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CONTINUUM MODELING OF STRESS-DRIVEN SURFACE DIFFUSION IN STRAINED ELASTIC MATERIALS

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ABSTRACT

The free energy of a deformable crystal is assumed to consist of elastic strain energy and surface energy, and the chemical potential for surface diffusion at constant temperature is obtained under this assumption. The result is applied in considering the phenomena of instability of a flat surface in a stressed material under fluctuations in surface shape, and the development of surface roughness due to the proximity of misfit dislocations to the free surface of the material.

INTRODUCTION

A characterizing feature of a homogeneous elastic body is that there is a well-defined *reference configuration* to which it returns when all applied loads are removed. While often viewed as being immutable, there are circumstances under which the shape of this configuration can change over time as, for example, in condensation/evaporation or diffusion processes. The focus here is on the particular mechanism of mass transport by surface diffusion. The discussion is limited to cases where the mass rearrangement is coherent, so that there is a well defined reference configuration at any time. The discussion will also be limited to processes with no net gain or loss of mass.

Mass transport by stress-driven diffusion is typically slow, and it can occur to a significant degree only when the process under consideration has the features of relatively high stress, high temperature and small size scale. These features are characteristic of strained-layer semiconductor material systems, of course, for which the magnitude of stress can exceed a gigapascal, the materials are grown or processed at temperatures of 500-600 C, and submicron physical dimensions are typical. Such systems provide the basis for the present discussion.

The systems considered are heterogeneously deformed and always in mechanical equilibrium. They are not in thermodynamic equilibrium, however, so they evolve in time in such a way as to decrease the system free energy. The surface field representing the tendency for the system to change the shape of its reference configuration is the chemical potential field [1,2]. Under circumstances for which this change can arise only through mass transport over the surface of the material, the chemical potential at a point on the surface is defined as the increase in Helmholtz free energy (isothermal potential energy) of the system due to addition of one atom at that point on the surface at fixed local strain. In general, material tends to diffuse down the chemical potential gradient along the surface. It must be recognized that the chemical forces involved are orders of magnitude greater than the mechanical forces. Nonetheless, it appears that stress can play a role in diffusion in cases where the gradients of chemical forces are very small. A development of concepts relevant to crystal growth is provided by Tsao [3], and various issues have been considered by Mullins and Sekerka [4], Leo and Sekerka [5] and Gurtin and Struthers [6].

The discussion proceeds in several steps. First, the chemical potential is defined as a function of position on the surface in terms of deformation and surface shape, under the assumption that the Helmholtz free energy of the system can change only as a result of a change in surface energy or elastic strain energy of the material. Then, the chemical

potential variations are examined for the case of an originally flat surface which becomes slightly wavy in order to determine the stability of a flat surface in a homogeneously stressed material under fluctuations in surface shape. The stability condition, which was obtained independently on the basis of quite different arguments by Srolovitz [7] and Grinfeld [8,9], is well known, and similar applications to strained layers have been developed more recently [10,11]. As an example of the influence of an *inhomogeneous* state of stress on chemical potential, the role of dislocations near the free surface in inducing surface roughness is considered. The dislocations are thought to represent interface misfit dislocations between a strained layer and its substrate, and the results are interpreted in the context of roughening of the surface of a strained epitaxial film due to the presence of interface misfit dislocations.

THE CHEMICAL POTENTIAL

To consider the phenomenon of stress-driven mass transport by surface diffusion in an elastic crystal, the bulk material and the material immediately adjacent to the surface are viewed as different phases of the same material [1]. The bulk material is idealized as an elastic continuum and the "surface" as a pre-stressed elastic membrane attached to the surface of the bulk material. The surface and bulk phases exert tractions on each other, they deform together, and they are described by different constitutive relations, in general. This situation is depicted in Figure 1 which shows some portion of the material with the phases separated from each other. To describe a two dimensional deformation process, fields in the bulk phase are referred to rectangular coordinates x_1, x_2 aligned with the unit base vectors e_1, e_2. Fields in the surface are referred to arclength s measured from some arbitrary point at any time. The surface unit normal is $e_n = n_i e_i$ and the surface unit tangent vector is e_s in the direction of increasing s. The traction exerted on the surface of the bulk phase by the surface phase is T and, of course, the bulk phase exerts an equal but opposite traction on the surface. The forces P_+ and P_- are required to balance internal surface tension at the boundaries of the surface.
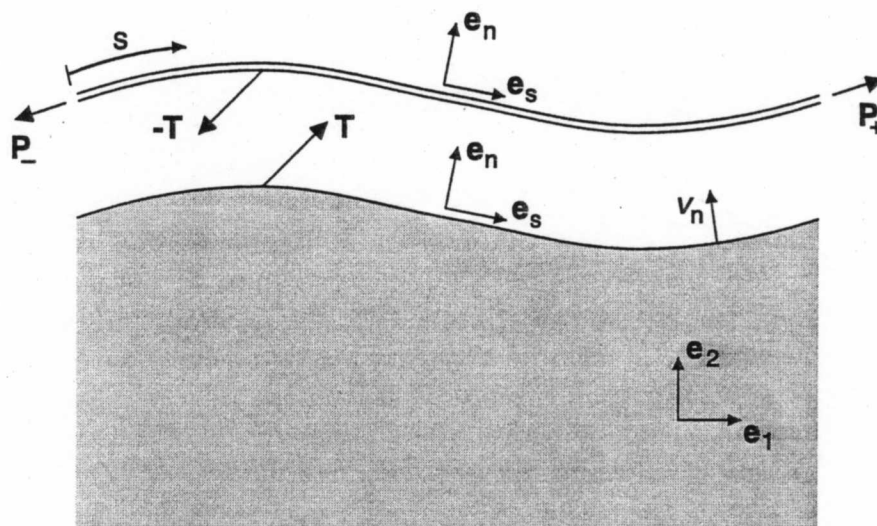

