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Rippling instability on surfaces of stressed crystalline conductors

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We report a surface morphological stability analysis for stressed, conducting crystalline solids without and with the simultaneous application of an electric field based on self-consistent dynamical simulations according to a fully nonlinear model. The analysis reveals that in addition to a cracklike surface instability, a very-long-wavelength instability may be triggered that leads to the formation of secondary ripples on the surface morphology. We demonstrate that the number of ripples formed scales linearly with the wavelength of the initial perturbation from the planar surface morphology and that a sufficiently strong electric field inhibits both the cracklike and the rippling instability.

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Morphological instabilities on surfaces of stressed solids and the resulting pattern formation are of major fundamental and technological significance toward improving materials function and reliability and developing innovative directed assembly processes for nanotechnology. Such a well-known phenomenon is the Asaro–Tiller–Grinfeld (ATG) instability,^{1–3} which leads to the formation of a regular pattern of cracklike grooves emanating from the surface of a stressed elastic solid and deepening by surface diffusion.^{4,5} Recently, we carried out an analysis of morphological stability of stressed solid surfaces under the simultaneous action of an electric field and reported that surface electromigration through the action of a sufficiently strong electric field can be utilized to inhibit the stress-induced ATG instability and prevent surface cracking;^{6,7} a linear stability theory⁶ predicted fairly accurately the current-induced stabilization of surface morphology in stressed elastic solids. However, complex aspects of surface morphological evolution and pattern formation, not accounted for by linear theory, still remain elusive.

The purpose of this letter is to analyze the surface morphological response of stressed solids both in the absence and under the simultaneous action of an electric field, focusing on response of planar surfaces to low-amplitude perturbations of very long wavelengths. Using self-consistent dynamical simulations according to a fully nonlinear model of surface morphological evolution, in conjunction with linear stability theory, we analyze the surface morphological stability of stressed crystalline conductors, such as the face-centered-cubic metals Al and Cu. We find that in addition to the ATG instability, a long-wavelength tip-splitting instability may be triggered forming a pattern of secondary ripples on the surface; rippling occurs in the absence of electric field application, as well as for weaker-than-critical applied electric fields. We characterize the rippled surface patterns as a function of the shape perturbation wavelength and we show that the surface can be stabilized against both ATG and rippling instabilities by application of a stronger-than-critical electric field.

Our morphological stability analysis for planar surfaces of stressed, electrically conducting solids under the simultaneous action of an electric field follows a fully nonlinear continuum model of surface mass transport.⁸ We consider a semi-infinite, single crystalline, conducting solid bounded by a planar surface ($y=0$) under a uniform uniaxial stress and an electric field of magnitudes σ_∞ and E_∞ , respectively, both along the x -direction in a Cartesian frame of reference.^{6,7} We parameterize the surface morphology according to the height function $y=h(x,t)$. An important element of our model is the anisotropy of surface diffusivity through the inhomogeneity $D_s=D_s(\theta)=D_{s,\min}f(\theta)$, where $D_{s,\min}$ is the minimum surface diffusivity and $f(\theta)\geq 1$ with $\theta=\tan^{-1}(\partial h/\partial x)$ is a properly parameterized anisotropy function.

The linear stability analysis of Ref. 6 yields the dispersion relation

$$\omega(\tilde{k}) = - \left(\frac{df}{d\theta} \bigg|_{\theta=0} \right) \Xi \tilde{k}^2 + 2f(\theta=0)\tilde{k}^3 - f(\theta=0)\tilde{k}^4, \quad (1)$$

where $\omega(\tilde{k})$ is the dimensionless frequency characteristic of the growth or decay of the initial perturbation from the planar morphology, with $\tilde{k}\equiv kl$, $l\equiv \gamma M/\sigma_\infty^2$, being the corresponding dimensionless wave number of a low-amplitude sinusoidal perturbation, and $\Xi\equiv E_\infty q_s^* l^2/(\gamma\Omega)$ is a dimensionless parameter that expresses the relative strength of the two externally applied forces;⁶ in the above equations, q_s^* is the surface effective charge, γ is the surface free energy per unit area, Ω is the atomic volume, and M is the elastic modulus. $\omega(\tilde{k})$ exhibits two maxima: at $\tilde{k}=0$ and at $\tilde{k}_{\max}=3/4+\{9-8\Xi(df/d\theta)_{\theta=0}/f(0)\}^{1/2}/4$. For $\Xi>\Xi_c$, $\omega(\tilde{k})<0$ for every $\tilde{k}>0$; $\Xi_c=f(0)/(df/d\theta)_{\theta=0}$. For $0<\Xi<\Xi_c$, the range of unstable wave numbers is $R(\Xi)\equiv\tilde{k}_{2,c}-\tilde{k}_{1,c}=2[1-\Xi(df/d\theta)_{\theta=0}/f(0)]^{1/2}$ with $\tilde{k}_{1,c}$ and $\tilde{k}_{2,c}$ being the roots of $\omega(\tilde{k})=0$ for $\tilde{k}>0$ and $\omega(\tilde{k})>0$ for $\tilde{k}_{1,c}<\tilde{k}<\tilde{k}_{2,c}$.

