Asymptotic derivation of the glued-wetting-layer model and contact-angle condition for Stranski-Krastanow islands

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(Received 19 June 1998)

We derive a generic mathematical model for Stranski-Krastanow island morphologies in strained solid films. We show that a class of boundary-layer transition models for the material properties across the film/substrate interface reduce to the ''glued-wetting-layer'' model in the limit of small transition-layer thickness. Our results provide an explicit derivation of the zero-contact angle condition for Stranski-Krastanow islands with isotropic properties. The glued-wetting-layer model is used to calculate a typical Stranski-Krastanow morphology and these results are combined with a specific boundary-layer transition model to determine a detailed solution for the wetting layer and the corner region. A consequence of our results is the equivalence of Stranski-Krastanow morphologies calculated from boundary-layer models in the limit of vanishing boundary-layer thickness. [S0163-1829(99)04604-4]

I. INTRODUCTION

In the growth of epitaxially-strained solid films the Stranski-Krastanow (SK) morphology, consisting of ''islands'' separated by a thin wetting layer, is a general feature in many systems such as Ge/Si.[1] It is generally understood that islands form as a mechanism of stress relaxation, and there have been a number of theoretical treatments of SK islands.[2–19] Some of the theoretical treatments have been based on atomistic calculations (see, for example, Refs. 2–4), and others on continuum theory. Of the theories using a continuum description, many use an imposed shape for the island such as a rectangle,[5] part of a pyramid,[6–12] or part of a circle.[13] In addition to the imposed-morphology theories, there have also been determinations of the island shape as a free-boundary problem where the shape is not restricted in any way.[14–19] Some of these theories use boundary-layer models for the material properties near the film/substrate interface[14–16] while others use a ''glued-wetting-layer'' model.[17–19]

In this paper we will consider a class of boundary-layer models and show that they all reduce to the glued-wetting-layer model in the limit of zero boundary-layer thickness. As such, the glued-wetting-layer model is a generic model for determining the island shape. This model has been used recently to determine the SK morphology.[17–19] An important result of our analysis is an explicit determination of the island shape near the island edge, which shows that the contact angle for the island must be zero. The zero contact angle for the island is consistent with the theoretical results of Srolovitz,[20] which show that the wetting angle at the island edge is not affected by the presence of stress.

The rest of the paper is organized as follows. In Sec. II we describe the equilibrium model for the SK morphology, which includes the possibility of boundary layer transitions in the material properties across the film/substrate interface. In Sec. III we determine the morphology in terms of solutions for the island, wetting layer, and the connecting corner. We then assemble the results in the form of a composite solution for the SK morphology. Finally, we summarize our work in Sec. IV.

II. EQUILIBRIUM MODEL

Consider a Stranski-Krastanow morphology consisting of a misfitting film with islands separated by thin wetting layers (see Fig. 1). We restrict ourselves here to two-dimensional morphologies (equivalent to parallel ridges in three dimensions) to keep the mathematical details as simple as possible. Our method could be extended to three-dimensional axisymmetric island shapes with little difficulty and to nonaxisymmetric shapes with more difficulty. We take the material to be a single component material or an alloy of fixed composition so that there are no interactions between composition and stress. We assume plane strain for the two-dimensional elasticity problem with isotropic elastic constants. We also consider the case of equal elastic constants in the film and substrate, which is a reasonable approximation for systems in which the film and substrate are elastically similar such as Ge/Si. Finally, we also assume isotropic surface energy, which means that the resulting island shapes do not contain facets.

The epitaxial film experiences a misfit strain ϵ_0 at the film/substrate interface $y=0$ due to the difference in lattice constants of the film and substrate. As has been

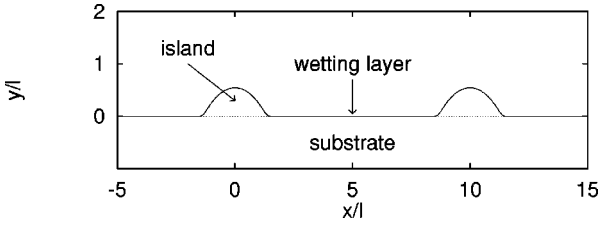

FIG. 1. A typical Stranski-Krastanow morphology as calculated using the glued-wetting-layer model. (The island spacing is $L/l=10$ and the island volume is $V/l^2=1$.)

established,[21–27] a strained planar film is unstable to the formation of surface bumps. These nonplanar morphologies result in an overall reduction in the total energy of the system. The length scale of the instability is set by the competing influences of surface energy (stabilizing) and strain energy (destabilizing). The nonplanar morphologies result in a nonuniform stress state for the film and substrate with the stress tensors given by $\boldsymbol{\sigma}^F$ and $\boldsymbol{\sigma}^S$, respectively.

