that capable of effectively contributing to relaxation of misfit stresses in crystalline films with twin boundaries [24,25], crystalline films deposited on amorphous substrates [26,27] as well as nanocrystalline and polycrystalline films (Fig. 1) [27-29]. Owing to the presence of the grain boundary phase in nanocrystalline and polycrystalline films, namely grain boundary disclinations play the role as misfit disclinations in such films (Fig. 1). The specific feature of

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the disclination micromechanism for relaxation of misfit stresses in nanocrystalline and polycrystalline films is that cores of grain boundary disclinations playing the role as misfit defects are located at existent grain boundaries (either at boundaries in film interior or at junctions of interphase and grain boundaries) and, do not induce any extra violations to the structure of the film/substrate interface.

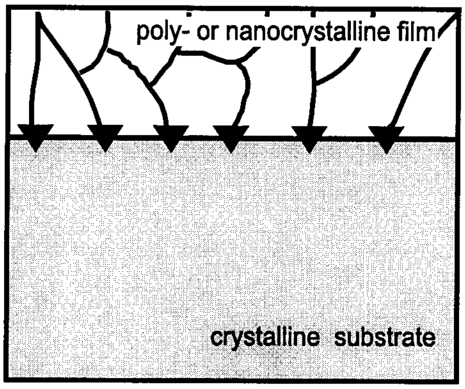

Figure 1. Misfit disclinations at junctions of film/substrate interface and grain boundaries in nanocrystalline (or polycrystalline) film.

The disclination micromechanism for relaxation of misfit stresses is of particular importance in nanocrystalline films, because of the fact that grain boundary disclinations can be intensively generated in nanocrystalline materials synthesized at highly non-equilibrium conditions (see, *e.g.*, [30]) and because of extremely high volume fraction of the grain boundary phase in nanocrystalline films. A theoretical description of grain boundary disclinations as misfit defects of a new type in nanocrystalline and polycrystalline films is in its infancy. Papers [27-29] just briefly discussed the key aspects of relaxation of misfit stresses via the formation of grain boundary disclinations in nanocrystalline and polycrystalline films. Papers [24-26] focused on some partial cases related to disclination configurations (dipoles, quadropoles, *etc.*) with self-screened stress fields in crystalline films with twin boundaries and crystalline films deposited on amorphous substrates. The aim of the present paper is to theoretically examine in detail the basic characteristics and the behavioral features of nanocrystalline and polycrystalline films with rows of misfit disclinations located at film/substrate interfaces (Fig. 1).

2. Model of Film/Substrate Boundary with Misfit Disclinations

Consider an interface between a nanocrystalline or polycrystalline film and a single crystalline substrate. In the chosen geometry the film is located in the area $-h \le x \le 0, -\infty < y < \infty, -\infty < z < \infty$, and the substrate is defined by $-\infty < x < -h, -\infty < y < \infty, -\infty < z < \infty$ (see Fig. 2). Any real interface between a nanocrystalline or polycrystalline film and a single crystalline substrate consists of many fragments each dividing the substrate and a grain of the film (Fig. 1). Different fragments of the interface are characterized by different misorientation parameters, in which case the interface serves as a source of spatially inhomogeneous stress fields associated with a spatially inhomogeneous distribution of its misorientation along

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the interface plane. In general, some fragments of the interface can be incoherent due to their "unfavorable" misorientation destroying the coherency of the interface [29].

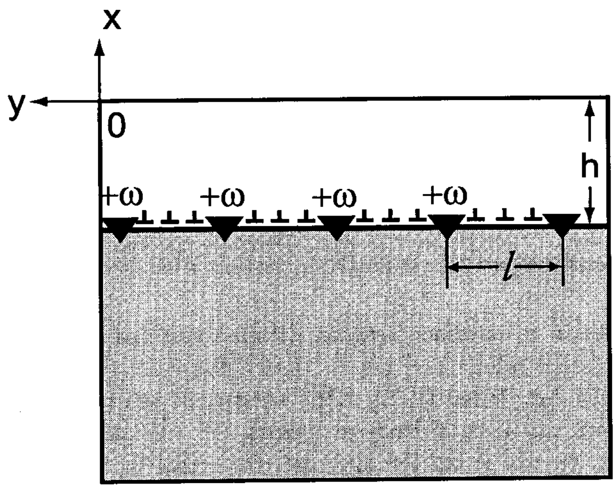

Figure 2. Schematic for film/substrate interface with coherency edge dislocations and misfit wedge disclinations $+\omega$.

