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The effect of surface stress and wetting layers on morphological instability in epitaxially strained films

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This paper investigates effects of surface stress and wetting layers on the morphological instability of a growing epitaxially strained dislocation-free solid film. Linear stability analysis of the planar film shows that the film, unstable due to lattice mismatch, is affected differently by surface stress for a film under compression than for one under tension and depends on whether the relative stiffness of the film to the substrate is less than or greater than $(1-2\nu)^{-1}$; here ν is Poisson's ratio. The presence of a wetting layer has the capacity to substantially stabilize the planar film. The critical thickness of the film below which the film is stable depends on the bulk elastic properties of film and substrate and increases with increase of the wetting potential. *© 2004 American Institute of Physics*. [DOI: 10.1063/1.1779953]

I. INTRODUCTION

The formation of nanoscale-island structures during the growth of epitaxially strained dislocation-free solid films has generated theoretical and experimental interest for the last decade. It is well known that a flat, strained, free surface is unstable with respect to sinusoidal surface perturbations having a wave number greater than a critical value.[1–3] More recently, this instability has been predicted and observed in thin films deposited on a substrate.[4] In this case the difference in lattice parameter between the film and substrate generates a stress that drives the instability. Spencer *et al.*[4] analyzed the morphological instability of a growing film subject to mismatch stresses using a continuum model, where surface of the film evolves by surface diffusion and the strained film was described by isotropic linear elasticity. They found that at low temperatures, where deposition flux is larger than the surface diffusion flux, the critical film thickness for instability depends on the deposition rate on the film. Unlike free surfaces on semi-infinite bodies, the presence of a substrate can affect the evolution of the instability. Spencer *et al.* ,[4] Freund and Jonsdottier,[5] and Shoykhet *et al.*[6] found that elastically hard substrates are stabilizing influences and, in the limit of a infinitely stiff substrate, the instability is completely suppressed below a critical film thickness.

The surface of a solid is fundamentally different from that of fluid,[7] because the presence of a crystalline lattice allows one to distinguish between the straining of a solid surface and the creation of new surface. Therefore, in addition to surface energy there is a surface stress, which can have either sign. The effect of surface stress on the equilibrium conditions at the crystal/melt interface of a three-dimensional (3D) crystal was investigated by Leo and Sekerka[8] using a variational approach along with the continuum mechanics suggested by Gurtin and Murdoch.[9] Later, Wu,[10] Freund,[11] Norris,[12] and Shenoy and Freund[13] computed the chemical potential of a crystal/vapor interface in the two-dimensional case in the presence of both bulk deformation and surface stress using a dynamical approach, which agrees with Leo and Sekerka in the equilibrium limit.

In most cases the effects of surface stress on the dynamics of interface evolution is small,[14] though this may not be the case for morphological evolution at the nanoscale. The extremely large curvatures of surfaces can lead to large stresses even if the surface stress is small. For example, it is well known that the lattice parameter of free standing nanoparticles can be different from the bulk. Moreover, Bimberg *et al.*[15] have shown that the singularities in the stress field induced by surface stress at facet junctions can be sufficient to stabilize against coarsening an array of quantum dots that are deposited on a surface. It is thus reasonable to investigate the effects of surface stress on the evolution of thin films deposited on substrates.

A complete model of thin film growth requires that, in addition to surface stress and misfit stresses, the effects of different elastic constants between the film and substrate be accounted for as well as the wetting interaction between the film and substrate. There have been a number of important studies that are of relevance to the complete model we develop. The effects of surface stress on the stability of the surface of a semi-infinite solid in two-dimensional case was examined by Wu *et al.*[16] They found that the conditions for stability of the surface are sensitive to the sign of the applied stress, i.e., the surface is flat (smooth) under tension, but rough under compression. The importance of this sign was

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also noted by Wu[17] for a film-substrate system. He studied the nonlinear effects of lattice mismatch on morphological and compositional instabilities of epitaxial layers. A current overview of surface-stress effects on the thermodynamics and kinetics of interfaces is given by Fried and Gurtin.[18]

Most films that are deposited on substrates wet the substrates to varying degrees. In one of the most well studied systems, Si-Ge, the film completely wets the substrate. By the Asaro-Tiller-Grinfeld instability islands form separated by regions of a thin wetted film. Thus, the growth of very thin films may be expected to be affected by the energetics of the wetting layer at the film-substrate interface. This layer would also be expected to play a particularly important role during the early stages of film growth.[19,20] Several experiments have found that Ge initially grows layer by layer on the Si(100)2×1 surface, up to a thickness of three atomic layers, after which islands appear. Tersoff[21] showed using model calculations that layer-by-layer growth is stabilized for up to three layers because it minimizes the strain energy associated with the surface dimerization. He also found that the chemical potential of a layer of atoms is a function of the wetting layer thickness. This is also the case with recent first principles calculations by Beck *et al.*[22] They found that the chemical potential of an atom on the surface is an increasing function of the wetting layer thickness. The models known from literature,[19,23–28] which account for the energetics of the film-substrate interface, involve surface energy as a function of the film thickness. This function vanishes if the film is much thicker than the width of the transition layer. The aim of the present work is to study quantitatively the effects on morphological instability of strained film of surface stress along with the presence of wetting layers.

