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THE EFFECT OF SURFACE STRESS ON THE STABILITY OF SURFACES OF STRESSED SOLIDS

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Abstract—The chemical potential associated with surfaces of stressed solids is found to consist of four terms, instead of the widely accepted two. The boundary conditions are also affected by the presence of a surface deformation-dependent surface stress. The stability of the surfaces of stressed solids is reinvestigated, using the revised equations. It is found that the stability condition is sensitive to the sign of the applied stress. © *1998 Acta Metallurgica Inc*.

1. INTRODUCTION

The first theoretical investigation of the stress-driven morphological instability in solids appears to have been given by Asaro and Tiller [1]. They examined the linear stability of a planar surface separating a stressed, two-dimensional semi-infinite solid from a fluid and found that the planar surface was unstable to small disturbances with wavelengths greater than a characteristic length. The same result was later rediscovered by Grinfeld [2] and Srolovitz [3]. The starting point of these theoretical investigations is the chemical potential Ψ given by

$$\Psi = (W - \Gamma_0 K)\Omega \tag{1}$$

where W is the strain energy density of the solid (evaluated on the surface in question), Ω the atomic volume, Γ_0 the assumed constant surface energy density, and K the mean curvature, all expressed in terms of a chosen referential configuration. The critical wavelength b_c governing the instability of the surface $Z_2 = 0$, bounding the elastic half-space $Z_2 < 0$, is

$$b_c = \frac{\pi E \Gamma_0}{(1 - \nu^2)T^2} \tag{2}$$

where E and ν are, respectively, Young's modulus and Poisson's ratio and T is the value of the horizontal stress in the solid. The elasticity solution associated with the above result satisfies the traction-free conditions along the perturbed planar boundary, i.e.

$$\tau_{NN} = 0, \quad \tau_{SN} = 0, \tag{3}$$

where S and N signify, respectively, the tangential and normal directions to the boundary. It is noted that b_c is not affected by the sign of T.

Stressing the importance of an assumed constant elastic surface stress (surface tension) Σ_0, Grilhe [4] replaced the first of equations (3) with, in terms of our notation,

$$\tau_{NN} = \Sigma_0 K \tag{4}$$

and obtained a new elasticity solution for the evaluation of W. Grilhe's modified critical wavelength b_{cg} is given by

$$b_{cg} = b_c(1 - \Sigma_0/Tb_c + \cdots) \tag{5}$$

which also makes use of equation (1).

In the context of finite elasticity and with the assumption that surface energy is a function of surface deformation, the completeness of the chemical potential, together with the associated governing equations, was re-examined by Wu [5]. It was found that, even after a reduction to linear elasticity, the expression (1) is incomplete. Moreover, even the modified condition (4) is still incomplete. The correct equations and conditions are presented in Section 2.1.

It has been commonly accepted that for solids surface tension is not the same as surface energy [6]. On the other hand it has also been not uncommon to find the two terms used in synonymous ways when applied to solids. One of the reasons for this ambiguity is perhaps due to the lack of known surface deformation-dependent surface energy expressions. The determination of surface energy is already a feat in itself [7]. We are not aware of any experimental or theoretical work that deals with the surface strain dependence of surface energy. Using an experimentally justified universal binding-energy–distance curve [8–11], a plausible surface energy expression is obtained in this paper. This is given in Section 2.2.

The stability of the surfaces of stressed solids is used as an example to illustrate the effect of the corrected equations. It is shown that the corrected critical wavelength b_{cw} is

$$b_{\mathrm{cw}} = b_{\mathrm{c}}\left(1 - \frac{4}{1-\nu}\epsilon_T - \frac{1-2\nu}{(1-\nu)^2}\epsilon_T^2 + \cdots\right) \tag{6}$$

where $\varepsilon_T = (1-\nu^2)T/E$. This result is to be compared with equations (1) and (5). The derivation for the above is given in Section 3.