Figure 1. Schematic of bulk and surface phases shown separated, illustrating the traction T through which these phases interact. The surface is moving with local normal speed v_n.

The deformation is described by a displacement vector $\mathbf{u}$ with component form $\mathbf{u} = u_1 e_1 + u_2 e_2$ in the bulk material and $\mathbf{u} = u_s e_s + u_n e_n$ in the surface layer. The

local curvature of the surface is denoted by κ, measured positive if the surface is concave to the normal direction. The strains in the bulk and surface phases are then

$$\epsilon_{ij} = \tfrac{1}{2}\left(u_{i,j} + u_{j,i}\right), \quad \epsilon_s = u_{s,s} - \kappa u_n \tag{1}$$

where the comma represents partial differentiation and repeated indices are summed, except for indices s and n.

Equilibrium of the bulk material requires that the stress field σ_{ij} be divergence free and that the stress be related to the traction according to Cauchy's stress principle,

$$\sigma_{ij,j} = 0, \quad \sigma_{ij} = \sigma_{ji}, \quad T_i = \sigma_{ij} n_j \tag{2}$$

For the two-dimensional deformations being considered here, the surface tension is denoted by $\sigma_s(s)$. Then, equilibrium of the surface requires that [12,13]

$$\sigma_s \kappa = T_n, \quad \sigma_{s,s} = T_s, \quad \sigma_s(s_\pm) = \pm P_s \tag{3}$$

where s_+ and s_- are the extreme values of s in the range of arclength of interest. For all of the problems considered here, the lateral boundaries at $s = s_\pm$ are either remote or symmetry boundaries, so that $\dot{u}_s = 0$ there.

Free energy of the material is assumed to exist in the form of elastic strain energy, represented by $U(\epsilon_{kl})$ and measured per unit volume of material in the reference configuration, and surface energy, represented by $U_s(\epsilon_s)$ and measured per unit area of surface in the same configuration. Thus, the total free energy is

$$\mathcal{F}(t) = \int_B U(\epsilon_{ij})\, dB + \int_S U_s(\epsilon_s)\, dS \tag{4}$$

where B is the area of the plane occupied by the bulk phase and S is the curve representing the surface. The reference configuration is that configuration for which the bulk phase is totally stress free, which is usually not a realizable state without application of external loading. The constitutive relations for the bulk and surface materials are contained in the definitions of U and U_s. In particular,

$$\sigma_{ij} = \frac{\partial U}{\partial \epsilon_{ij}}, \quad \sigma_s = \frac{\partial U_s}{\partial \epsilon_s} \tag{5}$$

The time rate of change of free energy due to change in the shape of the free surface described by the local normal velocity v_n is then

$$\dot{\mathcal{F}}(t) = \int_B \frac{\partial U}{\partial t}\, dB + \int_S U v_n\, dS + \int_S \frac{\partial U_s}{\partial t}\, dS - \int_S \kappa U_s v_n\, dS \tag{6}$$

The interpretation of the various terms in this result is relatively straight forward. The first term accounts for changes in the mechanical fields at a material particle as time goes on, the second term accounts for local changes in the amount of bulk material involved, the third term accounts for the deformation of the free surface, and the last term accounts for local changes in the amount of free surface. The stress power theorem applied for the bulk and surface phases separately yields

$$\int_S \sigma_{ij} n_j \dot{u}_i\, dS = \int_B \sigma_{ij} \dot{\epsilon}_{ij}\, dB, \quad -\int_S \sigma_{ij} n_j \dot{u}_i\, dS = \int_S \sigma_s \dot{\epsilon}_s\, dS \tag{7}$$

If these two expressions are added, and the equilibrium equations are taken into account, then it is found that

$$\int_B \frac{\partial U}{\partial \epsilon_{ij}} \dot{\epsilon}_{ij} \, dB + \int_S \frac{\partial U_s}{\partial \epsilon_s} \dot{\epsilon}_s \, dS = 0 \tag{8}$$