In Sec. II, using the results of Leo and Sekerka,[8] we derive the linearized equilibrium conditions in the sense of linear elasticity. Then, in Sec. III, we formulate the evolution problem. Section IV is devoted to linear stability analysis, while the stability results are discussed in Sec. V.

II. LINEARIZED EQUILIBRIUM CONDITIONS

In this section we give an equilibrium energy balance within a framework of small deformations. Consider a smooth two-dimensional surface $\mathcal{S}$ in three-dimensional space oriented by a choice of a smooth unit normal field $\mathbf{n}$. Following Gurtin and Jabbour,[29] we use the notation

$$\mathbf{L} = -\nabla_{\mathcal{S}}\mathbf{n}, \tag{2.1}$$

where $\nabla_{\mathcal{S}}$ is the surface gradient, tensor $\mathbf{L}$ is symmetric, and the mean curvature is defined by

$$\kappa = \mathrm{tr}\,\mathbf{L} = -\,\mathrm{div}_{\mathcal{S}}\mathbf{n}. \tag{2.2}$$

The effect of surface stress on crystal/melt equilibrium was considered by Leo and Sekerka.[8] For isotropic surface tension and constant pressure (say, zero) in the vapor the equilibrium energy balance within a framework of finite deformations at the reference interface $\mathcal{S}$ is

$$\omega_v - \kappa\gamma + [\mathrm{div}_{\mathcal{S}}(\hat{\mathbf{F}}^{\mathbf{T}}\cdot\hat{\mathbf{T}}) - \mathbf{F}^{\mathbf{T}}\cdot(\mathrm{div}_{\mathcal{S}}\hat{\mathbf{T}})]\cdot\mathbf{n} = 0. \tag{2.3}$$

Here ω_v is the bulk-phase grand potential density, measured per unit volume of the reference state, and $\kappa\gamma$ is a capillary pressure, where $\gamma = \gamma(\hat{\mathbf{E}})$ is the surface free-energy density per unit area of the reference state, while $\hat{\mathbf{E}}$ is the surface strain tensor. The remaining terms in Eq. (2.3) model the surface stress. Here $\mathbf{F}$ is the bulk deformation gradient tensor, $\hat{\mathbf{F}}$ is the surface deformation gradient, and $\hat{\mathbf{T}}$ is the first Piola-Kirchoff surface-stress tensor as defined by Gurtin and Murdoch.[9] Gibbs[7] first noted for solids that in addition to γ, which represents the excess free energy per unit area owing to the existence of a surface, there is the surface stress associated with the reversible work per unit area needed to elastically stretch a preexisting surface. Unlike γ, which is a positive scalar, the surface stress is a tensor with elements whose signs are not *a priori* determined.[30,31] For a general surface, this second-rank tensor can be diagonalized by reference to a set of principal axes. The diagonal elements are equal for a surface possessing a threefold or higher rotation-axis symmetry.[30] This means that the surface stress for these high symmetry surfaces is isotropic and can be taken as

$$\hat{\mathbf{T}} = f\mathbf{P}, \tag{2.4}$$

where a scalar f is equal to the magnitude of the change of the surface free energy per unit change in elastic strain of the surface and $\mathbf{P}$ is the projection operator onto $\mathcal{S}$

$$\mathbf{P} = 1 - \mathbf{n}\otimes\mathbf{n}. \tag{2.5}$$

To obtain the small-strain (linear) approximation of Eq. (2.3), set

$$\mathbf{F} = 1 + \mathbf{E} + \mathbf{U}, \quad \hat{\mathbf{F}} = \mathbf{P} + \hat{\mathbf{E}} + \hat{\mathbf{U}}, \tag{2.6}$$

where $\mathbf{E}(\hat{\mathbf{E}})$ and $\mathbf{U}(\hat{\mathbf{U}})$ are symmetric strain tensor and antisymmetric rotation tensor for the bulk (the surface), respectively. To obtain an equilibrium energy balance within a framework of small deformations, substitute Eqs. (2.6) and (2.4) into Eq. (2.3), and then take into account the following relations from Gurtin and Murdoch:[9]

$$\mathrm{div}_{\mathcal{S}}\mathbf{P} = \kappa\mathbf{n}, \quad \mathrm{div}_{\mathcal{S}}(\hat{\mathbf{E}})\cdot\mathbf{n} = \hat{\mathbf{E}}\cdot\mathbf{L}, \tag{2.7}$$

which result in

$$\omega_v - \kappa\gamma + f[\hat{\mathbf{E}}\cdot\mathbf{L} - \kappa(\mathbf{n}\cdot\mathbf{E}\mathbf{n})] = 0. \tag{2.8}$$

