Finite-time singularities in surface-diffusion instabilities are cured by plasticity

Ting-Shek Lo, Anna Pomyalov, Itamar Procaccia, and Jacques Zylberg
Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel
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A free material surface which supports surface diffusion becomes unstable when put under external nonhydrostatic stress. Since the chemical potential on a stressed surface is larger inside an indentation, small shape fluctuations develop because material preferentially diffuses out of indentations. When the bulk of the material is purely elastic one expects this instability to run into a finite-time cusp singularity. It is shown here that this singularity is cured by plastic effects in the material, turning the singular solution to a regular crack.

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We address the problem of an amorphous material with a free surface on which the material can diffuse such that the surface normal velocity is proportional to $\partial^2\mu/\partial b^2$, where μ is the local chemical potential and b is the parametrization of the interface. When the material itself is purely elastic, this phenomenon leads to an instability which was termed "thermal grooving" by Mullins [1], who discovered it. The phenomenon of grooving is equally present in crystals, where it provides an annoying mechanism for the failure of growing crystals [2,3], as it does in a range of amorphous solids that concern us here. Mullins considered the linear instability taking into account only the curvature dependence of the chemical potential. In fact, the chemical potential along the interface is strongly dependent on the elastic energy; linear stability analysis taking both effects into account [4] reveals that the surface is stable for short wavelengths but unstable for longer ones, with a usual "fastest growing mode" whose wavelength depends on the material parameters. The late stage of development of this instability was initially studied by a handful of researchers, namely Asaro and Tiller [5] and Grinfeld [6], and followed by many others [4,7–9]. The result is that the instability runs into a finite-time singularity, with the growing indentation forming a cusp. Clearly, this often explored [7,10,11] mathematical phenomenon cannot be physical, and its discovery leaves open the question of the physical mechanism that may cure the singularity.

The question of what might cure the finite-time singularity in the Asaro-Tiller-Grinfeld (ATG) instability remained dormant until recently when Brener and Spatschek proposed that inertial effect in the velocity of the moving boundary may tame the singularity [8]. These authors pointed out that without inertial effects the velocity of the tip v appears in one dimensionless combintation, i.e., vr_0^3/D, where r_0 is the radius of the tip and D the diffusion coefficient [of dimension length^4/time, and cf. Eq. (15)]. Therefore there is no mechanism to select v or r_0, and as r_0 decreases without limit, v increases without limit. Once inertial effects are taken into account the velocity appears also in the combination v/v_R where v_R is the Rayleigh wave speed. Thus a selection of both v and r_0 can happen. While clearly correct, the present authors stress that in many cases the surface diffusion is very slow, leading to small interface velocities which do not justify the incorporation of inertial terms. We focus here on such cases where the question of taming the cusp singularities remains open.

Here we propose that the generic mechanism for the taming of the ATG instability may be plastic deformation in the stressed material, especially near the putative cusp. To test and demonstrate this proposition we will employ the recently proposed theory of elastoplastic dynamics in amorphous systems [12]. To this theory, which is valid in the bulk of the material, we couple the surface diffusion, allowing the chemical potential to take its stress dependence from the elastoplastic theory. For concreteness we choose to explore this interesting physics on the inner surface of a hole which is stressed at infinity in a radial fashion. The surface diffusion modifies the shape of the slightly perturbed circular hole, leading eventually to a highly nonlinear morphology. With a sharpening interface due to the surface diffusion instability, stresses in the bulk increase rapidly, exceeding at some point in time the yield stress of the material, triggering plastic flows which are dissipated by the exertion of plastic work [12–14]. It is interesting to observe the coupling of both processes, namely surface diffusion and plasticity, as they become competitive and of opposite influence on the morphology, to a point where the finite time singularity is removed. In addition to shedding light on the late stage of the ATG instability we find that the elastoplastic theory employed here, which is sensitive to the plastic properties of matter, allows a natural understanding of this *a priori* seemingly hard problem.

