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A new relaxation mechanism in nanoscale films

I A Ovid'ko and A G Sheinerman

Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61,
Vasilyevskiy Ostrov, St Petersburg 199178, Russia

E-mail: ovidko@def.ipme.ru

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Abstract

A new mechanism of stress relaxation in heteroepitaxial films of nanoscale thickness is suggested and theoretically described. The mechanism represents nucleation of a 'non-crystallographic' partial dislocation (at the film–substrate interface) whose Burgers vector magnitude continuously grows during the nucleation process. It is shown that the new mechanism effectively competes with the standard nucleation of a perfect misfit dislocation at the free surface of the film and its further glide towards the film–substrate interface.

(Some figures in this article are in colour only in the electronic version)

Thin solid films are the subject of intensive research efforts motivated by their diverse technological applications and an interest in the fundamental physical phenomena occurring in these films. Both the structure and physical properties of flat and island films are strongly influenced by misfit stresses whose relaxation often occurs by the nucleation of misfit dislocations (MDs) in film–substrate composite solids (see, for example, [1–17]). MDs in flat films form if the film thickness exceeds a critical value, which depends on the misfit between the crystal lattice parameters of the film and the substrate (see, for example, the pioneering works [18–20], reviews [21, 22] and book [23]). In most cases, the critical thickness does not exceed 100 nm. That is, MDs commonly nucleate in solid films of nanoscale thickness (hereinafter called nanoscale films).

Two mechanisms for the formation of MDs in epitaxial films are considered as standard. The first mechanism incorporates the nucleation and subsequent expansion of MD segments produced by dislocations arising from the substrate and threading the film [19–23]. The second mechanism involves the nucleation of MD semi-loops at the film surface, their subsequent glide to the film–substrate interface and further expansion [21–23] (see the two-dimensional schematic illustration in figures 1(a)–(d)). Both mechanisms require that dislocations overcome a rather high energy barrier, which appears either due to the attraction between parallel threading dislocation segments or as a result of the attraction of MDs to the film surface. These mechanisms for MD formation are conventionally examined in estimates

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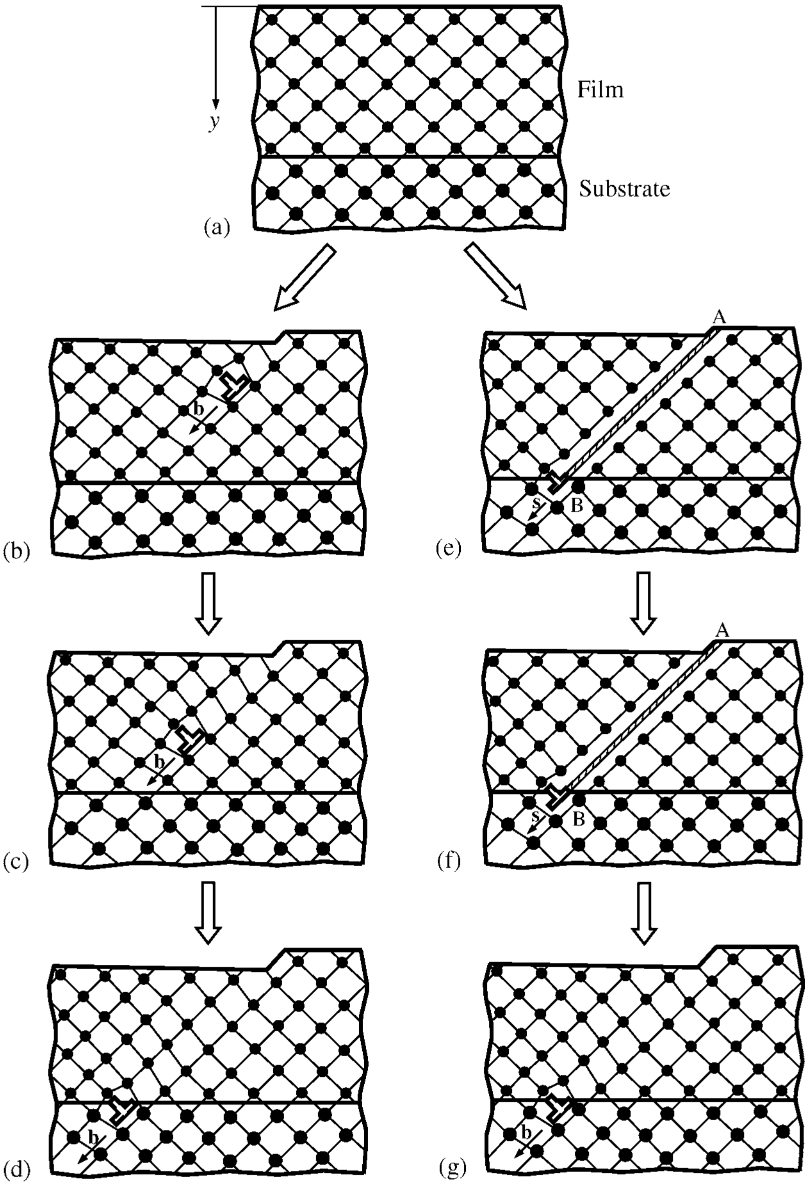

