Equilibrium island ridge arrays in strained solid films

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The equilibrium shape and chemical potential of an array of island ridges in an epitaxially strained solid film are determined from a continuum model describing the Stranski–Krastonow morphology of a thin layer on a substrate. This model incorporates the conditions for mechanical and chemical equilibrium, isotropic surface energy, and misfit strain. Solutions corresponding to periodic arrays of island ridges separated by wetting layers are found in the limit of island height much less than the island width. Our results describe how the island width, shape, and chemical potential vary as the distance between the ridges varies. The scaled island shape is shown to remain relatively constant as the distance between the islands increases. © *1999 American Institute of Physics.*
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I. INTRODUCTION

A heteroepitaxially strained film is created when a thin layer of one material is deposited upon a single-crystal substrate of a different material. If the film and the substrate have compatible crystal structures, then the deposited atoms of the film can assume the same crystal structure as the underlying substrate; in this case, the atoms of the film form a continuous extension to the crystal lattice of the substrate (a coherent interface). However, if the atomic sizes of the film and the substrate are different, the lattice of the film must be strained in order to align with the lattice of the underlying substrate. This mismatch strain affects the electronic band gap of the material, and enables strained films to be used in semiconductor devices.

The mismatch strain in the coherent film makes the film susceptible to the formation of strain relieving instabilities. One type of instability is the formation of misfit dislocations (see Ref. 1, and references therein). Another type of instability is morphological, where the surface of the film develops undulations to relieve the misfit strain.[2–14] For thin films, this instability may result in the Stranski–Krastonow island morphology, which consists of bumps (islands) surrounded by thin wetting layers (see Ref. 15). Recently, the electronic properties of films with arrays of such nanoscale islands (quantum dots) has generated significant interest. This article presents a relatively simple theory for describing the shape of elongated dots (quantum wires). These results could be useful in designing quantum wire morphologies with specifically desired properties.

In general, the morphology of a Stranski–Krastonow island depends on energetic factors, such as strain energy and surface energy, as well as kinetic factors, such as the rate of mass transport and surface diffusion. In this article, we describe the *equilibrium* morphologies of islands as an "end state" to which the morphology evolves. We find this equilibrium island shape by minimizing the total energy of the system subject to the constraint of constant island volume, or equivalently, we find the island shape with a constant chemical potential. There have been many theoretical treatments describing island morphologies using this approach, however, many of these approaches assume a particular shape or class of shapes for the islands.[16–23] But when the film and substrate materials are isotropic (above the roughening transition temperature), the shape of the island is not known, and must be determined from the solutions of a free boundary problem. So far, the theoretical results for this free boundary problem have focused on island ridges (quantum wires).[24–27] Island ridges possess finite height and width, and maintain a cross section which does not vary in the third direction, allowing the island ridge shape to be described in two dimensions. These elongated island ridges are energetically favorable at low film coverages and larger island volumes.[28] Also, elongated islands can dominate the film morphology in anisotropic materials.[29]

In this article we characterize periodic arrays of parallel island ridges. In particular, we determine how the shape and chemical potential of a ridge depend on the spacing between ridges. These results may have implications on the design and growth of quantum wire arrays devices. Furthermore, our solutions of island ridge morphologies may yield qualitative information relevant to fully three-dimensional islands. Our approach is based on the asymptotic theory presented by Spencer and Tersoff,[30] which describes the shape of a single, isolated, equilibrium island ridge characterized by a much smaller island height than island width. Here, we generalize these results to describe island ridge arrays with different spacings. Our results show that the scaled island shape and chemical potential are insensitive to the island spacing, except for closely spaced islands.

II. CONTINUUM MODEL

We use the glued wetting layer model[30] to describe the equilibrium island morphology. An infinitesimally thin wetting layer (perhaps only one atomic layer) coats the horizontal substrate surface and prevents substrate exposure. This thin wetting layer also generates well-defined island bound-

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aries and eliminates any transition layer calculations.[30] As in the previous work, we model the epitaxially strained system using isotropic linear elasticity and assume identical elastic constants in the film and substrate. This simplification is physically reasonable, since common film/substrate pairs such as Ge/Si have similar elastic constants. While Spencer and Tersoff have found solutions for a single isolated island ridge, we determine how the solutions are modified by periodic boundary conditions.

