Hyperdislocations in misfit dislocation networks in solid films

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Abstract

A theoretical model is suggested which describes a new type of topological defect in condensed matter, namely the hyperdislocations in networks of misfit dislocations at film/substrate interfaces. Formulae for elastic characteristics of misfit dislocation (MD) networks with hyperdislocations, such as elastic moduli and the hyperdislocation energy, are found. With these formulae, the anisotropy of the MD networks and the dependence of the hyperdislocation energy on the film thickness are analysed.

1. Introduction

Solid films exhibiting functional physical properties are the subject of intensive studies motivated by their diverse technological applications and the interest to in the fundamentals of the physical phenomena occurring in these films. Both the structure and the physical properties of the films are strongly influenced by the generation and evolution of misfit dislocations (MDs) and their configurations in film/substrate composite solids; see, e.g., [1–16]. In most cases MDs form a network at the interphase (film/substrate) boundary, whose geometry is sensitive to the crystallographic and material parameters of the adjacent film and substrate, and, in its turn, affects the physical phenomena in the solid films. For instance, a MD network at the film/substrate boundary serves as a stress source causing the formation of lattices of semiconductor quantum dots on the film free surface [13–15]. MD networks are commonly assumed to be regular, simplifying analysis of their behaviour. However, MD networks in real continuous and island films are strained and irregular; see a discussion in paper [15]. This arouses interest in examinations of strained and irregular MD networks. The main aim of this paper is to elaborate a theoretical model which describes elastic characteristics of strained MD networks containing hyperdislocations, topological defects of dislocation type, violating the translational order of periodic MD networks in the same way as conventional lattice dislocations violate the translational order of crystal lattices.

[1] http://www.ipme.ru/ipme/labs/ltdm/ovidko.html.
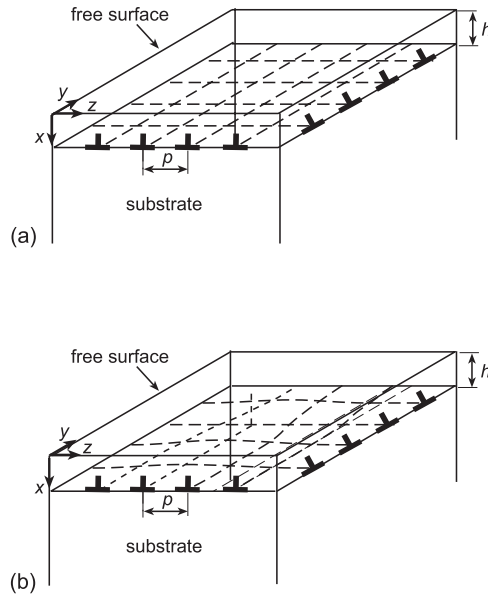
Figure 1. MD networks at a film/substrate boundary. (a) A defect-free network. (b) A network containing hyperdislocation.

2. Elastic moduli of a 2D network of misfit dislocations

Let us consider a model heteroepitaxial system consisting of a film of thickness h and a semi-infinite substrate. The film and the substrate are assumed to be isotropic solids having the same values of the shear modulus G and the same values of the Poisson ratio ν. The geometric mismatch at the film/substrate boundary is characterized by the misfit parameter $f = 2(a_s - a_i)/(a_s + a_f)$, where a_f and a_s are the crystal lattice parameters of the film and the substrate, respectively. Uniform elastic strains $\varepsilon_{yy}^f = \varepsilon_{zz}^f = f$ and misfit stresses $\sigma_{yy}^f = \sigma_{zz}^f = [2G(1 + \nu)/(1 - \nu)]f$, whose components are written in the coordinate system shown in figure 1, occur in the film due to the geometric mismatch at the interphase boundary.

A square network of MDs is formed at the film/substrate boundary, which consists of two orthogonal rows of MDs of the edge type (figure 1(a)). MDs induce stress fields that, in part, compensate for misfit stresses. The interspacing between neighbouring parallel dislocations is p; it corresponds to the minimum energy of the system. Burgers vectors of MDs are parallel with the film/substrate boundary and have the same magnitude b.

