# Dislocation Arrays at the Interface between an Epitaxial Layer and Its Substrate

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*Abstract:* The relationship between the film thickness and dislocation spacing in the interface dislocation arrays is studied by using a criterion based on the energy difference between the relaxed film configuration and a selected, partially relaxed or unrelaxed reference configuration. It is shown that arrays with lower dislocation density are formed in relaxation processes that are more gradual. Stability of arrays is examined, and new bounds of the stable range are constructed.

## 1. INTRODUCTION

Thin films constitute important parts of many electronic, optoelectronic, and magnetic devices. When the lattice parameters of the film and a substrate match, the film grows without a mismatch strain. If the lattice parameters differ, strain is needed to achieve perfect atomic registry across the interface (strained-layer epitaxy). The elastic energy stored in the film can cause the onset and propagation of structural defects in the layer. These defects are generally undesirable, since they can degrade electrical and optical performance of the layer and heterostructural device. If a dislocation is nucleated, for example as a half-loop from irregularities at the free surface, or if it extends from the substrate to the free surface of the layer, it is desirable that the dislocation expand into the configuration with a threading segment across the layer and a long misfit dislocation left behind at the interface between the layer and its substrate. The driving force provided by the misfit energy in the layer pushes the threading segment until it exits at the edges of the film. Only the misfit dislocation is left, which relaxes the strain in the layer and causes nonalignment between the layer and substrate lattices. The smallest layer thickness at which first misfit dislocation forms during epitaxial growth is known as the critical layer thickness. Comprehensive review of the subject can be found in Matthews [1], Nix [2], Fitzgerald [3], van der Merwe [4], and Freund [5].

If the layer is grown beyond its critical thickness and more dislocations enter, it becomes desirable to determine the relationship between dislocation spacing in the interface array and the layer thickness, for any given amount of initial mismatch strain, crystalline orientation, and material properties (Willis et al. [6, 7]; Jain et al. [8]; Gosling et al. [9]; [5]). A continuation of such studies is the objective of the present paper. In the analysis we use a criterion of strain relaxation, which is based on the difference between the energy of

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the relaxed film and the energy of selected reference configuration, with or without dislocations. This gives rise to a driving force for the transition between the two configurations. According to this criterion, the most dense array that could form in the film of a given thickness is the array created by simultaneous formation of all its dislocations. We then show that the arrays with lower dislocation density form in more realistic relaxation processes, with the gradual introduction of dislocations. Comparison with predictions based on the Frank and van der Merwe energy minimization criterion is also made. Stability of the arrays and the bounds which define the range of their stable configurations are subsequently examined. A new set of bounds is constructed. This analysis may be useful in a study of other more irregular dislocation structures.

Some important features of the process were not included in this paper, such as the lattice friction stress, possible dissociation of the threading dislocation into partial dislocations, and interaction of dislocations with other defects. An analysis based on the Peierls-Nabarro model of a threading dislocation was recently reported by Beltz and Freund [10]. The incorporation of elastic anisotropy and the differences between the elastic constants of the layer and the substrate were given by Gosling and Willis [11]. Dislocation arrays and compound arrays in buried and capped epitaxial layers were considered by Willis et al. [12] and Gosling et al. [13].

## 2. ENERGY OF A GENERAL STRAIGHT DISLOCATION ARRAY

An exact expression for the energy of a general straight dislocation array beneath the free surface of a semi-infinite body was derived by [6, 7]. For the array whose dislocations have Burgers vectors consisting of edge components $b_x$ and $b_y$, and screw component $b_z$ (Figure 1), the strain energy per unit length of a dislocation in the strip of width $p$, excluding the dislocation core, is

$$E^{\mathrm{d}} = -\frac{1}{2}\int_0^{h-\rho} [b_x\sigma_{xy}(x,0) + b_y\sigma_y(x,0) + b_z\sigma_{zy}(x,0)]\,dx - E_\rho. \tag{1}$$

The energy $E_\rho$ is the contribution from the tractions on the dislocation core surface of radius $\rho$. For a sufficiently small core radius ($\rho \ll h$), $E_\rho$ can be calculated by replacing the dislocation core with a cylindrical hole, whose surface is subjected to tractions of an isolated dislocation in an infinite homogeneous medium, along with the corresponding displacements. With a displacement discontinuity imposed along the cut along the $x$-axis from 0 to $h$, this is

$$E_\rho = \frac{1}{4}k\,[b_x^2 - b_y^2 - \frac{1}{2(1-\nu)}(b_x^2 + b_y^2)], \tag{2}$$

where $k = \mu/2\pi(1-\nu)$. The stresses $\sigma_{xy}(x,0)$, $\sigma_y(x,0)$, and $\sigma_{zy}(x,0)$ are listed in Appendix A. Upon substitution into equation (1) and integration, it follows that

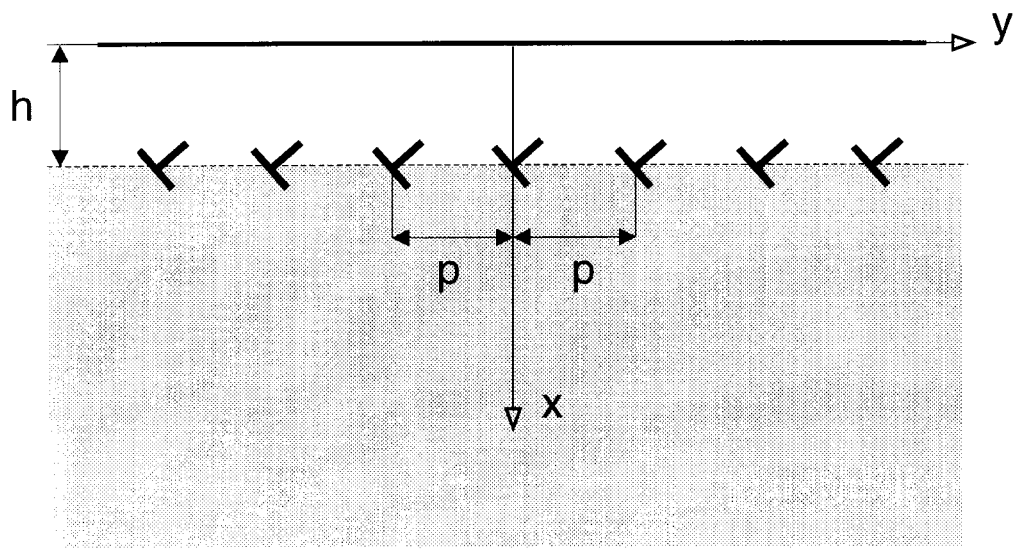


Fig. 1. An infinite array of dislocations with uniform spacing $p$ at the distance $h$ below the free surface of a semi-infinite body.

$$E^{\mathrm{d}} = \frac{k}{2}\left\{(b_x^2 + b_y^2)\left[\ln\frac{\mathrm{sh}\varphi_0}{\mathrm{sh}\rho_0} - \frac{\varphi_0^2}{2\mathrm{sh}^2\varphi_0} + \frac{1}{4(1-\nu)}\right]\right.$$
$$\left. +(b_x^2 - b_y^2)\left(\frac{1}{2} - \varphi_0\coth\varphi_0\right) + (1-\nu)b_z^2\ln\frac{\mathrm{sh}\varphi_0}{\mathrm{sh}\rho_0}\right\}. \tag{3}$$

The nondimensional variables $\varphi_0 = 2\pi h/p$ and $\rho_0 = \pi\rho/p$ are used. For a sufficiently small core radius, $\mathrm{sh}\rho_0$ can be replaced by $\rho_0$. Equation (3) is equivalent to the corresponding expression of [6, 7], which was given in terms of exponential functions.

