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MISFIT DISLOCATION CONFIGURATIONS AT INTERPHASE BOUNDARIES BETWEEN MISORIENTED CRYSTALS IN NANOSCALE FILM-SUBSTRATE SYSTEMS

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Abstract. A theoretical model is suggested which describes dislocation structures at interphase boundaries between misoriented crystal lattices of adjacent phases in film-substrate composite solids. The energy characteristics of such interphase boundaries are calculated in the model situation with infinite boundaries. The relationships between parameters of the equilibrium dislocation structure and geometry of the interphase boundaries are derived from the minimum energy criterion. These relationships are calculated and presented in the technologically interesting situations with $Si_{1-x}Ge_x$ film - Ge substrate and Cu film – Nb substrate composite systems.

1. INTRODUCTION

Interphase boundaries in composite solids (Fig. 1) strongly influence their mechanical, physical and chemical properties and represent the subject of intensive experimental and theoretical research; see, e.g., [1–20]. Interphase boundaries in crystalline composites are commonly characterized by the phase misfit between different crystalline lattices of the phases matched at these boundaries. Besides, in many cases, crystal lattices of the matched phases are misoriented and thereby cause the interphase boundaries to be characterized by the misorientation misfit. Thus, in the general situation, an interphase boundary carries both the phase and misorientation misfits between adjacent crystalline phases.

Of particular interest from both fundamental and applied viewpoints are interface structures and interface-controlled properties of film-substrate composites consisting of thin single crystalline films and thick substrates (Fig. 1a). Due to the misfits between films and substrates, interphase boundaries in film-substrate composites serve as sources of internal misfit stresses capable of causing structural transformations in films. In particular, the most effective and conventional mechanism for the misfit stress relaxation in films is the formation of misfit dislocations that are located at interphase boundaries and strongly influence their properties; see, e.g., [1–3,13–20]. In many cases, crystalline lattices of thin films and thick substrates matched at such boundaries have the same orientation and thereby are characterized by the only phase misfit. The formation and behavior of misfit dislocations in such film-substrate composites have been examined in detail in many papers; see, e.g., reviews [1,2,4] and book [3]. However, in general, crystalline lattices of films and substrates matched at interphase

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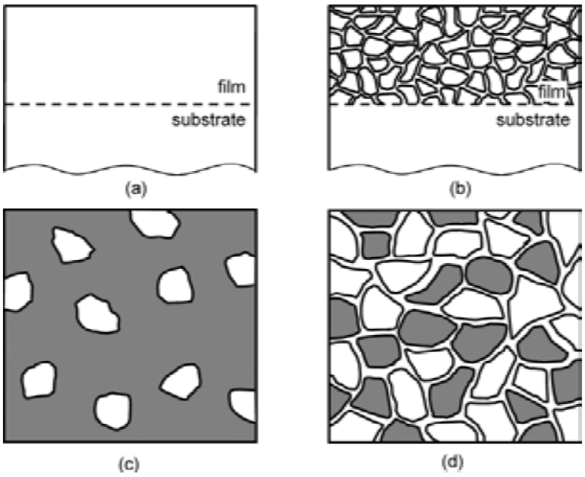

Fig. 1. Typical composite solids with interphase boundaries (schematically). (a) Composite consists of single crystalline film and substrate. (c) Composite consists of nanocrystalline film and substrate. (c) Bulk composite consists of a matrix and embedded nanoparticles. (d) Bulk nanocrystalline composite consists of nanocrystallites of different phases.

boundaries in film-substrate composites can be misoriented due to kinetic and other factors playing the role in the film growth process. As a corollary, there is high motivation in development of the theory of structural geometry (including arrangement of defects) of such boundaries. The main aim of this paper is to theoretically describe dislocation structures at interphase boundaries in film-substrate composites with the misoriented crystal lattices in the technologically interesting situation with low tilt misorientation and dilatational phase misfit.

2. DISLOCATION STRUCTURES AT INTERPHASE BOUNDARIES WITH LOW TILT MISORIENTATION BETWEEN ADJACENT CRYSTAL LATTICES OF SUBSTRATES AND FILMS OF INFINITE THICKNESS

Let us consider a model composite solid consisting of a semi-infinite substrate and a film of thickness h (Fig. 2). The film-substrate interface is supposed to be characterized by both low-angle tilt misorientation and dilatational phase misfit. The dilatational misfit is associated with difference in crystal lattice parameters between substrate and film having crystal lattices of the same type. For simplicity, we consider the case of one-dimensional misfit f, where the film and substrate crystal lattice parameters differ in the direction of the y-axis (see Fig. 2) but are the same in the direction of the z-axis. The interphase boundary tilt is described by a small misorientation angle θ ($\theta << 1$) made by adjacent crystal planes of the film and substrate crystal lattices (Fig. 2). Since the same crystallographic planes in the film and substrate are misoriented by different angles relative to the boundary plane (Fig. 2), the interphase boundary is of asymmetric type.