For the simplified case, in which $\mathcal{S}$ is a planar curve (in two-dimensional space), Eq. (2.8) agrees with that obtained by Fried and Gurtin.[18] The grand canonical free energy appearing in Eq. (2.8) is related to other free-energy functions and the chemical potential.[32] In the limit of a pure material containing vacancies and no dependence of the lattice parameter on vacancy concentration the grand canonical energy density in Eq. (2.8) can be replaced by difference of $\mathcal{E}$ that is a strain energy density and M that is a ratio of density of atoms in the crystal in the reference state over chemical potential of an atom on the surface.[33]

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$$M=\mathcal{E}-\kappa\gamma+f[\hat{\mathbf{E}}\cdot\mathbf{L}-\kappa(\mathbf{n}\cdot\mathbf{En})]. \tag{2.9}$$

This expression is valid for a surface on a semi-infinite solid. The effects of the molecular scale interactions on the chemical potential that are associated with the formation of a wetting layer are given below.

III. MODEL

A. Governing equations

Continuum elasticity theory[4] will be used to describe the stress state of the epitaxially strained film. The film/vapor surface is allowed to move due to the surface gradient of the chemical potential, which includes the influences of the strain energy, the surface energy, the surface stress, and the energy associated with the wetting layer. The stresses in both the film and in the substrate are governed by isotropic linear elasticity with an additional term in the film corresponding to misfit strain, generated by the difference in lattice spacings of the film and the substrate,[4]

$$\mathbf{T}=2\mu\left[\mathbf{E}+\frac{\nu}{1-2\nu}(\mathrm{tr}\,\mathbf{E})1-\frac{1+\nu}{1-2\nu}\mathbf{E}_0\right], \tag{3.1}$$

where μ is the elastic shear modulus and ν is Poisson's ratio. The misfit strain is $\mathbf{E}_0=\varepsilon 1$, where $\varepsilon=(a_f-a_s)/a_s$, a_f and a_s are the lattice spacings of the film and the substrate, respectively. The equilibrium conditions are assumed to be satisfied,

$$\mathrm{div}\,\mathbf{T}=0. \tag{3.2}$$

To ensure the coherency at the interface between the film and the substrate, continuity of both displacement $\mathbf{u}$ and the stress are required,

$$\mathbf{u}^F=\mathbf{u}^S, \quad \mathbf{T}^F\mathbf{n}=\mathbf{T}^S\mathbf{n}. \tag{3.3}$$

The force on the film surface balances zero pressure,

$$\mathbf{Tn}-f\,\mathrm{div}_{\mathcal{S}}\mathbf{P}=0, \tag{3.4}$$

or, taking into account Eq. (2.7),

$$\mathbf{Tn}-f\kappa\mathbf{n}=0. \tag{3.5}$$

The strains in the substrate far away from the film are required to decay to zero.

Following Mullins,[34] the evolution equation for the surface in the absence of vapor deposition is given by

$$V_n=\mathcal{D}\Delta_{\mathcal{S}}\mathrm{M}, \tag{3.6}$$

where V_n is the normal velocity of the surface, $\mathcal{D}$ is a constant related to the rate of surface diffusion, $\Delta_{\mathcal{S}}$ is the surface Laplacian, and M is a chemical potential.

1. *Remark* All equations are written in invariant (coordinate-free) form. If the substrate is planar, and the film surface (in a neighborhood of a point) can be uniquely projected onto this plane, then one can introduce the Cartesian coordinate system (x,y,z) with $z=0$ corresponding to substrate-film plane, and the free film surface can be written as $z=h(x,y,t)$.

B. Chemical potential

It is clear experimentally that intermolecular forces can lead to the formation of a thin wetting layer on the surface of a substrate. For example, in the Si-Ge system there exists a thin layer of Ge when deposited on Si(100) substrate. The existence of a thin layer is consistent with calculations of the energy of the wetting layer using empirical potentials[21] and first-principles density-functional approaches.[22] These calculations show that the energy of an atom on the surface of the wetting layer is a function of the wetting layer thickness. In the case of Ge on Si this dependence decays monotonically as a function of distance and asymptotically approaches a constant at about three to five atomic layers. In other cases, such as metals deposited on semiconductors, this force is of longer range and, as shown by Suo and Zhang,[26] are strong enough to compete with elasticity. They also established the specific dependence of the transition thickness on stress in the presence of different long-range forces. There have been various approaches proposed on how to incorporate these long-range forces into a continuum model. Chui and Gao[35] took the surface energy to be a function of height of the film and simulated the evolution of a thin film including surface diffusion and deposition. Spencer and Tersoff[24] were interested in the larger scale shapes of islands on surfaces and thus simplified the spatial dependence of the energy of the wetting layer to one in which a thin wetting layer is permanently attached to the substrate. Alternatively, Zangwill[36] and later Kukta and Freund[25] assumed that there is a narrow transition region through which the mismatched strain, but not the energy, changes continuously near the substrate. Ortiz *et al.*[19] suggested a model that accounts for the energetics of the film-substrate interface whose potential looks like

$$\Psi(h)=\eta h e^{-h/\delta}, \tag{3.7}$$

where η is a constant whose sign depends on the sign of the difference of interfacial energies of a film and substrate and δ measures the width of the transition layer.

