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Misfit strains and phase transformations in layered composite solids

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Abstract. General formulae are found for misfit strains and their energy density in multilayer solid composites. The effect of misfit strains on phase transformations (related to diffusional mixing) in layered composites is theoretically described with the help of the above general formulae. It is theoretically revealed here that misfit strains play a significant role in initiating solid-state amorphizing transformations. The dependence of the minimal critical thickness (which characterizes the amorphization processes) on misfit parameters in layered composites is found.

1. Introduction

Application of layered composite solids in micro- and nanoelectronics as well as in other areas of high technology commonly imposes strict demands on stability of their structure and properties. However, interphase boundaries as local structural imperfections (plane defects) and sources of misfit strains are capable of causing instability and degradation of the desired—from an applications viewpoint—properties of layered composites; see e.g. [1–8]. On the other hand, there are technologies which are based on the effects of microstructural and phase transformations at interphase boundaries in layered composites [9–15]. For instance, the effect of solid-state amorphizing transformations occurring in multilayer coatings serves as the basis for synthesis of amorphous metallic alloys (in particular, amorphous alloys with specific chemical compositions that cannot be obtained with the help of other technological methods of amorphous-alloy synthesis); see e.g. [9–13]. The significant role of interphase boundaries in processes occurring in layered composite solids is of great interest in experimental and theoretical studies of interphase boundaries and their contribution to the macroscopic properties of such solids. In such studies, up to now, the most attention in theoretical studies has been paid to the analysis of interphase boundaries in two-layer systems (mostly film/substrate systems), these being the simplest representatives of layer composites [2–8].

The role of misfit strains (induced by interphase boundaries) in structural and phase transformations in layered composites depends, in general, on many macroscopic factors (e.g., geometric dimensions of composites, temperature) as well as microscopic parameters which describe structural and chemical peculiarities of composites, and often cannot be directly identified by current experimental methods. As a corollary, at present, key micromechanisms and specific features of the structural and phase transformations in layered composites have not been unambiguously recognized in many cases.

The main aims of this paper are to calculate (in a general form) misfit strains and the strain energy density in multilayered composites with coherent interphase boundaries (section 2)

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and to theoretically describe the role of misfit strains in phase transformations in initially two-layer composites (section 3) with particular attention being paid to solid-state amorphizing transformations (section 4). A general discussion of the theoretical results of this paper will be given in section 5.

2. Misfit strains and energetic characteristics of multilayer composites

Let us consider a multilayered film deposited on a relatively thick substrate. Let N be the number of layers in the film (figure 1), and H and h_i $(i = 1, \ldots, N)$ be the substrate and ith-layer thicknesses, respectively, which have arbitrary magnitudes. In this situation, the total thickness of such a layered structure d is equal to $H + \sum_{i=1}^{N} h_i$, which is assumed to be much smaller than the other linear dimensions of the system. Let the misfit strain f_i be a characteristic eigenstrain (with respect to the substrate, where the eigenstrain is assumed to be equal to a zero value) for the ith layer. For definiteness, we consider hereinafter only the case with f_i being a two-dimensional misfit strain which is uniform within the ith layer. In these circumstances, the nonzero eigenstrain components $\varepsilon^0_{xx}(z) \equiv \varepsilon^0_{yy}(z) = \varepsilon^0(z)$ of the misfit eigenstrain tensor $\hat{\varepsilon}^0(z)$ can be written as follows:

$$\varepsilon^0(z) = \sum_{i=1}^{N} f_i \left\{ \Theta(z - z_{i-1}) - \Theta(z - z_i) \right\} \tag{1}$$

where $\Theta(z)$ is the Heaviside function, equal to 1, for $z > 0$, and 0, for $z < 0$; $z_i = \sum_{k=1}^{i} h_k$; $z_0 \equiv 0$.