Figure 1(a) shows results of the linear stability analysis (plots of dispersion relations) for $f(\theta)=1+A\cos^2[m(\theta+\phi)]$. The dimensionless parameters A and ϕ determine the anisotropy strength and the misorientation angle of a fast surface diffusion direction with respect to the applied electric field direction, respectively, and the integer parameter m is a symmetry parameter due to surface crystallographic

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FIG. 1. (Color online) (a) Dispersion relations showing the dependence of the dimensionless frequency, $\omega(\tilde{k})$, characteristic of the growth ($\omega > 0$) or decay ($\omega < 0$) rate of a shape perturbation from the planar surface morphology, on the dimensionless shape perturbation wave number, $\tilde{k}$, for $\Xi=0$, $\Xi=0.16 < \Xi_c$, and $\Xi=0.35 > \Xi_c$ with anisotropy parameters $A=12$, $m=3$, and $\phi=-15^\circ$, for which $\Xi_c=0.194$. Insets (1) and (2) show the evolution of surface morphologies for initial conditions represented by points A [$\Xi=0.16$ for $\tilde{k}=0.60$ ($\tilde{k}_{1,c} < \tilde{k} < \tilde{k}_{c,r}$) and $\tilde{\Delta}_0/\tilde{\lambda}=0.01$] and B [$\Xi=0.35$ ($\Xi > \Xi_c$) for $\tilde{k}=0.35$ and $\tilde{\Delta}_0/\tilde{\lambda}=0.01$]. The two vertical arrows mark the onset of the rippling instability, $\tilde{k}=\tilde{k}_{c,r}$, for the two cases. [(b) and (c)] Surface morphological evolution, $\tilde{h}(\tilde{x}, \tilde{t})$, starting from a sinusoidal perturbation from a planar surface morphology, $\tilde{h}(\tilde{x}, 0)=\tilde{\Delta}_0 \sin(\tilde{k}\tilde{x})$, at (b) $\Xi=0.0$ for $\tilde{k}=0.15$ ($\tilde{k} < \tilde{k}_{c,r}$) and $\tilde{\Delta}_0/\tilde{\lambda}=0.02$; and (c) $\Xi=0.16$ for $\tilde{k}=0.20$ ($\tilde{k} < \tilde{k}_{1,c}$) and $\tilde{\Delta}_0/\tilde{\lambda}=0.01$. The anisotropy parameters are the same with those that yielded the dispersion curves in (a). The evolution sequences are from the bottom to the top, the electric field is applied from right to left, and the stress is tensile and applied uniaxially parallel to the nominally flat surface (along x); $\tilde{t} \equiv t/\tau$ with $\tau \equiv k_B T^4 / (D_{s,min} \gamma \Omega)$. [(d) and (e)] Evolution of the perturbation amplitude, $\tilde{\Delta}(\tilde{t})$, (d) for case (b) and (e) for the cases in inset (1) of (a) and in (c); the solid lines and the symbols represent simulation results and results of linear stability theory [$\tilde{\Delta}(\tilde{t}) = \tilde{\Delta}_0 \exp(\omega \tilde{t})$], respectively.

orientation.⁶⁻⁹ For $\Xi=0$, i.e., for finite stress σ_∞ in the absence of electric field, $\omega(\tilde{k})$ is positive for all $\tilde{k} < \tilde{k}_c$, i.e., the planar surface is unstable for all perturbations with wavelength $\tilde{\lambda} > \tilde{\lambda}_c \equiv 2\pi/\tilde{k}_c$; $\tilde{\lambda} \equiv \lambda/l$. For a given parameter set, A , m , and ϕ , $R(\Xi)$ decreases as Ξ increases from 0 to Ξ_c , i.e., as E_∞ is increased from zero to some critical value. For $\Xi > \Xi_c$, R vanishes, i.e., $\omega(\tilde{k}) < 0$ for all $\tilde{k}$; therefore, a

stronger-than-critical E_∞ stabilizes fully the morphological response of a stressed solid at given σ_∞ .