Figure 1. Mechanisms for misfit stress relaxation in nanoscale films (two-dimensional schematic representation). (a)–(d) Standard relaxation mechanism is realized by (a) generation of a misfit dislocation at the free surface of the film and (b), (c) its further glide towards the film–substrate boundary where (d) the dislocation stops. (e)–(g) The new relaxation mechanism involves a nanoscale ideal shear. (e) A nanoscale ideal shear occurs along plane fragment AB and results in the formation of both a non-crystallographic partial dislocation with Burgers vector of infinitesimal magnitude s and stacking fault AB. (f) The Burgers vector magnitude s continuously increases and (g) reaches the magnitude b that characterizes a conventional misfit dislocation (perfect lattice dislocation).

and analyses of critical parameters—film thickness and misfit—of solid films, at which MDs are nucleated [21–23]. However, misfit stress relaxation in nanoscale films may also occur by a new alternative mechanism, namely the nucleation of a 'non-crystallographic' partial dislocation located at the film–substrate interface and characterized by a Burgers vector of magnitude s growing from zero to the magnitude b of a perfect lattice dislocation (figures 1(a), (e)–(g)). The main aim of this paper is to elaborate a theoretical model and give an energy analysis of the new relaxation mechanism in nanoscale films. We will show that the energy barrier for formation of MDs by the new mechanism is lower than that by the standard mechanism for certain ranges of film parameters.

Let us discuss the difference between the new relaxation mechanism and the standard mechanism incorporating the glide of MDs from the film surface towards the film–substrate interface. At the beginning action of the standard mechanism in a nanoscale film, a MD nucleates at the free surface of the film (figures 1(a) and (b)). Then the dislocation glides towards the film–substrate interface (figures 1(b) and (c)), where it stops (figure 1(d)). During the standard MD nucleation and glide processes (figures 1(a)–(d)), the magnitude b of its Burgers vector is always constant [21–23].

The new mechanism for MD nucleation (figures 1(a), (e)–(g)) operates as follows. First, a local momentary ideal shear (a rigid-body shear of the left part of the film relative to its right part) occurs along the nanoscale plane fragment AB (figure 1(e)). The momentary ideal shear is characterized by a small shear of magnitude s and produces a planar stacking fault AB of a finite nanoscopic length (figure 1(e)). The stacking fault ends at a 'non-crystallographic' partial dislocation characterized by a non-quantized Burgers vector $\boldsymbol{s}$ with quite a small magnitude $s \ll b$ (figure 1(e)). Then, due to the action of misfit stresses, the Burgers vector magnitude s of the partial dislocation continuously increases (figure 1(f)). Finally, the Burgers vector magnitude s reaches the Burgers vector magnitude b of a perfect dislocation (figure 1(g)), in which case the stacking fault disappears. (In general, the mechanism can stop at the stage shown in figure 1(f), in which case it produces a partial dislocation similar to those experimentally observed in heteroepitaxial films [24–27].)