Here we describe the equilibrium morphologies resulting from this instability. If the film is relatively thick, then the behavior is equivalent to that for a stressed, semi-infinite solid. In such thick films, an initially planar surface is unstable and evolves to form a cusped morphology with sharp cracklike features.[28–33] If the film is relatively thin and the film ''wets'' the substrate, then the equilibrium morphology consists of islands separated by thin wetting layers. We assume that the dominant mechanism of mass transport is by surface diffusion on the surface of the film in response to a chemical potential. Therefore, at equilibrium the morphology corresponds to constant chemical potential along the surface of the film $y=h(x)$. The conditions governing the equilibrium state can be found from a variational calculation that minimizes the total energy of the system at constant volume. Since the total energy consists of the surface energy and strain energy, the variational calculation gives

$$\mu=\gamma(h)\kappa+S(x,h)+n_y\gamma'(h) \quad \text{on} \quad y=h(x), \tag{2.1}$$

$$\boldsymbol{n}\cdot\boldsymbol{\sigma}=-\boldsymbol{n}\cdot\boldsymbol{\sigma}^m \quad \text{on} \quad y=h(x), \tag{2.2}$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}=0 \quad \text{in} \quad y<h(x), \tag{2.3}$$

and

$$\boldsymbol{\sigma}\to 0 \quad \text{as} \quad y\to-\infty. \tag{2.4}$$

In the above, $\boldsymbol{\sigma}^F=\boldsymbol{\sigma}-\boldsymbol{\sigma}^m$, $\boldsymbol{\sigma}^S=\boldsymbol{\sigma}$, μ is the chemical potential of the film surface, which is constant at equilibrium, $\gamma(h)$ is the surface energy on the film surface, κ is the curvature of the film surface, $S(x,h)$ is the strain-energy density evaluated at the film surface, $\boldsymbol{n}$ is the outward normal to the film surface, n_y is the y component of $\boldsymbol{n}$, and

$$\boldsymbol{\sigma}^m(y)=\begin{bmatrix}\sigma^m_{xx}(y) & 0\\ 0 & 0\end{bmatrix}, \tag{2.5}$$

where $\sigma^m_{xx}(y)$ is the misfit stress associated with a planar film. In addition, the strain energy density on the surface of the film $S(x,h)$ is given by

$$S(x,h)=\frac{(1-\nu)(1+\nu)}{2E}(\sigma^m_{xx}+\sigma_{xx}+\sigma_{yy})^2 \quad \text{on} \quad y=h(x), \tag{2.6}$$

where ν is Poisson's ratio and E is Young's modulus. For a planar film $S=S_0$ (constant). Equation (2.1) is in agreement with the results presented in Chiu and Gao.[14]

In Eqs. (2.1) and (2.5) the surface energy $\gamma(h)$ and the misfit stress $\boldsymbol{\sigma}^m(y)$ have been allowed to be general functions of the film thickness and distance from the film/substrate interface, respectively. For a sharp interface model of the film/substrate interface, these functions have step discontinuities at the interface (see Fig. 2): the misfit is a constant value ϵ_0 in the film and identically zero in the substrate; and the surface energy is γ_F if the film has finite thickness and γ_S if the substrate is exposed. For a wetting layer to be favored, the surface energy of the film must be less than that of the substrate.[34] The change in the properties across the interface is responsible for the establishment of the wetting layer on top of the substrate as exposing the substrate results in a larger surface energy, and hence a larger total energy for the system.