Inspired by the first-principles calculations of Beck *et al.*[22] in which the chemical potential of an atom on the surface of the wetting layer is determined, we augment the chemical potential given in Eq. (2.9) as follows:

$$\mathrm{M}=\mathcal{E}-\kappa\gamma+f\hat{\mathbf{E}}\cdot\mathbf{L}-f\kappa(\mathbf{n}\cdot\mathbf{En})+\Psi. \tag{3.8}$$

Here $\Psi=\Psi(h)$ is a wetting chemical potential, though not necessary of the form of Eq. (3.7). Since we are going to restrict ourselves by *linear stability analysis*, it is not necessary to commit to a specific $\Psi(h)$. A particular choice of the function $\Psi(h)$ will affect only the value of a constant, i.e., $\partial\Psi/\partial h$ evaluated at a certain point; thus, all admissible (rapidly decreasing) functions Ψ alter the stability condition through a single constant, and by varying this constant a family of wetting potential may be considered.

IV. LINEAR STABILITY ANALYSIS

The governing equations have a basic-state solution corresponding to a planar film $z=h_0$ with uniform epitaxial strain in the film:

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$$\tilde{u}_1^F = \tilde{u}_2^F = 0 \quad \tilde{u}_3^F = e_0 z, \tag{4.1}$$

where $e_0 = \varepsilon(1+\nu)/(1-\nu)$, and the state of a completely relaxed substrate is $\tilde{u}_j^S = 0$ for $j=1,2,3$.

Since the model is symmetric with respect to x and y, it is sufficient in linear stability theory to consider a 1D surface of a 2D film. We assume that ν has the same value for both the film and the substrate, but allow the shear moduli to differ, and perturb the basic-state solution as follows:

$$h = h_0 + \tilde{h}\exp(iax + \sigma t), \tag{4.2}$$

$$u_j^S = -i\tilde{u}_j^S(z)\exp(iax + \sigma t), \quad j = 1,3,$$

$$u_1^F = -i\tilde{u}_1^F(z)\exp(iax + \sigma t), \tag{4.3}$$

$$u_3^F = e_0 z + \tilde{u}_3^F(z)\exp(iax + \sigma t), \tag{4.4}$$

where σ is the growth rate and a is the wave number.

The linear system of equations for the disturbances to the displacement field is given by

$$B\partial_z^2\tilde{u}_1^F - Aa^2\tilde{u}_1^F - a\partial_z\tilde{u}_3^F = 0, \tag{4.5}$$

$$A\partial_z^2\tilde{u}_3^F - Ba^2\tilde{u}_3^F - a\partial_z\tilde{u}_1^F = 0, \tag{4.6}$$

$$B\partial_z^2\tilde{u}_1^S - Aa^2\tilde{u}_1^S - a\partial_z\tilde{u}_3^S = 0, \tag{4.7}$$

$$A\partial_z^2\tilde{u}_3^S - Ba^2\tilde{u}_3^S - a\partial_z\tilde{u}_1^S = 0, \tag{4.8}$$

where $A = 2(1-\nu)$, $B = 1-2\nu$.

The boundary conditions for the film interface at the substrate are as follows:

$$\tilde{u}_i^F = \tilde{u}_i^S = 0 \text{ on } z = 0, \tag{4.9}$$

$$\rho\partial_z\tilde{u}_1^F - \partial_z\tilde{u}_1^S - a(\rho\tilde{u}_3^F - \tilde{u}_3^S) = 0 \text{ on } z = 0, \tag{4.10}$$

$$\nu a(\rho\tilde{u}_1^F - \tilde{u}_1^S) + (1-\nu)(\rho\partial_z\tilde{u}_3^F - \partial_z\tilde{u}_3^S) = 0 \text{ on } z = 0, \tag{4.11}$$

at the film surface,

$$-2ae_0\tilde{h} + \partial_z\tilde{u}_1^F - a\tilde{u}_3^F = 0 \text{ on } z = h_0, \tag{4.12}$$

$$2\mu^F\nu(a\tilde{u}_1^F + \partial_z\tilde{u}_3^F) + 2\mu^F B\partial_z\tilde{u}_3^F - Bfa^2\tilde{h} = 0 \text{ on } z = h_0, \tag{4.13}$$

and in the substrate,

$$\tilde{u}_i^S \to 0, \quad \partial_z\tilde{u}_i^S \to 0 \text{ as } z \to -\infty, \tag{4.14}$$

where μ^F is a film shear modulus.