2. GOVERNING EQUATIONS

2.1. Finite plane elastostatics with surface strain dependent surface energy

As in Wu [5], we consider a two-dimensional material body with (two-dimensional) reference configuration B and (two-dimensional) deformed configuration b and designate by $\mathbf{Z} = Z_I\mathbf{e}_I$ and $\mathbf{z} = z_i\mathbf{e}_i$, respectively, the referential and spatial positions of a typical particle relative to a common origin 0 and common base $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. The referential and spatial positions of a typical particle are linked by

$$\mathbf{z} = \mathbf{\Phi}(\mathbf{Z}), \quad z_i = \Phi_i(Z_I) \text{ on } B, \tag{7}$$

and the associated deformation gradient tensor $\mathbf{F}$ is just

$$\mathbf{F} = \mathrm{Grad}\,\mathbf{\Phi}, \quad F_{iI} = \Phi_{i,I} = \partial\Phi_i/\partial Z_I. \tag{8}$$

It is assumed that the material body is composed of a homogeneous elastic material with strain-energy function $W(\mathbf{F})$ measured per unit volume in the referential configuration.

Let the bounding surface ∂B of B be parametrically represented by

$$\partial\mathbf{B}{:}\mathbf{Z} = \mathbf{X}(L) \tag{9}$$

where L measures the arc length along the boundary. The unit tangent $\mathbf{S}$ is

$$\mathbf{S} = \mathrm{d}\mathbf{X}/\mathrm{d}L \tag{10}$$

and the sense of L is fixed in such a way that, together with the outward normal $\mathbf{N}$ and $\mathbf{e}_3$, $(\mathbf{S}, \mathbf{N}, \mathbf{e}_3)$ is right-handed. It is convenient to express the unit tangent in terms of a single angle $\Theta(L)$ so that

$$\mathbf{S} = \cos\Theta\mathbf{e}_1 + \sin\Theta\mathbf{e}_2 \tag{11}$$

and

$$\frac{\mathrm{d}\mathbf{S}}{\mathrm{d}L} = K\mathbf{N}, \quad \frac{\mathrm{d}\mathbf{N}}{\mathrm{d}L} = -K\mathbf{S}, \tag{12}$$

where $K = \mathrm{d}\Theta/\mathrm{d}L$ is the curvature.

For an arbitrary point $\mathbf{Z}$ sufficiently close to a point $\mathbf{X}(L)$ on ∂B, it is convenient to introduce the shell-coordinates representation:

$$\mathbf{Z} = \mathbf{X}(L) + Y\mathbf{N}(L) \tag{13}$$

where Y measures the distance along $\mathbf{N}$. We have

$$\mathrm{d}\mathbf{Z} = [(1 - YK)\,\mathrm{d}L]\mathbf{S} + \mathrm{d}Y\mathbf{N} \tag{14}$$

which defines the metric associated with the curvilinear coordinates (L, Y). Subjecting equation (14) to the deformation (7), we obtain

$$\mathbf{F}(\mathbf{X} + Y\mathbf{N})\,\mathrm{d}\mathbf{Z} = \Lambda_{(S)}(L, Y)[(1 - YK)\,\mathrm{d}L]\mathbf{s} + \Lambda_{(N)}(L, Y)\,\mathrm{d}Y\mathbf{n}^d \tag{15}$$

where $\mathbf{s}$ and $\mathbf{n}^d$ are unit vectors, and, to the first order in Y,

$$\Lambda_{(S)}(L, Y) = \Lambda + \frac{\mathbf{FS}}{\Lambda}\cdot[\mathbf{N}\cdot\mathrm{Grad}\,\mathbf{F}]\mathbf{S}Y, \tag{16}$$

$$\Lambda_{(N)}(L, Y) = \Lambda_N + \frac{\mathbf{FN}}{\Lambda_N}\cdot[\mathbf{N}\cdot\mathrm{Grad}\,\mathbf{F}]\mathbf{N}Y, \tag{17}$$

in which

$$\Lambda = \Lambda_{(S)}(L, 0), \quad \Lambda_N = \Lambda_{(N)}(L, 0). \tag{18}$$

It can be easily checked that

$$\mathbf{FS} = \Lambda\mathbf{s}, \quad \mathbf{FN} = \Lambda_N\mathbf{n}^d \text{ on } \partial B \tag{19}$$

and $\mathbf{s}$, $\mathbf{n}^d$ are, in general, not orthogonal. It is now assumed that the material surface ∂B is characterized by an isotropic surface energy function $\Gamma(\Lambda)$, measured per unit surface area in the referential configuration. We may now write the total free energy of the system as

$$\Pi = \int_B W\,\mathrm{d}A + \int_{\partial B}\Gamma\,\mathrm{d}L, \tag{20}$$

and all the governing conditions can be deduced from a variational consideration of the above.