The energy for an isolated dislocation near a free surface (Freund [14, 15]) is obtained when $h \ll p$ in equation (3). This gives

$$E_0^{\mathrm{d}} = \frac{1}{2}k\left\{[b_x^2 + b_y^2 + (1-\nu)b_z^2]\ln\frac{2h}{\rho} - \frac{1}{4(1-\nu)}[(3-4\nu)b_x^2 - b_y^2]\right\}. \tag{4}$$

If the layer is bonded to the substrate, with dislocations at the interface, and if the initial uniform misfit strains are $\epsilon_y^{\mathrm{m}}$, $\epsilon_z^{\mathrm{m}}$, $\epsilon_{zy}^{\mathrm{m}}$, and the corresponding stresses $\sigma_y^{\mathrm{m}} = 2\mu(\epsilon_y^{\mathrm{m}} + \nu\epsilon_z^{\mathrm{m}})/(1-\nu)$, $\sigma_z^{\mathrm{m}} = 2\mu(\epsilon_z^{\mathrm{m}} + \nu\epsilon_y^{\mathrm{m}})/(1-\nu)$, $\sigma_{zy}^{\mathrm{m}} = 2\mu\epsilon_{zy}^{\mathrm{m}}$, the total elastic strain energy per unit length of a dislocation within the strip of width $p$ is

$$E = E^{\mathrm{d}} + E^{\mathrm{m}} + E^{\mathrm{d,m}}. \tag{5}$$

Here, $E^{\mathrm{d}}$ is the energy associated with dislocations alone, given by equation (3), and $E^{\mathrm{m}}$ is the energy associated with the misfit strain alone,

$$E^{\mathrm{m}} = \frac{1}{2}(\sigma_y^{\mathrm{m}}\epsilon_y^{\mathrm{m}} + \sigma_z^{\mathrm{m}}\epsilon_z^{\mathrm{m}} + 2\sigma_{zy}^{\mathrm{m}}\epsilon_{zy}^{\mathrm{m}})hp. \tag{6}$$

The interaction energy $E^{\mathrm{d,m}}$ is the work of uniform misfit stresses on dislocation jump displacements along the cut from the free surface to $x = h$; that is,

$$E^{\mathrm{d,m}} = -(\sigma_y^{\mathrm{m}} b_y + \sigma_{zy}^{\mathrm{m}} b_z)h. \tag{7}$$

During the layer deposition, all elastic accommodation is assumed to take place in the layer, with the substrate, being much thicker than the layer, essentially behaving as a rigid elastic half-space.

## 3. CONDITIONS FOR DISLOCATION ARRAY FORMATION

The dislocation array will not form at the interface if the process is not energetically favored. We can thus require as a necessary, but not sufficient condition, that $E \le E^{\mathrm{m}}$ for an array to form. The difference $\mathcal{F} = E^{\mathrm{m}} - E$ can be interpreted as the total driving force on each threading dislocation in the array, when all dislocations are imagined to simultaneously form [5]. In view of equation (5), we therefore have

$$\mathcal{F} = -(E^{\mathrm{d}} + E^{\mathrm{d,m}}), \tag{8}$$

where $E^{\mathrm{d}}$ is given by equation (3) and $E^{\mathrm{d,m}}$ is given by equation (7). If the array is at the interface, $\mathcal{F} \ge 0$. For arbitrary $\varphi_0$, the limiting condition $\mathcal{F} = 0$ gives the relationship between the layer thickness $h$ and dislocation spacing $p$. Actually, it gives the smallest dislocation spacing for which the array could exist in the film of a given thickness. The arrays with larger spacing could also exist at this film thickness, but they would be associated with the condition $\mathcal{F} > 0$. Alternatively, for a given dislocation spacing of the array, the condition $\mathcal{F} = 0$ specifies the smallest film thickness required to support the array at the interface. Thicker film could also support the considered array, but it would correspond to $\mathcal{F} > 0$. Since $E^{\mathrm{d}}$ is positive, in order that $\mathcal{F} \ge 0$, the interaction energy $E^{\mathrm{d,m}}$ must be negative, and its magnitude greater than or equal to $E^{\mathrm{d}}$.

In the limit $\varphi_0 \to 0$, the condition $\mathcal{F} = 0$ reduces to the Matthews-Blakeslee [16] equation for the critical film thickness, associated with the introduction of an isolated dislocation. In this case $\mathcal{F} = -(E_0^{\mathrm{d}} + E^{\mathrm{d,m}})$, where $E_0^{\mathrm{d}}$ is given by equation (4). If $\varphi_0 \to \infty$, that is, $h \gg p$, from equation (8) it follows that the smallest dislocation spacing of the interface array for a very thick layer is independent of $h$ and is given by $p = k\pi[2b_y^2 + (1-\nu)b_z^2]/(\sigma_y^{\mathrm{m}} b_y + \sigma_{zy}^{\mathrm{m}} b_z)$. Physically, the independence of $h$ is a consequence of the fact that for $h \gg p$ the stress field in the layer becomes essentially constant, and both energies, far ahead of and far behind the threading dislocation segments, are proportional to the layer thickness.

The misfit dislocation, far behind the threading dislocation segment, must be under a force directed away from the free surface so that misfit dislocations are not pulled out to the free surface. This force is given by the negative gradient of the energy difference

$E - E^{\mathrm{m}}$ with respect to the film thickness; that is, $F_x = \partial \mathcal{F}/\partial h$. Although this must be positive, the misfit dislocation will not advance into the substrate, since the external stress in a thick substrate is zero, and the free surface exerts only an attractive force on the misfit dislocation.

As an illustration, consider the layer and substrate which share the same cubic lattice and orientation, with the interface parallel to their (001) crystallographic planes. If the lattice parameters of the layer and substrate are $a_l$ and $a_s$, the fractional mismatch of the lattice parameter is $\epsilon^{\mathrm{m}} = (a_s - a_l)/a_l$. The associated misfit strain components are $\epsilon_y^{\mathrm{m}} = \epsilon_z^{\mathrm{m}} = \epsilon^{\mathrm{m}}$, $\epsilon_{zy}^{\mathrm{m}} = 0$, and the biaxial stress state is $\sigma_y^{\mathrm{m}} = \sigma_z^{\mathrm{m}} = \sigma^{\mathrm{m}} = 4\pi k(1+\nu)\epsilon^{\mathrm{m}}$, $\sigma_{zy}^{\mathrm{m}} = 0$. If the layer/substrate system is $\mathrm{Ge}_x\mathrm{Si}_{1-x}/\mathrm{Si}$, where $x$ is the fraction of lattice sites in the layer occupied by Ge atoms, the lattice parameters of the layer and substrate are $a_l = xa_{\mathrm{Ge}} + (1-x)a_{\mathrm{Si}}$ (approximately, by Vegard's rule), and $a_s = a_{\mathrm{Si}}$. Since $a_{\mathrm{Si}} = 5.4305$Å and $a_{\mathrm{Ge}} = 5.6576$Å, the misfit strain is $\epsilon^{\mathrm{m}} \approx -0.042x$. For $x = 0.25$, this gives $\epsilon^{\mathrm{m}} \approx -0.01$. The dislocation array consists of dislocations along $[1\bar{1}0]$ crystallographic direction on the (111) glide planes. The dislocation Burgers vector is along the $[0\bar{1}1]$, so that relative to the $(xyz)$ coordinate system $b_x = -b/\sqrt{2}$, $b_y = -b/2$, and $b_z = b/2$, where $b$ is equal to $a_l/\sqrt{2}$. Consequently, equation (3) becomes

$$E^{\mathrm{d}} = \frac{kb^2}{8}\Big[(4-\nu)\ln\frac{\mathrm{sh}\varphi_0}{\rho_0} - \frac{3\varphi_0^2}{2\mathrm{sh}^2\varphi_0} - \varphi_0\coth\varphi_0 + \frac{5-2\nu}{4(1-\nu)}\Big], \tag{9}$$

whereas equation (7) gives $E^{\mathrm{d,m}} = 2\pi k(1+\nu)\epsilon^{\mathrm{m}}bh$. The relaxation occurs because $E^{\mathrm{d,m}}$ is negative. (Relaxation actually proceeds with the formation of two orthogonal dislocation arrays; the other array consists of dislocations along [110] direction on the $(1\bar{1}1)$ glide planes. Since the incorporation of the contribution from the second array is straightforward, we proceed with the consideration of one array only.) With $\nu = 0.3$, and with the core radius $\rho$ equal to the length of the Burgers vector $b$, the critical layer thickness is $h_{\mathrm{cr}} = 19.25b$, where $b = 3.88$Å. This satisfies the condition $F_x > 0$, which requires $h > 5.66b$. The relationship between the dislocation spacing and the layer thickness, resulting from the condition $\mathcal{F} = 0$, is shown in Figure 2. The dislocation spacing $p$ tends to infinity when $h \to h_{\mathrm{cr}}$. The thickness $h_0 = 29.25b$ corresponds to a dislocation spacing $p_0 = -b/2\epsilon^{\mathrm{m}} = 50b$ at which the array completely relaxes the initial mismatch strain.