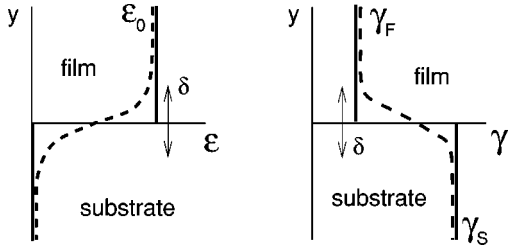

FIG. 2. Schematic of step discontinuity in properties across the film/substrate interface (solid lines). On the left, the misfit strain is ϵ_0 in the film and vanishes in the substrate. On the right, the surface energy is γ_F if the film covers the substrate and γ_S if the substrate is exposed. Wetting is promoted if $\gamma_F<\gamma_S$. The dashed curves represent a boundary-layer model for the variation in material properties across the interface as a smooth transition over a small length scale δ.

While the above sharp transitions have a clear physical origin due to the abrupt change in materials across the interface, it is difficult to implement these discontinuous properties to obtain a numerically convergent scheme for determining the equilibrium morphology. To circumvent these numerical difficulties, Chiu and Gao[14] used a boundary-layer model for the surface energy given by

$$\gamma(h)=\gamma_F+(\gamma_S-\gamma_F-\gamma_{FS})\exp(-y/\delta), \tag{2.7}$$

where δ is a transition-layer thickness, assumed to be small, and γ_{FS} accounts for the interfacial energy of the film/substrate interface. When $y\gg\delta$, $\gamma(h)\sim\gamma_F$, and the surface properties of the film are identical with the bulk properties and are not affected by the film/substrate interface. When $y=0$, the effective surface energy corresponds to that of an exposed substrate. By implementing this model numerically to mimic the influence of the substrate as the film becomes vanishingly thin, Chiu and Gao were able to calculate island morphologies during film deposition.

Kukta and Freund[15,16] have also used a boundary-layer model in the calculation of SK morphologies, but with a boundary-layer variation in the misfit instead of the surface energy. They suggested that the variation in the misfit could be represented as

$$\epsilon(y)=\epsilon_0\left(\frac{1}{\pi}\arctan(y/\delta)+\frac{1}{2}\right), \tag{2.8}$$

where ϵ_0 is the misfit strain in the film. Thus, the misfit is ϵ_0 when $y\gg\delta$ above the interface and the misfit is zero when $|y|\gg\delta$ below the interface. As in the work of Chiu and Gao, this boundary-layer transition represents a smooth regularization of the step transition of a material property (the mis-

fit). Kukta and Freund employed this model for a particular choice of small δ to calculate equilibrium island morphologies.

The idea of the boundary-layer model is that the step transition in properties is regularized over a thin transition region of width δ. If one considers the transition region to be of order of the lattice spacing, then the small-scale smooth variation might be construed as a reasonable continuum approximation to the small scale ''smearing'' of the interface over a few monolayers in thickness. Even so, the choice of the boundary-layer thickness and functional form for the transition, while physically motivated, is somewhat arbitrary unless information about the variation in properties for atomic-scale film thicknesses is available. Ideally, one would choose δ as being on the order of the lattice spacing and much smaller than the morphology scale; the macroscopic results would be independent of the choice of δ and the functional form for the transition layer.

The purpose of this paper is to show that there is a limiting ''generic model'' for a general class of boundary-layer models when $\delta \to 0$. This limiting model is the ''glued-wetting-layer'' model used in Spencer and Tersoff.[17–19] In this model, the effect of the step transition is retained by considering the limit of $\delta \to 0$ and the results are thus independent of the value of the boundary-layer thickness. The model permits the calculation of equilibrium island shapes, which are independent of the atomic scale details of the wetting layer. Viewed in this way, we suggest that the glued-wetting-layer model is a ''generic'' model for Stranski-Krastanow islands. We also show that a zero contact angle for the island edge is a generic feature for the morphology, independent of the particular transition-layer model chosen.