Consequently, the rate of change of free energy reduces to

$$\dot{\mathcal{F}}(t) = \int_S [U - \kappa U_s] \, v_n \, dS \tag{9}$$

The product $v_n \, dS$ can be interpreted as the atomic volume of the material, say Ω, times the number of atoms being added per unit time to the area dS (which has unit extent in the x_3 direction). Consequently, the chemical potential for the surface is [14]

$$\chi = [U - \kappa U_s] \, \Omega \tag{10}$$

Mass diffuses along the surface in response to a local gradient in chemical potential. The mass flux j, measured in number of atoms passing a point on the surface per unit time (per unit distance in the x_3 direction) is given by

$$j = -\frac{D_s c_s}{kT} \frac{\partial \chi}{\partial s} \tag{11}$$

where D_s is the surface diffusivity, c_s is the surface concentration of atom sites, k is Boltzman's constant, and T is the absolute temperature.

Conservation of mass at each point along the surface requires that the normal velocity is proportional to the divergence of the local surface flux. In the present context,

$$v_n = -\Omega \frac{\partial j}{\partial s} = \frac{D_s c_s \Omega^2}{kT} \frac{\partial^2}{\partial s^2} [U - \kappa U_s] \tag{12}$$

Thus, given the elastic strain energy density along the surface, the local curvature distribution along the surface, and the surface energy density, (12) yields the normal velocity of the surface. Note that U depends on the stress induced by the action of the surface tension, as well as the action of the applied loads.

Two applications of this general result are considered next. The first is concerned with the stability of the surface of a stressed solid under fluctuations in surface shape, and the second is concerned with the influence of interface misfit dislocations on the roughening of the surface of a strained film. Although the surface energy can depend on the local elastic strain and on the crystallographic orientation of the surface, U_s is assumed to be a constant γ for the cases considered here. The surface tension is assumed to have the same constant value, so these effects are included only in the most rudimentary way here.

STRAIN ALONG A SLIGHTLY WAVY SURFACE

Consider an elastic body with a flat, traction-free surface under conditions of plane strain deformation. The plane of deformation is the x, y plane, and the surface is $y = 0$ in the reference configuration. Suppose that an equilibrium stress field exists throughout the body, giving rise to a strain distribution $\epsilon_0(x)$ along the surface $y = 0$. If the surface

shape in the undeformed configuration is then changed to $y = h(x)$ with $|h'(x)| \ll 1$, the *additional* extensional strain along the surface due to the waviness of the surface is

$$\Delta\epsilon_{xx}(x) = \frac{2}{\pi} \int_{-\infty}^{\infty} \frac{[\epsilon_0(\xi)h(\xi)]'}{\xi - x} \, d\xi \tag{13}$$

where the prime denotes differentiation. The change in strain due to the slight waviness of the surface is represented as a distribution along the original, flat shape of the surface. The special case of a uniform strain along the free surface was discussed in detail by Gao [15].
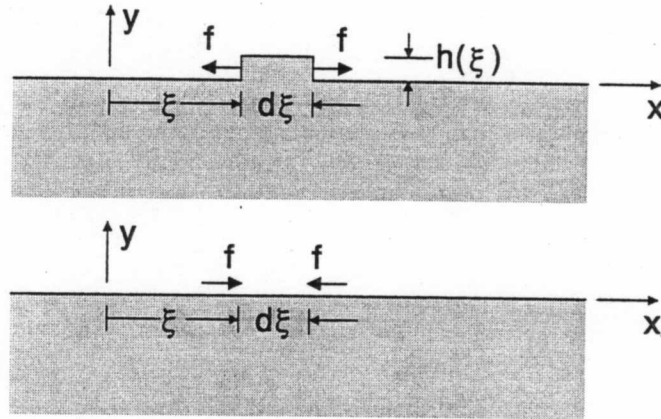

Figure 2. The superposition scheme leading to (13), involving the coherent attachment of a material element at a point with local strain $\epsilon_0(\xi)$ followed by relaxation of the forces needed to maintain that strain.

The expression (13) is derived by considering the process of coherently adding an infinitesimal strip of material of length $d\xi$ and thickness $h(\xi)$ to the flat surface at place $x = \xi$ in two steps, as depicted in Figure 2. This strip must be added with the same strain as the material to which it is being attached, or $\epsilon_0(\xi)$. As shown in Figure 2 (top), this strain must be maintained by forces of magnitude $f = Mh(\xi)\epsilon_0(\xi)$ where $M = 2\mu/(1 - \nu)$ is the plane strain extensional elastic modulus of the material with shear modulus μ and Poisson ratio ν. After the strip is attached, the forces maintaining this strain must be relieved, thereby altering the stress distribution in the bulk material. Because this force pair is essentially a dipole as shown in Figure 2 (bottom), the strain distribution induced throughout the body is that due to a surface force dipole. Superposition over the entire surface by integration leads to (13). The surface $y = 0$ is traction free, so the only contribution to the strain energy density along the surface is from the extensional strain along the surface. Thus,

$$U(x) = \tfrac{1}{2}M\left[\epsilon_0(x) + \Delta\epsilon_{xx}(x)\right]^2 \approx \tfrac{1}{2}M\left[\epsilon_0(x)^2 + 2\epsilon_0(x)\Delta\epsilon_{xx}(x)\right] \tag{14}$$

where only the term of lowest order in the small surface fluctuation is retained in the rightmost expression.