The main subject of this paper – the disclination micromechanism for relaxation of misfit stresses – is related to the role of interfaces as spatially homogeneous sources of misfit stresses generated due to the geometric mismatch between lattice parameters of the adjacent crystalline phases. With this taken into account, in order to distinguish the effects associated with misfit stresses, in this paper we will not consider any aspects related to spatially inhomogeneous distributions of misorientation that characterize interfaces between nanocrystalline or polycrystalline films and single crystalline substrates. In doing so, here and in the following we will focus our consideration on a model of interface as a semi-coherent interface which induces misfit stresses and contains misfit disclinations at junctions of grain boundaries and the interface (Fig. 2).

In the framework of our model, the interface as a source of misfit stresses is characterized by one-dimensional misfit (lattice mismatch) parameter

$$f = \frac{|a_2 - a_1|}{a_2}, \tag{1}$$

where a_1 denotes the substrate lattice parameter and a_2 the film lattice parameter. Here and in the following, the elastic strains (and other elastic fields, for example, misfit stresses) associated with the lattice mismatch are modeled as those induced by continuously distributed edge dislocations (as it is shown in Fig. 2) having infinitesimal Burgers vectors $\mathbf{db_c}$. These dislocations are known as coherency dislocations (CDs), *e.g.*, [31]. The misfit parameter f is related to CD linear density ρ_c and the magnitude of CD Burgers vector as follows:

$$\rho_c db_c = f, \tag{2}$$

It is well established that the relaxation of misfit stresses (and the corresponding diminishing of stored elastic energy) may be achieved as a result of the formation of misfit dislocations(MDs) at film/substrate interface, *e.g.*, [4-23]. In this paper, following [27-29], we

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consider misfit disclinations (MDDs) as the defects responsible for misfit stress compensation. In the first approximation, MDDs are modeled as wedge disclinations (with strength ω) that are periodically distributed along film/substrate interface, as it is schematically shown in Fig. 2. For definiteness it, it also assumed that $a_2 > a_1$ and initial misfit stresses in the film are compressive. This also dictates the positive sign for misfit wedge disclinations, *e.g.* $+\omega$. In the framework of our model, the disclination strength ω (accepted to be identical for all MDDs) serves as an important parameter of MDD array. In contrast to conventional situation with MDs whose Burgers vectors are quantized (they are strictly related to film lattice parameter), the disclination strength ω can change its magnitude to permit more flexible conditions for misfit stress relaxation.

3. Plastic Distortion of Coherent Dislocations and Wedge Disclinations

In our considerations an interface between a nanocrystalline or polycrystalline film and a single crystalline substrate cab be modeled as the interphase boundary containing defects of the two types: periodically distributed MDDs of the wedge type and CDs, continuously distributed edge dislocations with infinitesimal Burgers vectors. To calculate the elastic energy of such interphase boundary, we will apply the approach developed by Mura [32]. This approach is based on the concept of plastic distortion, which can be associated with any defect in elasto-plastic continuum. In this section we will obtain the plastic distortions for CD row distributed over the period l and for a single wedge disclination [1].

According to Mura [32] one can represent the plastic distortion for any isolated dislocation-disclination defect as follows:

$$\beta^*_{ij} = \delta_i(S)[-b_j - e_{jpq}\omega_p(x_q - x^0_q)], \tag{3}$$

where $\delta_i(S)$ denotes the three dimensional delta-function on the surface S ("i" is the index of the surface normal); $[-b_j]$ is the relative translation of the faces of this surface after cutting along it; $[-e_{jpq}\omega_p(x_q - x^0_q)]$ is the relative rotation of S-cut-faces ; e_{jpq} is the unit anti symmetrical tensor; ω_p is the Frank's pseudo vector of disclination; and x^0_q is the position of the rotation axis.