The model system that we consider here is an infinite two-dimensional isotropic elastoplastic sheet with a hole in the center whose radius is $R(\theta)$. For $r(\theta)<R(\theta)$ the system is void, whereas the elastoplastic material occupies the region $r(\theta)\geqslant R(\theta)$. The boundary is traction free, meaning that on the boundary $\sigma_{ij}n_j=0$, where $\boldsymbol{\sigma}$ is the stress tensor and $\mathbf{n}$ is the unit normal vector. The equations of acceleration and continuity are exact, reading

$$\rho\frac{\mathcal{D}\mathbf{v}}{\mathcal{D}t}=\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}, \tag{1}$$

$$\frac{\mathcal{D}\rho}{\mathcal{D}t}=-\rho\,\boldsymbol{\nabla}\cdot\mathbf{v}. \tag{2}$$

Here the full material derivative $\mathcal{D}$ is defined for an arbitrary tensor $\mathbf{A}$ as

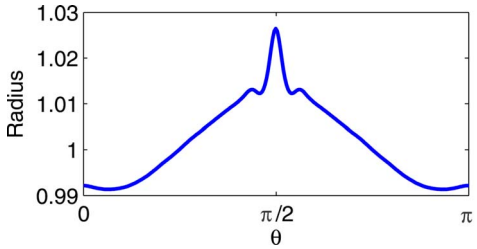

FIG. 1. (Color online) A typical half profile of the stressed interface under the action of surface diffusion and plasticity. To the bare eye the effect of plasticity is not seen here, and one needs to compare elastic and plastic solution in Figs. 2 and 3.

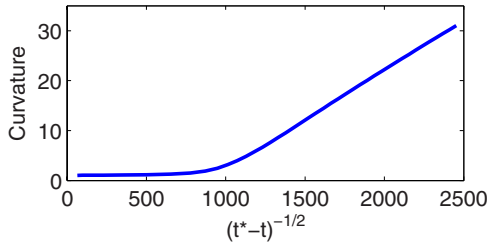

FIG. 2. (Color online) The tip curvatures of the elastic solution. This solution appears to approach a singularity at $t^*=5.37\times10^{-4}$.

$$\frac{\mathcal{D}\mathbf{A}}{\mathcal{D}t}=\partial_t\mathbf{A}+\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{A}+\mathbf{A}\cdot\boldsymbol{\omega}-\boldsymbol{\omega}\cdot\mathbf{A}, \tag{3}$$

where $\boldsymbol{\omega}$ is the spin tensor $\omega_{ij}\equiv\frac{1}{2}(\frac{\partial v_i}{\partial x_j}-\frac{\partial v_j}{\partial x_i})$. Reading Eq. (1) in radial coordinates we obtain

$$\rho\left(\frac{\partial v_r}{\partial t}+v_r\frac{\partial v_r}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_r}{\partial\theta}-\frac{v_\theta^2}{r}\right)=\frac{1}{r}\frac{\partial\tau}{\partial\theta}-\frac{1}{r^2}\frac{\partial}{\partial r}(r^2s)-\frac{\partial p}{\partial r}, \tag{4}$$

$$\rho\left(\frac{\partial v_\theta}{\partial t}+v_r\frac{\partial v_\theta}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_\theta}{\partial\theta}+\frac{v_rv_\theta}{r}\right)=\frac{\partial\tau}{\partial r}+\frac{1}{r}\frac{\partial s}{\partial\theta}-\frac{1}{r}\frac{\partial p}{\partial\theta}+\frac{2\tau}{r}. \tag{5}$$

Here s and τ are defined via the transformations

$$\sigma_{rr}=s_{rr}-p,\quad \sigma_{\theta\theta}=s_{\theta\theta}-p,\quad \sigma_{r\theta}=\tau,$$

$$s_{rr}=-s_{\theta\theta}=-s. \tag{6}$$

Note that our velocities are sufficiently small to allow neglecting the nonlinear terms $-v_\theta^2/r$ and v_rv_θ/r. On the other hand, nonlinear terms containing derivatives are retained since the derivatives are large.