We consider a general class of boundary-layer transitions depicted in Fig. 2 and described by

$$\gamma(h) = \frac{1}{2}(\gamma_F + \gamma_S) + \frac{1}{2}(\gamma_F - \gamma_S) f(y/\delta) \tag{2.9}$$

and

$$\epsilon(y) = \frac{1}{2}\epsilon_0[1 + f(y/\delta)], \tag{2.10}$$

where $f(y/\delta)$ is a general transition function with the following properties: (1) $f(y/\delta)$ increases monotonically from -1 as $y \to -\infty$ to $+1$ as $y \to +\infty$, so that the correct properties are recovered above and below the interface; and (2) $f(y/\delta)$ approaches the limiting value as $y \to +\infty$ as an algebraic power, i.e., we can write an expansion of the form

$$f(y/\delta) \sim 1 - A(\delta/y)^p + \cdots \quad \text{as} \quad (y/\delta) \to +\infty, \tag{2.11}$$

where A and p are positive constants. The above represents a general behavior far away from the interface and covers all behaviors with algebraic decay (but not exponential or logarithmic decay). We have chosen the same boundary-layer thickness and functional variation for the surface energy and misfit variations as representing a reasonable assumption that the atomic-scale variation of these quantities is due to the same atomic-scale ''smearing'' of the interface.

A prototype boundary-layer function that fits the above classification is the inverse tangent model used by Kukta and Freund[15,16] for the misfit, which corresponds to

$$f(y/\delta) = \frac{2}{\pi}\arctan(y/\delta), \tag{2.12}$$

which has the asymptotic behavior shown in Eq. (2.11) with $p = 1$ and $A = 2/\pi$. Note, however, that the exponential model of Chiu and Gao[14] does not satisfy the requirement that $f \to -1$ as $y \to -\infty$ (and, therefore, gives unphysical results if $y < 0$). Also, the limiting value as $y \to +\infty$ is approached exponentially and not algebraically. Thus, our analysis does not apply to the Chiu and Gao model, and it would also not apply to a hyperbolic tangent model for the transition layer with its exponential behavior. Nonetheless, our analysis does apply to a wide range of possible boundary-layer models, including all models that approach the limiting value inversely with distance to any finite power.

III. ASYMPTOTIC SOLUTIONS

We now consider Stranski-Krastanow solutions to the equilibrium conditions which consist of islands and wetting layers. The general idea is that we will describe the island and wetting layers in separate pieces, and then connect the pieces to obtain the final solution. Overall, Eq. (2.1) gives the morphology as a balance of the surface energy $[\gamma(h)\kappa]$, strain energy $[S(x,h)]$, and wetting effects $[n_y\gamma'(h)]$. Of these three terms, only some are relevant for the island or wetting layer. Since the island is much larger than the transition-layer thickness, the transition-layer effects will be irrelevant and the morphology will be governed by the balance of surface-energy and strain-energy terms. In the wetting layer, the film will be thin, and thus relatively flat, so curvature will be negligible. The morphology will be determined by a balance of the strain energy and the wetting effects. To join the island and wetting-layer solutions, we will need a description of the corner region, or contact angle, between the island and wetting layer. In this corner region all three terms will be important. We will show that a necessary condition to connect the island and wetting-layer solutions is that the island have a zero contact angle at its edge.

A. Island solutions

For the island, the local height of the film h is much larger than the transition-layer thickness δ. Thus, since $h/\delta \gg 1$, the boundary-layer transition for $\gamma(h)$ and $\boldsymbol{\sigma}^m(y)$ is not felt by the island. To leading order in δ the resulting equations for the island shape are

$$\mu = \gamma_F\kappa + S(x,h) \quad \text{on} \quad y = h(x), \tag{3.1}$$

$$\boldsymbol{n}\cdot\boldsymbol{\sigma} = -\boldsymbol{n}\cdot\boldsymbol{\sigma}^m \quad \text{on} \quad y = h(x), \tag{3.2}$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{\sigma} = 0 \quad \text{in} \quad y < h(x), \tag{3.3}$$

and

$$\boldsymbol{\sigma} \to 0 \quad \text{as} \quad y \to -\infty, \tag{3.4}$$

where

$$\boldsymbol{\sigma}^m = \begin{bmatrix} \sigma_{xx}^0 & 0 \\ 0 & 0 \end{bmatrix}, \tag{3.5}$$

$$S(x,h) = \frac{(1-\nu)(1+\nu)}{2E}(\sigma_{xx}^0 + \sigma_{xx} + \sigma_{yy})^2 \quad \text{on} \quad y = h(x), \tag{3.6}$$

and σ_{xx}^0 is the bulk-misfit stress in the film. These equations are identical to those describing the equilibrium of a semi-infinite strained film,[31] for which the interactions with the substrate are absent. To solve for the island shape the elasticity solution to the full SK morphology, including the wetting layer, is required. We postpone the calculation of these shapes until the full composite solution is formulated.