The misorientation and dilatational misfit of the substrate and film crystal lattices induce internal strains and stresses in both film and substrate. These strains and stresses can be modeled as those

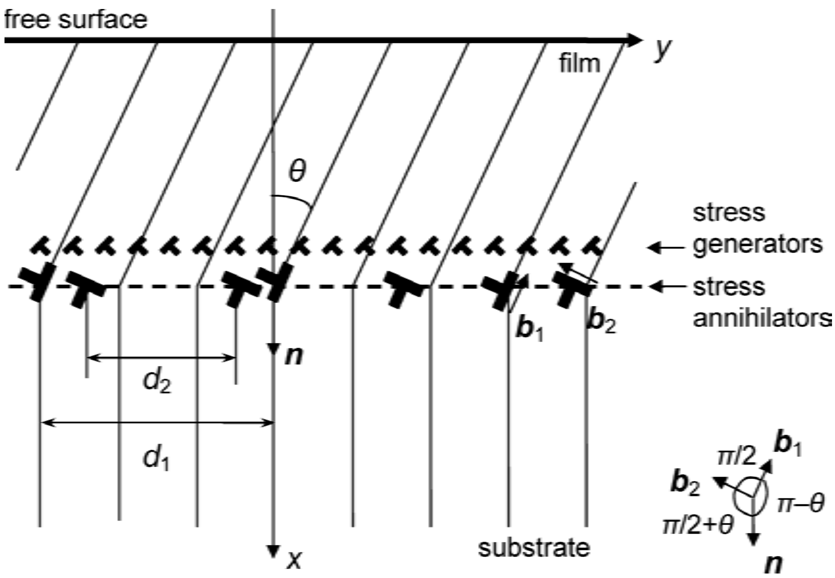

Fig. 2. Model of an interface between a semi-infinite substrate and a film, characterized by both low tilt misorientation and dilatational misfit.

created by ensembles of edge dislocations lying at the film-substrate interface. To find the characteristics (Burgers vectors and spatial arrangement parameters) of such dislocation ensembles at the film-substrate interface, first we consider the simplified situation where the film has an infinite thickness. In this situation, the interphase boundary (characterized by both dilatational misfit and tilt) represents an interface of two semi-infinite media. The dislocation representation of such an interface can be obtained using the Frank-Bilby theory [21].

Within this theory, dislocations forming a grain or interphase boundary structure can be divided into two groups: stress generators and stress annihilators. The origin of both dislocation types is illustrated as follows. A bicrystal with a tilt boundary can be created from a monocrystal by the following two-stage process. At the first stage, a top part of the monocrystal is bent by an angle θ, and the resulting strained state is modeled by a continuous distribution of virtual dislocations, called stress generators. At the second stage, additional dislocations (which are real, in contrast to stress generators) are introduced to release the stresses created at the first stage. Since these dislocations release the stresses induced by stress generators, they are referred to as stress annihilators.

The Frank-Bilby theory [21] allows one to find the net Burgers vector $\boldsymbol{B}$ of all the stress annihilators that intersect an arbitrary vector $\boldsymbol{p}$ lying in the boundary plane. The Burgers vector $\boldsymbol{B}$ is presented in terms of the operators $\mathbf{S_b}$ and $\mathbf{S_w}$, which transform a reference crystal lattice to the film and substrate crystal lattices, respectively. In the case of a tilt boundary, where the film and substrate crystal lattices are identical, $\mathbf{S_b}$ and $\mathbf{S_w}$ are the rotation operators. If a normal to the boundary plane is oriented from the film to the substrate, then the fundamental equation of the Frank-Bilby theory can be written as [21]

$$\boldsymbol{B} = \left(\mathbf{S_b^{-1}} - \mathbf{S_w^{-1}}\right)\boldsymbol{p}. \quad (1)$$

Here $\mathbf{S_b^{-1}}$ and $\mathbf{S_w^{-1}}$ are the inverse transformation operators.

To calculate the matrices $\mathbf{S_b^{-1}}$ and $\mathbf{S_w^{-1}}$ appearing in formula (1), let us choose the reference lattice. This choice defines the lattice in which the Burgers vector $\boldsymbol{B}$ is expressed [21]. We assume that the dislocations forming the interphase boundary belong to the film lattice. Then the reference frame coincides with the crystal lattice of the film, and we obtain: $\mathbf{S_w} = \mathbf{E}$, where $\mathbf{E}$ is the identity matrix. We define the misfit f as: $f = (a^f - a^s)/a^s$, where a^f and a^s are the crystal lattice parameters of the film and substrate, respectively, in the direction of the y-axis. The misfit value f is assumed to be low (f <<1).

An arbitrary basic vector of the film crystal lattice can be transformed to a basic vector of the substrate crystal lattice through the scaling by a factor of $1/(1+f)$ and rotation by the angle θ relative to the z-axis (Fig. 2). Therefore, in the coordinate system shown in Fig. 2, the operator $\mathbf{S_b}$ and $\mathbf{S_b^{-1}}$ inverse operator are written as follows:

$$\mathbf{S_b} = \frac{1}{1+f}\begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$\mathbf{S_b^{-1}} = (1+f)\begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (2)$$

With formula (2) and the relation f <<1, Eq. (1) can be rewritten as: , where

$$\mathbf{W} = \mathbf{S_b^{-1}} - \mathbf{E} = \begin{pmatrix} \cos\theta - 1 + f & \sin\theta & 0 \\ \sin\theta & \cos\theta - 1 + f & 0 \\ 0 & 0 & f \end{pmatrix}. \quad (3)$$