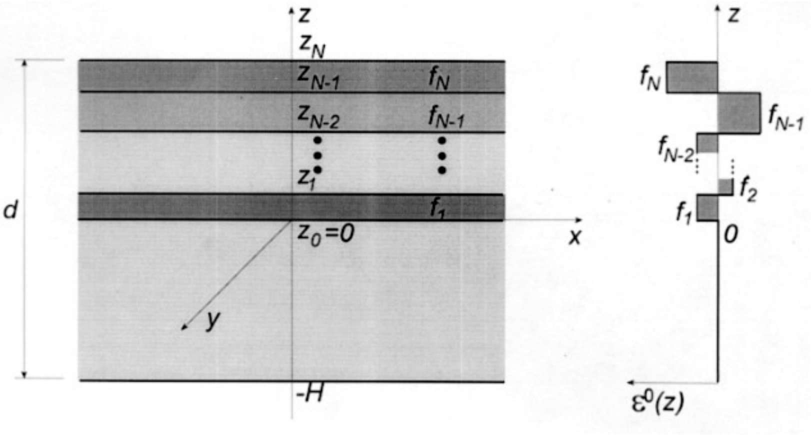

Figure 1. A multilayer composite consisting of a substrate and N layers characterized by eigenstrains f_i. The dependence $\varepsilon^0(z)$ is shown schematically on the right-hand side of the figure.

Let us assume that the outer surfaces of the multilayer composite (figure 1) are free of any external loading. The elastic properties of the substrate and layers are supposed to be identical.

Using the theory of eigenstrains [16], we can write the compatibility equation for the total strain tensor $\hat{\varepsilon}^t = \hat{\varepsilon} + \hat{\varepsilon}^0$ as follows:

$$\epsilon_{pki}\epsilon_{qlj} \nabla_k \nabla_l \hat{\varepsilon}^t_{ij} = 0 \tag{2}$$

where $\hat{\varepsilon}$ is the elastic strain tensor and ϵ_{pki} is the permutation tensor. In the case of a planar stressed state which is realized in the model situation discussed, both the total and elastic strains depend on the z-coordinate only. Therefore, equation (2) can be rewritten as

$$\frac{\partial^2}{\partial z^2}(\varepsilon_{ij} + \varepsilon^0_{ij}) = 0. \tag{3}$$

Equation (3) has the following solution:

$$\varepsilon_{ij}(z) = -\varepsilon^0_{ij}(z) + A_{ij} + B_{ij}z \tag{4}$$

where A_{ij} and B_{ij} are constants. From the structure of the tensor $\hat{\varepsilon}^0$, it is entailed that the nonvanishing components of $\hat{\varepsilon}$ are $\varepsilon_{xx}(z) = \varepsilon_{yy}(z) = \varepsilon(z)$, $\varepsilon_{zz}(z) = -2\nu\varepsilon(z)$, where ν is the Poisson ratio, $A_{ij} = A$, and $B_{ij} = B$.

The constants A and B can be found from the conditions that the average elastic stresses $\langle\sigma_{ij}\rangle$ and the average momenta $\langle z\sigma_{ij}\rangle$ are equal to zero [6]. These conditions result in the following equations:

$$\langle\varepsilon\rangle = \frac{1}{d}\int_{-H}^{z_N} \varepsilon(z)\,\mathrm{d}z = -\langle\varepsilon^0\rangle + A + B\langle z\rangle = 0 \tag{5}$$

$$\langle z\varepsilon\rangle = \frac{1}{d}\int_{-H}^{z_N} z\varepsilon(z)\,\mathrm{d}z = -\langle z\varepsilon^0\rangle + A\langle z\rangle + B\langle z^2\rangle = 0 \tag{6}$$

from which the constants are obtained as

$$A = \langle\varepsilon^0\rangle - \frac{\langle z\varepsilon^0\rangle - \langle z\rangle\langle\varepsilon^0\rangle}{\langle z^2\rangle - \langle z\rangle^2}\langle z\rangle \tag{7}$$

$$B = \frac{\langle z\varepsilon^0\rangle - \langle z\rangle\langle\varepsilon^0\rangle}{\langle z^2\rangle - \langle z\rangle^2}. \tag{8}$$

Introducing (7) and (8) into (4), one finds the following expression for the elastic strain $\varepsilon(z)$:

$$\varepsilon(z) = -\varepsilon^0(z) + \langle\varepsilon^0\rangle + \frac{\langle z\varepsilon^0\rangle - \langle z\rangle\langle\varepsilon^0\rangle}{\langle z^2\rangle - \langle z\rangle^2}(z - \langle z\rangle). \tag{9}$$