The final state of the film (figure 1(g)) relaxed by the new mechanism is identical to that (figure 1(d)) of the film relaxed by the standard mechanism. Therefore, the difference between the mechanisms cannot be identified by conventional *ex situ* experiments. Also, the new mechanism can hardly be identified by *in situ* x-ray topography, which is able to detect the moment of MD nucleation but not the exact geometry of the nucleation process. At the same time, the new relaxation mechanism in nanoscale films is analogous to that effectively operating in Gum Metal, a special titanium alloy with a low resistance to shear in certain crystallographic planes [28, 29]. Following [29], plastic flow in Gum Metal is carried by nanodisturbances, nanoscale dipoles of 'non-crystallographic' partial dislocations with continuously growing Burgers vector magnitudes. Also, a similar mechanism for plastic relaxation by nanoscale ideal shear events can operate in nanocomposites [30] and nanocrystalline metals [31] where conventional mechanisms for dislocation nucleation in nanoscale grains are suppressed (see, for example, [32–34]). The nucleation of lattice dislocations in nanoscale grains of nanocrystalline metals is energetically unfavourable, in particular due to the image forces causing a strong attraction of the dislocations to grain boundaries [35]. Similar image forces cause the strong attraction of MDs to the free surface of the film and thereby a high energy barrier for the standard MD nucleation at the surface (figures 1(a) and (b)) [21–23]. In contrast, the image forces are negligibly small in the case where a MD nucleates by the new mechanism far from the free surface (figures 1(a), (e)–(g)). This allows us to think that the new relaxation mechanism can operate in nanoscale films, although its experimental identification is difficult.

Let us calculate the energy characteristics of the new relaxation mechanism and compare them with those of the standard mechanism. To do so, consider a model nanoscale film of thickness H on a model semi-infinite substrate. The film and substrate are considered to be elastically isotropic crystalline solids with identical shear moduli G and Poisson ratios ν. The misfit f of the parameters a_s and a_f of the substrate and film crystal lattices, respectively, is assumed to be purely dilatational and defined as $f = (a_s - a_f)/a_f$.

First consider the standard formation of a MD via its glide from the film surface towards the film–substrate interface (figures 1(a)–(d)). We denote the film thickness as H and suppose that the MD is of the 60° type. Let us introduce a Cartesian coordinate system (x, y, z) whose $0xz$ plane coincides with the film surface with the y-axis directed inside the film. In this coordinate system, the MD line is distant by y from the free surface of the film and is supposed to have the direction $[\bar{1}, 0, 1]$ while the MD Burgers vector $\mathbf{b}$ is equal to $(b[\bar{1}, 1, 0]/\sqrt{2})\,\mathrm{sgn}\, f$. With these parameters, one can calculate the energy change ΔW_C that characterizes the standard MD nucleation (figures 1(a)–(d)) and is defined as the difference between the energies of the system in its final (dislocated) and initial (dislocation-free) states. In the spirit of the general theory of MDs [21–23], the energy change is given as:

$$\Delta W_C = \frac{D(b_e^2 + (1-\nu)b_s^2)}{2}\left[\ln\frac{2y}{b} + 1\right] - 2\pi D b(1+\nu)|f|y, \tag{1}$$

where $D = G/[2\pi(1-\nu)]$, while $b_e = b\sqrt{3}/2$ and $b_s = b/2$ are the magnitudes of the edge and screw components of the MD Burgers vector, respectively. The first term on the right-hand side of formula (1) describes the MD self-energy (including the energy of the dislocation core) and the second term specifies the energy of the interaction between the MD and the misfit stress field.

From formula (1) it follows that ΔW_C reaches its maximum value at some value $y = y_c$ of the coordinate y and is equal to the energy barrier that the MD has to overcome to be introduced into the film. For $y < y_c$, the MD is repelled from the film–substrate interface. For $y > y_c$, the MD is attracted to the film–substrate interface. The thickness y_c of the near-surface film region where the presence of MDs is energetically unfavoured is derived from the condition $(\partial \Delta W_C/\partial y)|_{y=y_c} = 0$ as $y_c = (4-\nu)b/(16\pi(1+\nu)|f|)$. (For typical values of $b = 0.3$ nm and $\nu = 0.3$, the thickness y_c approximately ranges from 2 to 20 nm, when $|f|$ diminishes from 0.01 to 0.001.) The corresponding magnitude W_b of the energy barrier is $W_\mathrm{b} = \Delta W_C(y = y_c) = -(4-\nu)\,(Db^2/8)\,\ln[8\pi(1+\nu)|f|/(4-\nu)]$.

