Nonlinear evolution equation for the stress-driven morphological instability

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A flat surface of stressed solid is unstable to small perturbations. This morphological instability is called Asaro–Tiller–Grinfeld instability. Nonlinear evolution of this instability will result in the formation of cusp singularities. This instability can be described by a continuum model with surface diffusion driven by a stress-dependent chemical potential. The stress and strain in the solid are coupled with surface morphology and an elasticity problem must be solved numerically. We derive a nonlinear approximation equation governing the evolution of this instability in which the stress-dependent chemical potential is expressed explicitly as a function of the surface morphology. Linear instability analysis using our equation shows the same results as the well-known Asaro–Tiller–Grinfeld instability result. Compared with the exact solution of the elasticity problem for cycloid surface obtained by Chiu and Gao, our nonlinear approximation has a much wider range of applicability than linear approximation. Numerical simulation using our nonlinear evolution equation shows that the surface evolves towards a cusplike morphology from small perturbations, which agrees very well with results obtained by solving the full elasticity problem. © 2002 American Institute of Physics. [DOI: 10.1063/1.1477259]

I. INTRODUCTION

The stress-driven morphological instability was first studied by Asaro and Tiller and later independently by Grinfeld, and Srolovitz. These authors studied the linear instability of a planar surface of a stressed solid to small perturbations and found that the planar surface is unstable for wave numbers less than a critical value. This instability is manifested by a mass transport via surface diffusion. The elastic energy in the solid is a destabilizing factor, while the surface energy is a stabilizing one. An important example of the stressed solid is the epitaxially strained solid film, in which the mismatch between the lattice constants in the film and the substrate causes misfit strain and stress in the film. In this context, the linear instability analysis performed by Grinfeld, Spencer et al., Freund and Jonsdottir showed that the difference between the elastic behaviors of the film and the substrate also affects the surface morphology by modifying the elastic energy. Additional work on linear instability was done by Gao, Nozieres, Grilhe, and others, taking into account such effects as anisotropic elasticity, gravity, and surface tension.

The nonlinear evolution of the stress-driven instability for a thick film results in the formation of deep, cusplike grooves. The formation of deep grooves or cusps was observed in experiments. Several researchers performed analyses in the weakly nonlinear regime or under the approximation of the grooves by prescribed functions. The first fully nonlinear analysis of this instability was performed numerically by Yang and Srolovitz. They showed that a planar surface of an elastically stressed solid can rapidly evolve into a cusplike morphology, which smooth tops and sharp, deep grooves. These grooves continue to sharpen as they grow deeper. Chiu and Gao were able to solve for the stress field analytically when the surface of the solid is of cycloid type. They showed that a cusped cycloid surface is energetically favorable when the surface wavelength exceeds a critical value and is stable once it develops. Spencer and Meiron performed the fully nonlinear bifurcation analysis. They tracked the branch of steady state solutions numerically and found that this branch terminates as the solutions form a cusp singularity. They also considered the evolution of the instability and found that the formation of cusps is a general feature. Kassner and Misbah also numerically analyzed the nonlinear evolution of a uniaxially stressed solid.

If the film is thin, its surface approaches the film–substrate interface before the formation of cusps. The different stress fields and the different surface energies of the film and the substrate affect the surface morphology and the film–substrate interface will be prevented from being exposed when the wetting criterion is satisfied. Stranski–Krastanow wetting islands will form in this case. The steady states of island shapes were studied by Spencer and Tersoff, Kukta and Freund, Spencer and his co-workers, and many other researchers. The nonlinear evolution of the surface of thin films and the formation of islands were studied by Chiu and Gao, and by Zhang and Bower. At later stage of the nonlinear evolution of the surface, dislocations will be created for further relaxation near the cusp tips where the stress concentrates. The reader may consult Gao and Nix for a review on the theoretical and experimental studies of the surface morphological instability in heteroepitaxial films.