### *3.1. Frank and van der Merwe Energy Criterion*

Frank and van der Merwe proposed that, for a given layer thickness $h$, dislocations in the array will arrange themselves by choosing the periodicity $p$ which minimizes the energy per unit area of the free surface. This energy is $E/p$, and the criterion requires

$$\frac{d}{dp}\Big(\frac{E}{p}\Big) = 0 \qquad \text{that is,} \qquad p\frac{dE}{dp} = E. \tag{10}$$

Since $E$ is given by equation (5), from the above condition it follows that

$$p\frac{dE^{\mathrm{d}}}{dp} = E^{\mathrm{d}} + E^{\mathrm{d,m}}. \tag{11}$$

The right-hand side of equation (11) is equal to $-\mathcal{F}$. Defining the force $f$ by

$$f = -p\frac{dE^{\mathrm{d}}}{dp}, \tag{12}$$

the Frank and van der Merwe energy condition can be expressed as

$$\mathcal{F} = f, \tag{13}$$

where

$$f = \frac{k}{2}\Big\{[(b_x^2 + b_y^2)\varphi_0 \coth\varphi_0 - 2b_y^2]\frac{\varphi_0^2}{\mathrm{sh}^2\varphi_0} + [2b_y^2 + (1-\nu)b_z^2]\varphi_0\coth\varphi_0 \\ -[b_x^2 + b_y^2 + (1-\nu)b_z^2]\Big\}. \tag{14}$$

It can be verified that $f$ is always positive (or equal to zero in the limit $\varphi_0 \to 0$) as expected, since from the criterion $E \le E^{\mathrm{m}}$, we know that $\mathcal{F}$ cannot be negative. A physical interpretation of $f$ can be given as follows. The force on a single threading dislocation entering alone into an epitaxial layer which already contains an array of spacing $p$ is the negative gradient of the specific energy with respect to dislocation density; that is, $\mathcal{G} = -d(E/p)/d(1/p)$ [9]. Indeed, if $n$ is the large number of dislocations in the array before one additional dislocation is inserted, the force can be written as $\mathcal{G} = nE(p) - (n+1)E(p+dp)$. Since dislocations distribute within the same domain, $np = (n+1)(p+dp)$. Thus, upon expanding, $\mathcal{G} = pdE/dp - E = \mathcal{F} - f$. The force $f$ is, therefore, the difference between the force $\mathcal{F}$ on a threading dislocation associated with a simultaneous formation of all dislocations in the array of spacing $p$ and the force $\mathcal{G}$ on a single dislocation when it alone enters an epitaxial layer already containing an array of spacing $p$. In the latter case, it is assumed that the array remains periodic upon the introduction of new dislocation by appropriate adjustment of its spacing (if necessary, by dislocation climb). Since $f$ is never negative, it follows that $\mathcal{F} \ge \mathcal{G}$ (equal sign applying only at infinitely large dislocation spacing). From this we can again conclude that the equilibrium spacing predicted by the Frank and van der Merwe criterion ($\mathcal{G} = 0$) must be greater than that obtained from the condition $\mathcal{F} = 0$. Indeed, if for an array $\mathcal{F} = 0$, then $\mathcal{G} < 0$, and one dislocation would tend to leave the array, which would increase the spacing among the remaining dislocations. The process would gradually continue until the condition $\mathcal{G} = 0$ is reached, which gives the equilibrium array configuration according to the Frank and van der Merwe criterion.

For the layer/substrate system under consideration, the predictions based on the condition $\mathcal{F} = f$, and the condition $\mathcal{F} = 0$, are shown in Figure 2. As previously discussed, for a given film thickness, a larger spacing is predicted by the Frank and van der Merwe criterion. If the array with dislocation spacing according to Frank and van der Merwe were formed by a simultaneous threading of all dislocations, the corresponding force $\mathcal{F}$ on the threading segments would not be zero, but large and positive. Arrays are observed which do not correspond to the minimum energy, or the most relaxed configuration, so that the

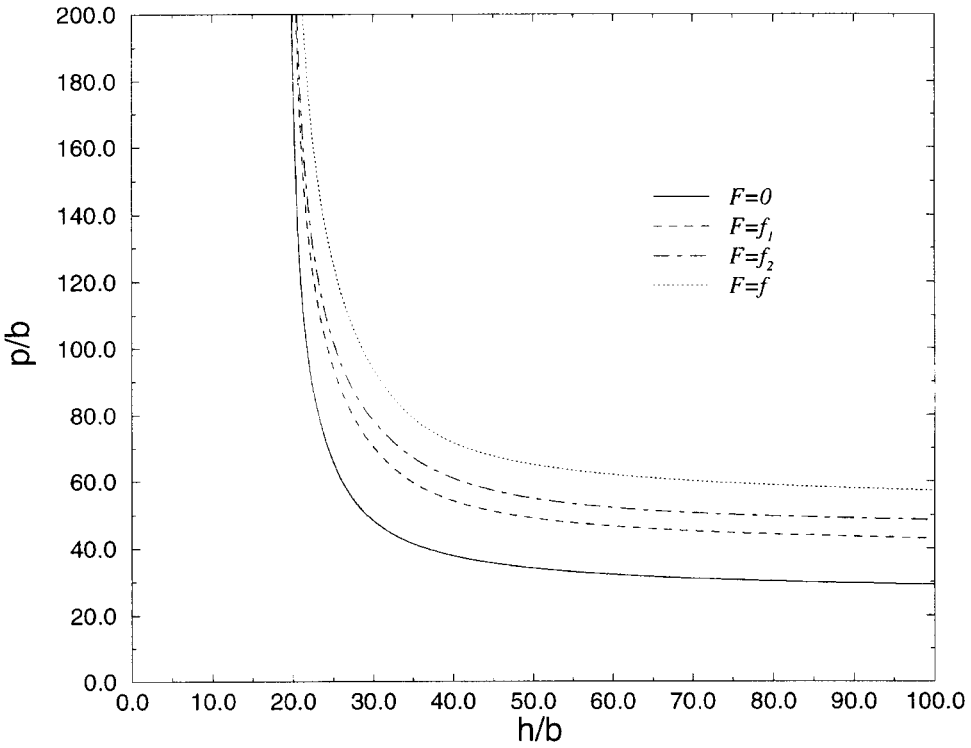


Fig. 2. Dislocation spacing $p$ versus layer thickness $h$ (scaled by the length of the Burgers vector) according to the condition based on simultaneous array formation, $\mathcal{F} = 0$; Frank and van der Merwe energy minimum condition, $\mathcal{F} = f$; and the conditions based on two different processes of gradual array formation, $\mathcal{F} = f_1$, and $\mathcal{F} = f_2$ ($0 < f_1 < f_2 < f$).

actual spacing may indeed be greater or smaller than that predicted by the Frank and van der Merwe criterion. One reason for this is that during the process of their gradual introduction, dislocations cannot easily readjust their positions to minimize the total energy [9]. Experiments, however, indicate that for a film thickness that exceeds the critical thickness by a factor of 2 or 3, the dislocation spacing is substantially greater than that predicted by the condition $\mathcal{F} = 0$ [5].

The critical layer thicknesses according to both criteria are identical [6]. The critical thickness according to the Frank and van der Merwe criterion follows from equation (13) in the limit $p \to \infty$, which implies that very few dislocations are introduced in the film. Since $f$ goes to zero as $p$ goes to infinity, the condition (13) reduces to $\mathcal{F} = 0$, which is the Matthews condition for the critical layer thickness. It is interesting to note that at this value of the layer thickness, the stationary value of the specific energy $E/p$, reached asymptotically in the limit $p \to \infty$, is actually a local energy maximum. There is also an energy minimum (being very slightly lower than the local energy maximum) which occurs at a large but finite value of the dislocation spacing. This was originally observed by [8]. However, by taking the critical film thickness to be just slightly smaller than that associated with the condition $\mathcal{F} = 0$, the value of the energy in the limit of infinite spacing

becomes an energy minimum, and a single dislocation can be deposited at the interface in a stable manner.