We consider a probe CD with Burgers vector $-db_c\mathbf{e}_y$, which is located at the point $(0, y_0)$, and choose the cut surface as a section $-h \le x \le 0, y = y_0$ of a plane parallel to ZOX plane with normal $\mathbf{n} = \mathbf{e}_y$. In this case the plastic distortion of a CD is as follows:

$$\beta^{*(c,0)}_{yy} = \delta_y(S)db_c, \tag{4}$$

where

$$\delta_y(S) = \int_{-\infty}^{+\infty}\int_{-h}^{0} \delta(x - x')\delta(y - y_0)\delta(z - z')dx'dz', \tag{5}$$

From Eq. (4) we obtain the plastic distortion for a single CD as follows:

$$\beta^{*(c,0)}_{yy} = db_c\delta(y - y_0)H(x + h), x \le 0, \tag{6}$$

where $H(x + h)$ is the Heaviside's function. For the row of CDs continuously distributed on the interphase boundary fragment of length (period) l, we get:

$$\beta^{*(c)}_{yy} = \int_0^l \rho_c\beta^{*(c,0)}_{yy}dy_0 = f \cdot H(x + h)\left\{\begin{array}{ll} 0, & y < 0 \\ 1, & 0 \le y \le l \\ 0, & l < y \end{array}\right\}, x \le 0 \tag{7}$$

[1]"Single" - because we are interested in the elastic energy per surface area YZ taking into account the periodicity of MDD row.

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The formulas for MDD plastic distortion can be derived from the general Equation (3) with the assumption that cut-surface is parallel with ZOX plane. For a single misfit disclination with strength ω and coordinates $(-h, 0)$, one can find the following non-zero components of plastic distortion tensor:

$$\beta^{*\omega}_{yy} = \delta_y(S)[-e_{yzx}\omega(x+h)] \tag{8}$$

and

$$\beta^{*\omega}_{yx} = \delta_y(S)[-e_{xzy}\omega y] \tag{9}$$

which finally can be transformed into:

$$\beta^{*\omega}_{yy} = -\omega(x+h)\delta(y)H(x+h), x \leq 0, \tag{10}$$

$$\beta^{*\omega}_{yx} = \omega y\delta(y)H(x+h) = 0. \tag{11}$$

To define the elastic energy associated with the interface containing MDDs we should use the plastic distortion of all defects located within the period l (Fig. 1) and elastic stresses of the defect system as a whole. This is the subject of the following sections.

4. Stresses of Coherent Dislocations and Periodic Array of Misfit Disclinations

The stress field of the array of continuously distrubuted CDs may be derived by integrating the stress field of a single edge dislocation placed near a free surface, *e.g.*, [33]. Using Eq. (2) we find the following non-zero components of misfit stresses:

$$\sigma^{(c)}_{yy} = -\frac{2fG}{1-\nu}H(x+h), x \leq 0, \tag{12}$$

$$\sigma^{(c)}_{zz} = -\frac{2fG\nu}{1-\nu}H(x+h), x \leq 0, \tag{13}$$

where f denotes the misfit parameter; G is the shear modulus; ν is the Poisson ratio, H(x+h) is the Heaviside's function.

The stress field of a single positive wedge disclination having coordinates $(-h, 0, z)$ (see Fig. 2) is [34]:

$$\sigma^{\omega}_{xx} = D\omega\left[\ln\frac{r_+}{r_-} + \frac{y^2}{r_+^2} - \frac{y^2}{r_-^2} + \frac{2xh(y^2-(x-h)^2)}{r_-^4}\right], \tag{14}$$

$$\sigma^{\omega}_{yy} = D\omega\left[\ln\frac{r_+}{r_-} + \frac{(x+h)^2}{r_+^2} - \frac{(x-h)^2}{r_-^2} + \frac{2h((x-h)^2(2h-x)+2y^2h-3y^2x)}{r_-^4}\right], \tag{15}$$

$$\sigma^{\omega}_{zz} = \nu(\sigma^{\omega}_{xx} + \sigma^{\omega}_{yy}), \tag{16}$$

$$\sigma^{\omega}_{xy} = D\omega\left[-\frac{(x+h)y}{r_+^2} + \frac{(x-h)y}{r_-^2} + \frac{2yh(h^2+y^2-x^2)}{r_-^4}\right]. \tag{17}$$