As it has been noted above, the interphase boundary under consideration is of asymmetric type. It is known [21] that the dislocation structure of such a boundary can be represented by two periodic sets of dislocations with the lines parallel to the rotation axis of the boundary. Let us denote the Burgers vectors of dislocations that belong to the two different sets as $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ and their separations as d_1 and d_2 (see Fig. 2). In this case, the Burgers vector $\boldsymbol{B}$ can be decomposed as follows [21]:

$$\boldsymbol{B} = (\boldsymbol{N}_1 \cdot \boldsymbol{p})\boldsymbol{b}_1 + (\boldsymbol{N}_2 \cdot \boldsymbol{p})\boldsymbol{b}_2, \quad (4)$$

where $N_i = (\boldsymbol{n} \times \xi_i)/d_i$, ($i$ = 1,2), ξ_i is the unit vector defining the dislocation line direction, and $\boldsymbol{n}$ is the normal to the boundary plane. Taking into consideration that $\boldsymbol{B} = \mathbf{W}\boldsymbol{p}$, Eq. (4) is re-written as:

$$\boldsymbol{Wp} = (\boldsymbol{N}_1 \cdot \boldsymbol{p})\boldsymbol{b}_1 + (\boldsymbol{N}_2 \cdot \boldsymbol{p})\boldsymbol{b}_2, \quad (5)$$

As equality (5) is valid for an arbitrary vector $\boldsymbol{p}$, it holds in the partial case $\boldsymbol{p} = \boldsymbol{N}_1$. To express the dislocation periods d_1 and d_2 in terms of the projections of the Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$, note that the vectors $\boldsymbol{N}_i$ lie in the boundary plane, and $\boldsymbol{N}_1 \parallel \boldsymbol{N}_2$. (The aforesaid follows from the definition of the vectors $\boldsymbol{N}_i$ and the relation $\xi_1 = \xi_2$). Then, from formula (5) we obtain the following vector equation:

$$\frac{\boldsymbol{b}_1}{d_1} + \frac{\boldsymbol{b}_2}{d_2} = \mathbf{W}\left(\boldsymbol{n} \times \xi_1\right). \tag{6}$$

In the coordinate system shown in Fig. 2, $\boldsymbol{n}$ = [100], ξ_1 = [001], and $\boldsymbol{n}\times\xi_1$. Projecting Eq. (6) onto the x- and y-axes and taking into account matrix expression (3) for $\mathbf{W}$, we rewrite formula (6) in the form of an equivalent system of equations as follows:

$$\begin{cases} \dfrac{b_{1x}}{d_1} + \dfrac{b_{2x}}{d_2} = -\sin\theta \\ \dfrac{b_{1y}}{d_1} + \dfrac{b_{2y}}{d_2} = 1 - \cos\theta - f \end{cases}. \tag{7}$$

Let us direct the Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ in such a way that $\boldsymbol{b}_1$ makes the angle θ with the boundary plane and $\boldsymbol{b}_2$ is perpendicular to $\boldsymbol{b}_1$ (Fig. 2). Also, for clarity, we assume that f>0 and the film crystal lattice is a cubic one. Then we have: b_1=b_2=b, and the Burgers vectors projections onto the x- and y-axis (see Fig. 2) are given as:

$$\begin{aligned} b_{1x} &= -b\sin\theta, \;\; b_{1y} = -b\cos\theta, \\ b_{2x} &= -b\cos\theta, \;\; b_{2y} = b\sin\theta. \end{aligned} \tag{8}$$

Substituting (8) to (7), we obtain:

$$d_1 = \frac{b}{1 + f - \cos\theta}, \;\; d_2 = \frac{b}{\sin\theta}. \tag{9}$$

Thus, we have found the Burgers vectors of dislocations-stress annihilators and the distances between these dislocations. To find the Burgers vectors and linear densities of dislocations-stress generators, let us assume that the examined interface of two semi-infinite media does not create long-range stress fields (hereinafter, we refer to the stress field as long-range, if it has non-zero component(s) at an infinite distance from the interface). To provide the absence of long-range stresses, the total Burgers vector of all the dislocations (both stress generators and stress annihilators) at the interface should be equal to zero [21]. With formula (1), the latter condition allows one to find the total Burgers vector of stress generators.

The stress generators are commonly represented as continuously distributed virtual dislocations with infinitesimal Burgers vectors [21]. With the condition that the sum Burgers vector of both stress generators and stress annihilators is the zero-vector, we find the stress generator distribution density. The right hand sides of the first and second equations (7) define the projections of the sum Burgers vector of stress annihilators (per unit length of the interphase boundary) onto the x- and y-axis, respectively. Thus, the expressions for the projections of the Burgers vectors of stress generators (per unit length of the interphase boundary) are given by the right hand sides of Eqs. (7), taken with the opposite sign. Since both the x- and y-projections of the stress generator Burgers vectors are non-zero in the considered case, the ensemble of stress generators can be represented as a continuous array of edge dislocations with infinitesimal Burgers vectors, inclined to the interface (Fig. 2). It is convenient to split such an array into two arrays formed by dislocations with infinitesimal Burgers vectors db_g $\boldsymbol{e}_x$ and –db_g $\boldsymbol{e}_y$ (Fig. 3). Then, taking into account Eqs. (7), the linear dislocation densities ρ_x and ρ_y are as follows:

$$\rho_x = \frac{\sin\theta}{dbg}, \;\; \rho_y = \frac{1 - \cos\theta - f}{db_g}. \tag{10}$$

Thus, we have found the characteristics of the arrays of both stress generators and stress annihilators in the simplified situation of an interface between two semi-infinite media. These characteristics will be used in next section as a basis of a theoretical analysis of interphase boundaries in thin film-substrate composites.