## 4. GRADUAL STRAIN RELAXATION

During the film growth beyond its critical thickness, dislocations gradually enter to form the misfit dislocation array at the interface between the film and its substrate. To uniformly relax the film, dislocations tend to form periodic arrays. A misfit dislocation already deposited at the interface on a particular glide plane relaxes the elastic strain on adjacent glide planes, reducing a tendency for another misfit dislocation there. The gradual relaxation is a difficult process, which involves time effects and the kinetics of dislocation nucleation and motion for any given temperature of the film growth. A simplified model of gradual relaxation was suggested by [5]. Imagine that in the process of the formation of an array of spacing $p$, at some instant the array of uniform spacing $2p$ is first formed. Denote the corresponding energy within the width $2p$ by $E(2p)$. The film is assumed to be thick enough for the energy difference

$$\mathcal{F}(2p) = 2E^{\mathrm{m}} - E(2p) = -E^{\mathrm{d}}(2p) - E^{\mathrm{d,m}} \tag{15}$$

to be positive. This is required to make the configuration energetically preferred relative to the film configuration without dislocations. The actual order by which dislocations entered the film to form the considered array is irrelevant for the present discussion, since the energy $E(2p)$ does not depend on that order. Thus, the value of $\mathcal{F}(2p)$ is also independent of the order, although $\mathcal{F}(2p)$ can be interpreted as a driving force on each threading dislocation in the array if all were to form simultaneously. For $\mathcal{F}(2p)$ to be positive, the film thickness must be greater than the thickness associated with the condition $\mathcal{F}(2p) = 0$.

A second set of dislocations is introduced by the glide of their threading segments along the planes midway between the glide planes of the first set. After this set is introduced, an array of dislocation spacing $p$ is formed. The corresponding elastic strain energy per unit length of dislocation, stored within the width $2p$, can be written as

$$2E(p) = E(2p) + E^{\mathrm{d}}(2p) + E^{\mathrm{d,m}} + E^{\mathrm{d,d}}(2p). \tag{16}$$

Here, $E(p)$ is the energy within the width $p$, given by equation (3), and $E^{\mathrm{d,d}}(2p)$ is the interaction energy between the two sets of dislocations (two arrays of spacing $2p$). The film of a given thickness will prefer the array of spacing $p$ rather than the array of spacing $2p$ if $2E(p) < E(2p)$, regardless of the order by which the second set is introduced. The difference

$$\mathcal{F}_1 = E(2p) - 2E(p) \tag{17}$$

is a driving force on each threading dislocation from the second set if all were introduced simultaneously. Substituting equations (15) and (16) into equation (17), we obtain

$$\mathcal{F}_1 = \mathcal{F}(p) - f_1, \quad f_1 = \frac{1}{2}E^{\mathrm{d,d}}(2p). \tag{18}$$

The force $\mathcal{F}(p)$ is given by equation (8). An expression for the interaction energy $E^{\mathrm{d,d}}(2p)$ can be conveniently obtained by using the fact that the elastic strain energy does not depend on the sequence by which dislocations are introduced in the array (alternatively, the interaction energy can be calculated by integration using the stress formulas listed in Appendix A). Thus, the energy within the width $2p$, associated with sequential formation of the array, given by equation (16), must be equal to the energy associated with simultaneous formation of the whole array, which is $2E(p) = 2E^{\mathrm{d}}(p) + E^{\mathrm{m}} + 2E^{\mathrm{d,m}}$. By equating this to the right-hand side of equation (16), we find

$$E^{\mathrm{d,d}}(2p) = 2[E^{\mathrm{d}}(p) - E^{\mathrm{d}}(2p)]. \tag{19}$$

Substituting equation (3), this becomes explicitly

$$E^{\mathrm{d,d}}(2p) = k\left\{[b_x^2 + b_y^2 + (1-\nu)b_z^2]\ln(\mathrm{ch}\frac{\varphi_0}{2}) + \frac{1}{8}(b_x^2 + b_y^2)\frac{\varphi_0^2}{\mathrm{ch}^2(\varphi_0/2)} - \frac{1}{2}(b_x^2 - b_y^2)\varphi_0\ \mathrm{th}\frac{\varphi_0}{2}\right\}. \tag{20}$$

For the previously considered layer/substrate system, equation (20) simplifies to

$$E^{\mathrm{d,d}}(2p) = \frac{kb^2}{4}\left[(4-\nu)\ln(\mathrm{ch}\frac{\varphi_0}{2}) + \frac{3\varphi_0^2}{8\mathrm{ch}^2(\varphi_0/2)} - \frac{1}{2}\varphi_0\ \mathrm{th}\frac{\varphi_0}{2}\right]. \tag{21}$$

It can be verified that this energy is always positive. It is also observed that $E^{\mathrm{d,d}}$ is a monotonically increasing function of $\varphi_0$, so that $E^{\mathrm{d,d}}(p) > E^{\mathrm{d,d}}(2p)$. The plot of the relationship between the dislocation spacing $p$ and the layer thickness $h$ associated with the condition $\mathcal{F}_1 = 0$, that is, $\mathcal{F}(p) = f_1$, is shown in Figure 2. For a given film thickness, the predicted dislocation spacing is greater in the case of sequential, rather than simultaneous, array formation associated with the condition $\mathcal{F}(p) = 0$.

An additional increase in predicted dislocation spacing is obtained if the relaxation process is more gradual. For example, imagine that, in the transition from the array of spacing $2p$ to the array of spacing $p$, an intermediate configuration is first reached which contains a periodic array of period $4p$. The dislocation spacing in this array is nonuniform, and it varies from $p$ to $2p$. The array is shown in Figure 3, if $p$ is replaced by $2p$. This configuration can be obtained by the introduction of a new dislocation between every second pair of dislocations of the array of spacing $2p$; that is, by an appropriate introduction of an array of spacing $4p$. The corresponding energy, within the width $4p$, is

$$E_2 = 2E(2p) + E^{\mathrm{d}}(4p) + E^{\mathrm{d,m}} + E^{\mathrm{d,d}}(2p). \tag{22}$$

The driving force for the transition from the configuration with the array of spacing $2p$ to the considered intermediate configuration is $2E(2p) - E_2$, which is assumed to be positive. The driving force from the intermediate configuration to the configuration with the array of spacing $p$ is $\mathcal{F}_2 = E_2 - 4E(p)$, which gives

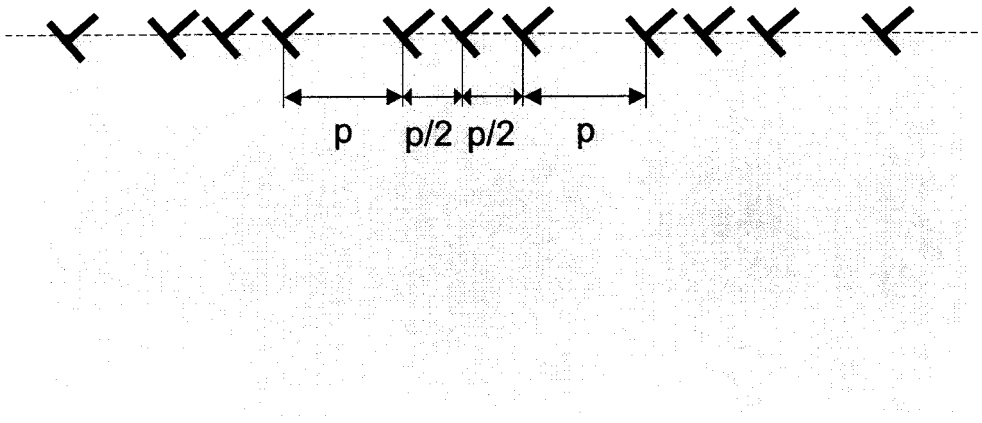


Fig. 3. An array of nonuniform dislocation spacing, which alters between $p$ and $2p$.

$$\mathcal{F}_2 = \mathcal{F}(p) - f_2 \qquad f_2 = 3E^{\mathrm{d}}(p) - 2E^{\mathrm{d}}(2p) - E^{\mathrm{d}}(4p) - E^{\mathrm{d,d}}(2p). \tag{23}$$

The plot of the relationship between the film thickness and the dislocation spacing, resulting from the condition $\mathcal{F}_2 = 0$, that is, $\mathcal{F}(p) = f_2$, is shown in Figure 2. The results demonstrate that, for a given film thickness, the predicted spacing is greater than that associated with the condition $\mathcal{F}_1 = 0$. Thus, the more gradual the relaxation process, the less dense is the array deposited at the interface.