Here $D = \dfrac{G}{2\pi(1-\nu)}$, G is the shear modulus, ω is the disclination strength, $r_+^2 = (x+h)^2 + y^2$, $r_-^2 = (x-h)^2 + y^2$, h is the distance between disclination and free surface.

The stress field of the periodic disclination array is calculated by summing the contributions of infinite number of MDDs and has the following simple form:

$$\sigma^{\Sigma\omega}_{xx} = D\omega\left[\frac{1}{2}\ln\frac{\cosh 2\pi(\tilde{x}+\tilde{h}) - \cos 2\pi\tilde{y}}{\cosh 2\pi(\tilde{x}-\tilde{h}) - \cos 2\pi\tilde{y}} - \pi(\tilde{x}+\tilde{h})\frac{\sinh 2\pi(\tilde{x}+\tilde{h})}{\cosh 2\pi(\tilde{x}+\tilde{h}) - \cos 2\pi\tilde{y}} + \right.$$

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$$\pi(\tilde{x}-\tilde{h})\frac{\sinh 2\pi(\tilde{x}-\tilde{h})}{\cosh 2\pi(\tilde{x}-\tilde{h})-\cos 2\pi\tilde{y}}+4\pi^2\tilde{x}\tilde{h}\frac{1-\cosh 2\pi(\tilde{x}-\tilde{h})\cos 2\pi\tilde{y}}{(\cosh 2\pi(\tilde{x}-\tilde{h})-\cos 2\pi\tilde{y})^2}\Bigg], \quad (18)$$

$$\sigma_{yy}^{\Sigma\omega}=D\omega\left[\frac{1}{2}\ln\frac{\cosh 2\pi(\tilde{x}+\tilde{h})-\cos 2\pi\tilde{y}}{\cosh 2\pi(\tilde{x}-\tilde{h})-\cos 2\pi\tilde{y}}+\pi(\tilde{x}+\tilde{h})\frac{\sinh 2\pi(\tilde{x}+\tilde{h})}{\cosh 2\pi(\tilde{x}+\tilde{h})-\cos 2\pi\tilde{y}}-\right.$$

$$\pi(\tilde{x}+3\tilde{h})\frac{\sinh 2\pi(\tilde{x}-\tilde{h})}{\cosh 2\pi(\tilde{x}-\tilde{h})-\cos 2\pi\tilde{y}}-4\pi^2\tilde{x}\tilde{h}\frac{1-\cosh 2\pi(\tilde{x}-\tilde{h})\cos 2\pi\tilde{y}}{(\cosh 2\pi(\tilde{x}-\tilde{h})-\cos 2\pi\tilde{y})^2}\Bigg], \quad (19)$$

$$\sigma_{xy}^{\Sigma\omega}=D\omega\left[-\pi(\tilde{x}+\tilde{h})\frac{\sin 2\pi\tilde{y}}{\cosh 2\pi(\tilde{x}+\tilde{h})-\cos 2\pi\tilde{y}}+\right.$$

$$\pi(\tilde{x}+\tilde{h})\frac{\sin 2\pi\tilde{y}}{\cosh 2\pi(\tilde{x}-\tilde{h})-\cos 2\pi\tilde{y}}-4\pi^2\tilde{x}\tilde{h}\frac{\sinh 2\pi(\tilde{x}-\tilde{h})\sin 2\pi\tilde{y}}{(\cosh 2\pi(\tilde{x}-\tilde{h})-\cos 2\pi\tilde{y})^2}\Bigg], \quad (20)$$

$$\sigma_{zz}^{\Sigma\omega}=D\omega\nu\left[\ln\frac{\cosh 2\pi(\tilde{x}+\tilde{h})-\cos 2\pi\tilde{y}}{\cosh 2\pi(\tilde{x}-\tilde{h})-\cos 2\pi\tilde{y}}-4\pi\tilde{h}\frac{\sinh 2\pi(\tilde{x}-\tilde{h})}{\cosh 2\pi(\tilde{x}-\tilde{h})-\cos 2\pi\tilde{y}}\right]. \quad (21)$$

Here $\tilde{x}=\frac{x}{l}, \tilde{y}=\frac{y}{l}, \tilde{h}=\frac{h}{l}$, and l is the period of the disclination row.