3. DISLOCATION STRUCTURES AT INTERPHASE BOUNDARIES WITH LOW TILT MISORIENTATION BETWEEN ADJACENT CRYSTAL LATTICES OF SUBSTRATES AND THIN FILMS

Let us consider the case of an interface between a semi-infinite substrate and a thin film of finite

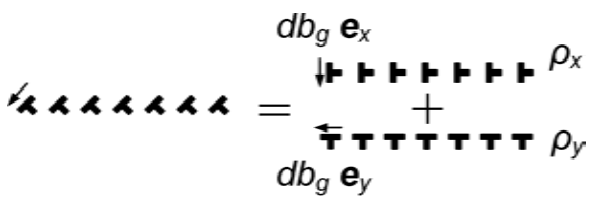

Fig. 3. Representation of an array of dislocations-stress generators with arbitrary Burgers vectors as a superposition of two dislocation arrays with the Burgers vectors oriented along the x- and y-axes. The dislocation densities ρ_x and ρ_y are defined by formula (10).

thickness h (Fig. 2). First, we examine the situation where the dislocation arrangement at the interface between a semi-infinite substrate and a thin film is identical to that at an interface between semi-infinite film and substrate, for the same values of f and θ. In this situation, in order to find the energetic characteristic of the interface, let us calculate the yy- and xy-components of both the stress field created by dislocations-stress annihilators (whose Burgers vectors and periods are given by formulae (8) and (9)) and the stress field of the dislocations-stress generators (whose linear densities are given by formulae (8)). By integrating the known expressions for the stress fields of a dislocation near a flat free surface [22], it is easily to prove that the first dislocation array (with the dislocation density ρ_x) does not create elastic stresses. At the same time, the second array is the well-known representation of a fully coherent interface [23], and its stresses, which are also the stresses of the stress generator system, can be written as

$$\sigma_{yy}^{g}=\begin{cases}\dfrac{2G\left(1-\cos\theta-f\right)}{1-\nu}, & x<h\\ 0, & x>h,\end{cases}\qquad \sigma_{xy}^{g}=0. \tag{11}$$

Here G is the shear modulus, and ν is the Poisson ratio. In the case of $\theta = 0$, formula (11) transforms to the expression [24] for the component of the stress tensor of a one-dimensional misfit in a film on a semi-infinite substrate. $\sigma_{yy}^{g} = -2Gf/(1-\nu)$ Thus, the stresses of dislocations-stress generators are presented as the sum of the stresses of orientational misfit (characterized by the angle θ) and the stresses of the dilatational misfit f.

The expressions for the yy- and xy-components of the total stress field of dislocations-annihilators are derived through the summation of the corresponding stress tensor components [22] of individual dislocations near a free surface. In doing so, we find:

$$\begin{aligned}\sigma_{yy}=\frac{G}{1-\nu}\sum_{k=1}^{2}\Bigg[&\frac{b_{kx}}{d_k}\sin Y_k\left(-\frac{1}{2A_k^-}+\frac{1}{2A_k^+}+\frac{X_k^-\sinh X_k^-}{2A_k^{-2}}-\frac{\left(X_k-3H_k\right)\sinh X_k^+}{2A_k^{+2}}+\frac{X_kH_k\cosh X_k^+}{A_k^{+2}}-\right.\\&\left.\frac{2X_kH_k\sinh^2 X_k^+}{A_k^{+3}}\right)+\frac{b_{ky}}{d_k}\left(\frac{\sinh X_k^-}{A_k^-}-\frac{\sinh X_k^+}{A_k^+}-\frac{X_k^-B_k^-}{2A_k^{-2}}+\frac{\left(X_k+3H_k\right)B_k^+}{2A_k^{+2}}+\right.\\&\left.\frac{X_kH_k\sinh X_k^+\cos Y_k}{A_k^{+2}}-\frac{2X_kH_kB_k^+\sinh X_k^+}{A_k^{+3}}\right)\Bigg],\end{aligned} \tag{12}$$

$$\begin{aligned}\sigma_{xy}=\frac{G}{1-\nu}\sum_{k=1}^{2}\Bigg[&\frac{b_{kx}}{d_k}\left(\frac{X_k^-B_k^-}{2A_k^{-2}}+\frac{X_k^-B_k^+}{2A_k^{+2}}+\frac{X_k^-\sinh X_k^-}{2A_k^{-2}}+\frac{X_kH_k\sinh X_k^+\cos Y_k}{A_k^{+2}}-\frac{2X_kH_k\sinh X_k^+}{A_k^{+3}}\right)+\\&\frac{b_{ky}}{d_k}\sin Y_k\left(-\frac{1}{2A_k^-}+\frac{1}{2A_k^+}+\frac{X_k^-\sinh X_k^-}{2A_k^{-2}}-\frac{X_k^+\sinh X_k^+}{2A_k^{+2}}-\frac{X_kH_k\cosh X_k^+}{A_k^{+2}}+\frac{2X_kH_kB_k^+\sinh X_k^+}{A_k^{+3}}\right)\Bigg].\end{aligned} \tag{13}$$

Here $X_i^{\pm}=2\pi\left(x\pm h\right)/d_i$, $X_i=2\pi x/d_i$, $H_i=2\pi h/d_i$, $A_i^{\pm}=\cosh X_i^{\pm}-\cos Y_i$, $B_i^{\pm}=\cosh X_i^{\pm}\cos Y_i-1$, and $i = 1,2$.

