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Misfit Dislocations in Thin Films on Plastically Deformed Substrates

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Abstract—A theoretical model describing the nucleation of misfit dislocations (MD) in interfaces between films and plastically deformed substrates with disclinations is proposed. The ranges of the parameters (disclination strength, density of the disclination ensemble, film thickness, and degree of misfit) within which MD nucleation is energetically favorable are found. It is shown that at certain strengths of disclinations and densities of their ensemble the critical thickness of the film on a plastically deformed substrate with disclinations can exceed that on an undeformed defect-free substrate by a few times. *© 2002 MAIK "Nauka/Interperiodica".*

1. INTRODUCTION

Thin-film heterostructures enjoy broad application in present-day micro- and nanoelectronics. The stability of the properties of heterostructures, which is of prime importance for their successful use in technology, depends substantially on the presence of defects and stress fields in the films (see, e.g., reviews [1–5] and monographs [6, 7]). For instance, the difference in the crystal lattice parameters between the substrate and film materials gives rise to the formation of internal stresses in films, more specifically, of misfit stresses which considerably affect the evolution of the structure and functional properties of the films. In particular, if the film thickness is in excess of a certain critical value, the misfit stresses become partially accommodated through the formation of misfit dislocations (MDs) in the interface separating the substrate and the film [1–16]. Such MDs disrupt the interface coherence, which can quite frequently degrade the functional properties of heterostructures. Recently, methods for increasing the critical film thickness on substrates were proposed based on the concept of formation of thin buffer layers of a given structure between films and substrates (see, e.g., [17–20]). An alternative method of increasing the critical thickness of films on substrates is proposed and studied theoretically in this paper. This method consists essentially in a preliminary plastic deformation of the substrate with the formation of edge dislocation walls and stress fields which suppress MD nucleation and, accordingly, increase the critical thickness of a film.

2. DISCLINATIONS IN PLASTICALLY DEFORMED SUBSTRATES

Plastic deformation of a crystal is frequently accompanied by the formation of edge dislocation walls in them (small-angle grain boundaries) [21, 22]. For instance, dislocation walls of one type form when the substrate is bent. Such walls actually represent small-angle grain boundaries, each of them crossing the substrate to terminate at the opposite free surface of the latter. Dislocation walls (small-angle boundaries) in substrates can substantially affect the misfit stress relaxation processes in epitaxial layers deposited on them. In particular, the formation of dislocation walls of one type in a plastically deformed substrate is capable of narrowing the ranges of the parameters (the film thickness and the degree of misfit) within which MD formation in the interface separating the film and the substrate is energetically favorable. To calculate the critical parameters for MD nucleation at the boundary between a plastically deformed substrate (containing dislocation walls) and a film, one has to determine the stress fields generated by the dislocation walls in the film. At distances in excess of the separation between neighboring dislocations in dislocation walls, the disclination component provides a major contribution to the stress fields of such dislocation walls. Therefore, to simplify the calculation of the stress fields created in a film by edge dislocation walls, we will approximate each such wall by a wedge disclination (which bounds the wall) near the film–substrate interface (Fig. 1). Generally speaking, each finite dislocation wall is bounded by two disclinations. The second disclination bounds the disloca-

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tion wall near the free substrate surface opposite to that on which a film is deposited. The stress fields of the second disclination are screened efficiently by the (nearest) free surface and, therefore, do not affect, in any way, dislocation nucleation in the film.

3. A FILM ON A SUBSTRATE WITH DISCLINATIONS: MODEL

Let us consider a system consisting of a semi-infinite substrate with disclinations and a film of thickness h (Fig. 1). The film and the substrate are assumed to be elastically isotropic solids with equal shear moduli G and equal Poisson ratios ν. We assume that the disclinations in the substrate are of the wedge type, have the same strength ω, and are the same distance p apart forming two infinite orthogonal rows at a distance d from the substrate surface (Fig. 1). We shall also assume that the substrate and film lattices are of the same type, the two basis vectors of each lattice lie in the interface plane and are pairwise parallel, and that the parameters of each lattice corresponding to these basis vectors are equal. (For instance, the crystal lattices of the Ge_xSi_{1-x}/Si system are mutually oriented as (001)[110] || (001)[110].) In this case, the boundary separating the substrate and film lattices is characterized by a two-dimensional dilatation misfit f determined from the relation $f = 2(a_1 - a_2)/(a_1 + a_2)$, where a_1 and a_2 are the lattice parameters of the substrate and the film, respectively.