Now we examine the new mechanism for MD nucleation (figures 1(e)–(g)). Let us consider a non-crystallographic partial 60° dislocation with the Burgers vector ($\boldsymbol{s} = s[\bar{1}, 1, 0]/\sqrt{2})\,\mathrm{sgn}\, f$ (where s ranges from 0 to b), located at the film–substrate interface and connected with the film surface by a stacking fault (figure 1(e)). The energy change ΔW_P, characterizing the formation of such a dislocation, is as follows:

$$\Delta W_P = \frac{(4-\nu)\,Ds^2}{8}\left[\ln\frac{2H}{s} + 1\right] - 2\pi D s(1+\nu)|f|H + \gamma(s/b)H\sqrt{2}, \tag{2}$$

where $\gamma(s/b)$ is the specific energy of the stacking fault associated with the partial dislocation with a Burgers vector magnitude s. The first term on the right-hand side of formula (2) describes the partial dislocation self-energy (including its core energy), the second term specifies the energy of its interaction with the misfit stress field, and the third term describes the stacking fault energy as a function of s. The first and second terms on the right-hand side of formula (2) are well defined and conventionally used in the theory of MDs in films. The dependences $\gamma(s)$ (figuring in the third term on the right-hand side of formula (2)) have been calculated for several materials and stacking fault planes using various computer simulation techniques (see, for example, [36–41]).

Let us use formula (2) in estimates of the energy barrier for MD nucleation by the new mechanism in typical metallic and semiconductor film/substrate systems. More precisely, we

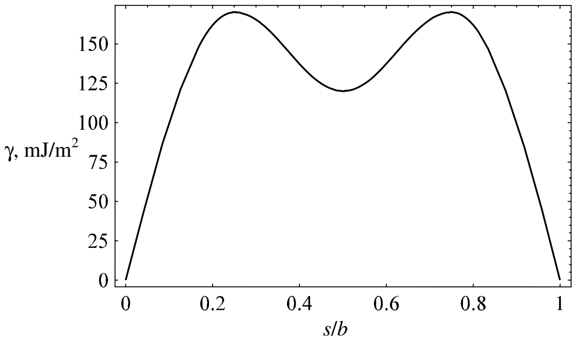

Figure 2. Dependence of the specific energy γ of a generalized stacking fault in nanocrystalline Ni on the normalized magnitude s/b of the dislocation Burgers vector (according to the approximate formula given in [44]).

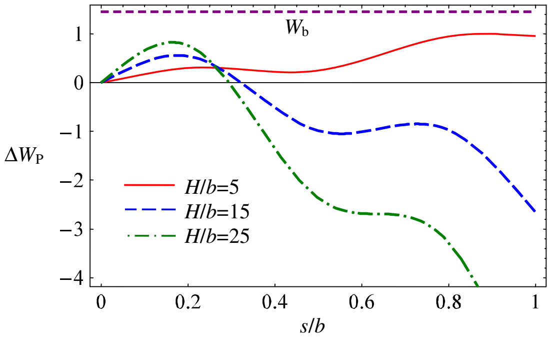

Figure 3. Dependences of energy change ΔW_P (characterizing the new relaxation mechanism) on dimensionless magnitude s/b of the partial dislocation Burgers vector for Ni/Cu systems. The horizontal line shows the value of the energy barrier W_b for MD formation by the standard mechanism. The energies ΔW_P and W_b are given in units of $(4-\nu)\,Db^2/8$.

consider the exemplary cases of a metallic 'Ni film/Cu substrate' system (showing remarkable magnetic properties) and semiconductor 'SiGe film/Si substrate' system (being of particular significance in semiconductor technologies).

In the case of a Ni/Cu system, we have [42, 43] $f = -0.026$, $G = 73$ GPa, $\nu = 0.34$, $b = 0.249$ nm. To estimate $\gamma(s)$, we take advantage of the following formula for the specific energy of the generalized stacking fault, suggested for nanocrystalline Ni [44]:

$$\gamma(s/b) = \begin{cases} \gamma_m \sin\dfrac{2\pi s}{b}, & s/b < 1/4, \\ \dfrac{\gamma_m + \gamma_0}{2} - \dfrac{\gamma_m - \gamma_0}{2}\cos\dfrac{4\pi s}{b}, & 1/4 \leqslant s/b < 3/4, \\ -\gamma_m \sin\dfrac{2\pi s}{b}, & 3/4 \leqslant s/b \leqslant 1. \end{cases} \tag{3}$$

Here γ_m and γ_0 are the maximum and minimum values of the specific energy $\gamma(s)$ of the generalized stacking fault that correspond to an unstable and stable stacking fault configuration, respectively; $\gamma_m \approx 0.17$ J m^{-2} and $\gamma_0 \approx 0.12$ J m^{-2}. The dependence $\gamma(s/b)$ is shown in figure 2.