STABILITY OF A FLAT SURFACE

Consider now the particular case when the material is subjected to a uniform tension or compression of magnitude σ_0 in the direction parallel to the interface. Suppose that the surface is initially sinusoidal with arbitrarily small but nonzero amplitude, say a_0, and with spatial wavelength λ, that is,

$$h(x, t) = a(t) \cos \frac{2\pi x}{\lambda} \tag{15}$$

where $a(t)$ is the time-dependent amplitude as shown in Figure 3. It is assumed that the change in shape of the free surface is effected by diffusive transport of mass over the surface, although other mechanisms of mass transport will lead to the same result.
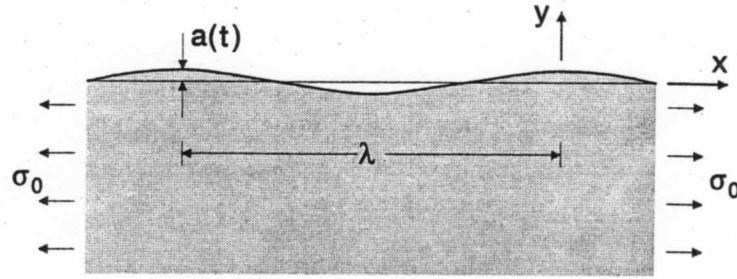

Figure 3. Schematic of a material with a wavy surface under plane strain tension or compression due to stress σ_0 parallel to the surface. The shape of the surface is given by (15).

For small amplitude fluctuation in surface shape, the equation (12) governing evolution of the surface shape is satisfied approximately if

$$\frac{\partial h}{\partial t}(x,t) = \frac{D_s c_s \Omega^2}{kT} \frac{\partial^2}{\partial x^2} \left[U(x,t) - \gamma \frac{\partial^2 h}{\partial x^2}(x,t) \right] \tag{16}$$

Because the strain energy density along the surface depends linearly on $h(x,t)$ through (14), this is a linear integro-differential equation for $h(x,t)$. With the assumption of a sinusoidal shape (15) and the uniform value of strain $\epsilon_0(\xi) = \sigma_0/M$, the integral (13) is readily evaluated to yield

$$U(x,t) = \frac{(1-\nu)\sigma_0^2}{4\mu} \left(1 - 8\pi \frac{a(t)}{\lambda} \cos \frac{2\pi x}{\lambda} \right) \tag{17}$$

It is noted in passing that a similar result can be obtained if the material is subjected to a biaxial stress state.

With the result in (17) for $U(x,t)$, the equation (16) governing the time-dependent shape of the surface is reduced to an ordinary differential equation for $a(t)$ which is most conveniently expressed in terms of nondimensional time τ, amplitude $\alpha(\tau)$ and wavelength ℓ defined by

$$\tau = \left(\frac{\sigma_0^2}{\gamma\mu} \right)^4 \frac{\gamma D_s c_s \Omega^2}{kT} t, \quad \alpha(\tau) = \frac{a(t)\sigma_0^2}{\gamma\mu}, \quad \ell = \frac{\lambda\sigma_0^2}{\gamma\mu} \tag{18}$$

The resulting equation for $\alpha(\tau)$ is

$$\alpha'(\tau) + \left(\frac{2\pi}{\ell} \right)^3 \left[\frac{2\pi}{\ell} - (1-\nu) \right] \alpha(\tau) = 0 \tag{19}$$

where the prime denotes differentiation. The solution of this equation satisfying the initial condition $\alpha(0) = \alpha_0$ is

$$\alpha(t) = \alpha_0 \exp \left\{ - \left(\frac{2\pi}{\ell} \right)^3 \left[\frac{2\pi}{\ell} - (1-\nu) \right] \tau \right\} \tag{20}$$

It is evident that the amplitude of the surface fluctuation will grow (decay) in time if the sign of the quantity enclosed in square brackets in the exponent of (20) is negative