When a film grows coherently on a substrate, the lattice misfit between the different phases and the disclinations in the substrate give rise to the formation of elastic strains in the film. For certain values of the parameters of the system (misfit f, film thickness h, distance d from the disclinations to the film–substrate interface, separation p between the disclinations, and disclination strength ω), the interface can transform to a semicoherent state characterized by MD nucleation (Fig. 2). To find the conditions favoring MD nucleation, we compare the energy of the system in the coherent state (without MDs) with that after a first single MD has formed in the system. In doing this, we assume that the positions of the disclinations in the substrate are fixed and are not affected by the MD nucleation. Within this model, the MD is an edge dislocation with the Burgers vector $\mathbf{b} = (b_l \mathbf{e}_l)$, where $\mathbf{e}_l$ is a unit vector parallel to the $0x_2x_3$ plane and forms an angle φ with the x_2 axis. This MD line lies on an m axis related to the coordinates x_2 and x_3 through the expressions $x_2 = x_2^0 - m\sin\varphi$ and $x_3 = x_3^0 + m\cos\varphi$, where x_2^0 and x_3^0 are constants (Fig. 2).

In the case of a film growing coherently on the substrate, the energy W_0 of the system is a sum of the energy W^f of proper film strains associated with the presence of a misfit, proper energy W^{ar} of two orthogonal rows of disclinations, and the energy W^{ar-f} with which the disclination rows interact with the misfit stresses:

$$W_0 = W^f + W^{af} + W^{ar-f}. \quad (1)$$

The energy W of a system with a single MD can be written as

$$W = W^f + W^{ar} + W^{ar-f} + W^d + W^{f-d} + W^{ar-d} + W^c, \quad (2)$$

where W^d is the proper MD elastic energy, W^{f-d} is the interaction energy between the MD and the misfit stresses, W^{ar-d} is the interaction energy between the MD and the disclination rows, and W^c is the MD core energy. (All the energies are reduced to a unit MD

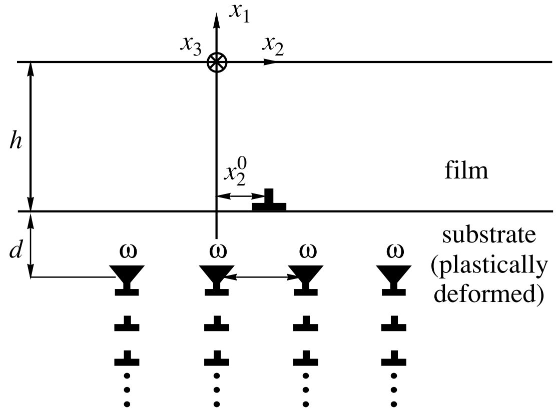

Fig. 1. Misfit dislocation in the interface between the film and a plastically deformed substrate. Wedge disclinations (triangles) bound dislocation walls of deformation origin. The disclination row along the x_3 axis is not shown.

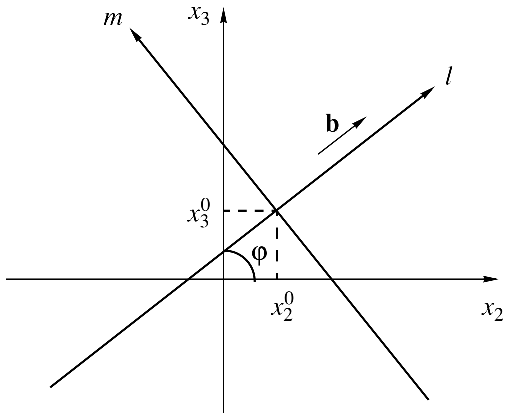

Fig. 2. Two coordinate frames on the plane. The Burgers vector of a dislocation is directed along the l axis, and the dislocation line coincides with the m axis.