Formulae (11)–(13) describe the interface, which does not create long-range stresses, so that far enough from the interface misfit stresses are completely relaxed. However, in finite-thickness films the full relaxation of misfit stresses is not always necessary. For example, it is well known that misfit stress relaxation via generation of misfit dislocations in very thin films might be energetically unfavorable. To describe partially relaxed interfaces, we suppose that the linear densities of dislocations-stress generators still obey relations (10) while the densities of dislocations-stress annihilators are smaller than those on composite consisting of semi-infinite film and substrate. More precisely, we divide the misfit f into two parts, f_0 ($f_0<f$), which is relaxed by dislocations-stress annihilators, and $f-f_0$, which is not relaxed by dislocations-stress annihilators. In this case, the Burgers vectors of dislocations-stress annihilators are still determined by formulae (8), while interdislocation distances d_1 and d_2 are obtained from formulae (9) with f replaced by f_0.

Varying the value of f_0, we can change the fraction of the dilatation misfit stress field relaxed by stress annihilators. In particular, if f_0 = 0, misfit stresses remain unrelaxed and a perfect coherent interface is formed. If $f_0 = f$, misfit stresses are completely relaxed at a large enough distance from the interface. Below we will perform the analysis of the dependences of the strain energy, accumulated in the film-substrate composite solid, on its structural and geometrical characteristics, when f_0 varies in the range $0<f_0<f$.

The strain energy of the film-substrate system can be presented as the sum of four terms. The first term describes the elastic self-energy of dislocations-stress annihilators. This energy is calculated as the work spent to generate the dislocations-stress annihilators in their own stress field (12) and (13). The second term describes the energy of the interaction between dislocations-stress annihilators and stress generators. It is calculated as the work spent to generate the dislocations-stress annihilators in the stress field of stress generators. The third term describes the core energies of dislocations-stress annihilators. Finally, the last term describes the self-energy of dislocations-stress generators.

First, we assume that the system of stress annihilators is a periodic one with a period D. This case is realized, if the ratio d_1/d_2 is a rational number. In this case, the specific energy W of the film-substrate composite solid (per unit area of its interface) can be written as:

$$W=\frac{1}{2D}\left[-\sum_{i=1}^{2}\sum_{j=1}^{n_i}\int_0^{h-r_0}\left\{\left(b_{ix}\sigma_{xy}\left(x,y=y_i^{(j)}\right)+b_{iy}\left[\sigma_{yy}\left(x,y=y_i^{(j)}\right)+2\sigma_{yy}^{g}\right]\right)\right\}\mathrm{d}x+2\left(n_1+n_2\right)W^c\right]+W^g, \quad (14)$$

where n_i denotes the number of dislocations belonging to the i-th set (i = 1,2) per one period D of the interface structure, r_0 the dislocation core radius, $y_i^{(j)} = (j - 1)d_i$ the coordinate of the j-th dislocation from the i-th set, W^c the dislocation core energy, and W^g the elastic self-energy of stress generators (per unit area of the interface).

The dislocation core energy is estimated by the known formula [25]

$$W^c=\frac{Gb^2}{4\pi\left(1-\nu\right)}. \quad (15)$$

The elastic self-energy W^g of stress generators (per unit area of the interface) is calculated as follows:

$$W^g=\frac{G\left(1-\cos\theta-f\right)^2h}{1-\nu}. \quad (16)$$

Substituting expressions (11)–(13), (15), and (16) into formula (14), after integration, we find:

$$\begin{aligned}W=&-\frac{G}{8\pi\left(1-\nu\right)D}\Bigg\{-2\left(n_1+n_2\right)b^2+\sum_{i=1}^{2}\sum_{j=1}^{n_i}\sum_{k=1}^{2}\Bigg[b_{ix}\Bigg(b_{kx}\Bigg(\ln\frac{A_k^-}{A_k^+}-\frac{X_k^-\sinh X_k^-}{A_k^-}+\frac{X_k^+\sinh X_k^+}{A_k^+}+\\&2H_k\left(\frac{X_k\cos Y_k^{(j)}+\sinh X_k^+}{A_k^+}-\frac{X_k\sin^2Y_k^{(j)}}{A_k^{+^2}}\right)\Bigg)+b_{ky}\sin Y_k^{(j)}\left(\frac{X_k^+}{A_k^+}-\frac{X_k^-}{A_k^-}-2H_k\left(\frac{1}{A_k^+}+\frac{X_k\sinh X_k^+}{A_k^{+^2}}\right)\right)\Bigg)+\\&b_{iy}\Bigg(b_{kx}\sin Y_k^{(j)}\left(\frac{X_k-3H_k}{A_k^+}-\frac{X_k^-}{A_k^-}+2H_k\left(\frac{1}{A_k^+}+\frac{X_k\sinh X_k^+}{A_k^{+^2}}\right)\right)+b_{ky}\Bigg(\ln\frac{A_k^-}{A_k^+}+\frac{X_k^-\sinh X_k^-}{A_k^-}-\\&\frac{\left(X_k+3H_k\right)\sinh X_k^+}{A_k^+}+2H_k\left(\frac{X_k\cos Y_k^{(j)}+\sinh X_k^+}{A_k^+}-\frac{X_k\sin^2Y_k^{(j)}}{A_k^{+^2}}\right)\Bigg)\Bigg)\Bigg]_{x=0}^{x=h-r_0}+\\&16\pi\left(1-\cos\theta-f\right)hb\left(-n_1\cos\theta+n_2\sin\theta\right)\Bigg\}+\frac{G\left(1-\cos\theta-f\right)^2h}{1-\nu},\end{aligned} \quad (17)$$

where $Y_k^{(j)}=2\pi y_i^{(j)}/d_k$, and the notation $f(t)\big|_{t=a}^{t=b}=f(b)-f(a)$ is used.