(positive). The discriminating wavelength is called the *critical wavelength* λ_{cr}, and it is given by

$$\lambda_{cr} = \frac{2\pi\mu\gamma}{(1-\nu)\sigma_0^2} \tag{21}$$

To consider the potential relevance of this result to strained-layer epitaxial systems, suppose that a value of the critical wavelength is calculated for the system parameters $\nu = 0.3$, $\sigma_0 = 10^9$ N/m^2, $\gamma = 1$ J/m^2 and $\mu = 50 \times 10^9$ N/m^2. The resulting value of critical wavelength is $\lambda_{cr} = 450$ nm, which falls within the range of interest in considering strained-layer systems with elastic mismatch strain on the order of one percent. For the case of biaxial tension, the critical wavelength is larger by a factor of $1 + \nu$.
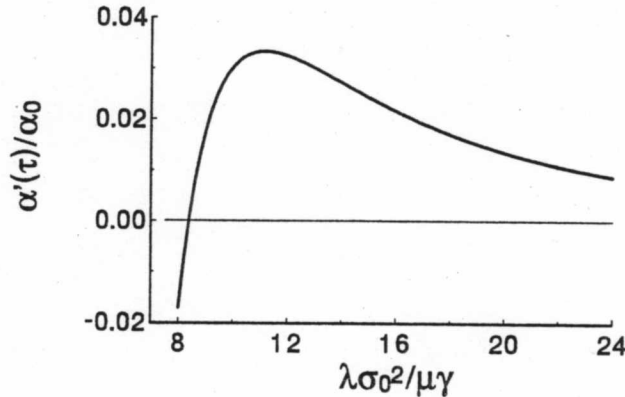

Figure 4. Normalized rate of growth of surface fluctuations versus wavelength as given by (20).

The rate of growth or decay of the amplitude of the fluctuation is given by the time-independent quantity $\dot{a}(t)/a_0$, which is plotted in the nondimensional form $\alpha'(\tau)/\alpha_0$ versus $\lambda\sigma_0^2/\mu\gamma$ in Figure 4 for $\nu = 0.3$. It is evident from this figure that the amplitude decays for $\lambda < \lambda_{cr}$. The highest rate of growth is seen to occur at a wavelength of $\frac{4}{3}\lambda_{cr}$, and it diminishes quite rapidly as wavelength increases beyond the maximum.

EQUILIBRIUM ROUGHNESS DUE TO MISFIT DISLOCATIONS

In the foregoing stability analysis, the consequence of mass rearrangement by surface diffusion is to perturb a spatially uniform stress field. In this section, attention is focused on a situation in which a *nonuniform stress field* induces mass rearrangement on the surface of a material. The analysis is motivated by an observation reported by Fitzgerald et al [16] on the surface topography of an InGaAs strained layer deposited on a GaAs substrate following partial strain relaxation by formation of interface misfit dislocations. They described ridges on the surface of the strained layer in which the elastic mismatch strain had been partially relaxed. Furthermore, the locations of the ridges correlated with the positions of interface misfit dislocations. It was suggested that perhaps the ridges played some role in the nucleation of the threading dislocations which propagated to produce the interface misfit dislocations. It appears, however, that a more likely sequence of events is that the misfit dislocations appeared *before* the surface ridges. Before relaxation, the surface is nominally flat and the strain in the layer is uniform. Thus, the chemical potential is uniform. Following formation of a misfit dislocation, the strain distribution along the surface becomes *nonuniform* and, consequently, the chemical potential develops a gradient along the surface. In response to this gradient, some mass rearrangement can occur over the surface to re-establish a shape with constant chemical potential (in the equilibrium limit). It is the point of

this section to demonstrate that this rearrangement can take the form of ridges on the surface of the material aligned with the underlying misfit dislocations. With reference to the equation (16) which describes the evolution of the surface shape, the long time limiting form of this equation governing the equilibrium shape (if such a shape exists) is

$$U(x) - \gamma h''(x) = \text{constant} \tag{22}$$

where the explicit dependence on time t has been suppressed. This condition provides an ordinary differential equation for the equilibrium shape of the surface. The value of the constant must be inferred from physical conditions of any particular case.
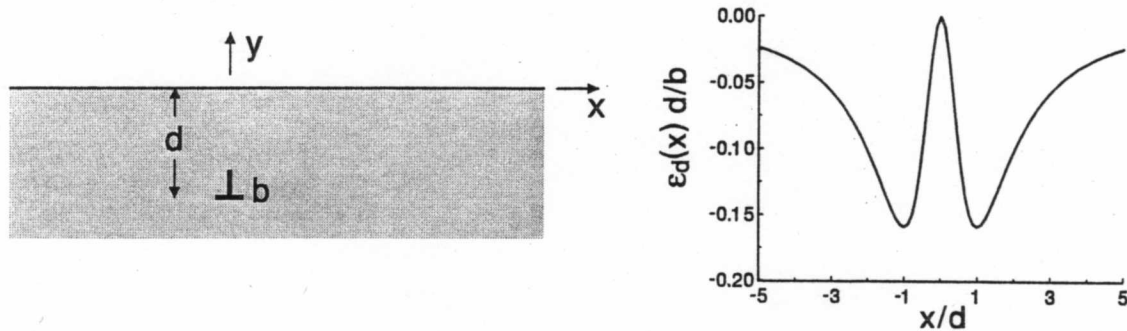

Figure 5. An edge dislocation at a depth d below the free surface of an elastic solid (left), and the extensional strain along the free surface induced by the dislocation (right).