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The dynamics of a surface of a stressed solid can be described by a continuum model with surface diffusion driven by a stress-dependent chemical potential. This chemical potential consists of two parts: surface energy and the contribution from elasticity. The elasticity contribution to chemical potential is equal to the elastic energy density on the surface. The elasticity problem is coupled with the surface shape, and generally there is no explicit solution to this problem. To avoid solving the elasticity problem, linear approximation was sometimes used at the early stage of the instability or for small island shapes. For example, it was used by Gao to compute the stress concentration at slightly undulating surfaces, by Tersoff and LeGoues to show the existence of an activation barrier for the nucleation of steps, by Spencer to simulate the time-dependent evolution of planar surface with small perturbations. For the nonlinear approximation, Spencer et al. derived an evolution equation governing the long-wave evolution of a stressed thin film on a rigid substrate. They found steady states with rounded-cusp peaks and smooth valleys. Nonlinear evolution using their equation showed steepening of the sides adjacent to the peak and widening of the valley. Their result is only valid for stressed thin films on rigid substrates, and is different from the deep cusp-like valley and smooth peak morphology observed in the experiments and numerical simulations for thick films.

In this article, we derive a nonlinear approximation equation for the surface morphology of an infinitely thick stressed solid. The stress-dependent chemical potential is expressed explicitly as a function of the surface morphology. We show that our equation describes the formation of deep cusp-like grooves and the results obtained by our equation agree very well with those obtained by solving full elasticity problem. Our equation and that of Spencer et al. are valid, respectively, for two extreme cases of the general epitaxially stressed films.

The rest of the article is organized as follows. In Sec. II we review the evolution equation and the elasticity problem. In Sec. III, we derive our nonlinear approximation equation and make a linear instability analysis using this equation. In Sec. IV, we compare our nonlinear approximation with the exact solution for a cycloid surface obtained by Chiu and Gao, and with the linear approximation. In Sec. V, we numerically simulate the evolution of small perturbations to a planar surface and compare our results with those of Spencer and Meiron obtained by solving the full elasticity problem. In Sec. VI, we summarize our findings.

II. FORMULATION

We consider a 2-dimensional semi-infinite stressed solid. The surface of the solid is assumed to be at \( y = h(x) \). The solid lies in the region \( y < h(x) \). The solid changes its surface morphology by mass transport via surface diffusion under the influence of a chemical potential. The chemical potential consists of two parts: surface energy and the contribution from elasticity. The evolution equation and the elasticity problem can be found, for example, in 1, 4, 6, 19, 22, 37. We use a formulation similar to that in 22.

The evolution equation can be written as

\[
\frac{\partial h}{\partial t} = D \frac{\partial}{\partial x} \left[ (1 + h^2)^{-1/2} \frac{\partial}{\partial x} \left( \mathcal{E} + \gamma \kappa \right) \right],
\]

where \( D \) is the diffusion constant, \( \gamma \) is the surface free energy density, \( \kappa \) is the surface curvature, and \( \mathcal{E} \) is the elastic energy density on the surface.

The stress and strain in the solid are described by isotropic linear elasticity. Plane strain is used for the 2-dimensional problem. The stress \( \{\sigma_{ij}\} \) is related to the strain \( \{\varepsilon_{ij}\} \) by the constitutive equations

\[
\sigma_{11} = \frac{E}{1 + \nu} \left( \varepsilon_{11} + \frac{\nu}{1 - 2\nu} (\varepsilon_{11} + \varepsilon_{22}) \right),
\]

\[
\sigma_{22} = \frac{E}{1 + \nu} \left( \varepsilon_{22} + \frac{\nu}{1 - 2\nu} (\varepsilon_{11} + \varepsilon_{22}) \right),
\]

\[
\sigma_{12} = \frac{E}{1 + \nu} \varepsilon_{12},
\]

\[
\sigma_{21} = \frac{E}{1 + \nu} \varepsilon_{21},
\]

where \( E \) is the Young modulus and \( \nu \) is the Poisson ratio. The stress tensor satisfies the equilibrium equations

\[
\frac{\partial \sigma_{11}}{\partial x} + \frac{\partial \sigma_{12}}{\partial y} = 0,
\]

\[
\frac{\partial \sigma_{21}}{\partial x} + \frac{\partial \sigma_{22}}{\partial y} = 0.
\]

On the surface \( y = h(x) \), we have the traction-free boundary condition

\[
\sigma_{11} n_1 + \sigma_{12} n_2 = 0,
\]

\[
\sigma_{21} n_1 + \sigma_{22} n_2 = 0,
\]

where \( (n_1, n_2) \) is the outward normal direction on the surface.