The dependences $\Delta W_P(s/b)$ for a Ni/Cu system are shown in figure 3. The horizontal dashed line shows the value of the energy barrier W_b for the formation of a perfect 60°

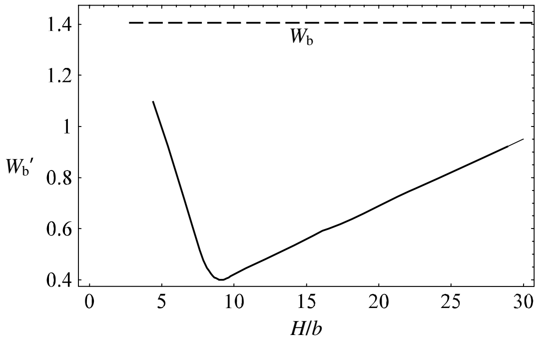

Figure 4. Dependence of the energy barrier W_{b}' (for the formation of a perfect MD by the new mechanism) on the normalized film thickness H/b for Ni/Cu systems. The horizontal line shows the value of the energy barrier W_{b} for MD formation by the standard mechanism. The energies W_{b}' and W_{b} are given in units of $(4-\nu)\,Db^2/8$.

dislocation by the standard mechanism. The energy W_{b} is shown for the case $H > y_c$ ($\approx 2.1b$ for Ni/Cu systems). If $H < y_c$, perfect MDs are repelled from the film to the surface, and the formation of stable MDs by the standard mechanism is not possible. As follows from figure 3, the dependences $\Delta W_P(s/b)$ have different characters, depending on H. However, if the length of the generalized stacking fault is not very great, the energy barrier for the formation of a perfect MD by the new mechanism (the barrier in question is equal to the highest value of ΔW_P within the interval $0 \leqslant s \leqslant b$) is smaller than the energy barrier W_{b} for MD formation by the standard mechanism. The necessary (although not sufficient) condition for the formation of a perfect MD by the new mechanism is $(\partial\Delta W_P/\partial s)|_{s=b} \leqslant 0$. As follows from figure 3, this condition is valid if the film is not very thin (see dashed and dotted curves in figure 3). At the same time, for very thin films, MD formation by the new mechanism is not possible (see the solid line in figure 3). This means that MD formation by the new mechanism is possible if the thickness of the film exceeds a critical value, as with the case of MD formation by the standard mechanism.

The energy barrier W_{b}' for the formation of a perfect MD by the new mechanism (W_{b}' is equal to the highest value of ΔW_P within the interval $0 \leqslant s \leqslant b$) is shown in figure 4 as a function of the normalized film thickness H/b, for a Ni/Cu system. The horizontal dashed line shows the value of the energy barrier W_{b} for MD formation by the standard mechanism in this system. The horizontal line is shown for the case $H > y_c$ where MDs generated by the standard mechanism are not repelled from the film to the surface. The curves $W_{\mathrm{b}}'(H/b)$ are shown for film thicknesses $H > 4.4b$ that satisfy the necessary condition $(\partial\Delta W_P/\partial s)|_{s=b} \leqslant 0$ of perfect MD formation by the new mechanism. From figure 4 it is seen that $W_{\mathrm{b}}' < W_{\mathrm{b}}$. This implies that the nucleation of a MD by the new mechanism is easier than its formation by the standard mechanism.

From figure 4 it also follows that the dependence of W_{b}' on H/b has a minimum at a film thickness of $H/b \approx 9$. Consequently, for film thicknesses $H > 9b$, the most energetically favourable mechanism for the formation of a perfect interphase MD involves the generation of a perfect MD at the distance $9b$ from the free surface by the new mechanism, followed by its glide towards the film–substrate interface.