After some algebra, we have

$$\langle\varepsilon^0\rangle = \frac{1}{d}\int_{-H}^{z_N} \varepsilon^0(z)\,\mathrm{d}z = \frac{1}{d}\sum_{i=1}^{N} f_i \int_{z_{i-1}}^{z_i} \mathrm{d}z = \frac{1}{d}\sum_{i=1}^{N} f_i h_i \tag{10}$$

$$\langle z\varepsilon^0\rangle = \frac{1}{d}\int_{-H}^{z_N} z\varepsilon^0(z)\,\mathrm{d}z = \frac{1}{d}\sum_{i=1}^{N} f_i \int_{z_{i-1}}^{z_i} z\,\mathrm{d}z = \frac{1}{2d}\sum_{i=1}^{N} f_i h_i (z_i + z_{i-1}) \tag{11}$$

$$\langle z\rangle = \frac{1}{d}\int_{-H}^{z_N} z\,\mathrm{d}z = \frac{z_N^2 - H^2}{2d} = \frac{z_N - H}{2} \tag{12}$$

$$\langle z^2\rangle = \frac{1}{d}\int_{-H}^{z_N} z^2\,\mathrm{d}z = \frac{z_N^3 + H^3}{3d}. \tag{13}$$

Introducing (1) and (10)–(13) into (9), we obtain the elastic strain distribution in the form:

$$\varepsilon(z) = \sum_{i=1}^{N} f_i \left\{\Theta(z - z_i) - \Theta(z - z_{i-1}) + \frac{h_i}{d^3}\left[d^2 + 3(H - z_N + 2z)\Psi_i\right]\right\} \tag{14}$$

where $\Psi_i = H - z_N + z_i + z_{i-1}$.

To illustrate the result found, let us consider two simple limiting cases.

First, let us discuss the case with $f_i \equiv f$ and $h_i \equiv h$—that is, the case of a thin single-layer film specified by both the thickness $h' = Nh$ and the misfit eigenstrain f, and deposited on a thick substrate with the thickness H. In this case, our general formula (14) is reduced to the following expression:

$$\varepsilon(z) = f\left\{-\Theta(z) + \frac{h'}{d} + \frac{3h'H(H-h')}{d^3} + \frac{6h'H}{d^3}z\right\} \tag{15}$$

which is well known in the theory of heteroepitaxial systems [6].

Second, let us consider the case with $h_i \equiv h$ and $f_i \equiv f$, if $i = 1, 3, \ldots, N-1$, and $f_i \equiv 0$, if $i = 2, 4, \ldots, N$, where N is an even number. This case corresponds to a superlattice deposited on a thick substrate. In the case discussed, the general expression (14) is transformed into the formula

$$\begin{aligned}\varepsilon(z) = f\Bigg\{ &\sum_{n=1}^{2(N-1)} (-1)^n \Theta[z-(n-1)h] \\ &+ (N-1)\frac{h}{d}\left[1 + \frac{3}{d^2}[H + h(N-3)](H - Nh + 2z)\right]\Bigg\}.\end{aligned} \tag{16}$$

The strain energy of the system (per unit surface square) can be written as

$$W = 2G\frac{1+\nu}{1-\nu}\int_{-H}^{z_N} \varepsilon^2(z)\,\mathrm{d}z \tag{17}$$

where G is the shear modulus. Substituting (14) into (17), after some cumbersome calculations, we find the following result:

$$\begin{aligned}W = 2G\frac{1+\nu}{1-\nu}\int_{-H}^{z_N} \Bigg\{ &\sum_{i=1}^{N} f_i^2 \left[\Theta(z - z_{i-1}) - \Theta(z - z_i)\right] \\ &+ \frac{2}{d^3}\sum_{i,j=1}^{N} f_i f_j h_j \left[\Theta(z - z_i) - \Theta(z - z_{i-1})\right]\left[d^2 + 3\Psi_j(H - z_N + 2z)\right] \\ &+ \frac{1}{d^6}\sum_{i,j=1}^{N} f_i f_j h_i h_j \\ &\times \left[d^4 + 3d^2(\Psi_i + \Psi_j)(H - z_N + 2z) + 9\Psi_i\Psi_j(H - z_N + 2z)^2\right]\Bigg\}\,\mathrm{d}z \\ = 2G\frac{1+\nu}{1-\nu} & \\ \times \Bigg\{ &\sum_{i=1}^{N} f_i^2 \int_{z_{i-1}}^{z_i} \mathrm{d}z - \frac{2}{d^3}\sum_{i,j=1}^{N} f_i f_j h_j \int_{z_{i-1}}^{z_i} \left[d^2 + 3\Psi_j(H - z_N + 2z)\right]\mathrm{d}z \\ &+ \frac{1}{d^6}\sum_{i,j=1}^{N} f_i f_j h_i h_j \\ &\times \int_{-H}^{z_N} \left[d^4 + 3d^2(\Psi_i + \Psi_j)(H - z_N + 2z) + 9\Psi_i\Psi_j(H - z_N + 2z)^2\right]\mathrm{d}z\Bigg\} \\ = 2G\frac{1+\nu}{1-\nu}\Bigg\{ &\sum_{i=1}^{N} f_i^2 h_i - \frac{1}{d^3}\sum_{i,j=1}^{N} f_i f_j h_i h_j (d^2 + 3\Psi_i\Psi_j)\Bigg\}.\end{aligned} \tag{18}$$