length.) For an MD to nucleate at the film–substrate interface, the energy W of the system with the MD must be less than the energy W_0 of the system without the MD:

$$W - W_0 = W^d + W^{f-d} + W^{ar-d} + W^c < 0. \quad (3)$$

To determine the ranges of parameters within which an MD can nucleate, we calculate (in the next section) the quantities W^d, W^{f-d}, W^{ar-d}, and W^c entering Eq. (3). As already pointed out, these quantities are the corresponding average linear energy densities per unit MD length. We note that the linear densities of the proper energy of an MD, its interaction energy with the elastic misfit stress field, and the MD core energy are the same at any point of the MD line. At the same time, the linear interaction energy density between the MD and a disclination row is different at different points of the MD line. Therefore, in our subsequent calculation of W^{ar-d}, we average this energy density over the MD line.

4. THE ENERGY OF A DISLOCATION IN A THIN-FILM SYSTEM WITH DISCLINATIONS

The proper energy W^d (per unit MD length) of an MD lying in the film–substrate interface is given by [23]

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

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

The elastic interaction energy W^{f-d} (per unit MD length) between the MD and the misfit stress fields is [23]

$$W^{f-d} = -4\pi(1+\nu)db_l hf. \quad (5)$$

The average interaction energy W^{ar-d} (per unit MD length) between the MD and two disclination rows is given by [24]

$$W^{ar-d} = -b_l\left\langle \int_{-h}^{0} \sigma_{ll}^{ar}(x_1, x_2 = x_2^0 - m\sin\varphi, x_3 = x_3^0 + m\cos\varphi)dx_1 \right\rangle_m, \quad (6)$$

where

$$\sigma_{ll}^{ar}(x_1, x_2, x_3) = \sigma_{22}^{ar}(x_1, x_2)\cos^2\varphi + \sigma_{33}^{ar}(x_1, x_3)\sin^2\varphi$$

is the component of the stress tensor generated by the two disclination rows; $\sigma_{22}^{ar}(x_1, x_2)$ and $\sigma_{33}^{ar}(x_1, x_3)$ are the stresses generated by disclination rows parallel to the x_2 and x_3 axes, respectively; and $\langle\ldots\rangle_m$ denotes averaging over the coordinate m along the MD line. To calculate the energy W^{ar-d}, we present the stresses $\sigma_{22}^{ar}(x_1, x_2)$ and $\sigma_{33}^{ar}(x_1, x_3)$ in the form

$$\sigma_{kk}^{ar}(x_1, x_k) = \sum_{n=-\infty}^{\infty}\sigma_{kk}^{\Delta}(x_1, x_k - np), \quad k = 2, 3, \quad (7)$$

where σ_{kk} is the component of the stress tensor generated by a disclination of strength ω with a line ($x_1 = -h - d$, $x_k = 0$). The stress $\sigma_{kk}^{\Delta}(x_1, x_k)$ can be expressed through the stress function $\chi(x_1, x_k)$ of this disclination as [25]

$$\sigma_{kk}^{\Delta}(x_1, x_k) = \frac{\partial^2\chi(x_1, x_k)}{\partial x_1^2}, \quad k = 2, 3. \quad (8)$$

Using Eqs. (6)–(8) and the expression [22]

$$\chi(x_1, x_k) = \frac{D\omega}{4}[(x_1 + h + d)^2 + x_k^2]\ln\frac{(x_1 + h + d)^2 + x_k^2}{(x_1 - h - d)^2 + x_k^2} \quad (k = 2, 3) \quad (9)$$

for the stress functions $\chi(x_1, x_2)$ and $\chi(x_1, x_3)$, we obtain

$$W^{ar-d} = -\frac{D\omega b_l d}{2}[\langle g((x_2^0 - m\sin\varphi)/p)\rangle_m\cos^2\varphi + \langle g((x_3^0 + m\cos\varphi)/p)\rangle_m\sin^2\varphi], \quad (10)$$

where

$$g(t) = \sum_{n=-\infty}^{\infty}\left[\ln\frac{d^2 + p^2(t-n)^2}{(2h+d)^2 + p^2(t-n)^2} - \frac{4h(h+d)(2h+d)/d}{(2h+d)^2 + p^2(t-n)^2}\right]. \quad (11)$$

