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Transitions from oscillatory to smooth fracture propagation in brittle metallic glasses

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We present a simple model to explain the transition from oscillatory to smooth crack propagation in brittle metallic glasses. We demonstrate that the smooth fracture propagation that is characteristic for higher temperature or higher crack opening velocities (for type 1 crack propagation) becomes unstable and oscillatory behavior is being observed. The characteristic feature size of the crack propagation may be at the nanometer scale and grows as the opening velocity decreases.

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Understanding crack propagation in materials and glasses in particular constitutes an interesting and very challenging problem. Glasses represent a good testing material for a theory of fracture because of the absence of microstructures, such as grain boundaries, elastic anisotropy, and lattice dislocations, which complicate the analysis of crystalline materials. Metallic glasses are particularly interesting, since they can be ductile as well as brittle, while most oxide glasses are brittle. Even when metallic glasses are macroscopically brittle, at the atomic scale their behavior is still controlled by viscoelasticity, while oxide glasses are atomically brittle.

A minimal model to describe oscillatory fracture propagation at the mesoscopic scale was proposed by Blumenfeld [1]. In Blumenfeld's model [1] the velocity of a crack oscillates from some minimum (nonzero) to a maximum value for an oscillatory behavior and is constant for a steady state case. Velocity oscillations in rapid fracture in thin brittle gels were recently observed by Livne *et al.* [2]. Models of crack propagation were recently proposed by several groups [3–8]. However, none of these models address the oscillatory crack propagation that creates a nanoscale periodic morphology at the atomistic scale. Such morphology was recently discovered on the fracture surface of a metallic glass [9]. To initiate fracture, a small seed crack was introduced at the edge of the glassy alloy, and was stretched by applying a uniform displacement at its vertical boundaries with moving speed of 0.01 mm/min. The characteristic feature size observed varied from 30 to approximately 200 nm. We propose a simple model to describe this oscillatory behavior based on the nonlinear response of the viscoelastic media.

The periodic fracture patterns can be created due to noncontinuous, possibly oscillatory (jerky) behavior of the crack tip. Here we present a simple model that describes oscillatory (jerky) crack propagation in metallic glasses and addresses crack propagation at the nanoscale. Our model characterizes time dependence of crack propagation and accounts for the tip dynamics in response to external uniform driving with a constant velocity. While we do not elaborate on the spatial structure of crack propagation, we demonstrate that the periodicity in crack propagation is strongly correlated with the ratio of the elastic-to-viscous properties and provide a path for experimental confirmation of our results.

We consider crack propagation under a tensile stress, the so-called mode one fracture. Until the applied stress reaches a critical value the system responds elastically. Once the critical value is exceeded the crack starts to propagate. We describe the motion of an infinitesimally small volume of material in the vicinity of the tip. As the tip moves, it deforms the vicinity by creating a deformation zone ϕ that is time dependent (equation for ϕ will follow). We propose the following equation to describe the motion of the crack tip with infinitesimal mass in the direction of the crack propagation:

$$\Gamma \dot{x} = k_{el}(v_0 t - x) - F_b, \tag{1}$$

where $\Gamma \dot{x}$ describes energy dissipation due to crack propagation, v_0 is the average crack propagation velocity that can be estimated from $v_t = v_0 \tan\theta$, v_t is the crack opening velocity, and θ is the opening angle.

The resistance force F_b can be described in the framework of linear elasticity [10] and we assume that it decays exponentially with the distance from the tip. We approximate $F_b = \int_0^\phi f(\Delta z) p(\Delta z) d(\Delta z)$ where $f(\Delta z)$ is the elastic force, $f = k_{el}\Delta z$, $p(\Delta z)$ is the probability density function (the probability of surfaces being separated by the distance $\Delta z \equiv z - z_{eq}$ at any given point along the crack propagation direction, where z_{eq} is the equilibrium distance between atoms) and is approximated by $p(\Delta z) = \frac{1}{\delta}\exp(-\Delta z/\delta)\Delta z$, and δ is the characteristic length of the viscous flow zone, $\delta \approx O(5-10\ \text{nm})$ involving approximately 20 atoms, corresponding to the width of the shear band [11].