B. Wetting-layer solutions

In the wetting layer, the film is thin (perhaps as thin as the transition layer) and relatively flat. We look for a scaling for the wetting layer solutions of the form

$$h(x) = \delta^n H(x), \tag{3.7}$$

where n is a scaling exponent to be determined. We substitute this scaling for the wetting-layer thickness into the chemical-potential balance [Eq.(2.1)] and look for a dominant balance of terms in which μ, S, and $\gamma'(h)$ are all $O(1)$. From the asymptotic behavior of the transition function the wetting term is $O(1)$ if $n = p/(p+1)$. Note that $0 < n < 1$ so the thickness of the wetting layer $O(\delta^n)$ is always much larger than the thickness of the transition layer $O(\delta)$. In effect, because of the derivative term $\gamma'(h)$, the wetting term becomes important even when the film thickness is still much greater than the transition-layer thickness.

An implication of the wetting-layer thickness being much larger than the transition-layer thickness is that the effect of the transition layer for the misfit is not present to leading order. Thus, with the same boundary-layer thickness and transition functions used to model the variation in the surface energy and misfit, only the surface energy is important to the wetting layer. Because the transition layer in the surface energy enters as a derivative, it dominates the contribution from the misfit-transition layer when δ is small. Therefore, it is sufficient to include a boundary-layer treatment in the surface energy and not the misfit to generate the wetting layer. This also suggests that the wetting-layer thickness found in the calculations of Kukta and Freund,[15,16] which use only a boundary layer for the misfit, would be different if they included a boundary-layer model for surface energy. (Overall, however, there would be little change in their calculated island shapes.)

Using the scaling for the wetting layer and the asymptotic behavior Eq. (2.11), the equilibrium condition Eq. (2.1) becomes

$$\mu = S(x,0) + \frac{1}{2}(\gamma_F - \gamma_S)\frac{Ap}{H(x)^{p+1}}. \tag{3.8}$$

Thus, given the stresses associated with a distribution of islands we can determine the scaled thickness of the wetting layer as

$$H(x) = \left[\frac{(\gamma_S - \gamma_F)Ap}{2[S(x,0) - \mu]}\right]^{1/(p+1)}. \tag{3.9}$$

In terms of the unscaled film thickness, the wetting layer is given by

$$h(x) = \delta^{p/(p+1)}\left[\frac{(\gamma_S - \gamma_F)Ap}{2[S(x,0) - \mu]}\right]^{1/(p+1)}. \tag{3.10}$$

For a given chemical potential for the film, $0 \leqslant \mu \leqslant S_0$.[19] The wetting layer adjusts its thickness in response to the strain energy according to Eq. (3.10). Since $S(x,0)$ is largest near the island and approaches a limiting value S_0 far away from an island, the wetting layer is thinnest near the island and approaches its equilibrium value of

$$h_0 = \delta^{p/(p+1)}\left[\frac{(\gamma_S - \gamma_F)Ap}{2(S_0 - \mu)}\right]^{1/(p+1)}, \tag{3.11}$$

far away from an island.

C. Corner solution

For the island, $h = O(1)$. For the wetting layer, $h = O(\delta^n) \ll 1$. These solutions are connected by a corner solution, which describes the island contact angle. In this local region, all of the terms in Eq. (2.1) contribute. We describe the corner solution in local variables as

$$x = x_0 + \delta^q \xi \tag{3.12}$$

and

$$h(x) = \delta^n \hat{h}(\xi), \tag{3.13}$$

where x_0 specifies a corner where island and wetting layer meet. Without loss of generality, we shall assume that we are describing a corner at the left edge of the island, so $\xi \to -\infty$ corresponds to the wetting layer and $\xi \to +\infty$ corresponds to the island. The choice of scaling for $h(x)$ is necessary to retain the transition-layer effect at leading order. The choice of q in the x scaling is made to include the curvature term at $O(1)$, which requires $q = n/2$. The leading-order corner solution $\hat{h}(\xi)$ is then described by a second-order ordinary differential equation

$$\mu = -\gamma_F \frac{d^2\hat{h}}{d\xi^2} + S(x_0,0) + \frac{1}{2}(\gamma_F - \gamma_S)\frac{Ap}{\hat{h}^{p+1}}. \tag{3.14}$$

The corner solution must match to the wetting layer as $\xi \to -\infty$ and must match the island as $\xi \to +\infty$.