In the first limiting case with $f_i \equiv f$, $h_i \equiv h$, and $N = 1$ (for simplicity), formula (18) gives

$$W = 2G\frac{1+\nu}{1-\nu}f^2 h\left(1 - h\frac{d^2 + 3H^2}{d^3}\right). \tag{19}$$

From (19), for $h \ll H \approx d$, we have the well known expression [5, 6] for the misfit energy in the simplest case of a thin film on a semi-infinite substrate:

$$W(h \ll H \approx d) \approx 2G\frac{1+\nu}{1-\nu}f^2h. \tag{20}$$

As a result, we have obtained a general expression (18) which can be effectively used for analysis of various models of misfitting multilayer composites. The above approach can also be directly generalized to the situation with different elastic moduli of the layer and substrate materials.

3. Misfit strains and phase transformations at interphase boundaries in layered composites

Let us consider with the help of the results obtained in the previous section a phase transformation occurring at the interphase boundary in a two-layer composite consisting of layers α and β. The phase transformation causes the pre-existing two-layer system to be transformed into a three-layer system with an intermediate layer (new phase) α–β (figure 2). Such phase transformations commonly result from diffusional mixing of atoms of the phases α and β; see e.g. [9–15]. In the context of our paper, we will examine the new three-layer composite as a misfitting system (characterized by two misfit parameters) with special attention being paid to the role of misfit strains in initiating the intermediate-layer formation—that is, the phase transformation at the interphase boundary in the pre-existing two-layer composite.

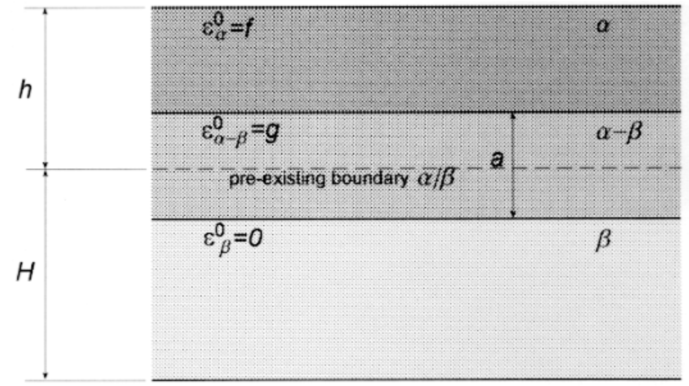

Figure 2. A three-layer composite consisting of 'edge' layers α and β and an intermediate layer (new phase) α–β. The pre-existing interphase boundary α/β is shown as a dashed line.

Let the thickness of the new three-layer system be $d = H + h$, in which case the new phase α–β forms an intermediate layer with the thickness a—that is, the layer between the initial film α and the substrate β characterized by the values $h - a/2$ and $H - a/2$, respectively, of the thickness (figure 2). Also, let us suppose that the eigenstrains of the dilatation misfit are f and g respectively in the layers α and α–β relative to the layer β characterized by the eigenstrain $\varepsilon^0 \equiv 0$.