Now we consider the situation where the value of d_1/d_2 is irrational. In this situation, the film/substrate interface has a quasiperiodic dislocation structure. To calculate the energy W of the film-substrate composite with a quasiperiodic interface, we model the quasiperiodic interface as its periodic approximant, a

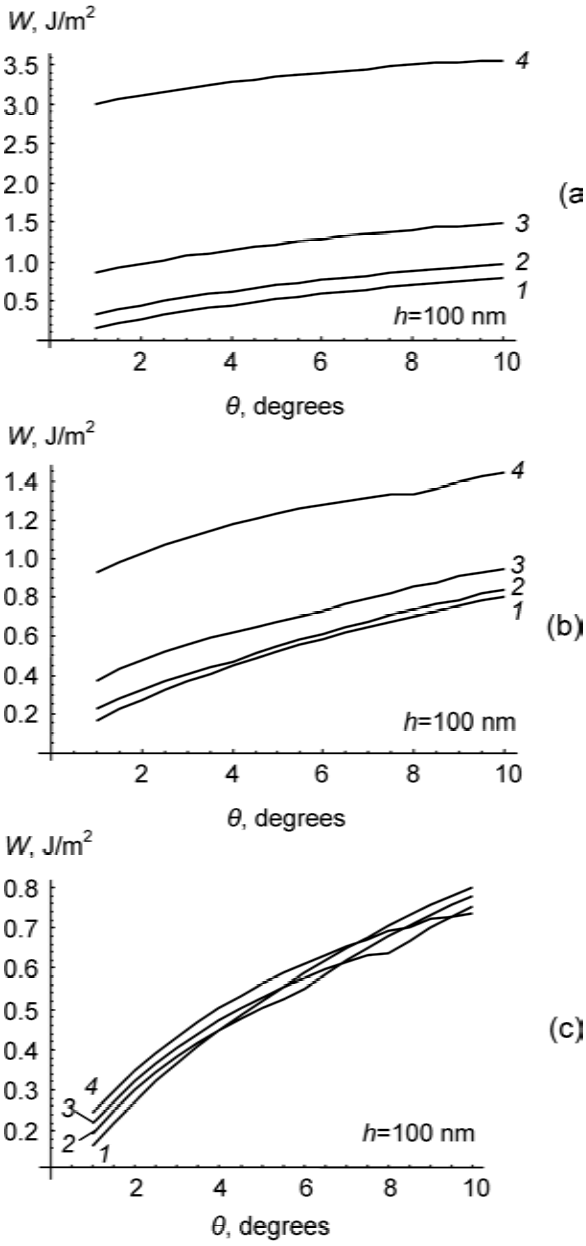

Fig. 4. Dependences of the specific energy W of the film-substrate $Si_{1-x}Ge_x$/Ge composite solid on the misorientation angle θ, for h = 100 nm and f = 0, 0.005, 0.01 and 0.02 (curves *1, 2, 3,* and *4*, respectively). (a) $f_0 = 0$; (b) $f_0 = 0.5f$; and (c) $f_0 = f$.

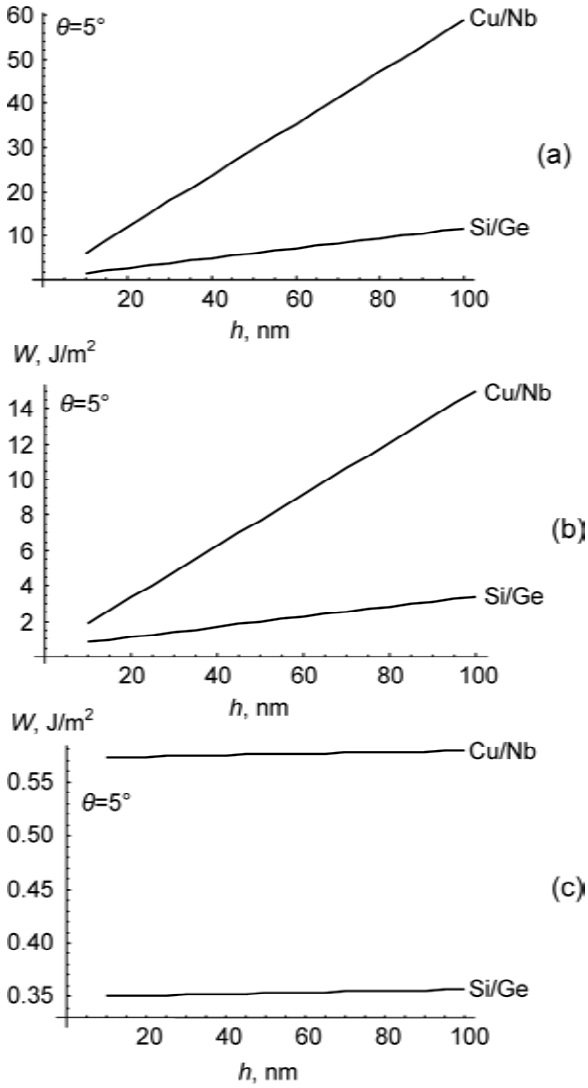

Fig. 5. Dependences of the specific energy W of the film-substrate Si/Ge and Cu/Nb composite solids with values of f = –0.04 and 0.09, respectively, on the film thickness h, for θ = 5°. (a) $f_0 = 0$; $f_0 = 0.5f$; and (c) $f_0 = f$.

periodic interface with a very large period (D=500d_1). In the framework of this model, formula (17) can be effectively applied to the cases of both periodic and quasiperiodic interfaces.