The outward normal vector on the film surface has the expression

\[
(n_1, n_2) = \left( -\frac{h_x}{\sqrt{1 + h_x^2}}, \frac{1}{\sqrt{1 + h_x^2}} \right).
\]

Therefore, the boundary condition on the surface can be written as

\[
-\sigma_{11} h_x + \sigma_{12} = 0,
\]

\[
-\sigma_{21} h_x + \sigma_{22} = 0.
\]

At infinity, we have

\[
\{\sigma_{ij}\} \rightarrow \begin{pmatrix} \sigma_0 & 0 \\ 0 & 0 \end{pmatrix} \text{ as } y \rightarrow -\infty,
\]

where constant \( \sigma_0 \) is the imposed uniaxial stress in the solid.
The elastic energy density is given by
\[\mathcal{E} = \frac{1}{2}\mathcal{E} = \frac{1}{2}\sigma_{11}\epsilon_{11} + \frac{1}{2}\sigma_{22}\epsilon_{22} + \sigma_{12}\epsilon_{12}. \tag{8}\]

Using the constitutive equations (2) and the boundary condition (6), the expression of the elastic energy density on the surface can be simplified as
\[\mathcal{E} = \frac{1 - \nu^2}{2E}(\sigma_{11} + \sigma_{22})^2. \tag{9}\]

Now we define a new stress tensor \(\tilde{\sigma}_{ij}\) and a new strain tensor \(\tilde{\epsilon}_{ij}\):
\[\tilde{\sigma}_{11} = \sigma_{11} - \sigma_0, \quad \tilde{\sigma}_{22} = \sigma_{22}, \ \tilde{\sigma}_{12} = \sigma_{12}, \quad \tilde{\sigma}_{21} = \sigma_{21}, \tag{10}\]
and
\[\tilde{\epsilon}_{11} = \epsilon_{11} - \frac{1 - \nu^2}{E}\sigma_0, \quad \tilde{\epsilon}_{22} = \epsilon_{22} + \frac{\nu(1 + \nu)}{E}\sigma_0, \tag{11}\]
\[\tilde{\epsilon}_{12} = \epsilon_{12}, \quad \tilde{\epsilon}_{21} = \epsilon_{21}.\]

Thus, the stress \(\tilde{\sigma}_{ij}\) and the strain \(\tilde{\epsilon}_{ij}\) still satisfy the constitutive equations (2) and the equilibrium equations (3).

On the surface \(y = h(x)\), the boundary condition [Eq. (6)] becomes
\[-\tilde{\sigma}_{11}h_1 + \tilde{\sigma}_{12} = \sigma_0h_x, \quad -\tilde{\sigma}_{21}h_2 + \tilde{\sigma}_{22} = 0. \tag{12}\]
Finally, at infinity, we have the condition
\[\tilde{\sigma}_{ij} \to 0 \quad \text{as} \quad y \to -\infty. \tag{13}\]

Therefore the elasticity problem in a stressed solid with traction-free boundary condition is equivalent to an elasticity problem in the solid without imposed stress but with a force acting on the boundary.

Now the elastic energy density on the surface [Eq. (9)] becomes
\[\mathcal{E} = \frac{1 - \nu^2}{2E}(\sigma_0 + \tilde{\sigma}_{11} + \tilde{\sigma}_{22})^2. \tag{14}\]

III. DERIVATION OF A NONLINEAR EQUATION

In this section, we derive our nonlinear evolution equation for infinitely thick stressed solids. We use the solution to the elasticity problem in half plane and impose appropriate boundary conditions on the surface. We also perform a linear instability analysis.