The strain energy density of the three-layer composite (figure 2) is given by formula (18), which can be rewritten in the situation discussed as follows:

$$W_2^c = W_1^c + 2G\frac{1+\nu}{1-\nu}f^2a\left\{\phi_0 + \phi_1\frac{a}{d} + \phi_2\left(\frac{a}{d}\right)^2 + \phi_3\left(\frac{a}{d}\right)^3\right\} \tag{21}$$

where

$$\phi_0 = -\frac{1}{2} + \left(1 - 2\frac{g}{f}\right)\frac{h}{d}\left(1 + 3\frac{H(H-h)}{d^2}\right) + \frac{g^2}{f^2}$$
$$\phi_1 = -\frac{1}{4}\left(1 + 3\frac{H^2 + h^2 - 4Hh}{d^2}\right) + \frac{g}{f}\left(1 - \frac{g^2}{f^2}\right)\left(1 + 3\frac{(H-h)^2}{d^2}\right)$$
$$\phi_2 = -\frac{3}{4}\left(1 - 2\frac{g^2}{f^2}\right)\frac{H-h}{d}$$
$$\phi_3 = -\frac{3}{16}$$

and W_1^c is the strain energy density of the pre-existing composite consisting of layers α and β only (see formula (19)).

Formula (21) is indicative of the fact that the strain energy density W_2^c depends, generally speaking, in a nonlinear way on the thickness a of the layer α–β as well as on the other parameters h, H, f and g of the three-layer composite. At the same time, in the limiting situation with an infinitely thick substrate ($H, d \to \infty$), the dependence of $\Delta W^c = W_2^c - W_1^c$ on a is linear:

$$\Delta W^c \approx 2G\frac{1+\nu}{1-\nu}f^2 a\left(\frac{g^2}{f^2} - \frac{1}{2}\right).$$

In this situation, ΔW^c does not depend on the film thickness h and, as a corollary, the intermediate-layer formation is energetically favourable ($\Delta W^c < 0$) or unfavourable ($\Delta W^c > 0$) depending on the ratio g^2/f^2. More precisely, the formation in question is energetically favourable ($\Delta W^c < 0$) at $g^2/f^2 < 1/2$—that is, at $|g| < |f|/\sqrt{2}$.

Now let us turn to the analysis of the situation with layers α and β having the same thickness—that is, $H = h$ and $d = 2h$. In this situation, $\phi_0 = -g/f + g^2/f^2$, $\phi_1 = 1/8 + g/f - g^2/f^2$, $\phi_2 = 0$, $\phi_3 = -3/16$, and, as a corollary,

$$W_2^c = W_1^c + 2G\frac{1+\nu}{1-\nu}f^2 a\left\{-\frac{g}{f} + \frac{g^2}{f^2} + \left(\frac{1}{8} + \frac{g}{f} - \frac{g^2}{f^2}\right)\frac{a}{d} - \frac{3}{16}\left(\frac{a}{d}\right)^3\right\}. \tag{22}$$

Here

$$W_1^c = \frac{G}{4}\frac{1+\nu}{1-\nu}f^2 h.$$

Let us examine with the help of (22) the initial stage of the intermediate-layer formation. In doing so, we focus our attention on the situations with $f > g > 0$ or $-f < -g < 0$, because the formation of the intermediate layer in other situations leads to the increase of the misfitting of a layered composite and, therefore, is definitely unfavourable from an energetic viewpoint. The intermediate layer at the initial stage of its formation is characterized by the thickness $a \ll d$. This allows us to neglect the term proportional to $(a/d)^3$ on the r. h. s. of formula (22). In doing so, from the reduced version of formula (22) (with the aforesaid term omitted) it is entailed that the intermediate-layer formation is energetically favourable ($\Delta W^c < 0$), if $h > h_c$, where the critical thickness

$$h_c \approx \frac{a}{2}\left(1 + \frac{f^2}{8g(f-g)}\right). \tag{23}$$

Formula (23), in particular, is indicative of the fact that there is a minimal critical thickness

$$h_{c,min} \approx \frac{3}{4}a \tag{24}$$

which corresponds to the situation with $g = f/2$. The critical thickness at $g \to 0$ is

$$h_c \approx \frac{a}{2}\left(1 + \frac{f}{8g}\right)$$

and it decreases with increasing g and increases with increasing f. When $g \to f$,

$$h_c \approx \frac{a}{2}\left(1 + \frac{f}{8(1 - g/f)}\right)$$

and it increases with increasing g and decreases with increasing f. The dependence of ΔW^c and h_c on f and g is shown schematically in figure 3.