As a first step, consider the elastic field of a single dislocation located a distance d from the initially flat, traction-free surface of a crystal. Eventually, the parameter d will be identified with the thickness of a strained layer. Furthermore, suppose that the dislocation is a pure edge dislocation with Burgers vector of magnitude b as shown in Figure 5. The only nonzero component of strain along the free surface is ϵ_{xx}, and an expression for this strain distribution is [17]

$$\epsilon_{xx}(x,0) = \epsilon_d(x) = \frac{2}{\pi} \frac{b\,d\,x^2}{(d^2 + x^2)^2} \tag{23}$$

A graph of this strain distribution due to the field of the dislocation alone is also shown in Figure 5. The strain energy density along the free surface is determined primarily by this strain distribution, but it also depends on the *additional* strain due to variations in the shape of the surface represented by the expression (13) and on the *additional* strain arising from the traction of interaction between the surface phase and the bulk phase represented by T_n in (3)$_1$. This last contribution is considered next.

In the simplest approximation, the surface energy and surface tension are equal in magnitude [1] so that $\sigma_s = \gamma$ in (3)$_1$. Furthermore, within the framework of small amplitude fluctuations, the curvature κ in (3) is given by $h''(x)$. Therefore, the normal traction induced on the surface of the bulk phase due to the curvature in the surface phase is $\gamma h''(x)$. The corresponding contribution to strain in the bulk phase is given by

$$\Delta\epsilon_{yy}(x) = \frac{\gamma h''(x)}{M} \tag{24}$$

With these contributions to the elastic strain along the surface identified, the strain energy density along the surface is

$$U(x) = \tfrac{1}{2} M \left([\epsilon_d(x) + \Delta\epsilon_{xx}(x)]^2 + \Delta\epsilon_{yy}(x)^2 \right) \approx \tfrac{1}{2} M \epsilon_d(x)^2 \tag{25}$$

It remains to solve the differential equation (22) for the shape of the surface, subject to the remote conditions that

$$h(x) \to 0 \quad \text{and} \quad h'(x) \to 0 \quad \text{as} \quad x \to \pm\infty \tag{26}$$

Consider first the approximation represented by the last form of the strain energy distribution in (25). The constant in (25) must be zero in this case and the governing differential equation is

$$h''(x) = \frac{M}{2\gamma}\epsilon_d(x)^2, \qquad m = \frac{Mb}{2\gamma}\frac{b}{d} \tag{27}$$

This equation poses an immediate difficulty. The right side is always positive, which implies that the curvature of the surface is always positive. However, there is no solution $h(x)$ to (27) which satisfies (26) *and* for which both $h(x)$ and $h'(x)$ are continuous. A solution for which the shape is continuous is easily obtained by direct integration, and it is shown in Figure 6. When all effects represented in the strain energy expression $(25)_1$ are taken into account, the equation (22) governing the shape of the surface in the reference configuration has the form of an integro-differential equation. This equation has been solved numerically, but the difference between the more complete solution and the result shown in Figure 6 is almost imperceptible. Thus, the discontinuity in slope at $x = 0$ must be rationalized on some other basis.
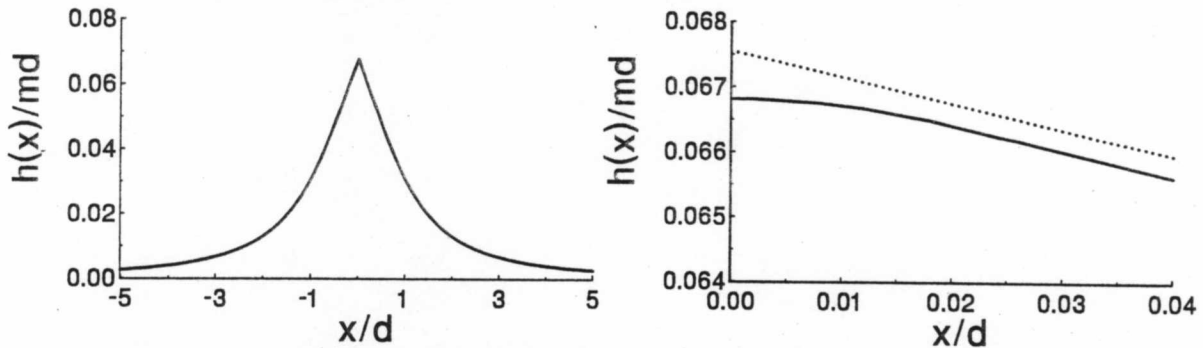

Figure 6. The equilibrium shape $h(x)$ of the surface of the material versus position along the surface obtained by solving the linear equation (27) (left). On the right, the solution of the nonlinear equation (29) for surface shape is shown as a solid curve. The dotted curve is from the graph on the left. The shape on the right is symmetric with respect to the point $x = 0$ and only the portion for $x \geq 0$ is shown. Note that the ordinate scales are exaggerated.