The velocity at the interface $\dot{R}(\theta)$ reads

$$\frac{\partial R}{\partial t}=\frac{v_\theta}{R}\partial_\theta R+v_r. \tag{7}$$

When the surface evolves, the stresses in the bulk evolve accordingly. A fundamental assumption of our elastoplastic theory is that the total rate of deformation $\mathbf{D}^{tot}\equiv\frac{1}{2}[\boldsymbol{\nabla}\mathbf{v}+(\boldsymbol{\nabla}\mathbf{v})^\dagger]$ can be represented as a linear combination of its elastic and plastic components [14],

$$\mathbf{D}^{tot}\equiv\mathbf{D}^{el}+\mathbf{D}^{pl}. \tag{8}$$

Here the elastic contribution $\mathbf{D}^{el}$ is assumed to be linearly dependent on the stress (linear elasticity),

$$D_{ij}^{el}\equiv\frac{\mathcal{D}\epsilon_{ij}}{\mathcal{D}t},\quad \epsilon_{ij}=-\frac{p\delta_{ij}}{2K}+\frac{s_{ij}}{2\mu}, \tag{9}$$

where K and μ are the two-dimensional bulk and shear moduli and p and s_{ij} are the pressure and the deviatoric stress tensor, respectively. The plastic rate of deformation, $\mathbf{D}^{pl}$, is determined by a set of internal fields which are discussed at length in [12] where the elastoplastic theory is presented in detail. For the purpose of this Brief Report it is enough to state that the tensorial field $\mathbf{m}$ acts as a "back stress" due to plastic deformations, and the scalar field χ is the effective temperature that controls the amount of configurational disorder in the elastoplastic materials. The constitutive relations that were derived for these fields read

$$D_{ij}^{pl}=e^{-1/\chi}\mathcal{C}(\tilde{s})\left(\frac{s_{ij}}{\tilde{s}}-m_{ij}\right), \tag{10}$$

$$\mathcal{D}m_{ij}/\mathcal{D}t=2e^{1/\chi}D_{ij}^{pl}-\Gamma(s_{ij},m_{ij})m_{ij}, \tag{11}$$

$$\mathcal{D}\chi/\mathcal{D}t=e^{-1/\chi}\Gamma(s_{ij},m_{ij})(\chi_\infty-\chi), \tag{12}$$

$$\Gamma(s_{ij},m_{ij})=s_{ij}D_{ij}^{pl}/e^{-1/\chi}, \tag{13}$$

$$\mathcal{C}(\tilde{s})=\frac{e^{-\tilde{s}}(2+\tilde{s})+\tilde{s}-2}{1+e^{-6(\tilde{s}-1.5)}}. \tag{14}$$

In these equations all the stresses were normalized by the yield stress of the material s_y, using $\tilde{s}=\sqrt{s_{ij}s_{ij}/2s_y^2}$. The function $\mathcal{C}(\tilde{s})$ has been chosen to make the material relatively brittle.

To this theory we need to couple now the surface diffusion, expressed in terms of the normal velocity, $v_n(\theta)$, on the boundary. Without the effects of elastoplasticity in the bulk the normal velocity satisfies

$$v_n=-\frac{D_s\Omega^2\delta}{k_BT}\frac{\partial^2\mu}{\partial b^2}, \tag{15}$$

where D_s is the surface diffusion constant, Ω the particle volume, and δ the number of particles per unit area. In solving the coupled problem the total normal velocity should be computed as a *sum* of this contribution and the one coming from Eqs. (4) and (5).

The chemical potential on the boundary, $\mu(\theta)$, is associated on the one hand with the destabilizing curvature and on the other hand with the stabilizing surface energy [3]

$$\mu=\mu_0-\gamma\kappa+\mathcal{E}. \tag{16}$$

Here μ_0 is the chemical potential of the unperturbed surface, the curvature $\kappa(\theta)=(R^2+2R'^2-RR'')/(R^2+R'^2)^{3/2}$, and the strain energy density $\mathcal{E}=\frac{1}{2}\sigma_{ij}\epsilon_{ij}$ [15]. γ is the surface energy.