In terms of the curvilinear coordinates (L, Y) of equation (13) and for linear elasticity, the strains and stresses may be denoted by $(\varepsilon_{SS}, \varepsilon_{NN}, \varepsilon_{SN})$ and $(\tau_{SS}, \tau_{NN}, \tau_{SN})$, respectively. They are the 2×2 portions of ε and τ, which are related by

$$\tau_{ij} = 2\mu\varepsilon_{ij} + \lambda\delta_{ij}\varepsilon_{kk} \tag{21}$$

where λ and μ are Lame constants. For the correct and complete chemical potential, we have

$$\Psi = \left[W - \Gamma K + \Sigma\frac{\partial\varepsilon_{SS}}{\partial Y} - \frac{\partial}{\partial L}(2\Sigma\varepsilon_{SN})\right]\Omega \tag{22}$$

where

$$W = \tfrac{1}{2}\tau_{ij}\varepsilon_{ij}, \tag{23}$$

$$\Gamma = \Gamma(\varepsilon), \quad \Sigma = \frac{\partial\Gamma}{\partial\varepsilon}, \quad \varepsilon = \varepsilon_{SS}(L, 0). \tag{24}$$

The boundary conditions for the elasticity problem to be solved are

$$\tau_{NN} = \Sigma k, \quad \tau_{SN} = (1 - \varepsilon)\frac{\mathrm{d}\Sigma}{\mathrm{d}L} \tag{25}$$

where

$$k = (1 - \varepsilon_{NN})K - \frac{\partial \varepsilon_{SS}}{\partial Y} + 2\frac{\partial \varepsilon_{SN}}{\partial L} \tag{26}$$

in which K is the curvature associated with ∂B. A detailed account of the above results may be found in Wu [5] where the development was based on the premise that the surface energy Γ is a function of the surface deformation, i.e. Λ of equation (18) or ε of equation (24). We are not aware of any known theoretical or experimental results dealing with the dependence of Γ on ε. However, it is commonly accepted that Γ and Σ are of comparable orders of magnitude [6]. A simple and plausible relation is established in the rest of the section based on certain known universal features of the equation of state of metals [8–11].

2.2. *Effect of surface strain on surface energy*

It has been shown in a series of papers by Rose *et al.* [8–11] that the metallic binding-energy–distance curves can be approximately scaled into a single universal relation in each of the following cases: (1) chemisorption on a metal surface; (2) metallic and bimetallic adhesion; and (3) the cohesion of bulk metals. In each case, the energy relation, expressed in terms of our notation, can be written as

$$E_T(a) = \Delta E_T E^*(a^*) \tag{27}$$

where $E_T(a)$ is the total energy as a function of the interatomic separation distance a, ΔE_T is the equilibrium binding energy, and $E^*(a^*)$ is an approximately universal function which describes the shape of the binding-energy curve. The dimensionless separation a^* is a scaled distance defined by

$$a^* = (a - a_e)/l \tag{28}$$

where a_e is the equilibrium separation and l is a scaling length characterizing the material(s) involved. A suitable choice for E^* is

$$E^*(a^*) = (1 + a^*)\,\mathrm{e}^{-a^*} \tag{29}$$

and the scaling length l may be determined from

$$l = \left[\Delta E_T \Big/ \left.\frac{\mathrm{d}^2 E_T(a)}{\mathrm{d}a^2}\right|_{a = a_e}\right]^{1/2}. \tag{30}$$

This result has been used by Gupta in an evaluation of the interface tensile strength–roughness relationship. Our purpose here is to deduce a surface strain-dependent toughness from the universal features of the above energy relation.