5. Elastic Energy of Interphase Boundary with Misfit Disclinations

In the framework of Mura's approach [32], the elastic energy associated with the distribution of defects in some material volume V (excluding the contribution of their cores) is approximately as follows:

$$\mathcal{E}=-\frac{1}{2}\int_{V^*}\beta_{kl}^*\cdot\sigma_{kl}dV, \quad (22)$$

where V^* denotes the material volume without core regions of the defects.

From Eqs. (7) and (10) to (17) it follows the expression for the elastic energy E (per unit of the interface area) of the film/substrate interface:

$$E=-\frac{1}{2l}\int_{-\infty}^{0}dx\int_0^l(\beta_{yy}^{*(c)}+\beta_{yy}^{*\omega})(\sigma_{yy}^{(c)}+\sigma_{yy}^{\Sigma\omega})dy. \quad (23)$$

On the other hand, the total energy of the system may be calculated as the sum of three components:

$$\mathcal{E}=\mathcal{E}^{\Sigma\omega}+\mathcal{W}+\mathcal{E}^f, \quad (24)$$

where $\mathcal{E}^{\Sigma\omega}$ is the energy of the disclination array; $\mathcal{W}$ is the energy of dislocation-disclination interaction; and $\mathcal{E}^f$ is the energy of CDs (or, in other words, the elastic energy associated with lattice mismatch). In context of this paper, we are interested mainly in the energy release due to the formation of MDD array, which can be defined as:

$$\Delta\mathcal{E}=\mathcal{E}-\mathcal{E}^f \qquad \text{or} \qquad \Delta E=E-E^f. \quad (25)$$

After some algebra by using the obtained formulas for defect plastic distortions and elastic stresses, we find the formula for the energy release ΔE (per unit of the interface area):

$$\Delta E=\frac{G}{4\pi(1-\nu)}\omega^2 l\Phi(\frac{h}{l})-\frac{G}{(1-\nu)}\omega f\frac{h^2}{l}, \quad (26)$$

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where G is the shear modulus, ν is the Poisson ratio, ω is the disclination strength, f is the misfit parameter, h denotes the film thickness, l is the distance (period) between disclinations in the array,

$$\Phi = \int_{-\tilde{h}}^{0} \left[\frac{1}{2}\ln\frac{\cosh 2\pi(\tilde{x}+\tilde{h})-1}{\cosh 2\pi(\tilde{x}-\tilde{h})-1} + \pi(\tilde{x}+\tilde{h})\frac{\sinh 2\pi(\tilde{x}+\tilde{h})}{\cosh 2\pi(\tilde{x}+\tilde{h})-1} - \right.$$

$$\left. \pi(\tilde{x}+3\tilde{h})\frac{\sinh 2\pi(\tilde{x}-\tilde{h})}{\cosh 2\pi(\tilde{x}-\tilde{h})-1} - 4\pi^2\tilde{x}\tilde{h}\frac{1}{\cosh 2\pi(\tilde{x}-\tilde{h})-1}\right](\tilde{x}+\tilde{h})d\tilde{x}$$

with $\tilde{h} = \frac{h}{l}$.

The first term on the r.h.s. of Eq. (26) is the energy of MDD array, and the second term on the r.h.s. of Eq. (26) is the interaction energy.

6. Results and Analysis

It follows from the consideration of Section 5 that the energy of the system depends on four variable parameters: MDD strength ω, the misfit parameter f, the film thickness h and the distance l between neighboring disclinations. The dependence of the normalized energy release $\Delta E^* = \frac{2\pi(1-\nu)}{(Gh)} \cdot \Delta E$ on MDD strength ω at fixed parameters f and $\frac{h}{l}$ is presented in Fig.3.