The normal-mode equation for the film surface can be rewritten as

$$\sigma\tilde{h} = -\mathcal{D}a^2(\tilde{\mathcal{E}} + \gamma_0 a^2\tilde{h} + fe_0 a^2\tilde{h} + w\tilde{h}), \tag{4.15}$$

where

$$\tilde{\mathcal{E}} = -2\mu^F e_0 a\tilde{u}_1, \quad w = \left.\frac{\partial\Psi}{\partial h}\right|_{h=h_0}, \tag{4.16}$$

and γ_0 is the surface energy of unstressed film. In arriving Eq. (4.15) the surface elastic constants are neglected and thus $\gamma(\hat{\mathbf{E}}) \approx \gamma_0 + f\hat{\mathbf{E}}$.

The solution of the system of linear ODEs (4.5)–(4.8) satisfying Eqs. (4.9) and (4.14) is given by

$$\tilde{u}_1^F = \alpha_1\cosh(az) + \beta_1\sinh(az) + \delta_2 z\cosh(az) + \delta_1 z\sinh(az),$$

$$\tilde{u}_3^F = \alpha_3\cosh(az) + \beta_3\sinh(az) - \delta_1 z\cosh(az) - \delta_2 z\sinh(az),$$

$$\tilde{u}_1^S = \alpha_1\exp(az) + \delta_3 z\exp(az),$$

$$\tilde{u}_3^S = \alpha_3\exp(az) - \delta_3 z\exp(az),$$

where

$$\delta_1 = a(i\alpha_1 + \beta_3)/C, \quad \delta_2 = a(i\beta_1 + \alpha_3)/C, \tag{4.17}$$

$$\delta_3 = a(i\alpha_1 + \alpha_3)/C, \quad C = 3 - 4\nu. \tag{4.18}$$

The coefficients α_1, α_3, β_1, and β_3 are found from the system (4.10)–(4.13) using "Maple 7."

The dispersion relation can be rewritten as follows:

$$\sigma = \mathcal{D}(a^3\mathcal{E}_0\tilde{u}_1^* - a^4\gamma_0 - a^4 fe_0 - wa^2), \tag{4.19}$$

where

$$\mathcal{E}_0 = (8\varepsilon^2\mu^F G^2)/A, \quad G = 1 + \nu, \tag{4.20}$$

$$\tilde{u}_1^* = \tilde{u}_1(h_0)/(2\varepsilon G\tilde{h}) = \mathcal{Z} + \frac{afB}{4\varepsilon\mu^F G}\mathcal{F},$$

$$\mathcal{Z} = \{\mu A^2 + (1 + 2B\mu - C\mu^2)ah_0 + (C + 2\mu B^2 + C\mu^2) \times \sinh(ah_0)\cosh(ah_0) + 2\mu A^2[\sinh(ah_0)]^2\}/d,$$

$$d = A^2 + a^2h_0^2(1 + 2\mu B - \mu^2 C) + 2\mu A^2\sinh(ah_0) \times \cosh(ah_0) + (C + 2\mu B^2 + \mu^2 C)[\sinh(ah_0)]^2,$$

$$\mathcal{F} = -\frac{1}{2Bd}\{(-1+\mu)[BC(-1+\mu) + 2a^2h_0^2(-1 - C\mu)] - B(C + 2B^2\mu + C\mu^2)\cosh(2ah_0) - 2A^2B\mu\sinh(2ah_0)\}, \tag{4.21}$$

and $\mu = \mu^F/\mu^S$ is the relative stiffness of the film to the substrate.

The dispersion relation (4.19) now can be rewritten as

$$\sigma/\mathcal{D} = a^3\mathcal{E}_0\mathcal{Z} + a^4\left(\frac{\mathcal{E}_0 fB}{4\epsilon\mu^F G}\mathcal{F} - \gamma_0 - fe_0\right) - a^2 w. \tag{4.22}$$

A negative (positive) f refers to a compressive (tensile) surface stress.[30] Note that both of the functions $\mathcal{Z}$ and $\mathcal{F}$ are bounded, and the function $\mathcal{Z}$ is positive for all values of μ and ah_0.

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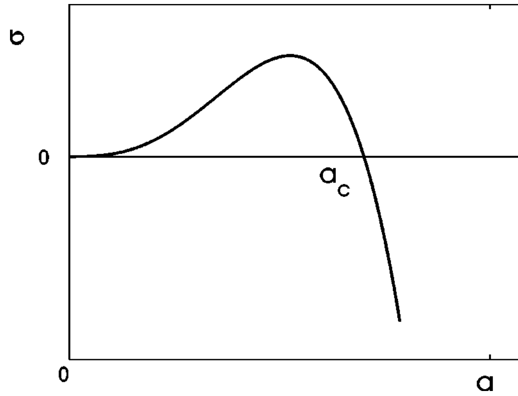

FIG. 1. Typical neutral stability curve, Eq. (5.1): the growth rate of perturbations σ as a function of disturbance wave number a.