## 5. STABILITY OF ARRAY CONFIGURATIONS

Consider a periodic array of spacing $p$ at the interface between the film and its substrate. If the film is sufficiently thick, additional dislocations will enter to relax the film. If the film is too thin, some dislocations will recede. For example, if enough dislocations enter so that, from the array of spacing $p$, an array of spacing $p/2$ is formed, the driving force for the transition is $E(p) - 2E(p/2) = \mathcal{F}(p) - E^{\mathrm{d,d}}(p)$. If the film resists the transition, this force must be negative; hence,

$$\mathcal{F}(p) < E^{\mathrm{d,d}}(p). \tag{24}$$

On the other hand, if the film is too thin, it may not support the array of dislocation density as high as $1/p$, and some dislocations will recede. Imagine that every second dislocation from the array leaves the film. The driving force for this recession is $-\mathcal{F}_1 = -\mathcal{F}(p) + E^{\mathrm{d,d}}(2p)/2$, as given by equation (18). If the recession is not preferred, the force must be negative, and

$$\mathcal{F}(p) > \frac{1}{2}E^{\mathrm{d,d}}(2p). \tag{25}$$

Combining the inequalities (24) and (25), we obtain the bounds which define the range of the $(p, h)$ values for which the array can stably exist at the interface, at least with regard to the considered perturbations in its structure. The bounds are shown in Figure 4, where they are designated by B1. Recall from Section 3 that the stable range was previously bounded from below by the condition $\mathcal{F} > 0$, which defines the lowest lower bound.

A higher lower bound can be obtained from the condition $\mathcal{F}_2 > 0$ associated with the recession in which every fourth dislocation leaves the array of uniform spacing $p$. From equation (23), we have

$$\mathcal{F}(p) > 3E^{\mathrm{d}}(p) - 2E^{\mathrm{d}}(2p) - E^{\mathrm{d}}(4p) - E^{\mathrm{d,d}}(2p). \tag{26}$$

On the other hand, a lower upper bound can be obtained by considering a possible transition of the array of spacing $p$ into the array of nonuniform spacing, which is obtained by the entrance of additional dislocation midway between every second pair of dislocations in the array of uniform spacing $p$ (Figure 3). The energy of this configuration, within the width $2p$, is $2E(p) + E^{\mathrm{d}}(2p) + E^{\mathrm{d,m}} + E^{\mathrm{d,d}}(p)$. Thus, if the transition should not occur,

$$\mathcal{F}(p) < E^{\mathrm{d,d}}(p) + E^{\mathrm{d}}(2p) - E^{\mathrm{d}}(p). \tag{27}$$

The bounds defined by (26) and (27) are also shown in Figure 4, designated there by B2, and they are within the previously defined bounds B1.

### *5.1. Stability Criteria of [9]*

Stronger stability conditions and restrictions on possible bounds can be obtained by using the analysis of [9], who introduced the criterion based on the conditions for the entrance, or recession, of a single dislocation from the periodic array. If the dislocation spacing can adjust so that the array maintains its periodicity upon the entrance of a new dislocation, the force on a threading dislocation entering the array would be $\mathcal{G} = \mathcal{F} - f$. Since the adjustment of spacing generally requires dislocation climb (which may not be operative at low temperatures), [9] assumed that dislocations in the array remain fixed as the new misfit dislocation deposits at the interface. The array is then considered to be stable if this deposition is resisted. The driving force on a threading dislocation midway between the two dislocations of the periodic array of spacing $p$ is the difference between the energies of the two configurations: the energy of the configuration with a periodic array and the energy of the same configuration with an inserted new dislocation. The latter is equal to the former, plus the energy of the added dislocation $E_0^{\mathrm{d}}$ given by equation (4), plus the work done to introduce the new dislocation against the stress of the existing array and the misfit stress, which is $E^{\mathrm{d,d}}(p) + E^{\mathrm{d,m}}$. Thus, the force to drive a dislocation into the array is

$$\mathcal{F}_{(+)} = -E^{\mathrm{d,d}}(p) - E^{\mathrm{d,m}} - E_0^{\mathrm{d}} = \mathcal{F}(p) - E^{\mathrm{d,d}}(p) + E^{\mathrm{d}}(p) - E_0^{\mathrm{d}}. \tag{28}$$

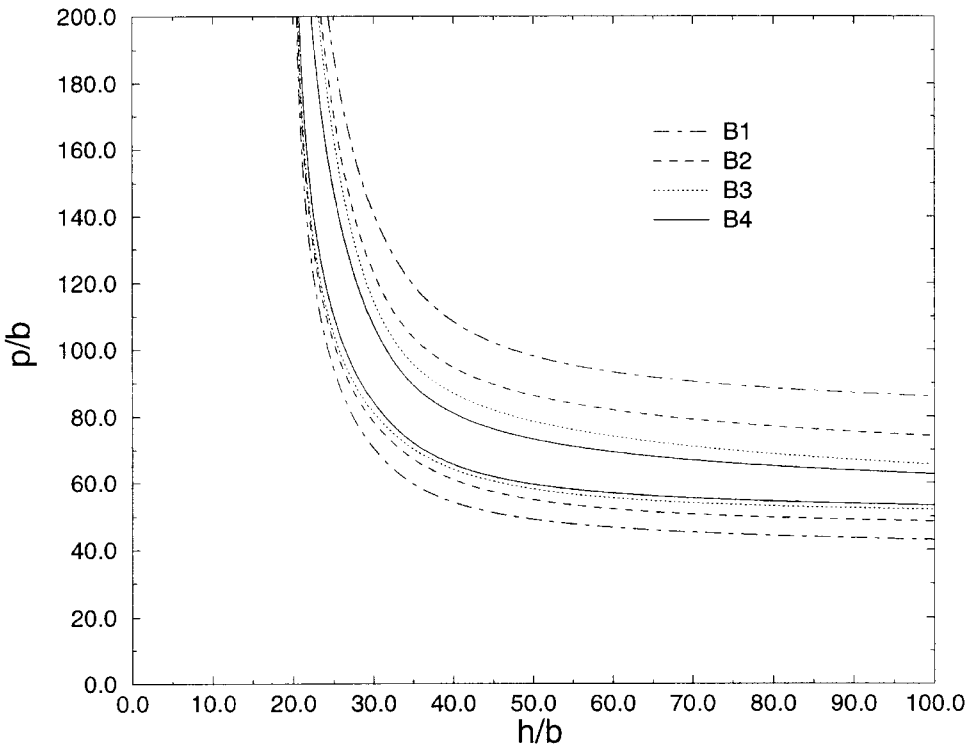


Fig. 4. Four sets of bounds (B1 through B4) which define range of stable array configurations with respect to assumed perturbations in the periodic array structure, as described in the text.

