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# Misfit Dislocation Dipoles in Nanodimensional Films with Periodically Modulated Composition

**I. A. Ovid'ko and A. G. Sheĭnerman**

*Institute for Problems of Mechanical Engineering, Russian Academy of Sciences, St. Petersburg, Russia*
*e-mail: ovidko@def.ipme.ru*

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**Abstract**—A model is suggested that describes the misfit defects of a new type—dislocation dipoles—in nanodimensional films with periodically modulated chemical composition. The critical thicknesses of such inhomogeneous films are determined, above which the formation of misfit dislocations or their dipoles becomes energetically favorable. It is shown that a critical thickness for the dislocation dipole nucleation can be smaller than that for the ordinary misfit dislocations. © *2002 MAIK "Nauka/Interperiodica".*

Nanodimensional films (nanofilms) with periodically modulated chemical compositions are promising materials for modern nano- and optoelectronic devices (see, e.g. [1]). Similarly to the case of films with homogeneous compositions, the misfit of the crystal lattice parameters between the inhomogeneous film and the substrate in such systems leads to the development of internal (misfit) stresses. In the case of homogeneous films, the misfit stresses are usually accommodated (relaxed) at the expense of formation of the misfit dislocations (see, e.g. [2–4]).

In inhomogeneous films with modulated composition, the crystal lattice parameters exhibit periodic oscillations. When the average lattice parameter of such a film coincides with that of the substrate, the misfit stresses exhibit alternating signs [5, 6]. An effective mechanism for the relaxation of such stresses is probably offered by nucleation of the misfit defects of a new type called the dislocation dipoles. The dislocation dipoles in a composition-modulated film of $Ga_{0.5}In_{0.5}P$ were observed in experiment [7]. It should be noted that similar defect configurations are effectively accommodating the internal misfit stresses in nanocrystalline films with a homogeneous composition [8].

The purpose of this study was to develop a theoretical model of misfit dislocation dipoles and to determine the critical parameters for the formation of misfit dislocations and their dipoles in the films with inhomogeneous composition.

Consider an isolated dipole formed by the edge dislocations spaced by a distance $p$, with the Burgers vectors $\mathbf{b}$ and $-\mathbf{b}$ (Fig. 1). The dislocations are situated at the interface between a semiinfinite substrate and a film with the thickness $H$. For certainty, we will consider the dipoles of 60° and 90° misfit dislocations similar to those observed in the aforementioned $Ga_{0.5}In_{0.5}P$ films [7]. In order to calculate the critical parameters for the nucleation of a misfit dislocation dipole, we will use the following assumptions of a model [5] describing composition inhomogeneities in the films free of misfit dislocations.

(i) The film and substrate are elastically isotropic solids possessing cubic crystal lattices and equal values of the shear modulus $G$ and the Poisson coefficient $\nu$.

(ii) The average crystal lattice parameter of the film with modulated composition coincides with the lattice parameter of the substrate.

(iii) The film composition modulation is the same through the entire film thickness.

(iv) The crystal lattice parameter $a$ of the film exhibits a sinusoidal variation with the coordinate $x$ along the film–substrate interface:

$$a = a_0(1 - \varepsilon_0 \cos\alpha x), \qquad (1)$$

where $a_0$ is the crystal lattice parameter of the substrate, $\varepsilon_0$ is the modulation amplitude, and $\alpha$ is the modulation frequency. The value of $\alpha$ is determined from the condition of minimum elastic energy of the film–substrate system, which is related to the crystal lattice misfit between the film and substrate. Under assumptions (i)–(iv), the misfit stresses related to modulation of the

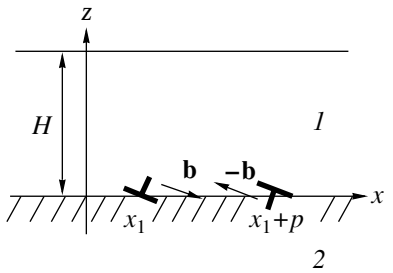


**Fig. 1.** A schematic diagram of the dislocation dipole formed at the interface between film (*1*) and substrate (*2*).

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crystal lattice parameter in the film can be calculated as described in [5].

Let us determine the conditions under which the nucleation of a misfit dislocation dipole at the film–substrate interface would energetically favorable. For this purpose, we will compare the energies of the system with and without such a dipole. In the absence of the misfit dislocations, the system energy includes only the that of elastic misfit deformation. When an isolated misfit dislocation dipole is formed, the energy $W$ per unit length represents a sum of four terms:

$$W = W^0 + W^{\mathrm{dip}} + W^{\mathrm{dip-f}} + 2W^{\mathrm{core}}, \qquad (2)$$

where $W^0$ is the energy of elastic misfit dislocations (per unit dislocation length), $W^{\mathrm{dip}}$ is the intrinsic energy of the misfit dislocation dipole, $W^{\mathrm{dip-f}}$ is the energy of interaction between the dipole and the elastic fields of misfit stresses, and $W^{\mathrm{core}}$ is the dislocation core energy. Nucleation of the misfit dislocation dipole is energetically favorable if this leads to a decrease in the total energy, that is, if $W - W^0 < 0$. Taking into account Eq. (2), this condition can be written as