Let us examine the elastic properties of a regular square network of MDs. In the coordinate system shown in figure 1, the nodes of the ideal (non-strained) MD network have coordinates (y_k, z_l), where $y_k = kp$, $z_l = lp$, with k and l being integers. In order to describe the effective elastic strains of the MD network, we will model it as a two-dimensional elastic medium by analogy with the case of strained lattices of quantum dots [17]. In doing so, a strained MD network results from the non-deformed MD network by displacing MD lines in the $0yz$ planes which keeps the MD lines continuous. The displacements of MDs from network nodes are described by a two-dimensional vector displacement field $u_i(x, y)$. The corresponding effective strains of the MD network are characterized by the strain tensor

$$\varepsilon_{ij} = (1/2)(u_{i,j} + u_{j,i}), \qquad i, j = y, z. \tag{1}$$

The corresponding tensor of effective stresses in a 2D network is defined as follows:

$$\sigma_{ij} = \frac{\partial w^{surf}}{\partial \varepsilon_{ij}}, \tag{2}$$

where $i, j = y, z$, and w^{surf} is the energy density (per unit area) of the heteroepitaxial system.

In general, the stresses σ_{ij} are in a non-linear relationship with the strains ε_{mn}. For definiteness and simplicity, hereinafter we restrict our consideration to the situation with low strains ($\varepsilon_{mn} \ll 1$). In doing so, the linear dependence of the stress tensor σ on the strain tensor ϵ is realized with a good accuracy. It can be found as the first-order term of the expansion of the tensor σ in power terms in ϵ. In the case of a square network of MDs discussed, three elastic constants, c_{11}, c_{12}, and c_{44}, figure in the linear relationship between the components of the tensors σ_{ij} and ε_{ij}:

$$\sigma_{yy} = c_{11}\varepsilon_{yy} + c_{12}\varepsilon_{zz} + o(\epsilon) \tag{3}$$

$$\sigma_{zz} = c_{11}\varepsilon_{zz} + c_{12}\varepsilon_{yy} + o(\epsilon), \tag{4}$$

$$\sigma_{yz} = 2c_{44}\varepsilon_{yz} + o(\epsilon). \tag{5}$$

In order to calculate the elastic moduli c_{11}, c_{12}, and c_{44}, we consider the MD network in the uniformly strained state characterized by strain: $\epsilon = \varepsilon_{yy}e_y e_y + \varepsilon_{zz}e_z e_z + \varepsilon_{yz}(e_y e_z + e_z e_y)$ (figure 2). The mean energy density (per unit area) w^{surf} of the system under consideration can be written as follows:

$$w^{surf} = \left(\frac{1}{p_1} + \frac{1}{p_2}\right)(W^d + W^{d-f} + W^c) + \frac{\sum_{i=1}^{\infty} W^{1-1}(ip_1)}{p_1}$$
$$+ \frac{\sum_{i=1}^{\infty} W^{1-1}(ip_2)}{p_2} + \frac{E^{1-2}}{p_1 p_2} + w_f^{surf}. \tag{6}$$

Here $p_1 = p(1 + \varepsilon_{yy})$, $p_2 = p(1 + \varepsilon_{zz})$, W^d denotes the proper linear energy density (energy per unit length of MD) of the MD, W^{d-f} the linear energy density that characterizes the interaction between the MD and the misfit stresses, W^c the dislocation core energy density, $W^{1-1}(r)$ the linear energy density that characterizes the interaction between two parallel MDs distant by r from each other, E^{1-2} the energy that characterizes the interaction between two MDs belonging to different orthogonal dislocation rows of the MD network, w_f^{surf} the energy density (per unit area) of misfit stresses.

The proper linear energy density W^d of MD is given as (for details, see [18] and the appendix)

$$W^d = \frac{Db^2}{2}\left[\ln\frac{2h}{b} - \frac{1}{2}\right], \tag{7}$$

where $D = G/[2\pi(1 - \nu)]$. The energy W^{d-f} that characterizes the interaction between the MD and the misfit stresses is as follows (for details, see [19] and the appendix):

$$W^{d-f} = -4\pi Db(1 + \nu)fh. \tag{8}$$

It is worth noting that the values of the energy density W^d (W^{d-f}) given by formula (7) (formula (8)) are the same for all MDs located at the interphase boundary. Both W^d and W^{d-f} are independent of the spatial arrangement of the MDs at the interphase boundary.