The governing equations, in the form of a nonlinear free boundary problem for the film surface $y=h(x)$, are the following. In the film and substrate, mechanical equilibrium is ensured by

$$(1-2\nu)\nabla^2\mathbf{u}+\nabla(\nabla\cdot\mathbf{u})=0 \quad \text{in both film and substrate,} \tag{2.1}$$

where $\mathbf{u}$ is the elastic displacement and ν is Poisson's ratio. At the surface of the film, we impose a traction-free boundary condition,

$$\mathbf{n}\cdot\sigma^F=0 \quad \text{on} \quad y=h(x), \tag{2.2}$$

where σ^F is the stress tensor in the film and $\mathbf{n}$ is the outward normal to the film surface. At the interface between the film and substrate, a force balance gives

$$\hat{y}\cdot\sigma^F=\hat{y}\cdot\sigma^S \quad \text{on} \quad y=0, \tag{2.3}$$

where $\hat{y}$ is the unit vector in the y direction. Continuity of displacement at the interface gives a misfit strain directed along the x axis[14]

$$E_{xx}^F=E_{xx}^S+\epsilon_m \quad \text{on} \quad y=0, \tag{2.4}$$

and a continuity of shear strain,

$$E_{xy}^F=E_{xy}^S \quad \text{on} \quad y=0, \tag{2.5}$$

where E_{ij} are the components of the strain tensor. Finally, the stresses decay to zero far into the substrate,

$$\sigma^S\to 0 \quad \text{as} \quad y\to-\infty. \tag{2.6}$$

The elasticity problem is completed by using the standard constitutive relations for isotropic linear elasticity.

We look for equilibrium solutions to the free boundary problem which represent a periodic array of island ridges. We look for symmetric islands, and take the island to be centered at $x=0$ and extend from $-W/2<x<W/2$, where W is the island width (to be determined). To find the island shape $y=h(x)$, we define a chemical potential μ, which is constant on the island surface at equilibrium. As in the ''glued wetting layer model,'' we assume that the islands are surrounded by a wetting layer of negligible thickness. Requiring a constant chemical potential on the surface of the island leads to the piecewise condition for the free boundary

$$\begin{cases} \mu=\gamma\kappa+S & \text{for } h(x)>0 \text{ (on the island)} \\ \qquad\quad \text{or} \\ h(x)=0 & \text{otherwise (on the wetting layer).} \end{cases} \tag{2.7}$$

In the earlier equation, μ is the chemical potential (in units of energy/volume), γ is the surface energy assumed to be constant, κ is the curvature of the film surface, and S is the strain energy density on the film surface, defined as
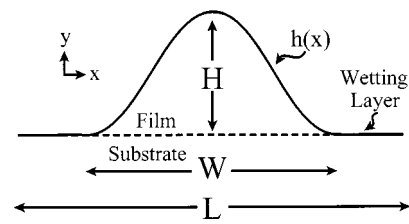

FIG. 1. Model configuration.

$$S=\tfrac{1}{2}\sigma_{ij}E_{ij} \quad \text{on} \quad y=h(x), \tag{2.8}$$

where repeated indices imply summation.

At the junction between island and wetting layer, a necessary connecting condition for Eq. (2.7) is that the surface slope of the film is zero[31]

$$\frac{\partial h}{\partial x}=0 \quad \text{at} \quad x=\pm W/2. \tag{2.9}$$

This condition is appropriate if the film is isotropic and the wetting layer is thin. For anisotropic materials and/or the Volmer–Weber morphology in which the wetting layer is absent, the island can have a nonzero contact angle and Eq. (2.9) would be modified (see below).

Finally, there are some symmetry conditions imposed upon the periodic surface morphology. Consider an array of symmetrical islands, each centered in a box of width L, as shown in Fig. 1. Due to the symmetry of the island shape and the existence of the wetting layer, displacement occurring at the edges of the periodic box and at the center of the island must occur only in the y direction

$$\mathbf{u}_x=0 \quad \text{at} \quad x=0,\pm L/2, \tag{2.10}$$

and

$$\frac{\partial\mathbf{u}_y}{\partial x}=0 \quad \text{at} \quad x=0,\pm L/2. \tag{2.11}$$

Furthermore, at the island peak, the surface is horizontal due to symmetry,

$$\frac{\partial h}{\partial x}(0)=0. \tag{2.12}$$

Equations (2.1)–(2.12) define the free boundary problem for the periodic array of islands. Our goal is to determine how the width W, shape $y=h(x)$, and chemical potential μ vary as the distance between islands varies.

Note that Eqs. (2.7) and (2.9) restrict the model to the Stranski–Krastonow morphology, where each island is surrounded by a thin wetting layer. When the film and substrate materials are isotropic and the wetting layer is thin, Spencer[31] has shown that Eqs. (2.7) and (2.9) correspond to a constant chemical potential on the film surface. For strongly anisotropic (faceted) islands, the contact angle condition [Eq. (2.9)] is not valid. Also, for isotropic Volmer–Weber morphologies in which there is no wetting layer, islands may have a nonzero contact angle; thus, Eq. (2.9) would not be appropriate in this situation. Moreover, the equilibrium Volmer–Weber case is more complicated than the Stranski–Krastonow case; in the Stranski–Krastonow

case, a wetting layer given by $h \approx 0$ corresponds to a balance of strain energy and wetting energy,[31] and thus a constant chemical potential. In the Volmer–Weber case, the $h = 0$ description for an exposed substrate surface does not represent an equilibrium configuration since the chemical potential is not constant. Thus, our model describes isotropic Stranski–Krastonow morphologies, but does not describe isotropic Volmer–Weber morphologies, even if the contact angle is zero.