Let a_1, a_2 and a_3 be the lattice constants of an orthorhombic crystal. If a is the interatomic separation distance in the a_3 direction, then $E_T(a)$ of equation (27) is the total energy between a couple of atoms divided by $a_1 a_2$. Thus $E_T(a)$ is the total energy per unit area in the referential (a_1, a_2)-plane. In applying equation (27), however, a_e of equation (28) should be replaced by a_3. Differentiating equation (27), we obtain

$$\sigma(a) = \frac{\partial E_T}{\partial a} = \frac{\Delta E_T}{l} a^*\,\mathrm{e}^{-a^*}, \tag{31}$$

$$\frac{\partial \sigma}{\partial a} = \frac{\partial^2 E_T}{\partial a^2} = \frac{\Delta E_T}{l^2}(1 - a^*)\,\mathrm{e}^{-a^*}, \tag{32}$$

where σ is the stress defined per unit area in the (a_1, a_2)-plane. In terms of a strain variable ε, we have

$$\frac{\partial \sigma}{\partial a} = \frac{1}{a_3}\frac{\partial \sigma}{\partial \varepsilon}, \quad \varepsilon = \frac{a - a_3}{a_3}. \tag{33}$$

Equating the last two expressions for $\partial\sigma/\partial a$ and setting $\varepsilon = a^* = 0$, we obtain

$$\Delta E_T = l^2 E/a_3 \tag{34}$$

where E is the modulus in the a_3 direction. The intrinsic toughness G_0 and the surface energy Γ_0, defined per unit area in the (a_1, a_2)-plane are given by

$$G_0 \equiv 2\Gamma_0 = \int_{a_3}^{\infty} \sigma(a)\,\mathrm{d}a$$

$$= E_T(\infty) - E_T(a_3) = \Delta E_T. \tag{35}$$

In particular, for a cubic lattice $a_1 = a_2 = a_3 = a_0$

$$\Gamma_0 = l^2 E/2a_0 \tag{36}$$

where E is Young's modulus.

Consider now a cubic lattice with lattice constant a_0. The crystal is deformed into an "orthorhombic system" with

$$a_1 = \Lambda_1 a_0, \quad a_2 = \Lambda_2 a_0, \quad a_3 = \Lambda_3 a_0, \tag{37}$$

where Λ_1, Λ_2 and Λ_3 are the principal stretch ratios associated with the deformation of the cubic lattice. Let $W(\Lambda_1, \Lambda_2, \Lambda_3)$ denote the strain energy density of the crystal. The stretch ratio Λ_3 of equation (37) is actually a function of Λ_1 and Λ_2 determined from

$$\left.\frac{\partial W}{\partial \Lambda_3}\right|_{\Lambda_3 = \Lambda_3^0(\Lambda, \Lambda_2)} = 0. \tag{38}$$

It is in this sense that a_3 of equation (37) is referred to as an equilibrium separation. We may now apply equations (27)–(35) to the orthorhombic system (37) to conclude that the surface energy Γ_0^* defined per unit area in the (a_1, a_2)-plane of equation (37) is

$$\Gamma_0^* = l^2 E/2a_3. \tag{39}$$

It follows that the surface energy Γ defined per unit area in the original (a_0, a_0)-plane is $\Lambda_1\Lambda_2\,\Gamma_0^*$, i.e.

$$\Gamma = \Gamma(\Lambda_1, \Lambda_2) = \frac{\Lambda_1\Lambda_2}{\Lambda_3^0(\Lambda_1, \Lambda_2)}\,\Gamma_0, \tag{40}$$

where Γ_0 is given by equation (36). For small to moderately large strains, one may use equations (23) and (38) to obtain

$$\Lambda_3^0 = 1 - \frac{\nu}{1-\nu}\,(\Lambda_1 + \Lambda_2 - 2). \tag{41}$$

The function $\Gamma(\varepsilon)$ of equation (24) may be deduced from the last two expressions. It is

$$\Gamma(\varepsilon) = \frac{1+\varepsilon}{1 - \dfrac{\nu}{1-\nu}\,\varepsilon}\,\Gamma_0. \tag{42}$$

The elastic surface stress (or surface tension) is just

$$\Sigma = \frac{\partial\Gamma}{\partial\varepsilon} = \Sigma_0\left(1 + \frac{2\nu}{1-\nu}\,\varepsilon + \cdots\right) \tag{43}$$

where $\Sigma_0 = \Gamma_0(1-\nu)$ is the constant portion of the surface stress.