Summation of the series in Eq. (11) yields

$$g(t) = \ln\frac{\cosh(2\pi d/p) - \cos(2\pi t)}{\cosh(2\pi(2h+d)/p) - \cos(2\pi t)} - \frac{4\pi h(h+d)}{pd}\frac{\sinh(2\pi(2h+d)/p)}{\cosh(2\pi(2h+d)/p) - \cos(2\pi t)}. \quad (12)$$

The energy W^c of the dislocation core is approximately equal to $Db^2/2$ [21].

Equations (3)–(5) and (10) yield the following necessary condition for MD nucleation:

$$\frac{b}{h}\left\{\ln\frac{2h-b}{b}+\frac{1}{2}-\frac{\omega d}{b}\operatorname{sgn}(b_l)\right.$$
$$\times[\langle g((x_2^0-m\sin\varphi)/p)\rangle_m\cos^2\varphi$$
$$\left.+\langle g((x_3^0+m\cos\varphi)/p)\rangle_m\sin^2\varphi]\right\}$$
$$<8\pi(1+\nu)\operatorname{sgn}(b_1)f. \quad (13)$$

5. THE CRITICAL PARAMETERS OF FILMS ON SUBSTRATES WITH DISCLINATIONS

To determine the ranges of parameters within which MD nucleation in the film–substrate interface is energetically favorable, we consider first the situation in which the projection of the MD line on the plane containing the disclination network is parallel to one of the disclination rows; i.e., $\varphi = s\pi/2$, where $s = -1, 0, 1, 2$. In this case, we have

$$\langle g((x_2^0-m\sin\varphi)/p)\rangle_m\cos^2\varphi = 0,$$

$$\langle g((x_3^0+m\cos\varphi)/p)\rangle_m\sin^2\varphi = g(x_3^0/p)$$

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. Hence, in the case under study, the ranges of the f and h parameters in which an MD can nucleate at the film–substrate boundary depend on the x_2^0 (or x_3^0) coordinate of the MD line relative to the disclination network. The values of x_2^0 and x_3^0 will be calculated below from the condition of the minimum of the energy W^{ar-d}.

Figure 3 plots the $g(x_k^0/p)$ relations ($k = 2, 3$) for various values of d/p and h/p. As seen from Fig. 3, for any values of d/p and h/p, the maxima of the $g(x_k^0/p)$ functions lie at points $x_k^0 = (j + 1/2)p$ and their minima are at $x_k^0 = \tilde{j}p$, where j and $\tilde{j}$ are integers, $k = 2$ if $\varphi = 0$ or π, and $k = 3$ for $\varphi = \pm\pi/2$.[1] Hence, the energy W^{ar-d} passes through a minimum at $x_k^0 = \tilde{j}p$ for $b_l = +b$ and at $x_k^0 = \tilde{j}p$ for $b_l = -b$. Substituting into Eq. (13) two different pairs of equalities, ($x_k^0 = p/2$, $b_l = +b$) and ($x_i^0 = 0$, $b_l = -b$) ($k = 2$ if $\varphi = 0$, π and $k = 3$ for $\varphi = \pm\pi/2$), we obtain the following relations for the critical values of the misfit:

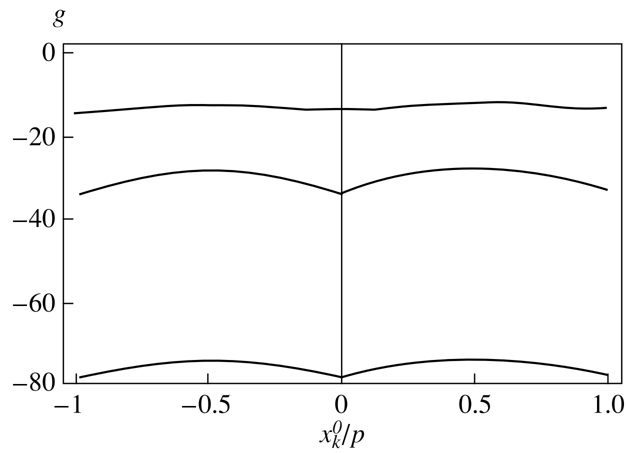

Fig. 3. Functions $g(x_k^0/p)$ plotted for the cases (top to bottom) $d/p = 0.2$, $h/p = 0.3$; $d/p = 0.05$, $h/p = 0.3$; and $d/p = 0.05$, $h/p = 0.5$.

$$8\pi(1+\nu)f^+ = \frac{b}{h}\left\{\ln\frac{2h-b}{b}+\frac{1}{2}+\frac{2\omega d}{b}\right.$$
$$\times\left[\ln\frac{\cosh\pi(2h+d)/p}{\cosh\pi d/p}\right.$$
$$\left.\left.+\frac{2\pi h(h+d)}{pd}\tanh\pi(2h+d)/p\right]\right\}, \quad (14)$$

$$8\pi(1+\nu)f^- = \frac{b}{h}\left\{-\ln\frac{2h-b}{b}-\frac{1}{2}+\frac{2\omega d}{b}\right.$$
$$\times\left[\ln\frac{\sinh\pi(2h+d)/p}{\sinh\pi d/p}\right.$$
$$\left.\left.+\frac{2\pi h(h+d)}{pd}\cosh\pi(2h+d)/p\right]\right\}. \quad (15)$$

In Eqs. (14) and (15), f^+ and f^- are the maximum and minimum values of the misfit f at which an MD with φ being a multiple of $\pi/2$and bl equal to $+b$ and $-b$, respectively, can nucleate in the film–substrate interface.

Figure 4 displays plots of $f^+(h/b)$ and $f^-(h/b)$ in the h/b vs. f coordinate frame for different values of ω. Nucleation of MDs with $b_l = b$ is energetically favorable for $f > f^+(h/b)$ (region I in Fig. 4). MDs with $b_l = -b$ can form for $f < f^-(h/b)$ (region III). Nucleation of

[1] Differentiation of Eq. (12) yields the same result.