We solve Eq. (3.14) by multiplying by $d\hat{h}/d\xi$ and integrating in ξ to obtain

$$\frac{1}{2}\gamma_F\left(\frac{d\hat{h}}{d\xi}\right)^2 = [S(x_0,0) - \mu]\hat{h} - \frac{1}{2}(\gamma_F - \gamma_S)\frac{A}{\hat{h}^p} + C. \tag{3.15}$$

To match the wetting-layer solution we require

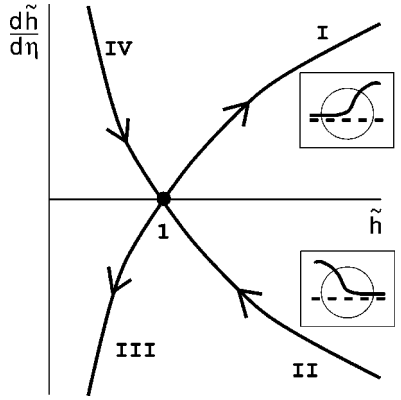

FIG. 3. Phase plane of corner solutions. All solution branches terminate at the equilibrium point corresponding to the wetting layer. Branches I and II correspond to corner solutions for the left edge and right edge of the island, respectively.

$$\lim_{x\to x_0} h_{\rm wet}(x) \sim \lim_{\xi\to-\infty} h_{\rm corner}(\xi). \tag{3.16}$$

Thus, using the wetting-layer solution (3.10), we find that the corner solution must match

$$\hat{h}(\xi)\to\hat{h}_\infty \ \text{ as } \ \xi\to-\infty, \tag{3.17}$$

where

$$\hat{h}_\infty=\left[\frac{(\gamma_S-\gamma_F)Ap}{2[S(x_0,0)-\mu]}\right]^{1/(p+1)}. \tag{3.18}$$

Substituting this into Eq. (3.15) gives

$$C=-\hat{h}_\infty\frac{p+1}{p}[S(x_0,0)-\mu]. \tag{3.19}$$

Using the above value for C we can graph the solutions to the differential equation in the phase plane. We introduce a rescaling for $\hat{h}$ and ξ according to

$$\hat{h}(\xi)=\hat{h}_\infty\tilde{h}(\eta), \tag{3.20}$$

where

$$\eta=\xi\sqrt{\frac{S(x_0,0)-\mu}{\gamma_F\hat{h}_\infty}} \tag{3.21}$$

to obtain

$$\frac{1}{2}\left(\frac{d\tilde{h}}{d\eta}\right)^2=\tilde{h}+\frac{1}{p\tilde{h}^p}-\frac{p+1}{p}. \tag{3.22}$$

The phase portrait of Eq. (3.22) is shown in Fig. 3. There are four solution branches which terminate at the equilibrium point $\tilde{h}=1$, $d\tilde{h}/d\eta=0$ (the wetting-layer solution). The asymptotic behaviors for the branches are

$$\frac{d\tilde{h}}{d\eta}\sim\pm\sqrt{2\tilde{h}} \ \text{ for } \ \tilde{h}\gg 1, \tag{3.23}$$

and

$$\frac{d\tilde{h}}{d\eta}\sim\pm\sqrt{\frac{2}{p\tilde{h}^p}} \ \text{ for } \ \tilde{h}\ll 1. \tag{3.24}$$

The branch labeled I corresponds to the corner solution at the left edge of an island, which matches the wetting layer ($\tilde{h}=1$) as $\eta\to-\infty$ and the island as $\eta\to+\infty$. Branch II describes the corner solution at the right edge of the island, which matches the wetting layer as $\eta\to+\infty$ and the island as $\eta\to-\infty$. Branches III and IV correspond to solutions in which the film thickness vanishes and are not relevant to matching the island.