Perhaps a more fruitful path toward resolving this dilemma could be based on the observation that the equation for $h(x)$ is enforced in the reference configuration, under the assumption that the curvature is everywhere small. The solution found obviously violates the assumption of small curvature in the neighborhood of $x = 0$, where the curvature becomes singular. Strictly, the condition for locating the equilibrium surface should be that the chemical potential is constant in the *current* configuration of the body. In the context of the present problem, the curvature in the current configuration, say κ^*, can be expressed in terms of the curvature κ in the reference configuration and the component of strain normal to the surface, which here is $\Delta\epsilon_{yy}(x,0)$ in (24), as

$$\kappa^* = (1 + \Delta\epsilon_{yy})\kappa \tag{28}$$

If this line of reasoning is pursued, the differential equation (27) governing $h(x)$ is modified to the form

$$\left(1 + \frac{\gamma}{M}h''(x)\right)h''(x) = \frac{M}{2\gamma}\epsilon_d(x)^2 \tag{29}$$

Although this equation can be solved without difficulty, it is clear from its form that the apparently slight modification resolves the problem. When the curvature is indeed small, the equation is the same as the original form (27) in all essential respects. When the curvature becomes large in magnitude, however, the nonlinear term on the left side comes into play. In a range of x in which curvature is large, mainly near $x = 0$, the equation is essentially $h''(x) = -M/\gamma$ which shows that the curvature is large in magnitude and negative. The effect is to smooth out the discontinuity in slope in $h(x)$ near $x = 0$. The result of actually solving the nonlinear equation is shown in Figure 6 (right), in which the abscissa is greatly expanded compared to that on the left to show the details. While inclusion of the nonlinear term in the governing equation makes it possible to find a solution with continuous slope $h'(x)$, as well as continuous $h(x)$, the difference in the maximum surface heights predicted by the two equations is about 1% of the total height, and the differences are imperceptible when plotted on the scale of Figure 6.

The same general approach can be followed in considering the roughening of the surface due to the presence of a periodic array of dislocations below the surface. For example, consider the case depicted on the left in Figure 7, which represents a periodic array of identical edge dislocations situated at a distance d below the initially flat surface and spaced at intervals of p. The strain distribution $\epsilon_{xx}(x, 0)$ induced along the surface due to this array of dislocations is given by [18]

$$\epsilon_d(x) = \frac{b}{d} \left[\frac{4\pi - 4\pi \cos \frac{2\pi x}{p} \cosh \frac{2\pi d}{p} - 2\frac{p}{d} \cos \frac{2\pi x}{p} \sinh \frac{2\pi d}{p} + \frac{p}{d} \sinh \frac{4\pi d}{p}}{2\frac{p^2}{d^2} \left(\cos \frac{2\pi x}{p} - \cosh \frac{2\pi d}{p} \right)^2} \right] \quad (30)$$

This strain distribution is also shown for the particular case of $p = 2d$ in Figure 7 (right).
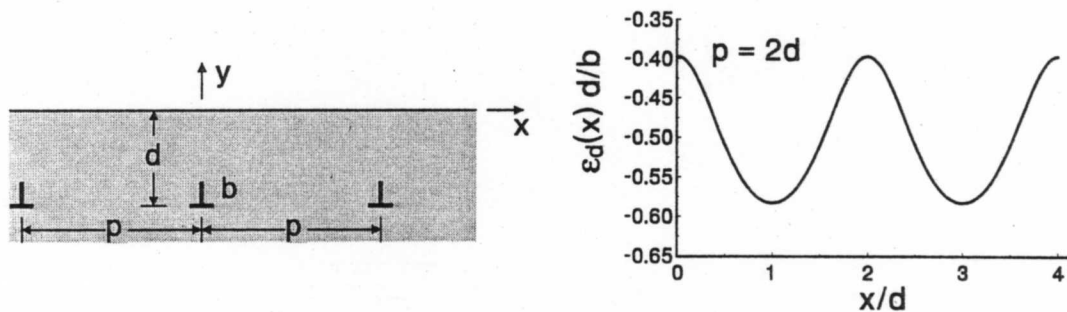

Figure 7. Periodic array of identical edge dislocations at depth d and spacing p (left), and the extensional strain along the surface induced by this array for the particular case with $p = 2d$ (right).

The differential equation (27) can also be solved for this strain distribution. One difference in the case of a periodic distribution of dislocations from that of an isolated dislocation is that the remote conditions (26) are no longer relevant. Instead, the equilibrium surface shape must be periodic, the slope of the surface shape must be continuous and mass must be conserved within each interval of length p. Consequently, any shape of the surface must satisfy the conditions

$$h(x) = h(p - x), \quad h'(0) = 0, \quad \int_0^p h(x)\, dx = 0 \quad (31)$$

These three conditions are sufficient to determine the constant in (22) plus the two constants of integration which arise. Of particular interest is the extent of surface roughening predicted. This result is presented in terms of difference between the maximum and minimum values taken on by $h(x)$ within each period along the surface. This difference is denoted by $\Delta h = h_{max} - h_{min}$ and, for the case of $p = 2d$, it has the value $\Delta h = 0.02\,md$.