III. ISLAND ARRAY SOLUTIONS

A. Conversion to semi-infinite elasticity problem

We now simplify the stress problem by adding an equivalent misfit strain to the substrate and converting the bimaterial problem to a single semi-infinite problem. To implement this, a new displacement field is defined which accommodates the misfit strain. For the displacement field, we assign

$$\mathbf{u} = \mathbf{u}^F \quad \text{in the film,} \tag{3.1.1a}$$

$$\mathbf{u} = \mathbf{u}^S + \epsilon_m \begin{bmatrix} x \\ \zeta y \end{bmatrix} \quad \text{in the substrate.} \tag{3.1.1b}$$

The corresponding transformation of stress is given by

$$\mathbf{T} = \sigma^F / \sigma_0 \quad \text{in the film,} \tag{3.1.2a}$$

$$\mathbf{T} = (\sigma^S + \sigma_m) / \sigma_0 \quad \text{in the substrate,} \tag{3.1.2b}$$

where σ_m is the uniaxial misfit stress of magnitude σ_0. For the case of equal elastic constants, the boundary conditions [Eqs. (2.3), (2.4), and (2.5)] are automatically satisfied with $\zeta = -\nu/(1-\nu)$ and $\sigma_0 = E\epsilon_0/[(1+\nu)(1-\nu)]$. The elastic problem is now determined by the single stress tensor $\mathbf{T}$ in the semi-infinite region of film and substrate.

B. Nondimensionalization

The system of equations is now nondimensionalized using characteristic scales for energy, stress, strain, and length, based on the solutions for a planar film. The characteristic scales are given by σ_0 for stress, S_0 for strain energy density and $l = \gamma/S_0$ for length. The system of nondimensional equations becomes

$$(1-2\nu)\nabla^2\mathbf{u} + \nabla(\nabla \cdot \mathbf{u}) = 0 \quad \text{in } y < h(x), \tag{3.2.1}$$

$$\mathbf{n} \cdot \mathbf{T} = 0 \quad \text{on } y = h(x), \tag{3.2.2}$$

$$\mathbf{T} \rightarrow \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{as } y \rightarrow -\infty, \tag{3.2.3}$$

$$\begin{cases} \mu = \kappa + S & \text{for } h(x) > 0 \text{ (on the island)} \\ h(x) = 0 & \text{otherwise (on the wetting layer)} \end{cases} \tag{3.2.4}$$

$$\partial h / \partial x (\pm W/2) = 0, \tag{3.2.5}$$

$$\partial h / \partial x (0) = 0, \tag{3.2.6}$$

$$\mathbf{u}_x = 0 \quad \text{at } x = 0, \pm L/2, \tag{3.2.7}$$

$$\partial \mathbf{u}_y / \partial x = 0 \quad \text{at } x = 0, \pm L/2, \tag{3.2.8}$$

where all variables are now nondimensional with respect to the appropriate length or energy scale.

By evaluation of Eq. (2.8) using the definitions provided in Sec. (III A) and the boundary conditions earlier, the value of S on the surface $y = h(x)$ in terms of T_{ij} can be determined as

$$S = [T_{xx} + T_{yy}]^2. \tag{3.2.9}$$

C. Scaling

We now consider solutions to the system corresponding to ''thin'' islands, such that the nondimensional island height, H, is much smaller than the nondimensional island width, W. A new scale of length, W, is chosen for the x and y coordinates. New unit axes are then defined, $\tilde{x} = x/W$ and $\tilde{y} = y/W$. The displacement vector $\mathbf{u}$ is scaled by W such that $\tilde{\mathbf{u}} = \mathbf{u}/W$. Also, consider the function $h(x)$ in terms of the island height, H. In this way, $h(x)$ is scaled as $\tilde{h}(\tilde{x}) = h(x)/H$. By definition, the shape of the island is $y = h(x)$. Scaling applied to this equation yields

$$\tilde{y} = \delta\tilde{h}(\tilde{x}),$$

where $\delta = H/W$. We shall look for solutions for which $H \ll W$, corresponding to $\delta \ll 1$.