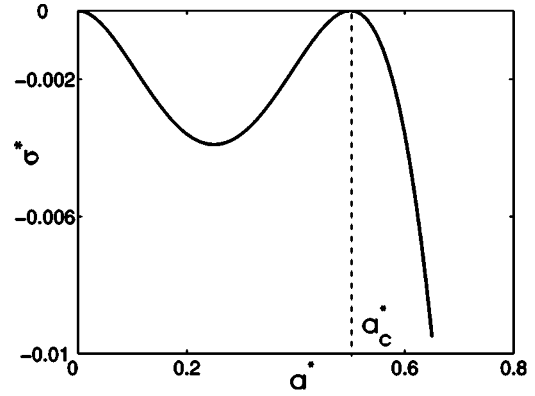

FIG. 2. Neutral stability curves for $\mu=1$, $w^*=0.25$.

V. STABILITY RESULTS

A. Surface stress and misfit only

This section is devoted to the study of the surface-stress influence only on morphological instability of the strained film and thus we take $w=0$. The dispersion relation (4.22) now looks like

$$\sigma/\mathcal{D} = a^3\mathcal{E}_0\mathcal{Z} + a^4\left[-\gamma_0 - \frac{2G\varepsilon f}{A}(1-B\mathcal{F})\right]. \tag{5.1}$$

The typical plot of neutral stability curve corresponding to that case is shown in Fig. 1.

If $\mu=1$, then $\mathcal{Z}\equiv\mathcal{F}\equiv 1$, and the dispersion relation has its simplest form

$$\sigma/\mathcal{D} = a^3(\mathcal{E}_0 - |\mathcal{E}_1|a), \tag{5.2}$$

where $\mathcal{E}_0$ is positive [see Eq. (4.20)]. The quantity $\mathcal{E}_1 = -(\gamma_0+2\nu e_0 f)<0$, because γ_0 is positive and f is generally the same order of magnitude as γ_0.[30] Though f might have either sign, it is multiplied by a small parameter proportional to the misfit ε, and therefore f does not affect on the sign of $\mathcal{E}_1$.

We introduce the length scale $l=\gamma_0/\mathcal{E}_0$, balancing surface energy per area and strain energy per volume, and the time scale, $\tau=\gamma_0^3/\mathcal{D}\mathcal{E}_0^4$. In dimensionless form Eq. (5.2) then looks like

$$\sigma^* = a^{*3} - \left(1 + 2\nu e_0\frac{f}{\gamma_0}\right)a^{*4}, \tag{5.3}$$

where $a^*=al$ and $\sigma^*=\sigma\tau$. The cutoff wave number corresponding to the nonzero solution of $\sigma^*=0$ satisfies

$$a_c^* = \gamma_0/(\gamma_0 + 2\nu e_0 f). \tag{5.4}$$

From Eq. (5.4) it follows that stabilization depends on the sign of a product $e_0 f$ in agreement with Wu *et al.*[16] (the importance of that sign was also mentioned by Wu[17]); they considered the case where $\mu=1$, and f is always positive and equal $\gamma_0/(1-\nu)$. More precisely, from Eq. (5.2) it follows that $a_c \approx 4\varepsilon^2(1+\nu)/(1-\nu)\gamma_0$ if $f=\gamma_0/(1-\nu)$. Up to the factor $1+\nu$, caused by additional term in Eq. (3.1) corresponding to the misfit strain, this coincides with Wu *et al.*[16]

For a compressed film, $\varepsilon>0$, the tensile surface stress slightly stabilizes the planar film, while compressive surface stress slightly destabilizes it. If the film is under tension, $\varepsilon<0$, the influence of the surface stress is opposite. Thus, for surface stress on the order of the surface energy, the surface stress will induce a small (about 5%) change in the critical wave number.

From Eq. (5.1) it follows that if the ratio of the shear modulii of substrate and film is not unity, $\mu\neq 1$, the influence of the surface stress is qualitatively the same as long as $1-B\mathcal{F}>0$, which holds if

$$\mu < (1-2\nu)^{-1}. \tag{5.5}$$

However, if $\mu>(1-2\nu)^{-1}$, the difference $1-B\mathcal{F}$ is negative for small magnitudes of ah_0 [i.e., for $a=O(1)$]. This means that if the film is much stiffer than the substrate, a_c increases for $\varepsilon f>0$ and decreases when $\varepsilon f<0$. The magnitude of that increase or decrease remains small as it was in the situation where $\mu=1$.

Substantial stabilization occurs when the substrate is stiffer than the film, $\mu<1$; here a_c tends to zero as $\mu\to 0$. This stabilization, due to elastic stiffness of the substrate, diminishes as the film thickness increases.[4] For the limiting case of a perfectly rigid substrate a_c is equal to zero if $h_c<l(1-\nu)$, and then the planar film is stable.