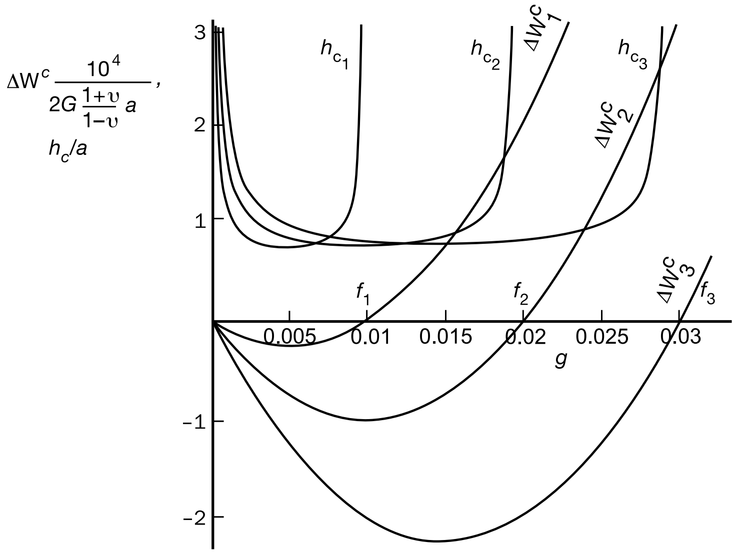

Figure 3. Dependences of ΔW^c and h_c on f and g (shown schematically).

Let us estimate numerically the value of h_c in the situation with nucleation of an intermediate layer—that is, the situation with the layer (as the layer of a new phase) characterized by the minimal thickness a_{min}. (The new phase should consist of, at least, several atomic layers, in which case a_{min} is commonly of the order of 1 nm.) Let the misfit parameter in the pre-existing two-layer system be $f = 0.01$. In these circumstances, for values of $g = 0.008$, 0.009 and 0.0099, from (24) we find the critical thicknesses $h_c \approx a_{min}$, $1.2a_{min}$, $500a_{min}$, respectively.

In our consideration, we have focused on the effect of misfit strains on phase transformations in layered composites. At the same time, in general, other factors also influence such transformations. First of all, the difference W^{a-c} between the free-energy (or another thermodynamic potential) densities of the pre-existing phases (α and β) and a new phase (α–β) usually plays an important role in phase transformations in layered composites. In these circumstances, any comparison of the quantitative estimates (e.g., values of h_c and $h_{c,min}$, the dependence of ΔW^c and h_c on f and g) obtained in this section using experimental data as well as other theoretical estimates seems to be unreasonable, because many other factors should be taken into account. A detailed labour-consuming analysis of the contribution of W^{a-c} to the energetic characteristics of intermediate-layer formation (figure 2), as well as other factors (different from misfit strains) affecting phase transformations of all types in layered composite solids, is beyond the scope of this paper. In the next section, we examine theoretically the only type of such transformations—namely the solid-state amorphizing transformations in layered composites, taking into account the misfit strain energy density and other energetic characteristics of the new phase—that are capable of influencing the amorphization processes.

4. Misfit strains and solid-state amorphization in layered composites

Solid-state amorphizing transformations occur in multilayer composite solids consisting of alternate layers, say, α and β, of elemental metals; see e.g. [9–13]. In these circumstances, layers of the new amorphous alloyed phase α–β nucleate at α/β interfaces due to diffusional mixing of atoms α and β. Recently, it has been experimentally revealed that solid-state amorphization does not occur in Ni/Ti multilayer composites having the crystalline layer thickness in a composite below some critical thickness h_c^{am} (which is several nanometres) [13]. We think that this experimental fact gives evidence of a strict relationship between misfit strains (whose contribution to the energy of a composite is dependent on the layer thickness; see sections 2 and 3) and the amorphization processes. More precisely, in the context of our previous consideration of the intermediate-layer formation in a film α/substrate β system, the amorphization occurs as a process with relaxation of misfit strains contributing to its driving force. In this section, we will theoretically examine with the help of results obtained in previous sections the effect of misfit strains on the solid-state amorphization in layered composites. In doing so, we also take into account both the energy density of crystal/glass interfaces resulting from the amorphization and the difference W^{a-c} between the free-energy densities of the (new) amorphous and (pre-existing) crystalline phases.