We apply the scalings to the entire system. For convenience, the $\tilde{\ }$ notation is dropped, and all variables are considered to be scaled

$$(1-2\nu)\nabla^2\mathbf{u} + \nabla(\nabla \cdot \mathbf{u}) = 0 \quad \text{in } y < h(x), \tag{3.3.1}$$

$$\mathbf{n} \cdot \mathbf{T} = 0 \quad \text{on } y = \delta h(x), \tag{3.3.2}$$

$$\mathbf{T} \rightarrow \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{as } y \rightarrow -\infty, \tag{3.3.3}$$

$$\begin{cases} \mu = \kappa + S & \text{for } h(x) > 0 \text{ (on the island)} \\ h(x) = 0 & \text{otherwise (on the wetting layer)} \end{cases} \tag{3.3.4}$$

$$\partial h / \partial x (\pm 1/2) = 0, \tag{3.3.5}$$

$$\partial h / \partial x (0) = 0, \tag{3.3.6}$$

$$\mathbf{u}_x = 0 \quad \text{at } x = 0, \pm \lambda, \tag{3.3.7}$$

$$\partial \mathbf{u}_y / \partial x = 0 \quad \text{at } x = 0, \pm \lambda. \tag{3.3.8}$$

In these equations, the nondimensional parameter λ is defined by $\lambda = L/2W$. Additionally, from the assumed island width and height, and the assumption of even symmetry, we have

$$h(\pm 1/2) = 0, \tag{3.3.9}$$

and

$$h(0) = 1. \tag{3.3.10}$$

D. Asymptotic solutions

We now consider asymptotic solutions to the system, where the island solutions are a perturbation of the trivial leading-order planar solution. We expand each variable (h, $\mathbf{T}$, μ, S, $\mathbf{u}$, and κ) in terms of the small parameter δ. For example

J. Appl. Phys., Vol. 86, No. 10, 15 November 1999

C. D. Rudin and B. J. Spencer   5533

$$h = h^{(0)} + \delta h^{(1)} + O(\delta^2). \tag{3.4}$$

These expansions are substituted into the scaled system. Terms of similar order are grouped together and the problems at each order of δ are solved sequentially.

E. Leading order problem

The leading order problem corresponds to a flat film of vanishing thickness. The leading order solution corresponds to a state of uniform stress. We thus look for solutions for $\mathbf{u}^{(0)}$ of the form $u_x^{(0)} = Ax + Cy + D$ and $u_y^{(0)} = By - Cx + E$ corresponding to uniform stress and strain. Substituting these equations into the leading order problem yields

$$u_x^{(0)} = x \quad \text{and} \quad u_y^{(0)} = -\nu y/(1-2\nu). \tag{3.5}$$

At leading order, the stress is uniform with $T_{xx}^{(0)} = 1$, and all other stresses zero. The island shape $h^{(0)}$ is undetermined at this order.

F. First order problem

The order δ problem is

$$(1-2\nu)\nabla^2 \mathbf{u}^{(1)} + \nabla(\nabla \cdot \mathbf{u}^{(1)}) = 0 \quad \text{in } y < 0, \tag{3.6.1}$$

$$\begin{cases} T_{xy}^{(1)} = T_{xx}^{(0)}(\partial h^{(0)}/\partial x) \\ T_{yy}^{(1)} = 0 \end{cases} \quad \text{on } y=0, \tag{3.6.2a} \tag{3.6.2b}$$

$$\mathbf{T}^{(1)} \rightarrow \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{as } y \rightarrow -\infty, \tag{3.6.3}$$

$$\mu^{(1)} = \kappa^{(1)} + S^{(1)} = -\frac{1}{W}h_{xx}^{(0)} + 2\frac{T_{xx}^{(1)}}{T_{xx}^{(0)}} \quad \text{on } y=0 \tag{3.6.4}$$

with the boundary conditions

$$\partial h^{(0)}/\partial x(\pm 1/2) = 0, \tag{3.6.5}$$

$$\partial h^{(0)}/\partial x(0) = 0, \tag{3.6.6}$$

$$u_x^{(1)} = 0 \quad \text{at } x = 0, \pm\lambda, \tag{3.6.7}$$

$$\partial u_y^{(1)}/\partial x = 0 \quad \text{at } x = 0, \pm\lambda, \tag{3.6.8}$$

$$h^{(0)}(\pm 1/2) = 0, \tag{3.6.9}$$

$$h^{(0)}(0) = 1. \tag{3.6.10}$$

The first-order problem is thus a coupled free-boundary/elasticity problem. The elasticity problem depends on $h^{(0)}(x)$ from boundary condition [Eq. (3.6.2a)], and $h^{(0)}(x)$ depends on the stress from the equilibrium condition [Eq. (3.6.4)].