If the introduction of new dislocation is resisted, then $\mathcal{F}_{(+)} < 0$, and

$$\mathcal{F}(p) < E^{\mathrm{d,d}}(p) - [E^{\mathrm{d}}(p) - E_0^{\mathrm{d}}]. \tag{29}$$

It was additionally proposed by [9] that the recession of a single dislocation from the array (creation of a vacancy in its periodic structure) should also be resisted. A simple way to calculate the force which tends to drive a dislocation out of the array, while all other dislocations remain fixed, is to imagine that a negative dislocation (whose Burgers vector is opposite to that of dislocations in the array) is introduced to annihilate one of dislocations from the array. The energy difference between the two configurations is then equal to the energy of the added negative dislocation, $E_0^{\mathrm{d}}$, plus the work done to introduce the negative dislocation against the stress of the existing periodic array and the misfit stress. This work is

$$\begin{aligned}\int_0^{h-\rho} [b_x\sigma_{xy}(x,0) + b_y\sigma_y(x,0) + b_z\sigma_{zy}(x,0)]\,dx \\ + 2E_\rho - E^{\mathrm{d,m}} = -2E^{\mathrm{d}}(p) - E^{\mathrm{d,m}}.\end{aligned} \tag{30}$$

Equation (1) was used to express the integral in equation (30) in terms of other introduced energy contributions. Thus, the force to drive dislocation out of the array is

$$\mathcal{F}_{(-)} = 2E^{\mathrm{d}}(p) + E^{\mathrm{d,m}} - E_0^{\mathrm{d}} = E^{\mathrm{d}}(p) - E_0^{\mathrm{d}} - \mathcal{F}(p). \tag{31}$$

An analogous expression was derived by [7] using a different procedure. A dislocation will not recede from the array if $\mathcal{F}_{(-)} < 0$; that is,

$$\mathcal{F}(p) > E^{\mathrm{d}}(p) - E_0^{\mathrm{d}}. \tag{32}$$

For the considered layer/substrate system, the bounds defined by equations (29) and (32) are shown in Figure 4, where they are designated by B3. These bounds are within the bounds B1. This was clear for the upper bounds, since $E^{\mathrm{d}}(p) - E_0^{\mathrm{d}}$ is positive. It was also expected for the lower bounds on physical grounds, since the array may be in a stable configuration with regard to the recession of every second dislocation from the array but in an unstable configuration with regard to a slighter disturbance due to recession of a single dislocation. For example, suppose the film is in the state corresponding to a point on the lower bound curve. With further film growth, dislocation spacing remains constant until the point on the upper bound curve is reached, at which instance a new dislocation can enter the film.

### *5.2. Further Bounds*

A new set of bounds which define a possible range of stable array configurations is constructed in this subsection by comparing the array configuration with two perturbed neighboring configurations, as follows.

#### 5.2.1. LOWER BOUND

Consider a perturbed array configuration which contains one dislocation at a distance $3p/2$ from the two neighboring dislocations, while the rest of the array has uniform spacing $p$ (Figure 5a). This configuration can be obtained from a perfectly periodic array of spacing $p$ by recession of two neighboring dislocations, and by injection of one new dislocation along the slip plane midway between the two receding dislocations. One may also think that one dislocation has receded, while one dislocation, ahead of or behind the receding dislocation, has subsequently positioned itself in the middle between the two dislocations of the perturbed array. The change of energy between the perturbed and unperturbed configurations can be calculated as follows. First, introduce a new dislocation midway between the two neighboring dislocations of the perfect array. As previously shown, the energy increases by $E_0^{\mathrm{d}} + E^{\mathrm{d,d}}(p) + E^{\mathrm{d,m}}$. Next, introduce two negative dislocations to annihilate two dislocations, ahead of and behind the inserted dislocation. This further increases the energy by $2[E_0^{\mathrm{d}} - 2E^{\mathrm{d}}(p) - E^{\mathrm{d,m}}]$, plus the interaction energy among the three dislocations, which is $E^{\mathrm{in}} = E^{(-,-)} + 2E^{(+,-)}$. It is shown in Appendix C that the interaction energy between the two negative dislocations is

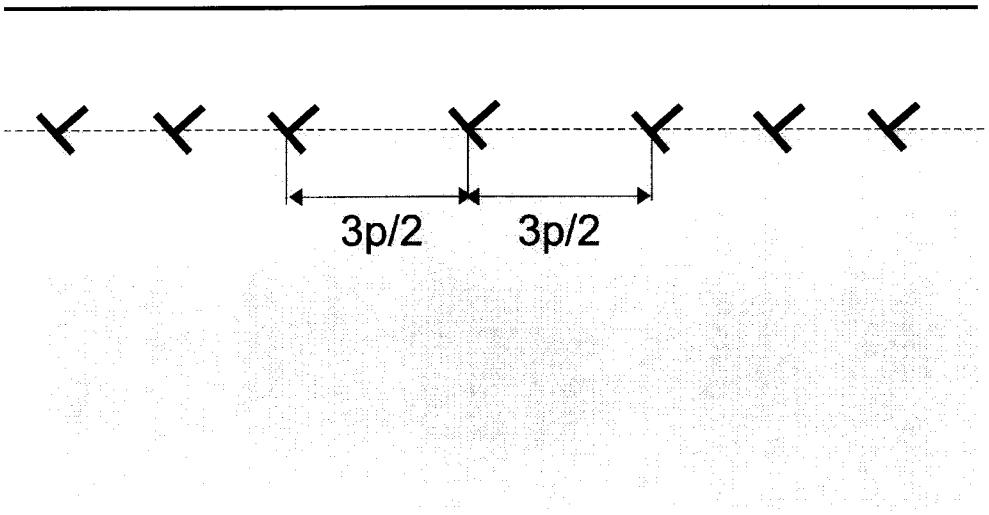


Fig. 5a. Perturbed array configurations used to derive the lower bound of the stable array configurations (designated by B4 in Figure 4).

$$E^{(-,-)} = \frac{k}{2}\Big\{[b_x^2 + b_y^2 + (1-\nu)b_z^2]\ln(1+\eta^2) - [(1+3\eta^2)b_x^2 - (3+\eta^2)b_y^2]\frac{\eta^2}{(1+\eta^2)^2}\Big\}, \tag{33}$$

where $\eta = 2h/p$. The interaction energy between the positive and negative dislocation $E^{(+,-)}$ is given by the same expression, with $\eta$ replaced by $2\eta$ and $k$ by $-k$. The force which drives the perfect array into the perturbed array is the negative of the corresponding energy change, which gives

$$\mathcal{F}_* = -\mathcal{F}(p) + 3[E^{\mathrm{d}}(p) - E_0^{\mathrm{d}}] - E^{\mathrm{d,d}}(p) - E^{\mathrm{in}}. \tag{34}$$

If the perturbation is resisted, $\mathcal{F}_* < 0$; that is,

$$\mathcal{F}(p) > 3[E^{\mathrm{d}}(p) - E_0^{\mathrm{d}}] - E^{\mathrm{d,d}}(p) - E^{\mathrm{in}}. \tag{35}$$

This defines a lower bound for the stable configuration of the perfect array (B4 in Figure 4) which is slightly higher than the lower bound B3 defined by (32). This was expected to be the case, since the symmetric configuration in Figure 5a is more relaxed than the configuration with the array containing the vacancy in its periodic structure, with the surrounding dislocations being fixed.

Since dislocation adjustment may require climb, it is supportive to the above consideration to give an additional or alternative interpretation of the condition $\mathcal{F}_* < 0$. Imagine that the periodic array of uniform spacing $p$ is completed, except for two missing dislocations next to each other. Denote the corresponding energy by $\mathcal{E}$. (Total energies of infinite

arrays are infinitely large, but their differences are finite, and will be needed only in this discussion.) If two dislocations enter and complete the perfect array, the energy becomes $\mathcal{E}_a$, and the driving force for this to occur would be $\mathcal{F}_a = \mathcal{E} - \mathcal{E}_a$. If, instead of two, only one dislocation enters, midway between the two missing dislocations of the perfect array, the energy is $\mathcal{E}_b$, and the corresponding force would be $\mathcal{F}_b = \mathcal{E} - \mathcal{E}_b$. If $\mathcal{F}_a > \mathcal{F}_b$, the case (a) is preferred, since then $\mathcal{E}_a < \mathcal{E}_b$. On the other hand, the force which would drive the configuration (a) into (b) is $\mathcal{F}_* = \mathcal{E}_a - \mathcal{E}_b = \mathcal{F}_b - \mathcal{F}_a$. Thus, the condition $\mathcal{F}_* < 0$ again gives $\mathcal{F}_a > \mathcal{F}_b$, which means that the perfect array (a) would be preferred to the perturbed array (b).