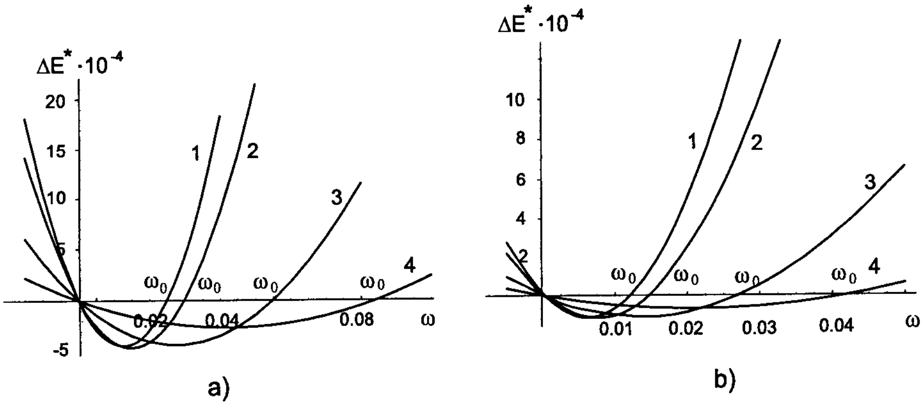

Figure 3. Dependence of the normalized energy release ΔE^* on disclination strength ω, for misfit parameter (a) $f = 0.01$, and (b) $f = 0.005$. Curves 1, 2, 3 and 4 correspond to the film thickness $h = 1.2l, 1.0l, 0.5l$ and $0.2l$, respectively, where l is the distance between neighboring disclinations.

It is obvious that ΔE^* is negative, if ω ranges from 0 to ω_0. Fig. 4 demonstrates the dependence of the optimal disclination strength ω_0 on the film thickness h in units l at constant misfit parameter f.

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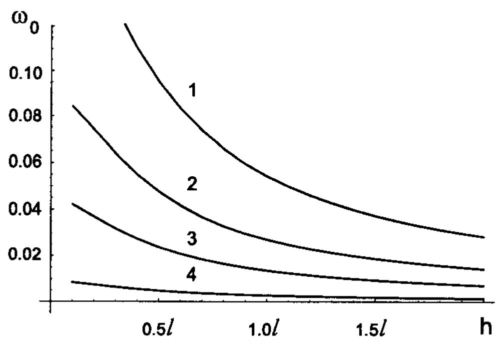

Figure 4. Dependence of optimal disclination strength ω_0 on film thickness h. Curves 1, 2, 3 and 4 correspond to misfit parameter $f = 0.02, 0.01, 0.005$ and 0.001, respectively.

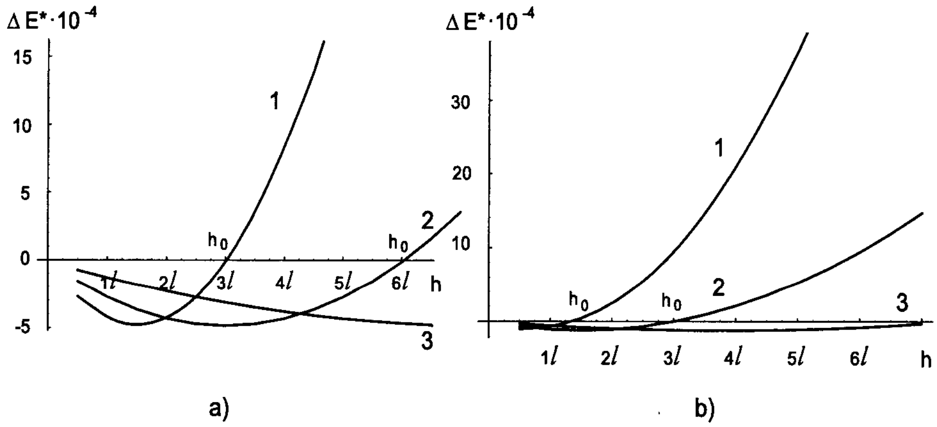

Figure 5. Dependence of the normalized energy release ΔE^* on film thickness h, for misfit parameter (a) $f = 0.01$, and (b) $f = 0.005$. Curves 1, 2 and 3 correspond to values of disclination strength $\omega = 0.01, 0.005$ and 0.002, respectively.