For the elasticity problem in the half plane \(y < 0\) with boundary condition
\[\sigma_{12} = p_1, \quad \sigma_{22} = p_2 \quad \text{on the surface} \quad y = 0, \quad \text{there is an explicit solution, e.g., see Appendix N in the book by Pimpinelli and Villain,}\tag{15}\]
Taking Fourier transform in \(x\):

For the surface \(y = 0\), we have
\[u_{1}(x, y) = \sum_k \hat{u}_1(y)e^{ikx}, \quad u_{2}(x, y) = \sum_k \hat{u}_2(y)e^{ikx}, \tag{16}\]
\[p_{1}(x) = \sum_k \hat{p}_1 e^{ikx}, \quad p_{2}(x) = \sum_k \hat{p}_2 e^{ikx}, \tag{16}\]
the solution can be written as
\[\hat{u}_1 = \frac{1 + \nu}{E} \frac{1}{|k|} \left[ |k|y + 2(1 - \nu) \right] \hat{p}_1 \]
\[\quad - i \left[ ky + (1 - 2\nu) \right] \frac{k}{|k|} \hat{p}_2 e^{i|k|y}, \tag{17}\]
\[\hat{u}_2 = \frac{1 + \nu}{E} \frac{1}{|k|} \left[ |k|y - (1 - 2\nu) \right] \frac{k}{|k|} \hat{p}_1 \]
\[\quad + \left[ |k|y - 2(1 - \nu) \right] \hat{p}_2 e^{i|k|y}. \tag{17}\]

The strain and stress tensors on the surface \(y = 0\) can be written as
\[\epsilon_{11} = - \frac{2(1 - \nu^2)}{E} H(p_1) + \frac{(1 + \nu)(1 - 2\nu)}{E} p_2, \tag{18}\]
\[\epsilon_{22} = \frac{2\nu(1 + \nu)}{E} H(p_1) + \frac{(1 + \nu)(1 - 2\nu)}{E} p_2, \tag{18}\]
\[\epsilon_{12} = \epsilon_{21} = \frac{1 + \nu}{E} p_1, \tag{18}\]
and
\[\sigma_{11} = - 2H(p_1) + p_2, \tag{19}\]
\[\sigma_{22} = p_2, \tag{19}\]
\[\sigma_{12} = \sigma_{21} = p_1, \tag{19}\]
where \(H(p_1)\) is the Hilbert transform of \(p_1\)
\[H(f) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(z)}{z - \xi} d\xi. \tag{20}\]

Going back to our problem, assume the solid surface \(h(x)\) has a small deviation \(\delta h\) from a flat surface \(h_0\), without loss of generality, assume \(h_0 = 0\). Expanding the strain and stress tensors in the power of \(\delta h\), we have
\[\tilde{\epsilon}_{ij} = \epsilon_{ij}^{(1)} + \epsilon_{ij}^{(2)} + \cdots, \tag{21}\]
\[\tilde{\sigma}_{ij} = \sigma_{ij}^{(1)} + \sigma_{ij}^{(2)} + \cdots. \tag{21}\]

Keeping the leading order terms, the boundary condition on the surface [Eq. (12)] becomes
\[\sigma_{12}^{(1)} = \sigma_0 h_x, \quad \sigma_{22}^{(1)} = 0. \tag{22}\]
From the solution formula (19), on the surface, we have
\[ \sigma_{11}^{(1)} = -2\sigma_0 H(h_x). \] (23)

The energy density on the surface [Eq. (14)] becomes
\[ E_s \approx \frac{1 - \nu^2}{2E} \sigma_0^2 [1 - 2H(h_x)]^2 - \frac{1 - \nu^2}{2E} \sigma_0^2 [1 - 4H(h_x)]. \] (24)

This is the linear approximation of the elastic energy on the solid surface which was used by the authors mentioned in the introduction.