Consider the corner solution corresponding to branch I. This solution already matches the wetting layer as $\eta\to-\infty$. The behavior as $\eta\to+\infty$ must match the island solution near the edge:

$$\lim_{x\to x_0} h_{\rm island}(x)\sim\lim_{\eta\to+\infty} h_{\rm corner}(\eta). \tag{3.25}$$

Thus, from integrating Eq. (3.23) in the limit of $\eta\gg 1$ (and $\tilde{h}\gg 1$) we have the corner solution behaving as

$$\tilde{h}(\eta)\sim\frac{1}{2}(\eta+B)^2 \ \text{ as } \ \eta\to+\infty, \tag{3.26}$$

where B is a constant of integration. Thus, the island edge must behave as

$$h(x)\sim\frac{S(x_0,0)-\mu}{2\gamma_F}(x-x_0)^2 \ \text{ as } \ x\to x_0. \tag{3.27}$$

The above result means that $h(x)\to 0$ quadratically at the island edge. It also means that the island will necessarily have a zero contact angle with

$$\frac{dh}{dx}=0 \ \text{ at an island edge.} \tag{3.28}$$

The zero contact-angle condition is robust. In the limit of $\delta\to 0$ the details of the contact angle are independent of the details of the transition region as evidenced by the independence of Eqs. (3.27) and (3.28) from the properties of the transition layer.

D. Composite solution

Having determined the behavior for the island, wetting layer, and connecting corner, we can formulate the composite solution for the SK morphology. Viewed on an $O(1)$ scale, the wetting layer and the corner solution appear to be vanishingly small. Thus, to leading order, the morphology appears as an island with a wetting layer of zero thickness. The conditions determining the morphology are:

$$\begin{cases} \mu=\gamma_F\kappa+S(x,h) \ \text{ for } \ h(x)>0 \ \text{ (on the island)} \\ \text{or} \\ h(x)=0 \ \text{ otherwise } \ \text{(on the wetting layer)} \end{cases} \tag{3.29}$$

$$\boldsymbol{n}\cdot\boldsymbol{\sigma}=-\boldsymbol{n}\cdot\boldsymbol{\sigma}^m \ \text{ on } \ y=h(x), \tag{3.30}$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}=0 \ \text{ in } \ y<h(x), \tag{3.31}$$

and

$$\boldsymbol{\sigma} \rightarrow 0 \quad \text{as} \quad y \rightarrow -\infty, \tag{3.32}$$

where

$$\boldsymbol{\sigma}^m = \begin{bmatrix} \sigma_{xx}^0 & 0 \\ 0 & 0 \end{bmatrix}, \tag{3.33}$$

and

$$S(x,h) = \frac{(1-\nu)(1+\nu)}{2E}(\sigma_{xx}^0 + \sigma_{xx} + \sigma_{yy})^2 \quad \text{on} \quad y = h(x). \tag{3.34}$$

Thus, Eq. (3.29) specifies that the SK morphology must satisfy either $h=0$ corresponding to the wetting layer or a condition of constant chemical potential on the island. This piecewise boundary condition for the free boundary is augmented by the edge conditions for the island from the corner solutions:

$$h(x) = 0 \quad \text{at an island edge}, \tag{3.35}$$

and

$$\frac{dh}{dx} = 0 \quad \text{at an island edge}, \tag{3.36}$$

where the location of the island edges must be determined as part of the solution to the free-boundary problem. Note that the above model corresponds to a constant chemical potential everywhere on the surface of the film, including the wetting layer. Once the solution to the above problem is determined, the thickness of the wetting layer can be determined by Eq. (3.10).

A typical SK morphology calculated with the glued-wetting-layer model (3.29)–(3.36) is shown in Fig. 1. For the calculation, we consider a periodic array of islands with spacing $L/l=10$ where the characteristic length scale $l = \gamma_F / S_0$ removes the dependence of the results on the misfit and surface energy. In general, one can find solutions corresponding to different island spacings and different island (two-dimensional) volumes as in Ref. 19. The calculations here are for an island volume $V/l^2=1$.