3. STABILITY OF SURFACES OF STRESSED SOLIDS

Consider the lower half-space defined by

$$Z_2 < h(Z_1) = a\cos\kappa Z_1 = a\cos\frac{2\pi Z_1}{b}, \tag{44}$$

where a is the amplitude and $b = 2\pi/\kappa$ is the wavelength of the bounding surface. The sinusoidal fluctuation of the surface is assumed to be small in the sense that $a\kappa \ll 1$. The half-space is uniformly stressed at infinity by $\tau_{11} = T$ and the boundary condition along $Z_2 = h(Z_1)$ is of the type specified by equation (25).

The following stress function [3] is introduced:

$$\Phi = \phi + \frac{T}{2}Z_2^2, \quad \phi = (A + B\kappa Z_2)\,\mathrm{e}^{\kappa Z_2}\cos\kappa Z_1, \tag{45}$$

where A and B are constants to be determined. The associated equilibrium stresses are:

$$\tau_{11} = T + \phi_{,22}, \quad \tau_{22} = \phi_{,11}, \quad \tau_{12} = -\phi_{,12} \tag{46}$$

where commas denote partial differentiation and $\phi(Z_1, Z_2)$ is biharmonic.

The kinematics associated with the boundary $Z_2 = h(Z_1)$ are defined by equations (10)–(12), and

$$\sin\Theta = -a\kappa\sin\kappa Z_1 + \ \ldots, \quad \cos\Theta = 1 + \cdots, \tag{47}$$

$$K = -a\kappa^2\cos\kappa Z_1 + \cdots. \tag{48}$$

It follows from equation (47) that the curvilinear components $(\tau_{SS}, \tau_{NN}, \tau_{SN})$ of the stress tensor are

$$\tau_{SS} = T + \phi_{,22} + \cdots, \quad \tau_{NN} = \phi_{,11} + \cdots,$$
$$\tau_{SN} = Ta\kappa\sin\kappa Z_1 - \phi_{,12} + \cdots. \tag{49}$$

The curvilinear components $(\varepsilon_{SS}, \varepsilon_{NN}, \varepsilon_{SN})$ of the strain tensor, for plane strain, are just

$$\begin{aligned}\varepsilon_{SS} &= \frac{1}{E}[(1-\nu^2)T \\ &\qquad + (1-\nu^2)\phi_{,22} - \nu(1+\nu)\phi_{,11} + \cdots],\\ \varepsilon_{NN} &= \frac{1}{E}[-\nu(1+\nu)T + (1-\nu^2)\phi_{,11} \\ &\qquad - \nu(1+\nu)\phi_{,22} + \cdots],\\ \varepsilon_{SN} &= \frac{1+\nu}{E}[Ta\kappa\sin\kappa Z_1 - \phi_{,12} + \cdots].\end{aligned} \tag{50}$$

The curvature k of the deformed boundary may be calculated from equation (26)

$$k = -\left\{\left[1 - \frac{(1+\nu)(2-\nu)T}{E}\right]a\kappa^2 - \frac{(1+\nu)\kappa^3}{E}[A - (1-2\nu)B]\right\}\cos\kappa Z_1. \tag{51}$$

Along the boundary $Z_2 = h(Z_1)$, the boundary conditions (25) must be satisfied. Making all the appropriate substitutions and retaining terms accurate to the order of $a\kappa$, we obtain

$$\left[1 + \frac{(1+\nu)\kappa\Sigma_0}{E}\right]\left(\frac{\kappa A}{aT}\right) - \frac{(1+\nu)(1-2\nu)\kappa\Sigma_0}{E}\left(\frac{\kappa B}{aT}\right) = \left[1 - \frac{(1+\nu)(2-\nu)T}{E}\right]\frac{\kappa\Sigma_0}{T}, \tag{52}$$

$$\left(\frac{\kappa A}{aT}\right) + \left(\frac{\kappa B}{aT}\right) + 1 = -\left[1 - \frac{(1-\nu^2)T}{E}\right] \times \frac{2\nu(1+\nu)\kappa\Sigma_0}{(1-\nu)E}\left[\left(\frac{\kappa A}{aT}\right) + 2(1-\nu)\left(\frac{\kappa B}{aT}\right)\right]. \tag{53}$$