G. Solution method for the first-order problem

Due to the periodic boundary conditions, the displacements are expected to be periodic on the interval $-\lambda \leq x \leq \lambda$. Thus, a general solution is assumed which is periodic in x with period 2λ, that is

$$\begin{bmatrix} u_x^{(1)} \\ u_y^{(1)} \end{bmatrix} = \sum_{n=1}^{\infty} \begin{bmatrix} F_n(y) \\ G_n(y) \end{bmatrix} \cos\frac{n\pi x}{\lambda} + \begin{bmatrix} H_n(y) \\ J_n(y) \end{bmatrix} \sin\frac{n\pi x}{\lambda}. \tag{3.7.1}$$

Using the boundary conditions from Eqs. (3.6.7) and (3.7.8), these equations can be simplified to

$$u_x^{(1)} = \sum_{n=1}^{\infty} H_n(y) \sin\frac{n\pi x}{\lambda}, \tag{3.7.2}$$

$$u_y^{(1)} = \sum_{n=1}^{\infty} G_n(y) \cos\frac{n\pi x}{\lambda}. \tag{3.7.3}$$

These equations are substituted into Navier's Eq. (3.6.1), yielding a system of equations as shown below [prime ("''") indicates differentiation with respect to y]

$$(1-2\nu)H_n''(y) - \gamma_n G_n'(y) - (2-2\nu)\gamma_n^2 H_n(y) = 0, \tag{3.7.4}$$

$$(2-2\nu)G_n''(y) + \gamma_n H_n'(y) - (1-2\nu)\gamma_n^2 G_n(y) = 0, \tag{3.7.5}$$

where $\gamma_n = n\pi/\lambda$. This is a linear ordinary differential equation system with constant coefficients.

Assuming a decaying exponential form for $H_n(y) = H_{0n}e^{\alpha_n y}$ and $G_n(y) = G_{0n}e^{\alpha_n y}$ consistent with boundary condition [Eq. (3.6.3)], the equations can be rearranged and expressed in terms of a linear system

$$\begin{bmatrix} (1-2\nu)\alpha_n^2 - (2-2\nu)\gamma_n^2 & -\gamma_n\alpha_n \\ \gamma_n\alpha_n & (2-2\nu)\alpha_n^2 - (1-2\nu)\gamma_n^2 \end{bmatrix}$$

$$\times \begin{bmatrix} H_{0n} \\ G_{0n} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{3.7.6}$$

Nontrivial solutions require the determinant of the coefficient matrix to vanish. This results in a fourth order polynomial for α_n: $(\alpha_n^2 - \gamma_n^2)^2 = 0$. The solutions are a pair of double roots, $\alpha_n = \pm\gamma_n$. The negative root violates boundary condition [Eq. (3.6.3)] and is discarded. Due to the presence of the double root $\alpha_n = \gamma_n$, the general form for the solution of $H_n(y)$ and $G_n(y)$ may be expressed as[32]

$$H_n(y) = H_{0n}e^{\alpha_n y} + H_{1n}ye^{\alpha_n y}, \tag{3.7.7}$$

$$G_n(y) = G_{0n}e^{\alpha_n y} + G_{1n}ye^{\alpha_n y}. \tag{3.7.8}$$

When these general forms are substituted into the system equations and boundary conditions [Eqs. (3.6.1) and (3.6.2)], the solutions for H_{1n}, G_{0n}, and G_{1n} may be expressed in terms of H_{0n}.

$$H_n(y) = H_{0n}\left[e^{\alpha_n y} + \frac{1}{2-2\nu}\alpha_n ye^{\alpha_n y}\right], \tag{3.7.9}$$

$$G_n(y) = H_{0n}\frac{1}{2-2\nu}[(1-2\nu)e^{\alpha_n y} - \alpha_n ye^{\alpha_n y}]. \tag{3.7.10}$$

We now substitute our general elasticity solution into the condition [Eq. (3.6.2a)]. Integrating against $\sin(m\pi x/\lambda)$, we determine the coefficients H_{0m} to be

$$H_{0m} = \frac{2(1+\nu)(1-\nu)}{\lambda E\gamma_m}\int_{-\lambda}^{\lambda}\sin\frac{m\pi x}{\lambda}\frac{\partial h^{(0)}}{\partial x}dx \tag{3.7.11}$$

for $m=1,2,...$. We now consider the equation for the free boundary [Eq. (3.6.4)]. The value for $T_{xx}^{(1)}$ at $y=0$ can now be determined as

$$T_{xx}^{(1)}|_{y=0} = \sum_{n=0}^{\infty} \frac{2\cos(\alpha_n x)}{\lambda} \int_{-\lambda}^{\lambda} \sin\frac{n\pi x}{\lambda} \frac{\partial h^{(0)}}{\partial x} dx. \tag{3.7.12}$$

This solution describes the elastic response to a general island shape $h^{(0)}(x)$. We substitute this expression into Eq. (3.6.4) for the free boundary to obtain an integro-differential equation for $\mu^{(1)}$ and $h^{(0)}(x)$

$$\mu^{(1)} = -\frac{1}{W} h_{xx}^{(0)} + 2\sum_{n=0}^{\infty} \frac{2\cos(\alpha_n x)}{\lambda} \int_{-\lambda}^{\lambda} \sin\frac{n\pi x}{\lambda} \frac{\partial h^{(0)}}{\partial x} dx. \tag{3.7.13}$$