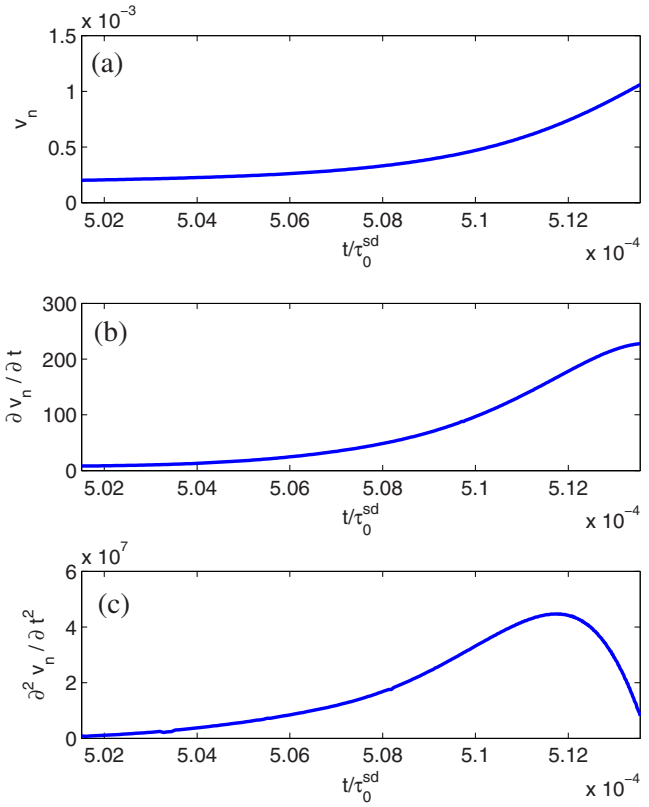

FIG. 3. (Color online) The tip velocity (a) and its first and second time derivatives [(b) and (c), respectively]. We see that the singularity is cured and the velocity decelerates due to the plastic effects.

In terms of these effects on the chemical potential one derives the equation for the normal velocity due to surface diffusion alone,

$$v_n = -\frac{D_s \Omega^2 \delta}{k_B T} \frac{\partial^2 \mu}{\partial b^2} \left[[-\gamma \kappa(\theta)] + \left(\frac{(1-\nu^2)}{2E} \sigma_{ij}^2(\theta) \right) \right], \tag{17}$$

where ν is the Poisson ratio and E Young's modulus. After nondimensionalization and projecting from v_n to v_r, one ends up with the following equation in terms of dimensionless quantities (denoted with the tilde):

$$\tilde{v}_r = -\partial_\theta \frac{1}{\sqrt{\tilde{R}^2 + \tilde{R}'^2}} \partial_\theta \left(-\tilde{\kappa}(\theta) + \frac{(1-\nu^2)}{2} \tilde{\sigma}_{ij}^2(\theta) \right). \tag{18}$$

As noted, we need to couple Eqs. (4), (5), and (18) to be solved together, such that the surface normal velocity is made from the sum of contributions coming from the bulk dynamics and the surface dynamics, respectively. This should be done while keeping the traction-free boundary conditions and the initial condition of a pure elastic solution of a slightly perturbed circle. In practice we used the fact that the elastic response is the fastest process in this problem. Accordingly, we solved first at each iteration the elastic part of the model (with $\mathbf{D}^{pl}=0$) to find the stress fields which are in agreement with the given interface, without taking into account any plastic deformation. Second, elastoplastic relaxation was allowed to take place, until the system reached elastoplastic equilibrium, allowing the interface to change. Here "equilibrium" means that $\mathbf{D}^{pl}$ is smaller than 10^{-4}. Lastly, a step of surface diffusion was allowed to take place using an adaptive time step such as to bound the maximal movement of the boundary by 10^{-4}. The last step changes the morphology of the boundary again, necessitating a recalculation of the elastic fields around the new boundary, etc. Since the effect on the velocity of the interface in the last two steps is additive, these steps (being infintesimal) also could be done simultaneously with impunity. We chose to separate the last two steps since the plastic and surface diffusion processes are nondimensionalized independently and have different normalization values of characteristic times and stresses.

In order to realize an infinite sheet it is convenient to transform the (r,θ) coordinate system through a conformal transformation to a finite domain (ζ,θ) with $\zeta \in [0,1]$,

$$\zeta(\theta) = R(\theta,t)/r. \tag{19}$$

In the finite space all the derivatives are redefined using the chain rule $\partial_{x_i} = \partial_{x_i} x_k \partial_{x_k}$. Explicitly

$$\frac{\partial}{\partial r} \to -\frac{\zeta^2}{R}\frac{\partial}{\partial \zeta}, \quad \frac{\partial}{\partial \theta} \to \frac{R'}{R}\zeta\frac{\partial}{\partial \zeta} + \frac{\partial}{\partial \theta}, \quad \frac{\partial}{\partial t} \to \frac{\dot{R}}{R}\zeta\frac{\partial}{\partial \zeta} + \frac{\partial}{\partial t}. \tag{20}$$