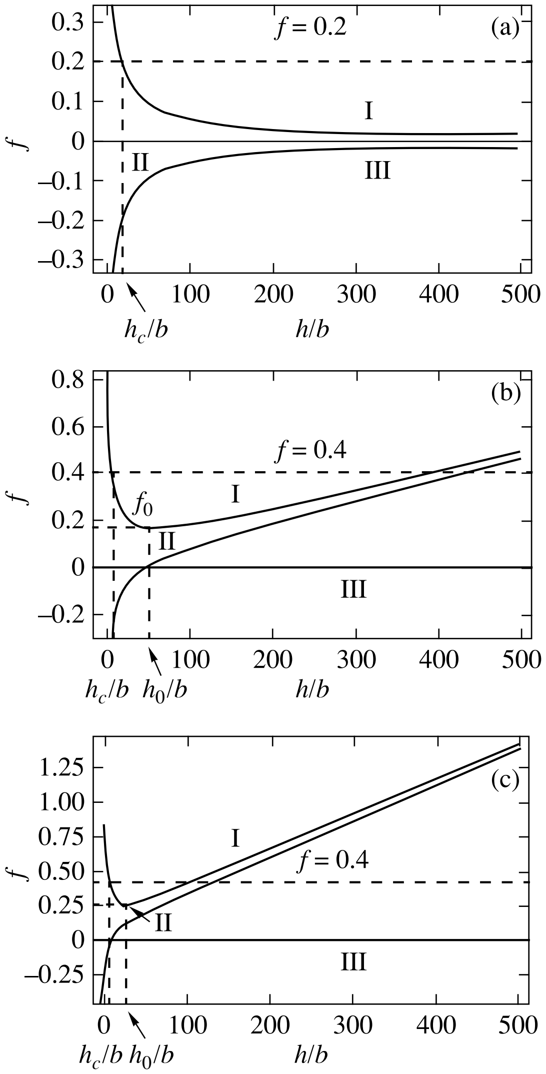

Fig. 4. Phase diagram of the system plotted in the (h/b, f) coordinate frame for the case of the MD Burgers vector parallel to the disclination network lines with parameters $d = 20b$, $p = 250b$, and (a) $\omega = 0$, (b) $\omega = 1°$, and (c) $\omega = 3°$. The lower and upper curves of f^- and f^+, respectively, separate region I, where MDs with $b_l = +b$ can nucleate, region II, where MDs do not nucleate, and region III of possible nucleation of MDs with $b_l = -b$. The values of f^+ and f^- are normalized against $1/[8\pi(1 + \nu)]$.

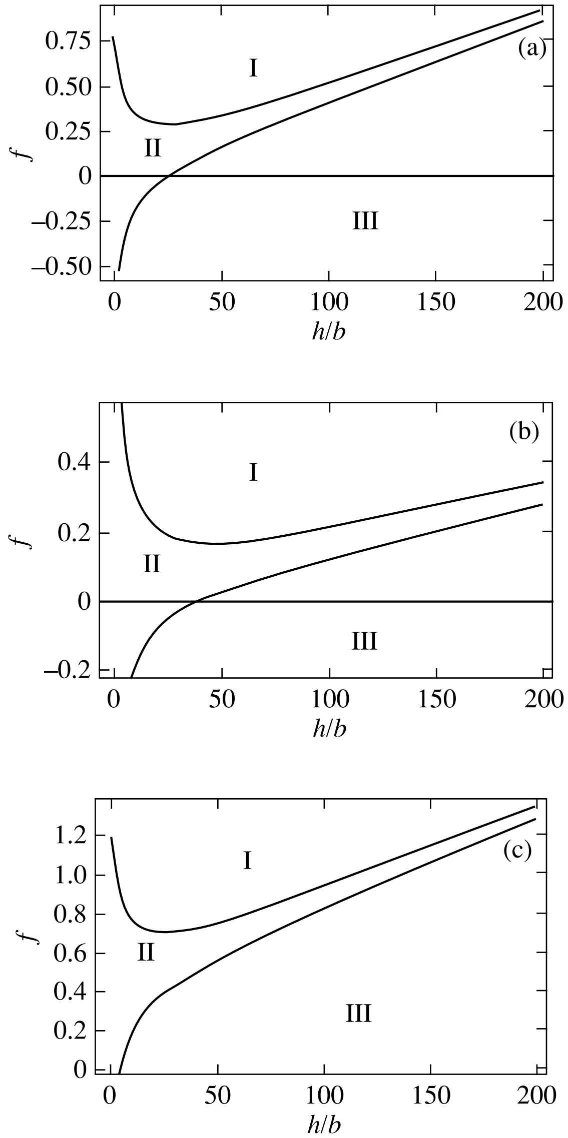

Fig. 5. Phase diagram of the system plotted in the (h/b, f) coordinate frame for the case of the MD Burgers vector parallel to the disclination network lines with parameters $\omega = 2°$ and (a) $d = 5b$, $p = 100b$, (b) $d = 5b$, $p = 300b$, and (c) $d = 50b$, $p = 100b$. The notation is the same as in Fig. 4.

MDs of both signs is energetically unfavorable for $f^-(h/b) < f < f^+(h/b)$ (region II). If the substrate has no disclinations ($\omega = 0$) (Fig. 4a), MDs can nucleate in a film of thickness h larger than a certain critical value h_c given by the intercept of the $f^+(h/b)$ (for $f > 0$) or $f^-(h/b)$ (for $f < 0$) curve with a horizontal line f = const. For $\omega > 0$, the $f^+(h/b)$ curve passes through a minimum (f_0) and, for $f < f_0$, the critical film thickness is given by the intercept of a horizontal line f = const with the $f^-(h/b)$ curve. As a result, for $f < f_0$ and $f \approx f_0$, the presence of disclinations in the substrate brings about a substantial increase (by a few times) of the critical thickness h_c compared with that for a film on a defect-free undeformed substrate. The critical thickness of a film reaches its maximum value h_0 for $f \longrightarrow f_0$, $f < f_0$. A comparison of Figs. 4b and 4c indicates that the value of h_0 for $\omega = 1°$ is larger than that for $\omega = 3°$.