To determine the island shape $h^{(0)}(x)$, we assume an expansion which automatically satisfies Eqs. (3.6.5) and (3.6.6)

$$h^{(0)}(x) = h_0 + \sum_{j=1}^{M} h_j \cos(2\pi j x). \tag{3.7.14}$$

We take M large enough that the solution converges. The task now is to determine the coefficients h_j from the free boundary Eq. (3.7.13). This equation is multiplied by $\cos(2\pi k x)$, $k\neq 0$, and integrated from $x=-1/2$ to $x=+1/2$ to obtain

$$0 = \frac{(\pi^2 k^2 h_k \lambda)}{2W} + \sum_{n=1}^{\infty} \sum_{j=1}^{M} (-2\pi j h_j) b_{j,n} a_{j,n}, \tag{3.7.15}$$

where

$$a_{k,n} = \begin{cases} \frac{1}{2} & \text{if } k=n/2\lambda \\ \frac{\sin\left(\frac{n\pi}{2\lambda}-\pi k\right)}{2\left(\frac{n\pi}{2\lambda}-\pi k\right)} + \frac{\sin\left(\frac{n\pi}{2\lambda}+\pi k\right)}{2\left(\frac{n\pi}{2\lambda}+\pi k\right)} & \text{if } k\neq n/2\lambda \end{cases}$$

$$b_{j,n} = \begin{cases} \frac{1}{2} & \text{if } j=n/2\lambda \\ \frac{\sin\left(\frac{n\pi}{2\lambda}-\pi j\right)}{2\left(\frac{n\pi}{2\lambda}-\pi j\right)} - \frac{\sin\left(\frac{n\pi}{2\lambda}+\pi j\right)}{2\left(\frac{n\pi}{2\lambda}+\pi j\right)} & \text{if } j\neq n/2\lambda \end{cases}.$$

To solve for the h_j's we express Eq. (3.7.15) as a linear system for the column vector of h_j's,

$$\mathbf{A}(W)\mathbf{h} = \mathbf{0}, \tag{3.7.16}$$

where each element of the matrix $\mathbf{A}$ is given by (j=column, k=row)

$$\langle \mathbf{A}(W)\rangle_{kj} = \frac{\delta(j,k)\lambda\pi^2 k^2}{2W} - \sum_{n=1}^{\infty} 2\pi j a_{k,n} b_{j,n}, \tag{3.7.17}$$

where

$$\delta(j,k) = \begin{cases} 1 & \text{for } j=k \\ 0 & \text{otherwise.} \end{cases}$$

The extra term on each diagonal entry, $j=k$, is due to the curvature term in Eq. (3.7.13). For nontrivial solutions, we require the determinant of the matrix $\mathbf{A}(W)$ to be 0. This determines W.

A Matlab[33] program was developed to numerically calculate the value of W corresponding to $\det(\mathbf{A})=0$ as a function of island spacing L (which appears in λ). For accuracy in the calculation of each matrix coefficient $\langle \mathbf{A}(W)\rangle_{kj}$, we required the infinite series term in Eq. (3.7.17) to converge. To assure this, the number of terms in the sum was incremented by factors of two until the relative contribution of the last half of the terms was less than 10^{-4} of the entire sum. For the sum [Eq. (3.7.14)] representing $h^{(0)}(x)$, we used a value of $M=4$ terms; in the next section, we will estimate the margin of error caused by such an approximation.

We found that for a given L, there was a single W such that $\det(\mathbf{A})=0$, and for which the free boundary problem had a nontrivial solution. To determine the shape, we consider the unnormalized values of h_j which correspond to the null vector of $\mathbf{A}$, $\mathbf{A}h_j^{un}=\mathbf{0}$. By considering the matrix problem $\mathbf{A}h_j^{un}=0$ as an eigenvalue equation, Matlab was used to find a null vector for h_j^{un} where $j=1,...,M$. The actual vector h_j may then be considered of the form $h_j=Ch_j^{un}$ for $j=1,...,M$, where C is a constant and h_0^{un} is arbitrary. Using the normalization conditions $h^{(0)}(\pm 1/2)=0$ and $h^{(0)}(0)=1$, we determine C and h_0^{un} as

$$C = \frac{1}{\sum_{j=1}^{M} h_j^{un}(1-(-1)^j)}, \tag{3.7.18}$$

and

$$h_0^{un} = \frac{1}{C} - \sum_{j=1}^{M} h_j^{un}. \tag{3.7.19}$$

The unnormalized island shape $h^{(0)un}(x)$ is constructed by substituting the values for h_0^{un} and h_j^{un}, $j=1,...M$ into the unscaled equivalent of Eq. (3.7.14).