The process of surface diffusion due to dislocations below the surface can also be considered when a uniform background strain is present, as in the case of strained epitaxial films. The equilibrium surface shape in this case is estimated by adding the uniform strain, say ϵ_u, to the strain energy expression (25) so that $U(x) \approx \frac{1}{2}M\left[\epsilon_d(x) + \epsilon_u\right]^2$, and then integrating the differential equation (22) subject to the conditions (31).

EVOLUTION OF SURFACE ROUGHNESS

While the discussion of the preceding section was focused on equilibrium surface shapes, a more complete analysis of the phenomenon of surface diffusion should lead to a description of the transient evolution of surface shape. Two ingredients are essential in a model intended to provide such a description. The first, which is represented by (12), gives the instantaneous motion of the surface in terms of a prescribed strain energy density U along the surface and a prescribed curvature κ of the surface. The complementary second ingredient gives the strain energy density along the surface for any prescribed surface shape. Equation (17) is a simple example of such a result. While the foregoing analysis of stability of the flat surface of a strained material appears to have these features, it is restricted in the respect that all fields, including strain energy density, are referred to the original flat shape of the surface rather than the current altered shape.
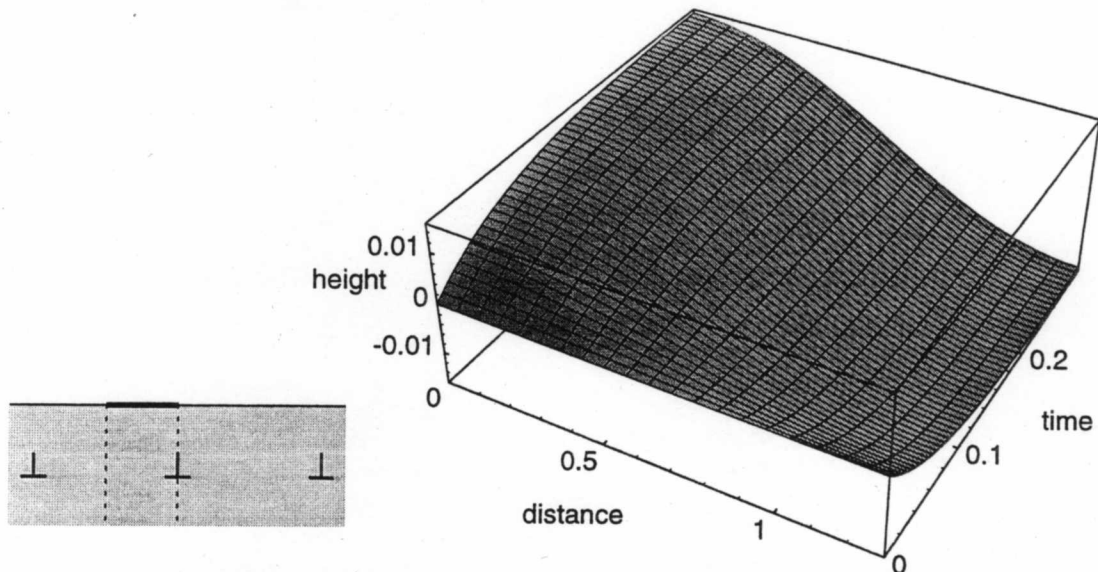

Figure 8. Time history of surface shape due to surface diffusion resulting from a periodic array of dislocations with Burgers vector b at depth d and spacing $3d$, plus a uniform background strain b/d. The portion of the material surface represented by this history is shown by the dark line on the inset.

The boundary value problem modeling this process is inherently nonlinear when posed in this way, and it appears that numerical implementation of the two ingredients is required for its solution. Work on this problem area is in its early stages, and no systematic study of these problems has yet been carried out. However, some results are now available and a preliminary sample is included here. Consider the case of a periodic array of edge dislocations as shown in Figure 7 (left) with spacing $p = 3d$,

which results in an average compressive strain along the surface of $-b/3d$. In addition, a uniform extensional strain $\epsilon_u = +b/d$ is superimposed on this field. The surface is initially flat, and then it is allowed to distort according to the transport equation (12). The step involving determination of the strain energy density along the surface in terms of surface shape is carried out by means of the numerical finite element method, and the step of integrating the surface evolution equation (12) is carried out by means of the Crank-Nicholson time integration algorithm. In Figure 8, normalized distance $= (1 - \nu)mx/d$, normalized height$= (1 - \nu)mh/d$ and normalized time$= \tau$ where m is defined in (27) and τ is defined in (18).

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