Now we compute the second order terms. The boundary condition at this order is
\[ \sigma_{11}^{(2)} = \sigma_{11}^{(1)} h_x - \frac{\partial \sigma_{12}^{(1)}}{\partial y} h, \]
\[ \sigma_{22}^{(2)} = \sigma_{22}^{(1)} h_x - \frac{\partial \sigma_{22}^{(1)}}{\partial y} h. \] (25)

Using the solution formula (17), we have on the surface
\[ \frac{\partial \sigma_{11}^{(1)}}{\partial y} = 3\sigma_0 h_{xx}, \]
\[ \frac{\partial \sigma_{22}^{(1)}}{\partial y} = -\sigma_0 h_{xx}, \] (26)
\[ \frac{\partial \sigma_{12}^{(1)}}{\partial y} = 2\sigma_0 H(h_{xx}). \]

Therefore the boundary condition becomes
\[ \sigma_{11}^{(2)} = -2\sigma_0 [hH(h_x)]_x, \]
\[ \sigma_{22}^{(2)} = \sigma_0 [hH(h_x)]_x. \] (27)

From the solution formula (19), we have on the surface
\[ \sigma_{11}^{(2)} = 4\sigma_0 H[hH(h_x)]_x + \sigma_0 (hH_{xx}). \] (28)

Keeping terms up to second order, the energy density on the surface [Eq. (14)] can be written as
\[ E_s \approx \frac{1 - \nu^2}{2E} \sigma_0^2 \left( \sigma_{11}^{(1)} + \sigma_{22}^{(1)} + 2\sigma_0 (\sigma_{11}^{(1)} + \sigma_{22}^{(1)})^2 \right. 
+ 2\sigma_0 \frac{\partial}{\partial y} \left( \sigma_{11}^{(1)} + \sigma_{22}^{(1)} \right) h_x 
\left. + 2\sigma_0 \sigma_{11}^{(2)} h + 2\sigma_0 \sigma_{22}^{(2)} \right). \] (29)

Using Eqs. (22), (23), (26), (27), and (28), we have
\[ E_s = \frac{1 - \nu^2}{2E} \sigma_0^2 \left( -4H(h_x) + 4h_x^2 + 8hh_{xx} 
+ 4H^2(h_x) + 8H[H(h_x)]_x \right). \] (30)

Therefore, omitting the O(\delta h^3) and higher order terms, the evolution equation becomes
\[ \frac{\partial h}{\partial t} = D \frac{\partial^2}{\partial x^2} \left( \frac{1 - \nu^2}{2E} \sigma_0^2 (-4H(h_x) + 4h_x^2 + 8hh_{xx} 
+ 4H^2(h_x) + 8H[H(h_x)]_x) - \gamma h_{xx} \right). \] (31)

Rescaling the length by the typical length scale
\[ l_0 = \gamma \frac{2E}{(1 - \nu^2)\sigma_0^2}, \] (32)
and the time by the typical time scale
\[ t_0 = \frac{(1 - \nu^2)\sigma_0^2}{D}, \] (33)

still using the notation x, h, and t, we have the nondimensional evolution equation
\[ \frac{\partial h}{\partial t} = \frac{\partial^2}{\partial x^2} \left( -4H(h_x) - h_{xx} + 4h_x^2 + 8hh_{xx} + 4H^2(h_x) + 8H[H(h_x)]_x \right), \] (34)

where the initial planar surface is \( h = 0 \). This is the main result of the present paper. It is valid for an infinitely thick stressed solid.

Equation (34) has a very nice variational form. It can be written as
\[ h_t = \mu_{xx}, \] (35)

where the chemical potential \( \mu \) is the variation of the total free energy of the solid:
\[ \sigma = \frac{\delta E_{\text{tot}}}{\delta h}. \] (36)

The total free energy \( E_{\text{tot}} \) is
\[ E_{\text{tot}} = E_{\text{el}} + E_{\text{surf}}, \] (37)
where \( E_{\text{el}} \) is the total elastic energy (here we use the state of the planar surface as the reference state for the energy):
\[ E_{\text{el}} = \int [-2H(h_x) + 4H^2(h_x) - 4h_x^2] dx, \] (38)
and \( E_{\text{surf}} \) is the surface free energy:
\[ E_{\text{surf}} = \int \frac{1}{2} h_x^2 dx. \] (39)

We will show in Sec. V that our Eq. (34) will result in the formation of cusplike valleys and smooth peaks for the nonlinear evolution of the surface. To see what the driving force is for the formation of this morphology, we first notice that the first term in Eq. (38) has an up-down symmetry. If we change \( h \) to \(-h\) it does not change. The second term in Eq. (38) tends to smooth the peak where \( h > 0 \) and sharpen the valley where \( h < 0 \) (note that the initial planar surface is \( h = 0 \)). The third term in Eq. (38) tends to sharpen the peak and smooth the valley. Therefore we can conclude that the second term must be the driving force for the cusp formation. The third term helps to determine the local structure of the cusp.