Returning to Eq. (3.7.14), and integrating from $x=-1/2$ to $x=1/2$ gives an expression for the chemical potential in terms of the shape coefficients.

$$\mu^{(1)} = \sum_{j=1}^{M} \sum_{n=1}^{\infty} \frac{-16j h_j}{n} b_{j,n} \sin\frac{n\pi}{2\lambda}. \tag{3.7.20}$$

Now, the coefficients in the expansion h_j, the width W, and the corresponding value of the chemical potential, $\mu^{(1)}$ can be determined for specific island spacing L. The value of W corresponding to specific L is determined numerically, and this result is used to numerically generate values for h_j and $\mu^{(1)}$.

IV. RESULTS

For a given film/substrate system, the length scale, stress scale, and energy scale are completely determined. The calculated nondimensional island shape is appropriate for islands with a much smaller island height H than island width W. For a given island ridge spacing L, we determine the island width W and the island shape. Since the calculation for the island shape is linear (at leading order), the island height
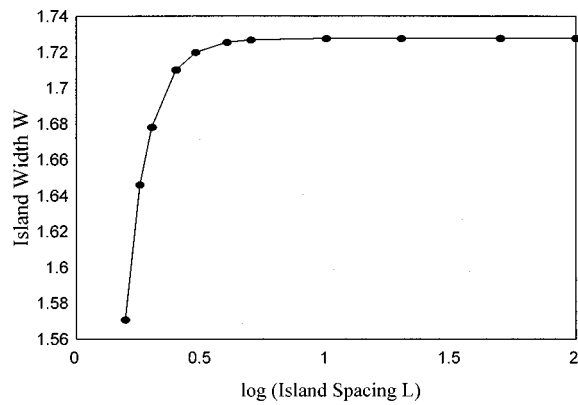
FIG. 2. Island width W vs log (island spacing L).

FIG. 4. Scaled morphological profile : Island height h vs x.

H is arbitrary. Thus, the results of our calculation describe small islands; a particular choice of H corresponds to a specific value of $\delta = H/W$. Since the unscaled island height depends linearly upon H, different H values are equivalent to different island volumes. For each island solution, there is a constant chemical potential on the surface. In our calculations, we determine $\mu^{(1)}$ as a function of the island separation. The actual nondimensional chemical potential can then be determined by $\mu = 1 + \delta \mu^{(1)}$, where $\delta = H/W$ depends on the island height.

Figure 2 illustrates the relationship of W to log L. Here, we can see that the equilibrium island width rapidly approaches a limiting value for large island separation. This limit is 1.7278, in agreement with the value 1.73 of Spencer and Tersoff.[30] For closely spaced islands (such that the island width approaches the island separation), W reaches a minimum at $L = W = \pi/2$, also in agreement with theoretical values for steady-state small amplitude periodic surfaces.[5]

A plot of $\mu^{(1)}$ versus log L is provided in Fig. 3. The chemical potential approaches a limiting value of -2.986 at large L. At small L, $\mu^{(1)}$ decays to zero.

The equilibrium solutions for the island profiles at $L = 100$ and $L = \pi/2$ are shown in Fig. 4. All solutions for intermediate values of L lie within these bounds, and rapidly approach the solution for $L = 100$ as L increases. These islands are scaled such that $H = 1$ and $W = 1$. We can see from
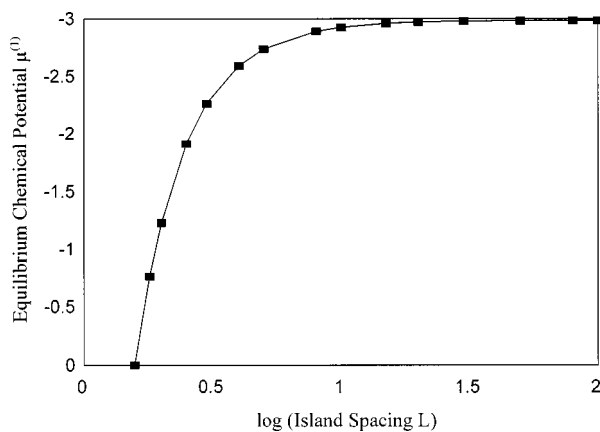
this figure that the scaled island shape does not seem to be significantly altered by the presence of nearby islands. In fact, as Fig. 4 shows, the island shapes are well approximated by a simple function determined in Ref. 30 for isolated islands. The wetting layer seems to provide the island with a morphological stability, in which the island width increases for large L, but the shape remains self-similar. In this way, the balance given between stress relaxation and surface energy seems to be fairly robust; when the distance between islands is altered, only a slight change in island width and a minute adjustment of chemical potential occurs. Since the effect of island spacing L seems to be so small, it would seem that the island shape determined by this simulation has some optimal properties that may be completely independent of L, W, H, $\mu^{(1)}$, etc. An exact solution to this problem has been determined (see Ref. 5 for example) for $L = W = \pi/2$ and is given by

$$h^{(0)}(x) = \tfrac{1}{2}[1 + 2 \cos(2 \pi x)] \quad \text{for } |x| \leqslant 1/2. \quad (4.1)$$

This solution is also presented in Fig. 4, in agreement with computed results. As suggested by Spencer and Tersoff,[30] this is also a close approximation for $L = \infty$ and $W \approx 1.73$. Since all calculated island shapes lie between these bounds, our analysis suggests that Eq. (4.1) is a close approximation for arbitrary island spacing L, using the corresponding island widths as determined in Fig. 2.