We remark again that the critical length b_c, (2), is the result of the approximation

$$\frac{\kappa A}{aT} = 0, \quad \left(\frac{\kappa A}{aT}\right) + \left(\frac{\kappa B}{aT}\right) + 1 = 0.$$

Grilhe's result, (5), is a consequence of replacing the first of the above with

$$\left(\frac{\kappa A}{aT}\right) = \frac{\kappa\Sigma_0}{T}.$$

In plane strain, the state of stresses $(\tau_{11}, \tau_{22}, \tau_{33}) = (T, 0, \nu T)$ is paired with $(\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}) = [\varepsilon_T,\ -(\nu/1-\nu)\varepsilon, 0]$ where

$$\varepsilon_T = (1-\nu^2)T/E. \tag{54}$$

In terms of ε_T and Σ_0 of equation (43), the expression b_c and the associated wave number κ_c may be written

$$b_c = \frac{2\pi}{\kappa_c} = \frac{\pi E \Gamma_0}{(1-\nu^2)T^2} = \frac{\pi \Gamma_0}{T\varepsilon_T} = \frac{\pi(1-\nu)\Sigma_0}{T\varepsilon_T}. \quad (55)$$

It is now convenient to scale the wave number κ by κ_c, so that

$$\kappa = \beta\kappa_c, \quad \frac{\kappa\Sigma_0}{E} = \frac{2\beta\varepsilon_\Gamma^2}{(1-\nu)^2(1+\nu)}. \quad (56)$$

The boundary conditions (52) and (53) may now be solved in terms of a power series of the small parameter ε_T. We have

$$\frac{\kappa A}{aT} = \frac{2\beta}{1-\nu}\varepsilon_T - \frac{6\beta}{1-\nu}\varepsilon_T^2 + \cdots, \quad (57)$$

$$\frac{\kappa B}{aT} = -1 - \frac{2\beta}{1-\nu}\varepsilon_T + \frac{2\beta(3+\nu)}{(1-\nu)^2}\varepsilon_T^2 + \cdots. \quad (58)$$

The chemical potential Ψ may now be computed from equation (22). Retaining terms linear in the amplitude a, we have

$$\begin{aligned}\frac{\Psi}{\Omega} = {} & \frac{1}{2}T\varepsilon_T - \left(\frac{1}{2}T\varepsilon_T\right)4a\kappa\left\{-\frac{\kappa B}{aT} - \frac{1}{2(1-\nu)}\frac{\kappa A}{aT}\right. \\ & - \frac{E\kappa\Sigma_0}{2(1+\nu)T^2} - \frac{\kappa\Sigma_0}{2(1-\nu)T}\left[\frac{\kappa A}{aT} + (3-2\nu)\frac{\kappa B}{aT}\right] \\ & \left. + \frac{\kappa\Sigma_0}{(1-\nu)T}\left[1 + \frac{\kappa A}{aT} + \frac{\kappa B}{aT}\right]\right\}\cos\kappa Z_1. \quad (59)\end{aligned}$$

Making use of equations (57), (58) and retaining terms accurate to the order of ε_T, we finally obtain

$$\begin{aligned}\frac{\Psi}{\Omega} = {} & \frac{1}{2}T\varepsilon_T\left[1 - 4a\kappa\left\{1 - \beta + \frac{4\beta}{1-\nu}\varepsilon_T\right.\right. \\ & \left.\left. + \varepsilon_T^2[4\beta^2 - (3+2\nu)\beta]\frac{1}{(1-\nu)^2}\right\}\cos\kappa Z_1\right]. \quad (60)\end{aligned}$$