In Spencer et al.,\textsuperscript{17} a nonlinear approximation equation for a stressed thin film on a rigid substrate was derived. It is
\[ \frac{\partial h}{\partial t} = \frac{\partial^2}{\partial x^2} \left( \left( h - 1 \right) h_{xx} + \frac{1}{2} h_x^2 \right). \] (40)

Using our scaling and neglecting the correction to curvature in their paper, it becomes
\[ \frac{\partial h}{\partial t} = \frac{\partial^2}{\partial x^2} \left( \frac{4}{1 - \nu} \left( h - 1 \right) h_{xx} + \frac{2}{1 - \nu} h_x^2 \right). \] (41)
It also has a variational form in which the contribution from elastic energy includes only the third term in our elastic energy expression \( ~38! \) with a different coefficient \( ~2/\sim 1! \). They found steady states with rounded-cusp peaks and smooth valleys. Nonlinear evolution using their equation showed steepening of the sides adjacent to the peak and widening of the valley. Their results agree with our energy analysis.

In both our Eq. (34) and theirs [Eq. (41)], the linear term \( h_{xx} \) in the chemical potential comes from the surface energy, other terms are the contribution from elasticity. Our equation has nonlocal terms representing the effect of the stressed semi-infinite solid, while their equation has an \( h h_{xx} \) term representing the effect of the stressed thin film on a rigid substrate. Notice that in our equation, \( h \) is the relative position of the solid surface from its average value, and in their equation, \( h \) is the height of the film. Our equation and theirs are valid, respectively, for two extreme cases of the general epitaxially stressed films.

Now we perform a linear analysis using our equation. Assume the planar surface has a small perturbation

\[ h = \varepsilon e^{ik_0 x + \omega t}, \]

where \( \varepsilon \) is very small. Here without loss of generality, we assume \( k_0 > 0 \).

Insert this expression of \( h \) into our Eq. (34), keeping the leading order terms of \( \varepsilon \), we obtain the dispersion relation

\[ \omega = 4k_0^2 - k_0^4. \]

Therefore the planar surface is unstable when

\[ k_0 < 4. \]

The most unstable mode which has the fastest growth rate is

\[ k_0 = 3. \]
In its original units, the planar surface is unstable when the wavelength satisfies
\[ \lambda > \lambda_{cr} = \frac{\pi E \gamma}{(1 - \nu^2) \sigma_0}, \] (46)
and the most unstable wavelength is
\[ \lambda_m = \frac{4 \pi E \gamma}{3(1 - \nu^2) \sigma_0^{\frac{3}{2}}}. \] (47)

This linear instability result is the same as the well-known Asaro–Tiller–Grinfeld linear instability result.

**IV. COMPARISON WITH EXACT SOLUTION FOR CYCLOID SURFACE**

In this section, we compare our nonlinear elastic energy density on the surface with the linear approximation and the exact solution for the cycloid surfaces which was found by Chiu and Gao.21

For cycloid surface
\[ x = \theta + \alpha \sin \theta, \quad h = \alpha \cos \theta, \] (48)
where \(0 < \theta < 2\pi\) and \(\alpha \leq 1\), Chiu and Gao found that the elastic energy density on the surface for a stressed solid is (after rescaling)
\[ \left( \frac{1 - \alpha^2}{1 + 2 \alpha \cos \theta + \alpha^2} \right)^2. \] (49)

Our nonlinear approximation is
\[ 1 - 4H(h_x) + 4h_x^2 + 8hh_{xx} + 4H^2(h_x) + 8H[hH(h_x)_x]. \] (50)
The linear approximation is
\[ 1 - 4H(h_x). \] (51)

Before the comparison, we plot some cycloid surfaces in Fig. 1. For \(\alpha = 1\), the surface has a cusp singularity and the elastic energy density on the surface is Dirac singular at the cusp tip.