Now let us consider flat $\mathrm{Si_{0.5}Ge_{0.5}}$ films on Si substrates, which are of particular interest for applications in semiconductor devices. We have failed to find in the literature any experimental data on the dependence $\gamma(s/b)$ for $\mathrm{Si_{0.5}Ge_{0.5}}$. (In the case of covalent materials,

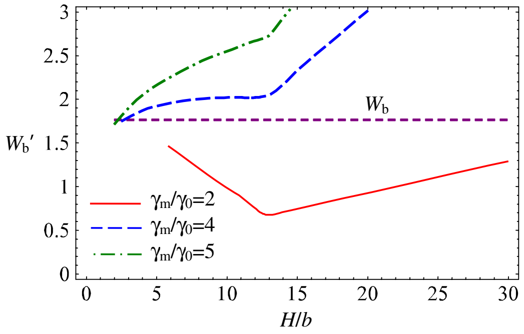

Figure 5. Dependences of the energy barrier W_b' (for the formation of a perfect MD by the new mechanism) on the normalized film thickness H/b for $Si_{0.5}Ge_{0.5}/Si$ systems. The horizontal line shows the value of the energy barrier W_b for MD formation by the standard mechanism. The energies W_b' and W_b are given in units of $(4 - \nu)\, Db^2/8$.

the dependences $\gamma(s/b)$ have been simulated for silicon [37, 41]. However, the results of these computer simulations are rather controversial and can hardly be used as a basis for our estimates of the dependence $\gamma(s/b)$ of SiGe alloy, because $\gamma(s/b)$ is, in general, highly sensitive to the chemical composition and temperature.) In these circumstances, in order to estimate the energy barrier W_b' for the formation of a perfect MD in a SiGe/Si system, in the first approximation, we will use the dependence of $\gamma(s/b)$ given by formula (3), put γ_0 equal to the specific stacking fault energy in SiGe ($\gamma_0 = 0.06$ [45]) and consider the cases where γ_m takes different values. Other parameters of $Si_{0.5}Ge_{0.5}/Si$ system, used in formula (3), are as follows: $f = -0.02$, $G = 45.6$ GPa, $\nu = 0.27$, $b = 0.392$ nm.

Figure 5 illustrates the energy barrier W_b' (for the formation of a perfect MD by the new mechanism in a $Si_{0.5}Ge_{0.5}/Si$ system) versus the normalized film thickness H/b, for various values of γ_m. The horizontal dashed line shows the value of the energy barrier W_b for MD formation by the standard mechanism in $Si_{0.5}Ge_{0.5}/Si$. As in figure 4, the horizontal line is shown for the case $H > y_c$ ($\approx 2.9b$ for $Si_{0.5}Ge_{0.5}/Si$), where MDs generated by the standard mechanism are not repelled from the film to the surface. The curves $W_b'(H/b)$ are shown for the film thicknesses which satisfy the necessary condition $(\partial \Delta W_P/\partial s)|_{s=b} \leqslant 0$ of perfect MD formation by the new mechanism. As follows from figure 5, $W_b' < W_b$, if the value of the parameter γ_m is small enough (see the lower curve in figure 5). In the case under consideration, the formation of a perfect MD in a SiGe/Si system can occur by the new mechanism. At the same time, if the value of γ_m is high (see two upper curves in figure 5) we have: $W_b' > W_b$. In this case, the formation of a perfect MD in a SiGe/Si system by the new mechanism is not likely. Thus, with the absence of valid data on the energies $\gamma(s/b)$ of generalized stacking faults in SiGe, it is not yet clear whether the new mechanism can operate in SiGe/Si systems or not. Clarification of this issue requires further computer simulations of generalized stacking fault energies and/or experimental *in situ* observations of MD nucleation in SiGe films.

Thus, in this paper a new relaxation mechanism in strained nanoscale films—the nucleation of 'non-crystallographic' partial MDs with a continuously growing Burgers vector magnitude (figures 1(e)–(g))—has been suggested. According to our analysis of the energy characteristics of this mechanism, it can effectively compete with the standard relaxation mechanism (figures 1(a)–(d)) in a wide range of parameters of heteroepitaxial films. In this context, degradation of the functional physical properties of solid films associated with MD formation should be experimentally examined and theoretically described in the future, with the features of the new relaxation mechanism taken into account. Of special importance will be experimental *in situ* observation of the MD nucleation events in nanoscale films with various compositions and geometric parameters. This potentially allows one to identify the conditions at which either the standard or the new relaxation mechanism is dominant.

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