$$W^{\mathrm{dip}} + W^{\mathrm{dip-f}} + 2W^{\mathrm{core}} < 0. \qquad (3)$$

In order to calculate the energy $W^{\mathrm{dip}}$ of the misfit dislocation dipole depicted in Fig. 1, we have used the stress functions [9] for an edge dislocation near the free surface. The $W^{\mathrm{dip-f}}$ value was calculated using the exact formulas [5] for the field of misfit stresses in a film with periodically modulated composition. According to [10], the dislocation core energy is $W^{\mathrm{core}} \approx Gb^2/[4\pi(1-\nu)]$. Substituting this expression for $W^{\mathrm{core}}$ and the known expressions for $W^{\mathrm{dip}}$ and $W^{\mathrm{dip-f}}$ into inequality (3), we arrive at the following condition for the misfit dislocation dipole nucleation: $H > H_c$, where $H_c$ is the critical film thickness determined from the relationship

$$8\pi(1+\nu) f_e = \frac{b_x}{H_c}\left\{\frac{(1+(b_z/b_x)^2}{2}\left[\ln\frac{2H_c}{b} - \ln\frac{p^2+4H_c^2}{p^2} + 1\right]\right. \qquad (4)$$

$$\left. + \frac{2H_c^2[(b_z/b_x)^2(12H_c^2+p^2) - (4H_c^2+3p^2)]}{(4H_c^2+p^2)^2}\right\}.$$

Here, $f_e = \varepsilon_0(0.158 + 0.0047 b_z/b_x)\sin\pi p/T$ and $T = 2\pi/\alpha$ is the period of the crystal lattice parameter modulation in the film. An analysis of formula (4) shows that the critical thickness $H_c$ has a minimum at $p = T/2$.

An equation for determining the critical thickness $H_c$ (above which the nucleation of a single dislocation at the film– substrate interface is possible) can be derived in the same manner as it was done for determining $H_c$. Figure 2 shows the critical film thicknesses $\tilde{H}_c$ and $H_c$ for the nucleation of 60° and 90° misfit dislocations and their dipoles at the film–substrate interface plotted versus the parameter $8\pi(1+\nu)\varepsilon_0$ for $p = T/2$. The plots of $H_c(\varepsilon_0)$ for single dislocations (solid curves in Fig. 2) coincide.

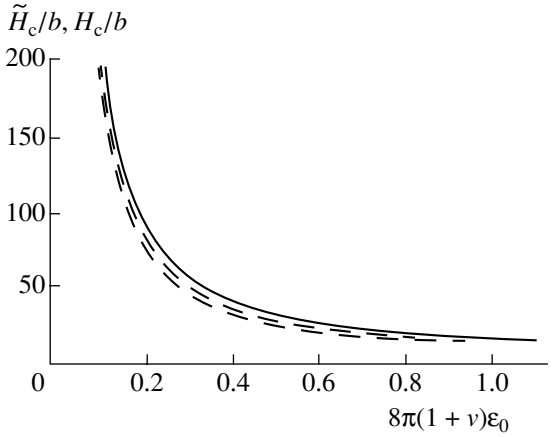


**Fig. 2.** Dependence of the critical film thickness $\tilde{H}_c/b$ on the modulation amplitude $\varepsilon_0$ for the nucleation of 60° and 90° single misfit dislocations ($H_c/b$, coinciding solid curves) and the 60° and 90°o misfit dislocation dipoles ($H_c/b$, upper and lower dashed curves, respectively).

An analysis of Fig. 2 allows us to draw the following conclusions. First, the critical thicknesses $\tilde{H}_c$ and $H_c$ for the nucleation of single misfit dislocations and their dipoles in the films with modulated compositions decrease with increasing modulation amplitude $\varepsilon_0$. Second, the critical thicknesses $\tilde{H}_c$ and $H_c$ for the nucleation of 90° misfit dislocations and dipoles are smaller than the analogous values for the 60° dislocations. Third, the critical thicknesses $\tilde{H}_c$ for the nucleation of single misfit dislocations in the films with modulated composition is greater than the analogous value for the formation of dipoles of such dislocations. Thus in a sufficiently thin film with modulated composition ($H < H_c$), neither misfit dislocations nor their dipoles form in the film. As the film thickness increases so as to fall within the interval $H_c < H < \tilde{H}_c$, a misfit dislocation dipole can form in the system. The further increase in the film thickness makes possible the formation of both individual misfit dislocations and their dipoles. In addition, the calculations show that the formation of misfit dislocation dipoles in inhomogeneous films is energetically more favorable than the formation of single misfit dislocations. The last conclusion agrees with the experimental data [7] on the dislocation dipoles formed in nanodimensional $Ga_{0.5}In_{0.5}P$ films with modulated compositions.

Thus, we have theoretically analyzed the conditions for nucleation of the misfit dislocations and their dipoles in films with inhomogeneous compositions. It

was demonstrated that the critical thickness and the activation energy for the formation of dislocation dipoles is smaller than the analogous values (critical thickness and activation energy) for single misfit dislocations. Therefore, the dislocation dipoles may be typical elements of the defect structures of films with inhomogeneous compositions, which agrees with the experimental data reported in [7].

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