The dislocation core energy density W^c is approximately equal to $Db^2/2$ [20]. The energy density $W^{1-1}(r)$ of the interaction between the parallel MDs may be calculated in the same way as the energy density W^{d-f}. It is given by the formula [21]

$$W^{1-1}(r) = \frac{Db^2}{2}\left[\ln\frac{4h^2 + r^2}{r^2} + \frac{4h^2(4h^2 + 3r^2)}{(4h^2 + r^2)^2}\right]. \tag{9}$$
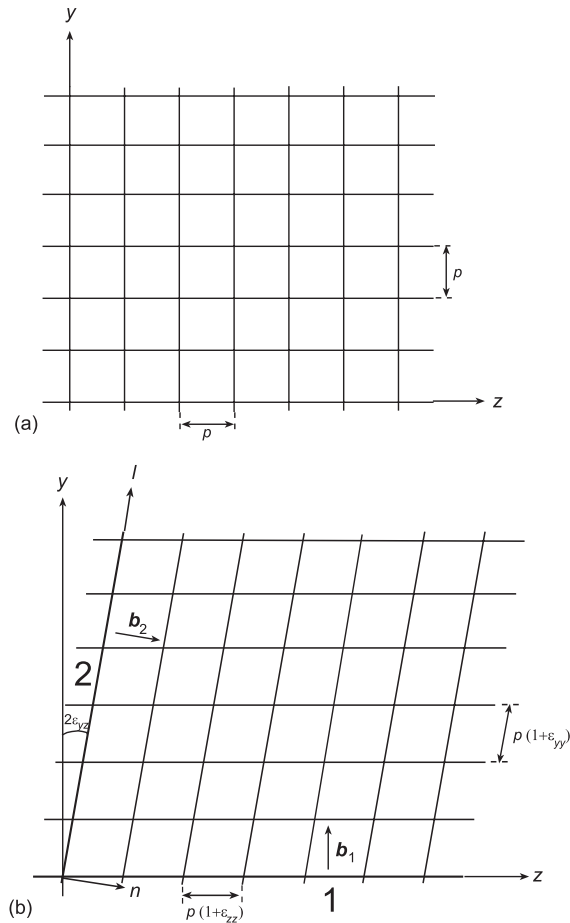
Figure 2. MD networks in (a) non-strained and (b) uniformly strained states.

In order to calculate the energy E^{1-2} of the interaction between MDs belonging to different dislocation rows, for definiteness, we consider two MDs, 1 and 2 (figure 2(b)), whose lines intersect at a point with coordinates $y = z = 0$. Let the dislocations 1 and 2 have Burgers vectors $\boldsymbol{b}_1 = b\boldsymbol{e}_y$ and $\boldsymbol{b}_2 = b\boldsymbol{e}_n$, respectively, with the unit vector $\boldsymbol{n}$ being normal to the line of MD 2. In these circumstances, the energy E^{1-2} that characterizes the interaction between MDs 1 and 2 can be calculated using the following formula [22]:

$$E^{1-2} = -b \int_0^h \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}l\, \sigma_{nn}^d. \tag{10}$$

Here l is the coordinate along the line of MD 2 ($l = y/\cos\alpha$), $\sigma_{nn}^d(x, y)$ is the component of the stress tensor of MD 1, and $\alpha = 2\varepsilon_{yz}$ denotes the angle between axes l and y.

The stress σ_{nn}^d can be written in terms of the components σ_{yy}^d, σ_{zz}^d, and σ_{yz}^d of the stress tensor of MD 1 as follows:

$$\sigma_{nn}^d = \sigma_{zz}^d \cos^2\alpha + \sigma_{yy}^d \sin^2\alpha - \sigma_{yz}^d \sin 2\alpha. \tag{11}$$

Here $\sigma_{yz}^d = 0$, and the stress tensor components σ_{zz}^d and σ_{yy}^d of a MD in a half-space are obtained from the stress field [22] of a dislocation in a two-phase medium by putting the elastic moduli

of one of the phases equal to zero. The stresses σ_{zz}^d and σ_{yy}^d are given by the following formulae:

$$\sigma_{zz}^d(x, y) = 2\nu Db\left\{\frac{x_1}{r_1^2} - \frac{x_2}{r_2^2} + 2h\left(-\frac{1}{r_2^2} + 2\frac{x_2^2}{r_2^4}\right)\right\}, \tag{12}$$