### 5.2.2. UPPER BOUND

A lower upper bound can be obtained by considering a perturbed array configuration shown in Figure 5b. This configuration can be obtained from the perfectly periodic array of spacing $p$ by recession of one dislocation, and by symmetric injection of two new dislocations at the distance $p/3$ from the receding dislocation. Alternatively, one may consider that a perfect array was created, except for one missing dislocation, and that the competition is taking place whether one more dislocation will enter and complete the perfect array or whether two dislocations will symmetrically enter to form the perturbed array in Figure 5b. Imagine that a negative dislocation is introduced to cancel one dislocation from the perfect array, and two additional dislocations are then injected. The energy change relative to the perfect configuration is equal to the energy of the added negative dislocation, $E_0^d$, plus the work done to introduce the negative dislocation against the stress of the perfect array and the misfit stress, which is given by equation (30), plus the energy associated with the introduction of the two dislocations. This is $2E_0^d + 2E^{d,m}$, plus the interaction energy of the two dislocations with the perfect array $2E^{int}(p/3)$, plus the interaction energy among the three added dislocations, $E^{in} = E^{(+,+)} + 2E^{(+,-)}$. Thus, the force that would drive the perfect array into the perturbed array is

$$\mathcal{F}^* = \mathcal{F}(p) + 3[E^d(p) - E_0^d] - 2E^{int}(\frac{p}{3}) - E^{in}. \tag{36}$$

The interaction energy $E^{+,+}$ is given by equation (33), with $\eta = 3h/p$. The interaction energy $E^{(+,-)}$ is given by the same expression, with $\eta$ replaced by $2\eta$ and $k$ by $-k$. The interaction energy associated with the introduction of dislocation at a distance $y$ from the dislocation in the array is obtained from the general expression derived in Appendix B by substituting $x = h$. This gives

$$E^{int}(y) = k[b_x^2 I_x + b_y^2 I_y + (1-\nu)b_z^2 I_z], \tag{37}$$

where

$$I_x = I_z - \frac{\varphi_0 \,\mathrm{sh}2\varphi_0}{\mathrm{ch}2\varphi_0 - \cos\psi} + \frac{\varphi_0^2(1 - \mathrm{ch}2\varphi_0 \cos\psi)}{(\mathrm{ch}2\varphi_0 - \cos\psi)^2} \tag{38}$$

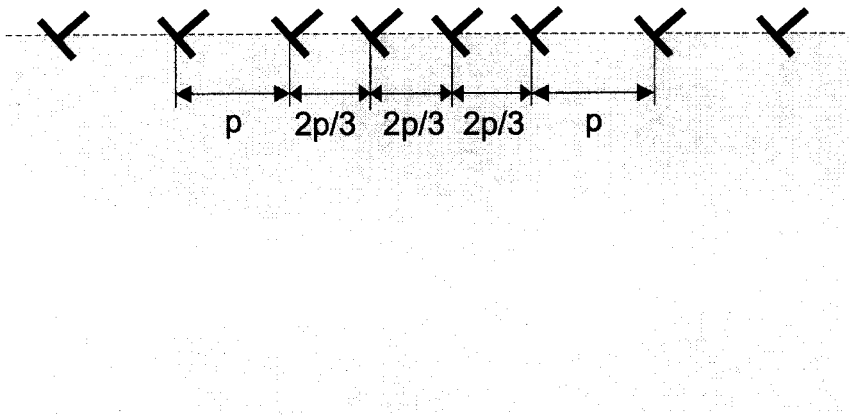


Fig. 5b. Perturbed array configurations used to derive the upper bound of the stable array configurations (designated by B4 in Figure 4).

$$I_y = I_x + \frac{2\varphi_0 \,\mathrm{sh}2\varphi_0}{\mathrm{ch}2\varphi_0 - \cos\psi} \tag{39}$$

$$I_z = \frac{1}{2} \ln \frac{\mathrm{ch}2\varphi_0 - \cos\psi}{1 - \cos\psi}. \tag{40}$$

In equations (38)-(40), $\varphi_0 = 2\pi h/p$, and $\psi = 2\pi y/p$. The interaction energy $E^{\mathrm{int}}(p/3)$ follows for $\psi = 2\pi/3$.

The perturbation is resisted if $\mathcal{F}^* < 0$; that is,

$$\mathcal{F}(p) < 2E^{\mathrm{int}}(\frac{p}{3}) + E^{\mathrm{in}} - 3[E^{\mathrm{d}}(p) - E_0^{\mathrm{d}}]. \tag{41}$$

This defines an upper bound for the stable configuration of the perfect array (B4 in Figure 4) which is lower than the upper bound B3 defined by (29), since the symmetric configuration in Figure 5b is more relaxed than the perfect array configuration with an additional dislocation exactly midway between the two dislocations of the array. It is interesting to note that the four lower bounds shown in Figure 4 are closer to each other than the four upper bounds, so that bounds are more sensitive to perturbation modes involving the entrance of new dislocations than the recession of some dislocations.

From a purely energetic point of view, which does not take into account possible mechanisms by which configurations can alter, the stable configuration would be unique and given by the Frank and van der Merwe criterion. The corresponding curve is always between the upper and lower bound of any considered set of bounds, since $f$ in equation (13) is always between these bounds. However, during the film growth, dislocations may

be entering in such a way that the minimum energy spacing cannot actually be attained at a given film thickness, since complete readjustment of already taken dislocation positions would be required (either by climb, or recession of some and entrance of other dislocations). In view of this, any spacing between derived upper and lower bounds could in principle correspond to a given film thickness, depending on the sequence or the order by which dislocations entered in the process of film growth. Inevitably, the dislocation spacing will be more or less nonuniform, although dislocations will try their best to form as nearly as possible into periodic arrays, and to minimize the total energy of the system. Furthermore, the order by which dislocations enter depends on the location and strength of available dislocation sources. The rate of film growth has also an obvious effect on dislocation spacing that is eventually taken by the array at the final film thickness.

## 6. CONCLUSION

We have shown in this paper that dislocation spacing in the interface arrays between an epitaxial layer and its substrate increases with an increasing tendency toward a gradual dislocation formation. This is illustrated in Figure 2, where the relationship between the film thickness and dislocation spacing is shown for the simultaneous introduction of the whole array, and for two different sequences of gradual formation of the same array. We have subsequently examined the range of stable array configurations with respect to assumed perturbations in the structure of the array. Three new sets of bounds are derived and compared in Figure 4 with the original bounds obtained by [9]. The results presented are conveniently expressed in terms of the driving force $\mathcal{F}$, which represents the energy difference between the relaxed film configuration and the film configuration without dislocations. The only other quantities that appear are the various dislocation interaction energies. Explicit expressions for these are derived in each case. In the appendixes, we list in a compact form the expressions for relevant stress components due to the dislocation arrays considered in the present work. It is believed that the results so obtained can be helpful in dealing with more irregular dislocation structures that occur during film growth.

## APPENDIX A

The required stress components along vertical planes containing a dislocation from the array can be obtained from the general formulas listed in Appendix B. They can be conveniently written as

$$\sigma_{xy}(x,0) = \frac{\pi k b_x}{2p}\left[\frac{\vartheta}{\mathrm{sh}^2(\vartheta/2)} - \frac{\varphi}{\mathrm{sh}^2(\varphi/2)} + \frac{2\varphi_0}{\mathrm{sh}^2(\varphi/2)}A(\varphi)\right] \tag{A.1}$$

$$\begin{aligned}\sigma_y(x,0) = \frac{\pi k b_y}{2p}\Big[4(\coth\frac{\vartheta}{2} - \coth\frac{\varphi}{2}) - \frac{\vartheta}{\mathrm{sh}^2(\vartheta/2)} \\ + \frac{\varphi}{\mathrm{sh}^2(\varphi/2)} + \frac{2\varphi_0}{\mathrm{sh}^2(\varphi/2)}A(\varphi)\Big]\end{aligned} \tag{A.2}$$

$$\sigma_{zy}(x,0)=\frac{\mu b_z}{2p}\left(\coth\frac{\vartheta}{2}-\coth\frac{\varphi}{2}\right), \tag{A.3}$$

where $A(\varphi)=1-(\varphi-\varphi_0)\coth(\varphi/2)$.