For a comprehensive investigation of the morphological stability of planar surfaces within the fully nonlinear model, we carried out systematically self-consistent dynamical simulations of surface morphological evolution guided by the results of the linear stability theory, such as those of Fig. 1(a). Our computational approach combines a Galerkin boundary-integral method with a front tracking method and has been described in detail in Refs. 6–9. In our numerical simulations, we start with a low-amplitude sinusoidal morphology, $\tilde{h}(\tilde{x}, 0) = \tilde{\Delta}_0 \sin(\tilde{k}\tilde{x})$ with $\tilde{\Delta}_0 \ll 1$, and monitor the surface morphological evolution for a given set of parameters, Ξ , A , m , and ϕ , over a broad region of parameter space; the tildes are used to denote dimensionless quantities, where lengths are made dimensionless with the length scale l , i.e., $\tilde{h} \equiv h/l$, etc. Our numerical simulations have revealed a surface morphological instability that is not predicted by the linear stability theory. This is a very long-wavelength rippling instability that leads to the formation of a pattern of secondary ripples in the surface morphology.

This long- $\tilde{\lambda}$ rippling instability occurs both without and with the simultaneous application of the electric field (i.e., both for $\Xi=0$ and for $0 < \Xi < \Xi_c$). Figure 1(b) shows such a rippling instability for $\Xi=0$ with the corresponding amplitude evolution, $\tilde{\Delta}(\tilde{t})$, shown in Fig. 1(d): a pattern of secondary ripples forms on top of the regular pattern of surface grooves, which form due to the ATG instability. A comparison of the simulation results with those of linear stability theory in Fig. 1(d) shows close agreement between theory and simulation until the initiation of the secondary (tip-splitting) instability that facilitates the ripple formation; beyond such tip splitting, the introduction of additional wavelengths into the surface morphology results in subsequent faster modes in the growth of the surface shape perturbation. These faster modes accelerate the surface morphological evolution toward surface cracking compared to the rates due to the ATG instability in the absence of rippling. Our simulations, over a broad range of parameters (A , m , ϕ , and $\tilde{k}$) for $\Xi < \Xi_c$, indicate that the rippling instability is triggered as a result of long-wavelength perturbations beyond a critical wavelength $\tilde{\lambda}_{c,r}$, i.e., $\tilde{\lambda} > \tilde{\lambda}_{c,r}$ corresponding to $0 < \tilde{k} < \tilde{k}_{c,r} \equiv 2\pi/\tilde{\lambda}_{c,r}$. Numerically computed critical wave numbers, $\tilde{k}_{c,r}$, for the onset of the rippling instability are marked by the two vertical arrows in Fig. 1(a) (for $\Xi=0$ and for $\Xi=0.16 < \Xi_c$). For the parameter range examined, we find consistently that $\tilde{k}_{1,c} < \tilde{k}_{c,r}$.

The general picture that emerges from these findings, in conjunction with the results of Ref. 6, determines the surface morphological response as a function of initial shape perturbation wavelength and defines, in general, four regions over the spectrum of wave numbers: (1) stable response for $\tilde{k} > \tilde{k}_{2,c}$ at $0 < \Xi < \Xi_c$ (or $\tilde{k} > \tilde{k}_c$ at $\Xi=0$), (2) only ATG instability for $\tilde{k}_{c,r} < \tilde{k} < \tilde{k}_{2,c}$ at $0 < \Xi < \Xi_c$ (or $\tilde{k}_{c,r} < \tilde{k} < \tilde{k}_c$ at $\Xi=0$), (3) coupled ATG and secondary rippling instability for $\tilde{k}_{1,c} < \tilde{k} < \tilde{k}_{c,r}$ at $0 < \Xi < \Xi_c$ (or $0 < \tilde{k} < \tilde{k}_{c,r}$ at $\Xi=0$), and (4) only rippling instability for $0 < \tilde{k} < \tilde{k}_{1,c}$ at $0 < \Xi < \Xi_c$. Representative results of surface morphological evolution in regions (3) and (4) are shown in inset (1) of Fig. 1(a) and in