To demonstrate how the actual unscaled shapes change with L, we consider islands of equal volume, where volume is given by the area under $y = h^{(0)}(x)$. To retrieve the unscaled solution, we combine the formula for the unscaled island surface $y_{\text{unscaled}} = H h^{(0)}(x)$ with a definition for (two-dimensional) island volume,
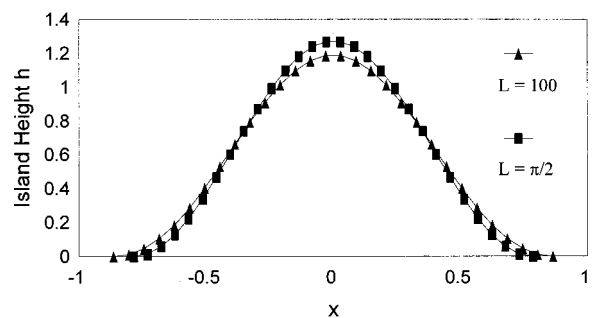

FIG. 3. Equilibrium chemical potential $\mu^{(1)}$ vs log (island spacing L).

FIG. 5. Morphological profile with constant island volume.

TABLE I. Estimate of error in solutions.

L	$W(M=4)$	$W(M=2)$	% Difference in W
$\pi/2$	$\pi/2$	$\pi/2$	0.00
1.8	1.6461	1.6469	0.05
2	1.6782	1.6798	0.09
2.5	1.7101	1.7125	0.14
3	1.7199	1.7277	0.16
4	1.7254	1.7283	0.16
5	1.7268	1.7298	0.17
8	1.7276	1.7305	0.17
10	1.7277	1.7306	0.17
15	1.7277	1.7307	0.17
20	1.7277	1.7306	0.17
30	1.7278	1.7307	0.17
50	1.7277	1.7307	0.17
80	1.7277	1.7306	0.17
100	1.7278	1.7307	0.17

L	$\mu^{(1)}(M=4)$	$\mu^{(1)}(M=2)$	% Difference in $\mu^{(1)}$
$\pi/2$	0	0	0.00
1.8	-0.7648	-0.7659	0.14
2	-1.2294	-1.2322	1.23
2.5	-1.9134	-1.9200	0.34
3	-2.2626	-2.2711	0.37
4	-2.5915	-2.6018	0.40
5	-2.7374	-2.7484	0.40
8	-2.8908	-2.9026	0.41
10	-2.9256	-2.9376	0.41
15	-2.9597	-2.9718	0.41
20	-2.9716	-2.9838	0.41
30	-2.9801	-2.9922	0.41
50	-2.9844	-2.9966	0.41
80	-2.9859	-2.9981	0.41
100	-2.9862	-2.9984	0.41

$$V = \int_{-1/2}^{1/2} h^{(0)}(x)\,dx \tag{4.2}$$

which yields $y_{\text{unscaled}} = H h^{(0)} = [V/(W C h_0^{un})] h^{(0)}$, and $x_{\text{unscaled}} = W x$. Results are shown in Fig. 5 for constant volume $V=1$ with $L=\pi/2$ and $L=100$. The island shape does vary slightly, due to the increase in W with increasing L. With L large, an island is somewhat broader and shorter than a corresponding island of the same volume with smaller L, but the overall change is small.

The value of $M=4$ used in these trials was chosen to approximate the solutions for larger M. In order to estimate the error, we compare results from two different values of M and show that W and $\mu^{(1)}$ have converged. Values for W and $\mu^{(1)}$ were calculated for each L at $M=4$ and $M=2$. (See Table I for these results.) The percent difference between the two measurements for each W was less than 0.2% in every case, and the percent difference for each measurement of

$\mu^{(1)}$ was beneath 0.5% in every case. Because of the smallness of this error, the $M=4$ results appear to have sufficient accuracy.

V. CONCLUSION

Asymptotic and numerical solutions to a model of periodic Stranski–Krastonow island morphologies yields results for the equilibrium shapes, widths, and chemical potentials of small aspect ratio island arrays. It has been shown that island shapes are not significantly altered by island separation, and appear to be remarkably self-similar. The relationship between island width and island separation has been established, as well as the relationship between chemical potential and island separation.

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