B. Wetting layer and misfit only

Now let f be equal to zero and let $w\neq 0$ in Eq. (5.2). Consider first the simplest case, $\mu=1$. The dispersion relation looks like

$$\sigma^* = a^{*3} - a^{*4} - w^* a^{*2}, \tag{5.6}$$

where $w^*=w\gamma_0/\mathcal{E}_0^2$. The neutral curve for $w^*=0.25$ is shown in Fig. 2; here $a_c^*=0.5$.

By varying the relative stiffness μ one changes the location of the local maximum as is shown in Fig. 3(b).

The presence of a wetting layer can completely stabilize the planar film if $w^*\geqslant\mathcal{Z}^2/4$. The critical value of wetting constant w^*, w_c^*, above which the film is stable, depends on both relative stiffness μ and the film thickness. This is shown in Figs. 3 and 4. In Fig. 3(a) the thickness $h_0^*=h_0/l$ is fixed, and w_c^* decreases as the substrate becomes stiffer. In Fig. 3(b) the corresponding critical wave number is shown; for a rigid substrate, $\mu\to 0$, a_c^* approaches zero, and is nearly constant for $\mu>5$. If the substrate is stiffer than the film, as it is for

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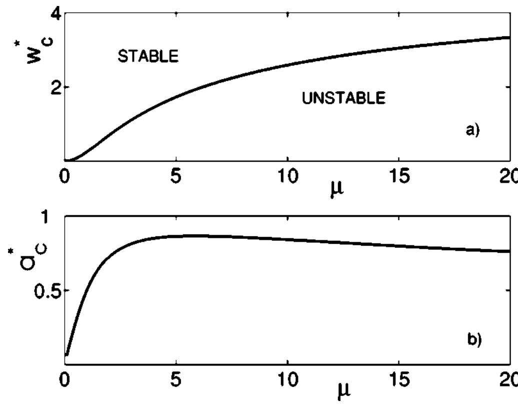

FIG. 3. Wetting layer vs relative stiffness for $h_0^*=0.1$, $\nu=1/3$, $\gamma_0=1927$, and $\varepsilon=0.0418$ (a) and (b) the corresponding critical wave number.

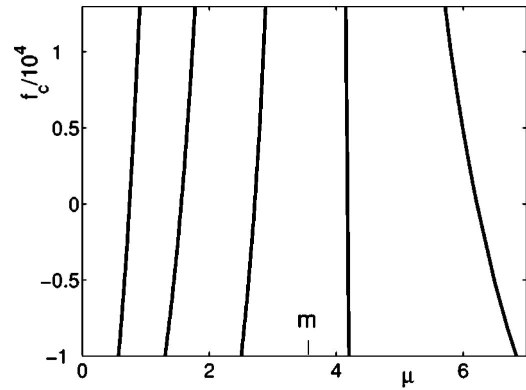

FIG. 5. Critical value of the surface stress magnitude vs stiffness ratio μ for $\varepsilon=0.0418$, $h_0^*=0.1$, $\gamma_0=1927$, and $w=0.15$, 0.5, 1, 1.5, and 2.5 from left to right. Stability corresponds to the left of a given curve.

Ge on Si, then decreasing of the film thickness stabilizes the film [see the dashed curve in Fig. 4(a)]. If the film is stiffer, as it is for GaAs on Si, then the effect of thickness is different [see the solid curve in Fig. 4(a)]. The corresponding critical wave number is shown in Fig. 4(b) does not change much if the film is relatively thick. If the film is thin for Ge on Si, it is a slightly increasing function, while for GaAs on Si it has small oscillations. A sufficient condition for complete stabilization is given by $w^* > 1/4\max\{1,\mu^2\}$.

C. Surface stress, wetting layer, and misfit

Let now consider the full model, taking into account the surface stress, the wetting layer, and the misfit stress. For $\mu=1$ the characteristic equation has its simplest form and looks like

$$\sigma^* = a^{*3} - \left(1 + 2\nu e_0 \frac{f}{\gamma_0}\right) a^{*4} - w^* a^{*2}. \tag{5.7}$$

The values of the wetting constant that lead to complete stabilization and the corresponding critical wave number are found from Eq. (5.7)

$$w_c^* = [4(1+2\nu e_0 f/\gamma_0)]^{-1}, \quad a_c^* = [2(1+2\nu e_0 f/\gamma_0)]^{-1}, \tag{5.8}$$

where $e_0=\varepsilon(1+\nu)/(1-\nu)$. From Eq. (5.8) follows that when $f\varepsilon>0$, there is a stabilization due to the surface stress, while if $f\varepsilon<0$ there is a destabilization. Figure 5 illustrates the fact that this dependence on the sign of the product $f\varepsilon$ holds for $\mu<m\approx(1-2\nu)^{-1}$. However, when the film is much stiffer than the substrate, $\mu>m$, as it is usually, for example, for GaAs on Si, the influence of surface stress is different; to get a stabilization the signs of f and ϵ must be opposite. The two right curves in Fig. 5 have negative slope. Stable regions in Fig. 5 are to the left of the curves.