The comparison of the energy density of the exact solution, linear approximation, and nonlinear approximation are shown in Fig. 2. For a very small \(\alpha = 0.02\), both the linear and the nonlinear approximation match the exact solution very well. For \(\alpha = 0.1\), there is a small difference between the linear approximation and the exact solution, the nonlinear approximation still match the exact solution very well. For \(\alpha = 0.3\), the difference between the linear approximation and the exact solution is large, the nonlinear approximation is still good. For \(\alpha = 0.5\), the difference between the linear approximation and the exact solution is even larger, but the nonlinear approximation is still acceptable.

We also compare the errors in the second derivative of the elastic energy density, which describes the dynamics of the surface, using linear approximation and nonlinear approximation. We plot the maximum relative errors in Fig. 3. For example, if we want the error to be less than 20%, the maximal \(\alpha\) we can choose is \(\alpha = 0.055\) (max curvature \(= 0.06\)) in the linear approximation and is \(\alpha = 0.245\) (max curvature = 0.43) in the nonlinear approximation. When \(\alpha = 0.5\) (max curvature = 2), the errors are large in both the linear and nonlinear approximation, but the nonlinear approximation still provides a good qualitative agreement with the exact solution (see Fig. 4). Thus, our nonlinear energy density has a much wider range of applicability than the linear approximation.

**V. NONLINEAR EVOLUTION USING OUR EQUATION**

The fully nonlinear evolution of small perturbations of the flat surface of a stressed solid was first studied by Yang...
and Srolovitz\textsuperscript{19,20} and later by Spencer and Meiron.\textsuperscript{22} They showed that the evolution of the small perturbations will result in the formation of cusps and they solved the full elasticity problem numerically. However, their results are slightly different: Yang and Srolovitz found formation of small bumps adjacent to the deep groove; Spencer and Meiron found a branch of steady states. This is because they chose different amplitudes of the initial perturbations. Though both of them used small initial perturbations to a flat surface, the amplitude of the perturbations used by Y and and Srolovitz is larger than that used by Spencer and Meiron.

In this section, we simulate the nonlinear evolution of small perturbations of the flat surface of a stressed solid using our nonlinear equation (34). We use the initial perturbations used by Spencer and Meiron and compare our results with theirs. The scale we use for our equation is the same as the scale they used.

We use pseudospectral method in our computation. Let

\[ h(x) = \sum_{k=1}^{N_0} C_k \cos kx, \]  

the equation becomes

\[ \frac{\partial C_k}{\partial t} = \lambda_k C_k - k^2 f_k, \]  

where

\[ \lambda_k = 4k^3 - k^4, \]  

and

\[ f_k = 4h_k^2 + 8hh_{xx} + 4H(h_k) + \frac{1}{2} H[H(h_k)], \]

\[ = \sum_{k=1}^{N_0} f_k \cos kx. \]  

We use trapezoidal rule for the time discretization for the linear part and compute the nonlinear part explicitly, the numerical scheme is

\[ \frac{C_k^{n+1} - C_k^n}{\Delta t} = \lambda_k C_k^{n+1} + C_k^n - k^2 \left( \frac{3}{2} f_k^n - \frac{1}{2} f_k^{n-1} \right), \]  

where \( f_k^{n+1} = f_k^0 \).

As in Spencer and Meiron’s paper,\textsuperscript{22} we choose \( N_0 \) large enough to make sure the contribution from high Fourier modes is

\[ \left( \sum_{N_0/2 < k < N_0} |C_k|^2 \right)^{1/2} < 10^{-3}. \]  

If it becomes larger than \( 10^{-3} \), we increase the number of Fourier modes \( N_0 \) and decrease the time step to keep \( \Delta t/N_0^{-4} \) constant. In our numerical examples, we choose \( N_0 = 50 \sim 100 \).

Initially, we use the same small perturbations as those used by Spencer and Meiron,\textsuperscript{22}

\[ h(x,0) = \frac{\sqrt{2}}{100} \cos k_0 x, \]  

where \( k_0 = 0.3, 1.5, 3, 3.8, \) and 5.