Using formulae (17), we have analyzed the dependences of the specific energy W of the film-substrate composite solid on its geometric and structural parameters in the exemplary cases of $Si_{1-x}Ge_x$/Ge and Cu/Nb systems. Elastic moduli and crystal lattice parameters in $Si_{1-x}Ge_x$ films, should vary with continuous change of parameter x characterizing its chemical composition. For simplicity, in a description of the $Si_{1-x}Ge_x$ phase, we have used parameters of pure Si, the namely G = 51 GPa, ν = 0.28, and $b = a_f/\sqrt{2}$. This approximation seems to be rather correct, because silicon and germanium (two border cases of the $Si_{1-x}Ge_x$ alloy) have close values of the elastic constants (for Ge, one has: G = 47 GPa, ν = 0.27). Lattice parameter a_f of the $Si_{1-x}Ge_x$ film continuously varies with the change of x from the value of 5.43 Å for pure silicon to 5.66 Å for pure germanium. Consequently misfit parameter ranges from f = 0 (for Ge/Ge system) to $f \approx -0.04$ (for Si/Ge composite). In the case of Cu film deposited onto Nb substrate, we used the following char-

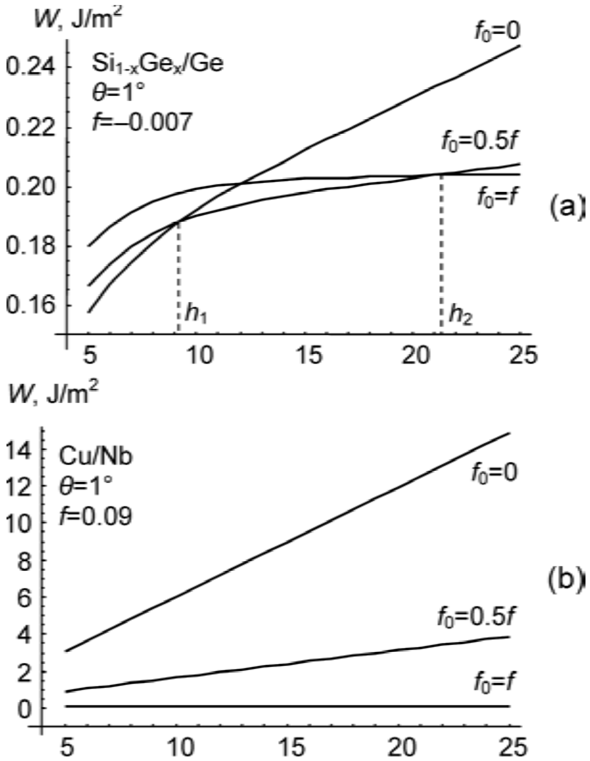

Fig. 6. Dependences of the specific energy W of the film-substrate composite solid on the film thickness h, for $\theta = 1°$ and different values of f_0. (a) $Si_{1-x}Ge_x$/Ge system with $f = -0.007$; (b) Cu/Nb system with $f = 0.09$.

acteristic values of parameters: $G = 48$ GPa, $\nu = 0.34$, $a_f = 3.61$Å, $a_s = 3.30$Å, $b = a_f/\sqrt{2}$, and $f \approx 0.09$.

Fig. 4 shows the dependence of the specific energy W of $Si_{1-x}Ge_x$/Ge system on the misorientation angle θ, for different values of f_0 and f. As is seen in Fig. 4, the energy W grows with an increase in the misorientation angle θ and/or misfit f. Besides, the misfit stress relaxation by formation of interphase dislocations leads to an overall decrease of the energy W. This tendency is strongest at high values of misfit f (see curves *3* and *4* in Figs. 4a and 4b).

Fig. 5 plots the dependences of the specific energy W of Si/Ge and Cu/Nb systems on the film thickness h, for $\theta = 5°$ and different values of f_0 and f. The dependences $W(h)$ in Figs. 5a and 5b are close to linear ones, because the self-energy of stress generators depends on the film thickness in a linear way. Comparison of figures 5a and 5b shows that the partial relaxation of misfit stresses significantly decreases the specific energy W of the film-substrate composite solid. In the case of the complete relaxation of misfit stresses (Fig. 5c), the energy W depends on the film thickness very weakly,