Complete stabilization is insured when

$$w^* > \frac{\max\{1,\mu^2\}}{4(1+(1-B\mathcal{F})e_0 f/\gamma_0)}; \tag{5.9}$$

in particular, it means that $w^*>[4(1+e_0 2\nu f/\gamma_0]^{-1}$ for $\mu \in [0,1]$, and $w^*>\mu^2[4(1+e_0(3-\mu)\nu f/\gamma_0]^{-1}$ for $\mu\in[1,3]$. Since $w=\partial\Psi/\partial h$ at $h=h_0$ it means that to control stability for a large family of wetting potentials, it is enough to be able to control only the constant w.

Dependence of the critical film thickness on the stiffness ratio and the misfit is illustrated in Fig. 6. Figure 6(a) shows that the increase of the wetting constant increases the h_c

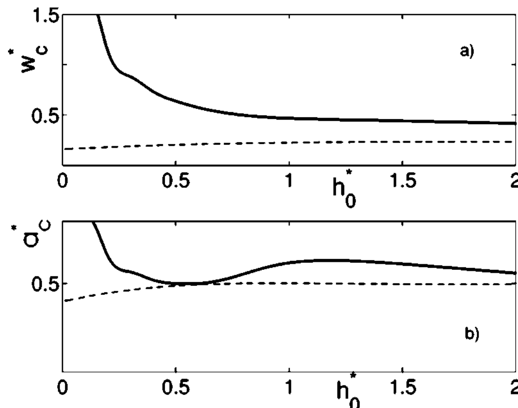

FIG. 4. Wetting layer vs h_0^* for $\mu=0.8$ (dashed curve) and for $\mu=5$ (solid curve) (a) and (b) the corresponding critical wave number.

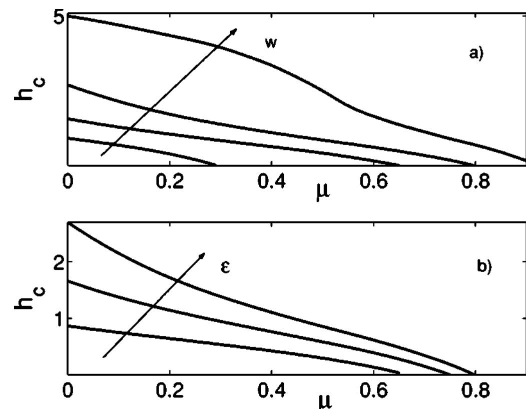

FIG. 6. h_c vs μ, $f=\gamma_0=1927$, (a) for fixed $\varepsilon=\varepsilon_0=0.0418$ and varied $w=0.02$, 0.1, 0.15, and 0.2 (as shown) and (b) for fixed $w=0.15$ and varied $\varepsilon=-4\varepsilon_0$, $-\varepsilon_0$, ε_0.

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below which the film is stable. Figure 6(b) shows dependence of h_c on the sign of $f\varepsilon$, where the constant f is fixed and positive. The upper curve corresponds to positive value of ε and therefore, the positive value of the product $f\varepsilon$. The other curves in Fig. 6(b) correspond to negative values of ε. As was the case without wetting the layer (see Sec. V A), an increase of $f\varepsilon$ (including either sign) has a stabilizing effect, and in the presence of a strong enough wetting potential this stabilization is complete.

VI. CONCLUSIONS

The effects of surface stress and wetting layers on morphological instability of epitaxially strained solid film have been investigated. Linear stability analysis shows that these effects are dependent on the relative stiffness $\mu=\mu^F/\mu^S$ of the film to the substrate. As two relevant examples one can think about Ge on Si ($\mu=0.83$) and GaAs on Si ($\mu=4.76$).

In the absence of wetting layers for small stiffness ratio, $\mu<(1-2\nu)^{-1}$ (for Ge on Si), when the film is compressed, tensile surface stress slightly stabilizes the planar film, and when the film is under tension the compressive surface stress stabilizes. For $\mu>(1-2\nu)^{-1}$ (for GaAs on Si) the situation is opposite, i.e., to stabilize a compressed film, the surface stress must be also compressive.

Wetting layers stabilize the planar film in all cases. For complete stabilization in the absence of the surface stress one must have $w^*\geqslant \mathcal{Z}^2/4$, where function $\mathcal{Z}$ depends on both the relative stiffness and the film thickness; w_c^* monotonically increases with μ.

In the presence of both the surface stress and wetting layers there is a critical value of the film thickness below which the film is stable. This value increases with w, and its dependence on surface stress is shown in Fig. 6.

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