At $\zeta=0$ all the derivatives vanish and on the boundary $\zeta=1$ the time derivatives are estimated by linear extrapolation in the ζ direction. For the sake of numerical stability small viscosity terms were added to the acceleration components. The coupled equations were solved using $K=100$ and $\mu=50$. Since the speed of sound is orders of magnitude larger than the velocity of the interface, we could safely neglect the effects of Eq. (2), giving up on seeing the sound waves. The initial condition on the perturbed circle were

$$R(t=0,\theta) = 1 + 0.01\cos 2\theta, \tag{21}$$

the stress at infinity was chosen to be $\sigma_\infty = 0.9 s_y$. The Poisson ratio ν in Eq. (18) is 1/3. The surface diffusion equations contain fourth-order derivatives, calling for spectral techniques for sufficiently stable evaluation. All the other derivatives were computed by finite differences.

The typical morphology of the unstable interface is shown in Fig. 1. The elastic solution for the finite-time singularity is well established and was reproduced in our numerics. The curvature κ in the growing cusp first grows exponentially and rapidly switches to a faster regime that agrees with the growth law

$$\kappa(t) \propto (t^* - t)^{-1/2}. \tag{22}$$

To make this growth obvious we plotted the curvature of the elastic solution in Fig. 2 as a function of $(t^*-t)^{-1/2}$ with $t^* = 5.37 \times 10^{-4}$. Once plasticity is allowed to intervene, it prevents the finite-time singularity by blunting the tip and by dissipating the stress.

On the boundary, the smoothening of the interface in the vicinity of the cusp via blunting is the "cure" of the singu-

larity. The ever-increasing curvature occurring in the elastic solution is prevented in the plastic solution by the plastic flow induced by stress concentration. The avoidance of the singularity is shown by the deceleration in the tip velocity, see Figs. 3(b) and 3(c).

It is important to stress that although the plasticity in the bulk succeeds to cure the finite-time cusp singularity, the role of surface diffusion is far from being negligible. Without it, the stressed circle would remain stable to small shape fluctuations, as was demonstrated recently in [16]. The surface diffusion makes the circle unstable, and the instability results in the growth of a groove. Without plasticity in the bulk the solution loses its meaning at $t=t^*$, whereas now, with plasticity playing its useful role, the solutions continue to exist at times $t>t^*$, in a form of a lengthening groove, or crack, whose tip is protected from cusping by the plastic effects. At some point the crack will increase its velocity due to the Griffith mechanism, and then the problem becomes inertial again.

[1] W. W. Mullins, J. Appl. Phys. **28**, 333 (1957).
[2] R. H. Torii and S. Balibar, J. Low Temp. Phys. **89**, 391 (1992).
[3] M. A. Grinfeld, J. Nonlinear Sci. **3**, 35 (1992).
[4] W. H. Yang and D. J. Srolovitz, Phys. Rev. Lett. **71**, 1593 (1993).
[5] R. J. Asaro and W. A. Tiller, Metall. Trans. **3**, 1789 (1972).
[6] M. A. Grinfeld, Sov. Phys. Dokl. **31**, 831 (1986).
[7] X. Yang and E. Weinan, J. Appl. Phys. **91**, 9414 (2002).
[8] E. A. Brener and R. Spatschek, Phys. Rev. E **67**, 016112 (2003).
[9] F. Barra, M. Herrera, and I. Procaccia, Europhys. Lett. **63**, 708 (2003).
[10] A. Pimpinelli and J. Villain, *Physics of Crystal Growth* (Cambridge University Press, New York, 1998).
[11] C. H. Chiu and H. Gao, Int. J. Solids Struct. **30**, 2983 (1993).
[12] E. Bouchbinder, J. S. Langer, and I. Procaccia, Phys. Rev. E **75**, 036107 (2007); **75**, 036108 (2007).
[13] E. Bouchbinder, T. S. Lo, and I. Procaccia, Phys. Rev. E **77**, 025101 (2008).
[14] E. Bouchbinder, J. S. Langer, T.-S. Lo, and I. Procaccia, Phys. Rev. E **76**, 026115 (2007).
[15] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity*, 3rd ed (Pergamon, London, 1986).
[16] E. Bouchbinder, T.-S. Lo, I. Procaccia, and E. Shtilerman, Phys. Rev. E (to be published).