The glued-wetting-layer model constitutes an ''outer'' solution: on the scale of the island, the wetting layer appears to have zero thickness. To determine the small-scale structure of the wetting layer and the details of the island edge a specific choice of a transition model (δ, A, p) is required. For purposes of illustration we use the inverse-tangent transition model given by Eq. (2.12) with $\delta/l=0.001$. We also choose the surface energy of the substrate to be 50% larger than that of the film: $(\gamma_S - \gamma_F)/\gamma_F = 0.5$. The wetting-layer solution is then found from our ''outer'' solution using Eq. (3.10). Using the value of the strain-energy density at the island edge $S(x_0,0)$ from the outer solution we determine the solution for the corner by integrating Eq. (3.22) numerically. These results are shown for the right edge of an island in Fig. 4. Each piece (island, wetting layer, and corner) is a locally valid solution. We construct a uniformly valid solution for the entire problem by forming the composite solution

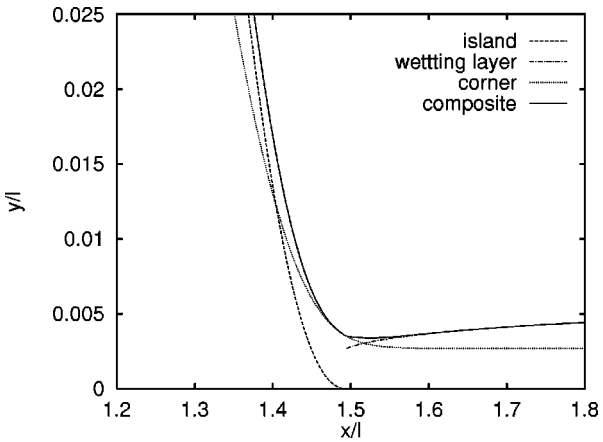

FIG. 4. Details of the island edge (right side). Shown are the separate solutions for the island and wetting layer together with the local solution for the corner region. The composite solution (see text) provides the uniformly valid solution for the entire surface.

$$h_{\text{composite}} = h_{\text{island}} + h_{\text{corner}} - h_{\text{island/corner}} \quad \text{for the island}, \tag{3.37}$$

and

$$h_{\text{composite}} = h_{\text{wet}} + h_{\text{corner}} - h_{\text{wet/corner}} \quad \text{for the wetting layer}, \tag{3.38}$$

where $h_{\text{island/corner}}$ and $h_{\text{wet/corner}}$ are the terms matched between island and corner solutions [Eq. (3.17)], and wetting layer and corner solutions [Eq. (3.27)], respectively. Figure 4 shows the composite solution for the entire surface, which describes the smooth transition from the island to the wetting layer.

The composite solution shown in Fig. 4 is essentially that which would be found with a full calculation involving the boundary-layer model. Thus, our results give two important conclusions regarding the correspondence of boundary-layer models and the glued-wetting-layer model: (1) The glued-wetting-layer model is the generic limiting model for a wide class of boundary-layer transition models in the limit of vanishing boundary-layer thickness. These results are independent of the transition-layer details. (2) Since any boundary-layer transition model in this class will give equivalent results in the limit of small boundary-layer thickness, our results can also be viewed as a validation of boundary-layer models in the calculation of SK morphologies. We have shown that in the limit of vanishing boundary-layer thickness the macroscopic SK morphologies are equivalent.

IV. SUMMARY

We have derived the equilibrium conditions for the Stranski-Krastanow (SK) morphology for a class of boundary-layer transition models for the change in material properties across the interface in the limit of small boundary-layer thickness. We have found that these models reduce to the ''glued-wetting-layer'' model of Spencer and Tersoff,[17] which consists of islands of constant chemical potential separated by wetting layers of vanishing thickness. A particular feature of this analysis is an explicit derivation of the

zero contact angle condition for SK islands. The glued-wetting-layer model enables relatively straightforward calculation of equilibrium SK island morphologies that is independent of the atomic-scale physics which produces the wetting layer. This ''outer'' solution for the morphology can be combined with a specific transition layer model to determine the detailed microstructure of the wetting layer and the corner region. A consequence of our results is the equivalence of SK morphologies calculated from boundary-layer models in the limit of vanishing boundary-layer thickness.

ACKNOWLEDGMENT

This research was supported by NSF Grant No. DMS-9622930.

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