$$\sigma_{yy}^d(x, y) = Db\left\{3\frac{x_1}{r_1^2} - 2\frac{x_1^3}{r_1^4} - 3\frac{x_2}{r_2^2} + 2\frac{x_2^3}{r_2^4} + 2h\left[-\frac{1}{r_2^2} + 8\frac{x_2^2}{r_2^4} - 8\frac{x_2^4}{r_2^6} - 2h\left(3\frac{x_2}{r_2^4} - 4\frac{x_2^3}{r_2^6}\right)\right]\right\}, \tag{13}$$

where $x_{1,2} = x \mp h$, $r_{1,2}^2 = x_{1,2}^2 + y^2$. With (11)–(13) substituted into formula (10) and the relationship $dl = dy/\cos\alpha$ taken into account, we have

$$E^{1-2} = 4\pi Db^2 h\left(\nu\cos\alpha + \frac{\sin^2\alpha}{\cos\alpha}\right). \tag{14}$$

For small deformations ($\varepsilon_{yy} \ll 1$, $\varepsilon_{zz} \ll 1$, $\alpha = 2\varepsilon_{yz} \ll 1$), formula (14) can be rewritten in the following form:

$$\frac{E^{1-2}}{p_1 p_2} = 4\pi Db^2 h\left(\frac{\nu}{p_1 p_2} + \frac{2(2-\nu)}{p^2}\varepsilon_{yz}^2\right). \tag{15}$$

With (7)–(9) and (15) substituted into formula (6), we get

$$w^{surf} = \frac{Db^2}{2}\left\{g(2\pi h/p_1) + g(2\pi h/p_2) + \frac{8\pi\nu h}{p_1 p_2} + \frac{16\pi(2-\nu)h}{p^2}\varepsilon_{yz}^2\right\} + w_f^{surf}, \tag{16}$$

where

$$g(u) = \frac{u}{2\pi h}\left(\ln\frac{2h}{b} - 8\pi(1+\nu)f\frac{h}{b} + \ln\frac{\sinh u}{u} + u\coth u - \frac{u^2}{2\sinh^2 u}\right). \tag{17}$$

Substitution of (16) and (17) into the condition $\partial w^{surf}/\partial\varepsilon_{yy}|_{\epsilon=0} = 0$ (or its equivalent $\partial w^{surf}/\partial\varepsilon_{zz}|_{\epsilon=0} = 0$) results in the following relationship:

$$8\pi(1+\nu)f\frac{h}{b} - \ln\frac{2h}{b} = \ln\frac{\sinh t}{t} + 3t\coth t - \frac{5t^2}{2\sinh^2 t} - 1 - \frac{t^3\coth t}{\sinh^3 t} + 4\nu t, \tag{18}$$

where $t = 2\pi h/p$. From (2)–(5) and (16)–(18) we find the elastic constants:

$$c_{11} = \frac{\partial^2 w^{surf}}{\partial\varepsilon_{yy}^2}\bigg|_{\epsilon=0} = \frac{\partial^2 w^{surf}}{\partial\varepsilon_{zz}^2}\bigg|_{\epsilon=0} = \frac{4\pi Db^2 h}{p^2}\beta, \tag{19}$$

$$c_{12} = \frac{\partial^2 w^{surf}}{\partial\varepsilon_{yy}\varepsilon_{zz}}\bigg|_{\epsilon=0} = \frac{4\pi\nu Db^2 h}{p^2}, \tag{20}$$

$$c_{44} = \frac{1}{2}\frac{\partial^2 w^{surf}}{\partial\varepsilon_{yz}^2}\bigg|_{\epsilon=0} = \frac{2(2-\nu)}{\nu}c_{12}, \tag{21}$$

where

$$\beta = \frac{-\sinh^4 t + 2t\sinh 2t\sinh^2 t - 8t^2\sinh^2 t + 4t^3\sinh 2t - t^4(1 + 2\cosh^2 t)}{4t\sinh^4 t}. \tag{22}$$

The dependence of the parameter β on the parameter $t = 2\pi h/p$ is shown in figure 3. As follows from figure 3, β increases from 0 to 1 with t rising from 0 to ∞. As $t \to 0$ ($p \to \infty$), we have $\beta \to 0$, in which case $c_{11}/c_{12} \to 0$, and $c_{11}/c_{44} \to 0$. That is, the MD network is extremely anisotropic. For instance, the strain ε_{yy} along the y-axis produces only the stress σ_{zz} perpendicular to the y-axis and does not induce any stress (σ_{yy}) along this axis.