Figure 5 presents the phase diagram of the system in the (h/b, $8\pi(1 + \nu)f$) coordinates for different distances d from the disclinations to the interface and different distances p between the disclinations. As seen from Fig. 5, an increase in d or a decrease in p shifts region

II, where MDs do not nucleate, toward larger misfits, while, at the same time, bringing about a decrease in h_0.

Now, we consider the case where the projection of the MD line onto the plane containing a disclination network is not parallel to any of the disclination rows ($\varphi \neq n\pi/2$, where n is an integer). To analyze this case, one has to calculate the quantities $\langle g(x_2^0 - m\sin\varphi)\rangle_m$ and $\langle g(x_3^0 + m\cos\varphi)\rangle_m$ entering Eq. (14). In view of the periodicity of the function $g(t)$, as well as accepting the conditions $\sin\varphi \neq 0$ and $\cos\varphi \neq 0$, we obtain

$$\langle g((x_2^0 - m\sin\varphi)/p)\rangle_m = \langle g((x_3^0 + m\sin\varphi)/p)\rangle_m = \frac{1}{2\pi}\int_{-\pi}^{\pi} g(t)dt = -\frac{4\pi h(h+2d)}{pd}. \tag{16}$$

Substituting Eq. (16) into Eq. (13), we obtain the following two equations for the minimum (f'^{+}) and maximum (f'^{-}) values and of the misfit f for which the nucleation of MDs with $\varphi \neq n\pi/2$ and b_l equal to $+b$ and $-b$, respectively, is possible in the film–substrate interface:

$$8\pi(1+\nu)f'^{+} = \frac{b}{h}\left(\ln\frac{2h-b}{b} + \frac{1}{2} + \frac{4\pi\omega h(h+2d)}{bp}\right), \tag{17}$$

$$8\pi(1+\nu)f'^{-} = \frac{b}{h}\left(-\ln\frac{2h-b}{b} - \frac{1}{2} + \frac{4\pi\omega h(h+2d)}{bp}\right). \tag{18}$$

As follows from Eqs. (17) and (18), an increase in ω or d or a decrease in p shifts the $f'^{+}(h/b)$ and $f'^{-}(h/b)$ curves toward larger values of f.

To find the ranges of parameters within which MDs with any Burgers vector (either parallel or not parallel to the disclination network rows) do not nucleate, the f^{-}, f^{+}, f'^{-}, and f'^{+} were plotted vs. h/b in the same coordinate frame (not displayed here). It was found that the parameter region in which MDs with a Burgers vector oriented arbitrarily in the interface plane do not nucleate coincides with the region where nucleation of MDs with Burgers vectors parallel to one of the disclination rows is not possible (region II in Fig. 4b).

6. CONCLUSION

Thus, we carried out a theoretical study of the conditions favoring nucleation of misfit dislocations in thin films on plastically deformed substrates containing disclination ensembles. It was shown that disclinations present in the substrate affect the ranges of the parameters (film thickness h and misfit f) in which film growth without MD nucleation is energetically favorable. For certain values of f (depending on the disclination strength ω, distance p between the disclinations, and distance d from the disclinations to the interface), the critical thickness of a film on a substrate with disclinations substantially exceeds the critical thickness of a film grown on an undeformed defect-free substrate. Increasing the parameter d or ω or decreasing the parameter p shifts the (h, f) region in which MDs do not nucleate toward larger values of f. The results obtained indicate a possibility of effectively increasing the critical thickness of single-crystal films through preliminary plastic deformation of their substrates.

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