Let us consider the formation of an intermediate amorphous layer α–β in an initially two-layer system consisting of crystalline layers α and β (figure 2). The amorphous-layer formation is accompanied, in particular, by the occurrence of two crystal/glass interfaces. Following the model of [17] of crystal/glass interfaces, the total energy density E_i^{tot} of a crystal/glass interface can be represented as the sum of the two basic terms, E_i^{dil} and E_i^{dis}, which are related to the dilatation misfit (originating from the difference between the mean interatomic distance in the amorphous phase and the crystal lattice parameters of the adjacent crystalline phases) and disorder-induced distortions (originating from distortions of the adjacent amorphous phase), respectively. In the context of our paper, in the theoretical examination of the amorphous-layer formation in a pre-existing two-layer crystalline composite, we will operate with dilatation misfit strains induced by crystal/glass interfaces and their energy density E_i^{dil} by means of methods developed in previous sections, in which case it is identified as the energy density W_2^c. At the same time, the energy density E_i^{dis} will be taken into account as a parameter contributing to the energetic criterion for the amorphous-layer formation (see below).

Let us consider the amorphous layer at the initial stage of its nucleation in a two-layer composite. It is characterized by the minimal thickness a_{min}, the dilatation misfit energy density W_2^c, and the energy density $E_{am}(a_{min})$ (per unit area) which is the sum of its proper free-energy density $W^{a-c}a_{min}$ and the energy density $2E_i^{dis}$ of two (new) crystal/glass interfaces ($E_{am}(a_{min}) = W^{a-c}a_{min} + 2E_i^{dis}$). The energy density $E_{am}(a_{min})$ is included in the energetic criterion for amorphous-layer formation, which is as follows:

$$\Delta W^c + E_{am}(a_{min}) < 0. \tag{25}$$

With criterion (25) taken into account, we find after some analysis the following formula for the critical thickness h_c^{am}:

$$h_c^{am} \approx \frac{a}{2(1-E)}\left(1 + \frac{f^2}{8g(f-g)}\right) = \frac{h_c^{cr}}{1-E} \tag{26}$$

where

$$E = \frac{E_{am}(1-\nu)}{2G(1+\nu)ag(f-g)} < 1 \tag{27}$$

and h_c is given by formula (23). In general, h_c^{am} can take widely varying values, depending on E_{am}. In particular, the amorphization does not occur in composites with high values of E_{am} (and, therefore, high values of h_c^{am}).

Let us discuss the effect of the terms $W^{a-c}a_{min}$ and E_i^{dil} (which are treated here as parameters) on the amorphization. The traditional viewpoint on the solid-state amorphization in layered composites, which does not take into account misfit strains, is that the driving force for the amorphization is associated with a negative W^{a-c} [9]. Within the framework of these representations, the amorphization occurs if $W^{a-c} < 0$, and does not occur if $W^{a-c} > 0$. However, recently, amorphization has been experimentally observed in immiscible Y/Mo multilayer composites characterized by $W^{a-c} > 0$ [11]. This is indicative of the crucial effect of interfaces on the amorphization. In the paper [11], this effect was analysed by the methods of thermodynamics, operating with the fraction of interfacial atoms as the key factor. However, the approach of [11] does not allow one to explain the experimentally revealed [13] existence of the minimal critical thickness h_c^{am} for the amorphization in Ni/Ti multilayer composites. As a corollary, in the context of the theoretical results obtained here, we think that misfit strains play a very important role in the amorphization processes and should definitely be taken into account in any description of the processes in question.

5. Concluding remarks

Here we have calculated in a general form both misfit strains and their energy density in multilayer solid composites. The results of these calculations can be effectively used in examinations of the structural stability and the effect of misfit strains on the macroscopic properties of layered composites. Thus, a general formula (18) for the misfit energy density has been applied in this paper to the analysis of the role of misfit strains in initiating phase transformations in layered composites, which are related to diffusional mixing in the vicinity of interphase boundaries. This role has been revealed to be important, with misfit strains crucially influencing the formation of new phases in layered composites.

Solid-state amorphizing transformations in layered composites have been theoretically examined here as phase transformations affected by misfit strains. It has been found that there is a minimal critical thickness h_c^{am} which characterizes the solid-state amorphization in layered composites: composites consisting of layers with thicknesses whose values are above (or below, respectively) h_c^{am}, are amorphized (or are not amorphized, respectively). The experimental data [11] on the crucial role of interfaces in the amorphization processes in layered composites and the experimental data [13] on the existence of the minimal critical thickness h_c^{am} in Ni/Ti multilayer composites are in agreement with the theoretical results obtained in this paper. These results, indicating the special role of interphase boundaries (plane defects) in amorphization processes in layered composites, supplement the theoretical representations [18–21] of the important contribution of defects to solid-state amorphization processes in crystals.

Acknowledgments

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