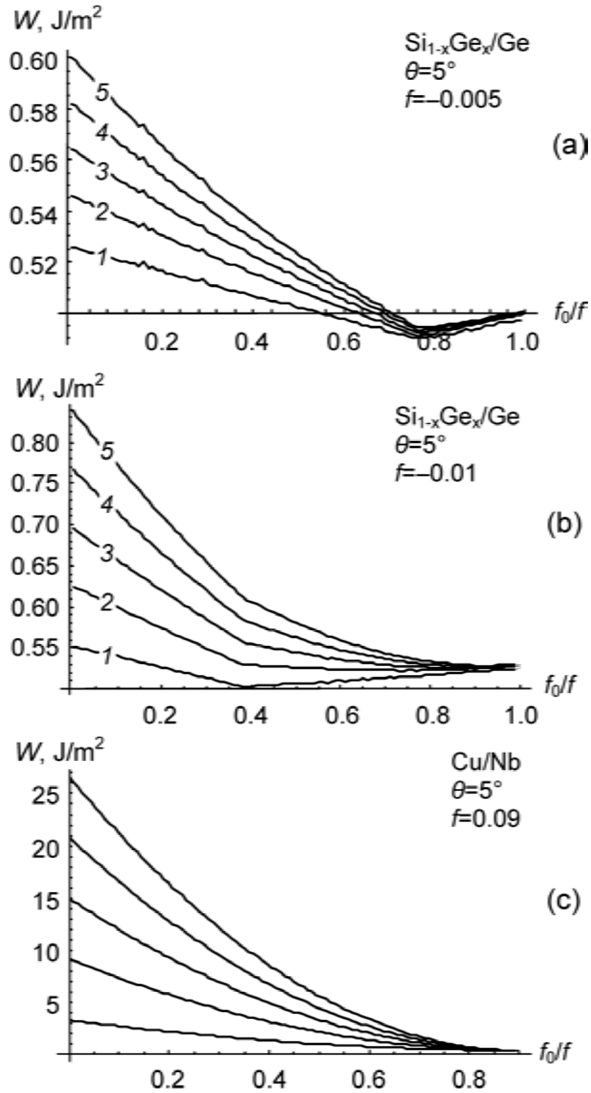

Fig. 7. Dependences of the specific energy W of the film-substrate composite solid on the parameter f_0, for $\theta = 5°$, h = 5, 15, 25, 35, and 45 nm (curves *1, 2, 3, 4,* and *5*, respectively). (a) $Si_{1-x}Ge_x$/Ge system, $f = -0.005$; (b) $Si_{1-x}Ge_x$/Ge system, $f = -0.01$; (c) Cu/Nb system, $f = 0.09$.

because the elastic stresses dramatically fall with rising the distance from the interface.

It is known that the typical mechanism of misfit stresses relaxation – the generation of misfit dislocations – is not energetically favorable in very thin films at $\theta = 0$; see, e.g., [1,2]. A similar effect also comes into play in the examined case of $Si_{1-x}Ge_x$/Ge composite with non-zero tilt misorientation θ at certain values of parameters. Fig. 6a presents the dependences $W(h)$ of $Si_{1-x}Ge_x$/Ge composite in the range of small values of the film thickness h, for $\theta = 1°$, $f = -0.007$ and different values of f_0. As follows from Fig. 6a, among three dislocation structures of the interface (corresponding to the cases of $f_0 = 0$, $f_0 = 0.5f$, and $f_0 = f$), the structure with $f_0 = 0$ is energetically favorable at very small values of the film thickness ($h<h_1$). For intermediate values of the film thickness h ($h_1<h<h_2$), the structure with $f_0 = 0.5f$ has the lowest energy. For comparatively large values of the film thickness h ($h>h_2$), the complete relaxation of misfit stresses ($f_0 = f$) is energetically favorable. These different behaviors are exhibited by $Si_{1-x}Ge_x$ film – Ge substrate composite, depending on the film thickness h. In contrast, for Cu film - Nb substrate composite characterized by large value of misfit parameter, the complete relaxation is energetically favorable at all realistic values of the film thickness (Fig. 6b).

In general, the parameter f_0 may take any value from the range $0<f_0<f$, depending on geometric parameters and component phases of a film-substrate composite. Therefore, in order to determine the values of f_0 that minimize the energy W, we need to analyze the dependences $W(f_0)$, for any given value of h. Fig. 7 shows such dependences in the situations with $Si_{1-x}Ge_x$/Ge and Cu/Nb composites, for $\theta = 5°$ and different film thicknesses h. It is easily seen that, for $Si_{1-x}Ge_x$/Ge composite with low misfit (Fig. 7a), the curves have pronounced minimum near $f_0 \approx 0.8f$. As film thickness h increases, the minimum of $W(f_0)$ moves to larger values f_0. For higher value of misfit parameter (Fig. 7b), the minimum exists only for ultra-thin films (see curve *1*). When the film thickness h becomes sufficiently large, the function $W(f_0)$ reaches its minimum when its argument approaches a limiting value close to f. This behavior is explained by the natural tendency to completely relax the misfit stresses in comparatively thick films through the formation of interphase dislocations. When the misfit parameter reaches very high values (as with Cu/Nb system characterized by $f = 0.09$, Fig. 7c), the minimum value of the specific energy corresponds to the case of $f_0 = f$ in the whole range of film thickness values.

4. CONCLUDING REMARKS

Thus, in this paper, dislocation structures at interphase boundaries between misoriented crystal lattices of adjacent phases in film-substrate composite solids have been theoretically described in the situation with low tilt misorientation and dilatational phase misfit. We have calculated the energy characteristics of such interphase boundaries in the model situation with infinite boundaries. With the minimum energy criterion, we have found the relationships between characteristics (Burgers vectors and spatial arrangement parameters) of the equilibrium dislocation structure and geometric parameters (tilt misorientation angle θ and dilational misfit f) of the interphase boundaries. The suggested general approach is illustrated by calculations of the aforesaid relationships in practically interesting cases of $Si_{1-x}Ge_x$ film - Ge substrate and Cu film – Nb substrate composite systems.

The discussed dislocation structures at interphase boundaries between misoriented crystal lattices of adjacent phases in film-substrate composites are worth being experimentally examined and theoretically described in detail in the future. Of special importance would be a systematic experimental analysis of the dislocation structures in film-substrate composites with various compositions and geometric parameters. Besides, the theoretical approach elaborated in this paper for a description of dislocation structures at infinite interphase boundaries between misoriented crystallites of different phases can be used as a basis for a theoretical study of dislocation structures at interphase boundaries of finite extent. This study would be of crucial importance for a description of the structural and behavioral features of nanocomposites where nanoscale interphase boundaries exist and crystal lattices of the adjacent phases are often misoriented.

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