If we treat the amplitude of equation (44) as a function of time, $a(t)$, then the surface evolution governed by surface diffusion satisfies

$$\frac{\partial h}{\partial t} = D\frac{\partial^2}{\partial Z_1^2}(\Psi/\Omega), \quad (61)$$

where D is a positive diffusion constant. It follows that

$$\begin{aligned}a = {} & 4\kappa^3\left(\frac{1}{2}T\varepsilon_T\right)D\left\{1 - \beta + \frac{4\beta}{1-\nu}\varepsilon_T\right. \\ & \left. + \varepsilon_T^2[4\beta^2 - (3+2\nu)\beta]\frac{1}{(1-\nu^2)}\right\}a, \quad (62)\end{aligned}$$

and the flat surface becomes unstable if

$$\beta < \beta_c = 1 + \frac{4}{1-\nu}\varepsilon_T + \frac{17-2\nu}{(1-\nu)^2}\varepsilon_T^2 \quad (63)$$

or, equivalently,

$$b > b_{cw} = b_c\left[1 - \frac{4}{1-\nu}\varepsilon_T - \frac{1-2\nu}{(1-\nu)^2}\varepsilon_T^2\right], \quad (64)$$

where b_c is given by equation (2). It is seen that a tensile applied stress enhances the instability whereas a compressive applied stress inhibits the instability region. It is important to note that the change is brought about by the correct equations (22)–(26), not merely the inclusion of the surface stress in the form of equation (14). Finally, in the context of epitaxially-strained solid films [12–14] it is not uncommon to find ε_T as large as ±4%.

4. SUMMARY AND DISCUSSION

Flat surfaces of stressed solids are unstable against diffusional perturbations with wavelengths larger than the critical wavelength b_c given by equation (2). In fact the maximally unstable mode has the wavelength $b = b_m = (4/3)b_c$. This result, however, is independent of the sign of the underlying stress. Using a refined chemical potential and an explicit surface deformation-dependent surface energy, we have readdressed the instability phenomenon and obtained a new critical wavelength that is sensitive to the sign of the underlying stress. It is found that tensile stresses (positive ε_T) enhance the instability while compressive stresses (negative ε_T) inhibit the instability. The full implication of the full chemical potential on the nonlinear evolution of the surface remains to be calculated. It would be premature to predict at this point the exact nature of the equilibrium surface morphology resulting from the refined potential. It suffices to say that the outcome would be quite different from that of Spencer and Meiron [15].

It is well known that bulk strain plays an important role in determining surface morphology [16, 17]. The continuum approach presented in this paper ignores, by necessity, the presence of different surface steps. Based on molecular dynamics simulations, the effect of the sign of the underlying bulk strain on semiconductor surface roughness was investigated by Xie *et al.* [18]. It was found that the surface is flat (smooth) under tension but rough under compression.

The study employed $Ge_{0.5}Si_{0.5}$ films grown on Ge_xSi_{1-x} cap layers which, in turn, were grown on compositionally graded buffer layers. The cap layers are therefore treated as the substrate in the following discussion. Using $a_{Si} = 0.5433$ nm and $a_{Ge} = 0.5660$ nm, we compute the effective lattice spacing for the substrate $a_s = xa_{Ge} + (1-x)a_{Si} = 0.5433 + 0.0227x$. The effective lattice spacing for the film is just $a_f = 0.5546$ nm. The misfit strain in the film, considered as a function of x and denoted by $\varepsilon_T(x)$, is just

$$\varepsilon_T(x) = (a_s - a_f)/a_f = -0.02(1 - 2x),$$

ranging from 2% tensile on a 100% Ge substrate to 2% compressive on a 100% Si substrate. Substantial surface roughness was found for the film under 2% compression, while no detectable roughness was observed for films under tensile strains of up to 2%. Based on the atomic force micrographs given in the paper, the most pronounced wavelength for the roughness is in the range of 0.05–0.1 μm. Inserting $\Gamma_0 = 1\ \mathrm{J/m^2}$, $E = 160$ GPa, $\nu = 1/4$ and $\varepsilon_T = \pm 0.02$ into equation (55) yields $b_c = 0.046\ \mu$m. The refined critical wavelength turns out to be $b_{cw} = (1 \mp 0.107)$ $0.046\ \mu$m, where the signs apply to $\varepsilon_T \pm 0.02$. The maximally unstable mode has the wavelength $b_m \simeq 4/3\, b_{cw} = (1 \mp 0.107)\, 0.0612\ \mu$m. For a 2% compressive strain, $b_m \simeq 0.0677\ \mu$m. It is hoped that a nonlinear evolution calculation based on our refined theory would lead to the desired steady film profile.

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