$c_{11} \to 0$ at $p \to \infty$, because the linear energy density W^{1-1} that characterizes the interaction between parallel MDs, given by formula (9), approaches 0 in the limit of $p \to \infty$.
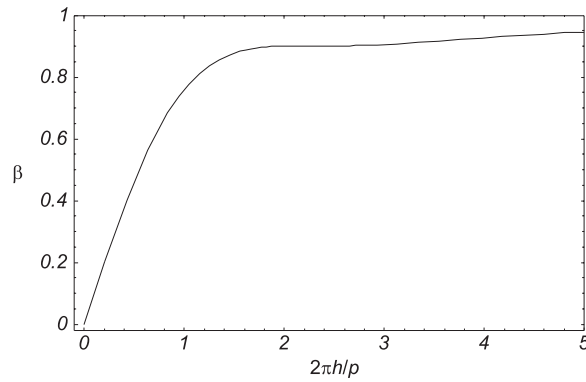
Figure 3. The dependence of the parameter β on $2\pi h/p$.

At the same time, the linear energy E^{1-2} that characterizes the interaction between MDs belonging to different dislocation rows, given by formula (14), does not depend on p. As a corollary, MDs belonging to different dislocation rows interact elastically, even if $p \to \infty$. Due to this interaction, the elastic moduli c_{12} and c_{44} have non-zero values at $p \to \infty$.

The situation with a low-density network of MDs is realized at $h > h_c$ and $h \approx h_c$ with h_c being the critical film thickness for generation of one MD in the film. In the situation with large t ($t > 1$) and the corresponding intermediate values of p/h ($p/h < 2\pi$), we have $\beta \approx 1$. The situation with a high-density network of MDs is realized when h exceeds h_c by more than a factor ranging from 1.5 to 2, depending on the misfit parameter f. At $\beta \approx 1$, the anisotropy of the MD network is not significant compared to that of the low-density MD network.

3. The energy of a hyperdislocation (cellular dislocation) in a misfit dislocation network

Let us calculate the energy of a hyperdislocation in the MD network, using formulae for the elastic constants c_{11}, c_{12}, and c_{44} (see the previous section). We assume that the hyperdislocation is formed due to 90° bending of one of the MD lines, in which case the curved MD line enters the film free surface (figure 1(b)). In doing so, for definiteness, we will consider a high-density MD network ($p/h < 2\pi$) characterized by $\beta \approx 1$. In order to estimate in the first approximation the energy of the hyperdislocation, we will examine it in the elastically isotropic medium (MD network) characterized by the mean 2D shear modulus G_d and the Poisson ratio ν_d. Formulae (3)–(5) and the following 2D analogue of Hooke's law:

$$\sigma_{ij} = \frac{2G_d}{1 - \nu_d}[(1 - \nu_d)\varepsilon_{ij} + \nu_d \varepsilon_{kk}\delta_{ij}] \tag{23}$$

(where $i, j = y, z$; $\varepsilon_{kk} = \varepsilon_{yy} + \varepsilon_{zz}$, and δ_{ij} is the Kronecker symbol) result in the following expressions: $\nu_d = c_{12}/c_{11} \approx \nu$, $G_d = \gamma c_{44}$, with γ being the factor taking into account anisotropy ($\gamma \sim 1$). It is worth noting that the elastic constants G_d, ν_d, c_{11}, c_{12}, and c_{44} are those of a two-dimensional medium; hence their units are different from the units of three-dimensional elastic constants.

Equation (23) formally coincides with Hooke's law for the 3D medium in the plane stress state. Therefore, the elastic energy E_{sd}^{el} of the hyperdislocation in a 2D network of MDs is given by a formula similar to expression [20] for the elastic energy of a conventional dislocation (per its unit length) in a 3D infinite medium, where ν_d is replaced by $\nu_d/(1 + \nu_d)$ (for details,

see [23]):

$$E_{sd}^{el} = \frac{D'p^2}{2} \ln \frac{R}{p}.$$ (24)

Here $D' = G_d(1+\nu_d)/(2\pi)$, and R is the screening length for the hyperdislocation stress field. As follows from formulae (20), (21), and (24), the elastic energy E_{sd}^{el} of a hyperdislocation in a MD network runs parallel with the film thickness h.

The total energy of the hyperdislocation consists of three terms:

$$E_{sd} = E_{sd}^{el} + E_{sd}^{c} + E_{segm}.$$ (25)

Here E_{sd}^{c} denotes the hyperdislocation core energy, and E_{segm} the energy that characterizes the formation of the MD segment perpendicular to the film free surface (figure 1(b)).