The simulation results are shown in Figs. 5 and 6. Fig. 5 shows the evolution of amplitude of the surface for various \( k_0 \). The amplitude, which has been used by Spencer and Meiron,\textsuperscript{22} is defined by

\[ A = \sqrt{\frac{k_0}{2\pi}} \int_0^{2\pi/k_0} h^2(x) dx. \]  

Initially \( A = 0.01 \). Fig. 6 shows the evolution of small perturbations of flat surface with those unstable wave numbers \( k_0 = 0.3, 1.5, 3, 3.8 \). From these pictures, we can see that at the early stage, the surface growth obeys the linear theory. For perturbations with wave number \( k_0 < 4 \), the perturbations increase and gradually the most unstable mode \( k_0 = 3 \) dominates. For perturbations with wave number \( k_0 > 4 \), the perturbations decay and finally the surface goes back to the initial flat surface. For the unstable case \( k_0 < 4 \), at the later stage where the nonlinear theory applies, the surface evolves to a cusplike morphology.

These results are very similar to those of Spencer and Meiron,\textsuperscript{22} except that in their results, there is a band of wave numbers \( k_0^2 < k_0 < 4 \) (\( k_0 = 3.8 \) is in that band) in which the perturbations evolve to steady states. In our model, there is no steady state solution for the unstable wave numbers \( k_0 < 4 \), and all small perturbations evolve to cusps. However, there exists a branch of steady states for the stable wave numbers \( k_0 > 4 \) with higher energy than that of a flat surface (see Fig. 7).
As did Spencer and Meiron\textsuperscript{22} and Yang and Srolovitz,\textsuperscript{20} we monitor the minimum curvature radius to estimate when the cusp singularity forms. The value of the curvature radius is computed after rescaling in $x$ such that one period is $2\pi$ as in Fig. 6. For the most unstable mode $k_0 = 3$, the evolution of minimum curvature radius is shown in Fig. 8, the cusp forms when $t \approx 0.063$. In Spencer and Meiron’s paper,\textsuperscript{22} this time is $t \approx 0.073$. In our numerical simulations, we compute the evolution of surface until the minimum radius of curvature is of order $10^{-2}$.

FIG. 6. Evolution of small perturbations of flat surface. (a) Initially the wave number of the perturbation is $k_0 = 0.38$. The surface is plotted at time increments of 0.014325 until $t=0.1146$. The last one is $t=0.1149$. (b) Perturbation wave number $k_0 = 3$, time increments 0.0074 until $t=0.0592$, the last one is $t=0.06297$. (c) Perturbation wave number $k_0 = 1.5$, time increments 0.0148 until $t=0.1184$, the last one is $t=0.1282$. (d) Perturbation wave number $k_0 = 0.3$, time increments 0.1852 until $t=1.2964$, the last one is $t=1.4594$. In case (d), initially the growth rate is very small. After the most unstable mode $k_0 = 3$ is invoked, it grows very fast.

FIG. 7. (a) Branch of the steady states (extending to $k_0 = \infty$). (b) Steady-state solutions. $k_0 = \infty$ corresponds to the case when the linear term involving Hilbert transform is deleted from the equation.
VI. SUMMARY

We derived a nonlinear evolution equation for stress-driven morphological instability via surface diffusion in two-dimensional stressed solids in the absence of deposition. We obtained a nonlinear approximation for the elastic energy density along the surface, which serves as the chemical potential due to elasticity for surface diffusion, and which was either computed numerically or approximated by a linear function of small perturbation in the literature. Linear instability analysis using our equation shows the same result as the well-known Asaro–Tiller–Grinfeld instability result. Compared with the exact elastic energy density expression for cycloid surface obtained by Chiu and Gao, our nonlinear approximation has a wider range of applicability than that of a flat surface. Our nonlinear evolution equation can be used for further analysis of the formation of cusps. Our nonlinear approximation can also be used to analyze or compute other interesting physical phenomena such as the formation of equilibrium islands or the nucleation of dislocations, combined with other mechanisms.

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FIG. 8. Evolution of minimum radius of curvature $R$ for the most unstable mode $k_0 = 3$. 