Along vertical planes midway between the two dislocations from the array, the stresses are

$$\sigma_{xy}(x,\frac{p}{2})=\frac{\pi k b_x}{2p}\Big[-\frac{\vartheta}{\mathrm{ch}^2(\vartheta/2)}+\frac{\varphi}{\mathrm{ch}^2(\varphi/2)}-\frac{2\varphi_0}{\mathrm{ch}^2(\varphi/2)}B(\varphi)\Big] \tag{A.4}$$

$$\sigma_y\left(x,\frac{p}{2}\right)=\frac{\pi k b_y}{2p}\left[4\Big(\mathrm{th}\frac{\vartheta}{2}-\mathrm{th}\frac{\varphi}{2}\Big)+\frac{\vartheta}{\mathrm{ch}^2(\vartheta/2)}-\frac{\varphi}{\mathrm{ch}^2(\varphi/2)}-\frac{2\varphi_0}{\mathrm{ch}^2(\varphi/2)}B(\varphi)\right] \tag{A.5}$$

$$\sigma_{zy}\left(x,\frac{p}{2}\right)=\frac{\mu b_z}{2p}\left(\mathrm{th}\frac{\vartheta}{2}-\mathrm{th}\frac{\varphi}{2}\right), \tag{A.6}$$

where $B(\varphi)=1-(\varphi-\varphi_0)\mathrm{th}(\varphi/2)$.

The nondimensional variables $\vartheta$, $\varphi$, and $\varphi_0$ are defined in Appendix B. Multiplying equations (A.4)-(A.6) with $-b_x$, $-b_y$ and $-b_z$, respectively, an integration in $x$ from 0 to $h$ gives the interaction energy $E^{\mathrm{d,d}}(p)$. The expression is given by equation (20), in which $\varphi_0/2$ is replaced by $\varphi_0$.

## APPENDIX B

This appendix gives the general expression for the interaction energy associated with the introduction of an additional dislocation into the periodic array, anywhere between two dislocations in the array; that is,

$$E^{\mathrm{int}}(x,y)=-\int_0^x[b_x\sigma_{xy}(x,y)+b_y\sigma_y(x,y)+b_z\sigma_{zy}(x,y)]\,dx. \tag{B.1}$$

The stress components appearing in equation (B.1) can be obtained from the general formulas for the stress distribution due to dislocation arrays near bimaterial interface (Lubarda [17]). They are compactly written as

$$\sigma_{xy}=\frac{\pi k b_x}{p}\,T_x+\frac{\pi k b_y}{p}\,T_y\sin\psi \tag{B.2}$$

$$\sigma_y=\frac{\pi k b_y}{p}\,Y_y+\frac{\pi k b_x}{p}\,Y_x\sin\psi \tag{B.3}$$

$$\sigma_{zy}=\frac{\pi k(1-\nu)b_z}{p}\left(\frac{\mathrm{sh}\vartheta}{C}-\frac{\mathrm{sh}\varphi}{A}\right), \tag{B.4}$$

where

$$T_x = \frac{D\vartheta}{C^2} - \frac{B\vartheta}{A^2} - \frac{2\varphi_0(\varphi-\varphi_0)}{A^3}(B-\sin^2\psi)\mathrm{sh}\varphi \tag{B.5}$$

$$T_y = \frac{1}{A} - \frac{1}{C} + \frac{\vartheta\ \mathrm{sh}\vartheta}{C^2} - \frac{\varphi\ \mathrm{sh}\varphi}{A^2} + \frac{2\varphi_0(\varphi-\varphi_0)}{A^3}(B+\mathrm{sh}^2\varphi) \tag{B.6}$$

$$Y_x = \frac{1}{A} - \frac{1}{C} + \frac{\vartheta\ \mathrm{sh}\vartheta}{C^2} - \frac{(\varphi-4\varphi_0)\ \mathrm{sh}\varphi}{A^2} - \frac{2\varphi_0(\varphi-\varphi_0)}{A^3}(B+\mathrm{sh}^2\varphi) \tag{B.7}$$

$$Y_y = \frac{2\mathrm{sh}\vartheta}{C} - \frac{2\mathrm{sh}\varphi}{A} - \frac{D\vartheta}{C^2} + \frac{B(\varphi+2\varphi_0)}{A^2} - \frac{2\varphi_0(\varphi-\varphi_0)}{A^3}(B-\sin^2\psi)\mathrm{sh}\varphi. \tag{B.8}$$

The following abbreviations were used: $A = \mathrm{ch}\varphi - \cos\psi$, $B = \mathrm{ch}\varphi\cos\psi - 1$, $C = \mathrm{ch}\vartheta - \cos\psi$, and $D = \mathrm{ch}\vartheta\ \cos\psi - 1$. The nondimensional variables are $\vartheta = 2\pi(x-h)/p$, $\varphi = 2\pi(x+h)/p$, $\varphi_0 = 2\pi h/p$, and $\psi = 2\pi y/p$.

Substitution of equations (B.2)-(B.4) into equation (B.1) gives, upon integration (in which the integrals without a closed-form solution cancel out), the following expression for the interaction energy:

$$E^{\mathrm{int}}(x,y) = k\left[b_x^2 I_x + b_y^2 I_y + b_x b_y I_{xy} + (1-\nu)b_z^2 I_z\right], \tag{B.9}$$

where

$$I_x = I_z - \frac{1}{2}\frac{\varphi\ \mathrm{sh}\varphi}{\mathrm{ch}\varphi-\cos\psi} + \frac{1}{2}\frac{\vartheta\ \mathrm{sh}\vartheta}{\mathrm{ch}\vartheta-\cos\psi} + \varphi_0(\varphi-\varphi_0)\ \frac{1-\mathrm{ch}\varphi\ \cos\psi}{(\mathrm{ch}\varphi-\cos\psi)^2} \tag{B.10}$$

$$I_y = I_x + \frac{\varphi\ \mathrm{sh}\varphi}{\mathrm{ch}\varphi-\cos\psi} - \frac{\vartheta\ \mathrm{sh}\vartheta}{\mathrm{ch}\vartheta-\cos\psi} \tag{B.11}$$

$$I_{xy} = \vartheta\ \sin\psi\ \left(\frac{1}{\mathrm{ch}\vartheta-\cos\psi} - \frac{1}{\mathrm{ch}\varphi-\cos\psi}\right) \tag{B.12}$$

$$I_z = \frac{1}{2}\ln\frac{\mathrm{ch}\varphi-\cos\psi}{\mathrm{ch}\vartheta-\cos\psi}. \tag{B.13}$$

An analogous expression was derived by [13] in their study of periodic arrays of dislocation dipoles and strain relaxation in capped layers.

## APPENDIX C

The interaction energy between two dislocations, both at depth $h$ below the free surface of a semi-infinite body and at the horizontal distance $y$ from each other, is

$$E^{(1,2)} = -\int_0^h \left[b_x^{(2)}\sigma_x^{(1)}(x,y) + b_y^{(2)}\sigma_y^{(1)}(x,y) + b_z^{(2)}\sigma_{zy}^{(1)}(x,y)\right] dx. \tag{C.1}$$

One dislocation has the Burgers vector $\mathbf{b}^{(1)}$, and the other $\mathbf{b}^{(2)}$. Upon substitution of Head's expressions into equation (C.1), the integration gives

$$\begin{aligned} E^{(1,2)} &= \frac{k}{2}\left\{\left[b_x^{(1)}b_x^{(2)} + b_y^{(1)}b_y^{(2)} + (1-\nu)b_z^{(1)}b_z^{(2)}\right]\ln(1+\eta^2)\right. \\ &- (b_x^{(1)}b_y^{(2)} - b_y^{(1)}b_x^{(2)})\frac{2\eta^3}{(1+\eta^2)^2} \\ &- \left.\left[(1+3\eta^2)b_x^{(1)}b_x^{(2)} - (3+\eta^2)b_y^{(1)}b_y^{(2)}\right]\frac{\eta^2}{(1+\eta^2)^2}\right\}, \end{aligned} \tag{C.2}$$

where $\eta = 2h/y$. The energy $E^{(-,-)}$ of Section 5, equation (33), is obtained from equation (C.2) by taking $\mathbf{b}^{(1)} = \mathbf{b}^{(2)} = -\mathbf{b}$, and $y = p$. The energy $E^{(+,-)}$ is obtained if $\mathbf{b}^{(1)} = -\mathbf{b}^{(2)} = \mathbf{b}$, and $y = p/2$.

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