The energy release ΔE^* as function of the film thickness h at fixed f and ω is given in Fig. 5. The found dependencies again demonstrate the presence of the range $(0, h_0)$ where the energy release is negative. The dependence of the optimal thickness h_0 on disclination strength ω is shown in Fig. 6, for some fixed values of misfit parameter f.

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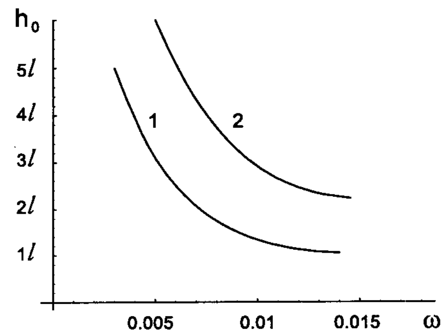

Figure 6. An optimal film thickness as function of disclination strength. Curves 1, 2 correspond to misfit parameter $f = 0.005$ and 0.01, respectively.

7. Discussion and Conclusions

Thus in this paper the formation of misfit disclinations in nanocrystalline and polycrystalline films has been theoretically examined. The energy and stresses of a thin solid film with a periodic array of misfit disclinations of wedge type at interphase boundary (distant by h from free surface of the film) (see Fig. 2) have been calculated. From our calculations it follows that there is no critical thickness for misfit disclination generation in thin films. That is, the formation of misfit disclinations is more energetically favorable than the coherent state of interphase (film/substrate) boundary at any value of the film thickness. It is contrasted to the situation with "conventional" misfit dislocations see, *e.g.*, [4-23] whose formation in a thin film is energetically favorable compared to the coherent state, only if the film thickness exceeds some critical value. At the same time, following calculations of this paper, there is an optimal film thickness at which the presence of misfit disclinations in a thin film becomes energetically unfavorable. Thus the new micromechanism for relaxation of misfit stresses – generation of misfit disclinations – is an effective alternative to the standard micromechanism – generation of misfit dislocations – in polycrystalline and nanocrystalline films characterized by low values of film thickness, in particular, in films with nano-scale thickness. The effective action of the disclination micromechanism for relaxation of misfit stresses in nanocrystalline films can be responsible for experimentally observed (see [35] and references therein) fact that residual stresses, by particle, are absent in nanocrystalline films and coatings synthesized by thermal spray methods. In the framework of the model suggested here, efficiency of misfit disclinations as defects causing relaxation of misfit stresses decreases with film thickness. Either the coherent state of interphase boundary or the formation of conventional misfit dislocations is more energetically favorable than the formation of misfit disclinations in films with thickness exceeding the optimal thickness discussed. As with disclinations in polycrystalline and nanocrystalline bulk solids (*e.g.*, [30]), misfit disclinations are assumed to be generated at junctions of interfaces. This is a rather important specific feature of the new micromechanism for relaxation of misfit stresses, because generation of misfit disclinations at existent junctions of interphase and grain boundaries does not induce any extra violations of the interphase boundary structure. In contrast, the "standard" generation of misfit dislocations leads to occurrence of violations of the interphase boundary structure at misfit dislocation cores, and, as a corollary, to degradation

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of the functional properties of interphase boundaries. The micromechanism for relaxation of misfit stresses, examined in this paper, is based on the concept of disclinations, which has been effectively used also in theoretical description of glassy structures (*e.g.*, [36]), grain boundary structures [37-40], solid state amorphizing transformations [41], and plastic deformation processes in solids (*e.g.*, [34,42,43]); see also papers in this volume. In this context, the model considered here, from a methodological viewpoint, serves as one more example of the effective application of the disclination theory in materials science and solid state physics.

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