Fig. 1(c), respectively, for $\Xi=0.16 < \Xi_c$ and parameters A , m , and ϕ that yielded the dispersion curves of Fig. 1; the corresponding $\tilde{\Delta}(\tilde{r})$ evolution is shown in Fig. 1(e). Inset (1) in Fig. 1(a) shows that surface grooving at the original valleys of the initial perturbed morphology (ATG instability), which leads eventually to surface cracking, occurs simultaneously with tip splitting that gives rise to secondary ripple formation. On the other hand, Fig. 1(c) shows tip splitting and ripple formation on a surface, the early morphological evolution of which (prior to ripple formation) is characterized by amplitude decay of the original perturbation; in this case, surface cracking is the outcome of a rippling instability. In any case, a strong electric field, $\Xi > \Xi_c$, inhibits both the ATG and the rippling instability for any shape perturbation wavelength. A representative result of such stable response is shown in inset (2) of Fig. 1(a) at $\Xi > \Xi_c$ and a $\tilde{k}$ that would lead to a coupled ATG and secondary rippling instability in the absence of electric field application. It should be mentioned that our numerical simulations have validated the Ξ_c predictions according to the linear stability theory, with an error in the theoretical prediction up to 5%. Using the definition of Ξ , Ohm's law, thermophysical properties representative of Al at room temperature, and tensile stresses typical of Al interconnects,⁸ a Ξ value over the range $0.16 \leq \Xi \leq 0.3$ yields a current density j over the range $1.6 \times 10^6 \text{ A/cm}^2 \leq j \leq 3.2 \times 10^6 \text{ A/cm}^2$.

Finally, we characterize the morphology of the surfaces that undergo rippling instability, regions (3) and (4), focusing on the number of ripples, N , generated per original perturbation wavelength as a function of the wavelength, $\tilde{\lambda}$. The simulation results are summarized in Fig. 2. The analysis is based on fast Fourier transform (FFT) of the surface profile as it evolves. Representative results are shown in inset (1) of Fig. 2 for a surface profile, initially and after its driven morphological evolution, and in inset (2) of Fig. 2 for the corresponding FFT-generated power spectra. Most importantly, we find that N increases linearly with the wavelength of the initial perturbation scaled with the maximally unstable wavelength, i.e., $N \sim \tilde{\lambda}/\tilde{\lambda}_{\max}$ or equivalently $N \sim \tilde{k}_{\max}/\tilde{k}$. Figure 2 shows this dependence for three different parameter sets together with a straight-line fit that confirms the linear scaling result.

In conclusion, we reported a morphological instability in stressed solids that leads to the formation of a secondary pattern of ripples on the surface. Such shorter-wavelength ripples on an initially long-wavelength perturbation of a planar solid surface can accelerate surface cracking acting cooperatively with an ATG instability or they may induce surface cracking under conditions that do not trigger ATG instabilities according to linear theory. The critical wavelength for the onset of this secondary rippling is not pre-

FIG. 2. (Color online) Number of ripples, N , per original perturbation wavelength as a function of the initial perturbation wavelength scaled with the maximally unstable wavelength, $\tilde{\lambda}/\tilde{\lambda}_{\max}$, for parameters $\Xi=0.16$, $A=12$, $m=3$, and $\phi=-15^\circ$ (circles); $\Xi=0.125$, $A=12$, $m=2$, and $\phi=-35^\circ$ ($\times$ -marks); and $\Xi=0.14$, $A=12$, $m=3$, and $\phi=-15^\circ$ (diamonds). The straight line is a least-squares fit to the simulation results. Inset (1) shows the initial (at $t=t_0=0$) and evolved (at $t=t_1$) surface morphologies. The initial conditions correspond to point C in Fig. 1(a): $\Xi=0.16 < \Xi_c$ and $\tilde{k}=0.35 < \tilde{k}_{1,c}$. Inset (2) shows the power spectra of the two surface profiles from inset (1), characterized by a single one and by three wavelengths, respectively ($N=3$).

dicted by linear theory, but it has been computed numerically; the numerical simulations also give a linear scaling with the perturbation wavelength for the characterization of the rippled surface pattern. Our analysis adds this rippling instability to the mechanisms of stress relaxation through surface pattern formation that may lead to surface cracking. Our findings contribute to a fundamental understanding toward the prevention or healing of cracks in stressed solid surfaces through simultaneous application of electric fields and motivate their testing and validation through carefully designed experimental studies.

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