The hyperdislocation core energy in the standard approximation [20] is $E_{sd}^{c} \approx D'p^2/2$. The energy E_{segm} of the MD segment (figure 1(b)) is derived from the energy [24] of a prismatic dislocation loop perpendicular to a free surface as [24]

$$E_{segm} = \frac{Db^2h}{2}\left[\ln \frac{2h}{b} + \frac{[1 - 2\nu(6 - 11\nu + 8\nu^3)]\ln 2}{(1 - 2\nu)^2} - \frac{1}{4}\right].$$ (26)

It should be noted that the energy E_{segm} at low values of h/b essentially depends on the Poisson ratio, and can be either positive or negative. With (20), (21), (24), and (26) substituted into formula (25), we find the total energy of the hyperdislocation:

$$E_{sd} = \frac{Db^2h}{2}\left\{4\gamma(1+\nu)(2-\nu)\left(\ln \frac{R}{p} + 1\right) + \ln \frac{2h}{b} + \frac{[1 - 2\nu(6 - 11\nu + 8\nu^3)]\ln 2}{(1 - 2\nu)^2} - \frac{1}{4}\right\}.$$ (27)

Notice that a hyperdislocation in a two-dimensional MD network represents a point defect, unlike conventional dislocations in bulk crystals. Therefore, the hyperdislocation energy is given by formula (27) which has a typical form for energies of point defects in condensed media, in contrast to the case for conventional dislocations, which are characterized by linear energy densities.

As follows from formula (27), the energy E_{sd} grows more rapidly with rising h compared to the energy density W^d of MDs located at the film/substrate boundary ($W^d \propto \ln(h/b)$). As a corollary, the formation of hyperdislocations can occur only in thin films.

4. Concluding remarks

Thus, in this paper, we have theoretically examined topological defects of the new type, hyperdislocations in MD networks (figure 1(b)). We have found formulae for elastic characteristics of MD networks with hyperdislocations, such as elastic moduli and the hyperdislocation energy. According to our theoretical analysis, MD networks exhibit essential anisotropy whose degree increases with rising density of MDs. The energy of a hyperdislocation in a MD network formed in film of thickness h grows rapidly with rising h; as a result, the formation of hyperdislocations is possible only in thin films. Hyperdislocations cause irregularities in spatial arrangement of MDs, which induce a stress distribution in film/substrate composites, which, in turn, strongly affects the functional properties of solid films. In this context, of special importance will be experimental identification of the structural and behavioural features of MD networks containing hyperdislocations (figure 1(b)). These features should be definitely taken into consideration in further experimental and theoretical study of solid films, because of their fundamental significance and potential use in technological

applications. The results of the theoretical analysis of this paper can used be also in studies of ordered ensembles of semiconductor quantum dots as well as vortices in superconductors, superfluids, ferromagnetic materials, etc.

Acknowledgments

Appendix

The proper energy density (per unit length of MD) W^d of a MD is calculated as the work spent in generation of the MD (or, in other words, the transfer of the MD from the film free surface $x = 0$ to its position at the interphase boundary) in its stress field. For instance, the proper linear energy density W^d of the MD with dislocation line ($x = h$, $y = 0$) is calculated using formula [22] as follows:

$$W^d = -\frac{b}{2} \int_0^{h-r_c} \sigma_{yy}^d(x, y = 0)\, dx. \tag{A.1}$$

Here r_c is the dislocation core radius, and σ_{yy}^d is the yy-component of the MD stress field tensor, given by formula (13). With (13) substituted into formula (A.1), for $h \gg b$ and $r_c = b$, we have the known [18] formula (7) (see the text) for the proper linear energy density W^d of the MD.

The energy density (per unit length of MD) W^{d-f} that characterizes the interaction between the MD and the misfit stresses is calculated as the work spent in generation of the MD (or, in other words, the transfer of the MD from the film free surface $x = 0$ to its position at the interphase boundary) in the misfit stress field σ_{ij}^f:

$$W^{d-f} = -b \int_0^h \sigma_{yy}^f(x, y = 0)\, dx. \tag{A.2}$$

Substitution of the expression $\sigma_{yy}^f = [2G(1 + \nu)/(1 - \nu)]f$ into formula (A.2) yields the known [19] formula (8) (see the text) for the interaction energy W^{d-f}.

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