Thus,

$$F_b = \frac{k_{el}}{\delta}\int_0^\phi \Delta z p(\Delta z) d(\Delta z)$$
$$= \frac{k_{el}}{\delta}\int_0^\phi \Delta z e^{-\Delta z/\delta} d(\Delta z) = k_{el}\delta[1 - e^{-\phi/\delta}(1 + \phi/\delta)].$$

The proposed form of the resistance force F_b is consistent with the expression for separation potential suggested by Xu and Needelman [12] and with assumptions of the elastic chain models [13]. The expression for F_b has some similarities with the expression for the normal and shear work separation between the interfacial surfaces [14,15]. We do not take into consideration the effects of nonlinearity (hyperplasticity) recently suggested by Buehler *et al.* [16] that may not

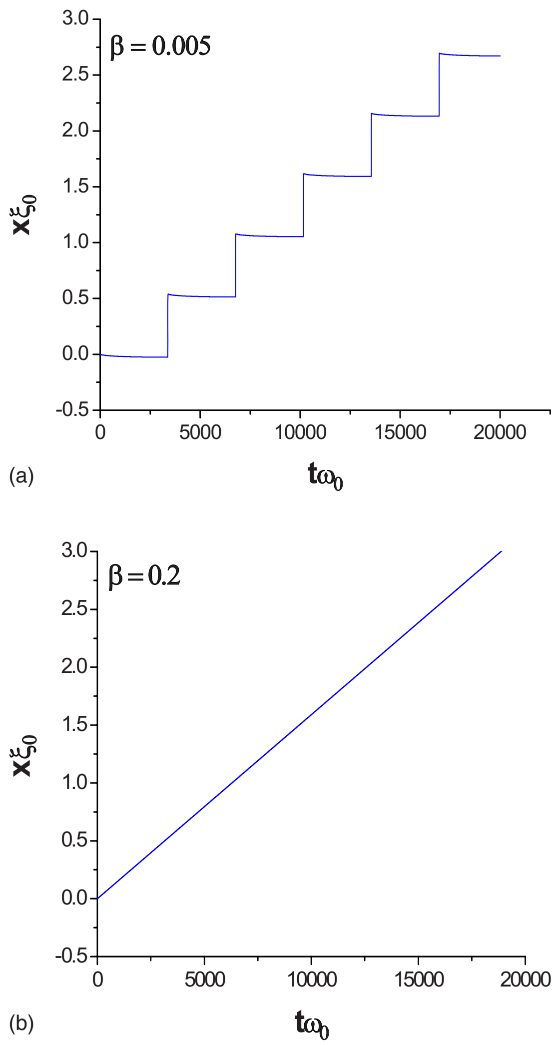

FIG. 1. (Color online) A typical behavior of the tip ξ for a variety of β values. The parameter values are $\dot{\xi}_0=1.59\times10^{-4}$; $\delta_0=10^2$; $D=10^{-3}$; (a) $\beta=0.005$, and (b) $\beta=0.2$.

be significant for brittle materials on the nanometer scale.

The effect of viscosity is taken in consideration through the equation for ϕ and is related to a Kelvin-Voigt model for viscoelasticity. Substituting the expression for F_b into Eq. (1) leads to

$$\Gamma\dot{x}=k_{el}(v_0t-x)-F_0[1-e^{-\phi/\delta}(1+\phi/\delta)], \tag{2}$$

where $F_0\equiv k_{el}\delta$.

We now derive the equation for ϕ based on the following considerations. We presume a generic form $\dot{\phi}=-\frac{\phi}{\tau_\phi}+v_0$ and $\frac{1}{\tau_\phi}=\frac{1}{\tau_m}+\frac{1}{\tau_{tip}}$. Here τ_m is the characteristic relaxation time of the material expressed by the Maxwell relaxation time, $\tau_m=\frac{\eta}{G}$, where η is the viscosity and G is the shear modulus. τ_{tip} is the relaxation time due to the tip motion and can be approximated as $\tau_{tip}^{-1}\approx\frac{|\dot{x}|}{a}$, where $|\dot{x}|$ is the velocity of the tip and a is the characteristic interatomic length of the material. Defining $B\equiv\frac{1}{\tau_m}$, we obtain the following equation for ϕ:

$$\dot{\phi}=-\left(B+\frac{|\dot{x}|}{a}\right)\phi+v_0. \tag{3}$$

It is interesting to note that the form of Eq. (3) can be related to the Kelvin-Vogt model for viscoelastic fluids with B corresponding to the ratio of the shear modulus G to the viscosity coefficient η. A similar form of the equations has been used to describe dry friction ([17,18], and references therein), although there are also significant differences [see, for example, Ref. [17] and Eqs. (2) and (3) in our model]. Moreover, for fracture propagation the mass of the tip is negligible (the overdamped dynamics) while the effect of inertia on frictional dynamics is often considerable.

We estimate the range of the parameters. We assume $v_t\approx O(10^{-7})$ m/s, $\theta\approx10^{-2}$, thus $v_0\approx O(10^{-5})$ m/s. The value of the lattice constant a is approximated as $a\approx2.5\times10^{-10}$ m and we assume $\delta\approx O(5\times10^{-9})$ m. The value of k_{el} can be estimated as $k_{el}\approx E\delta$, where E is the Young modulus. Assuming $E\approx O(5\times10^{10})$ Pa, we obtain $k_{el}\approx O(2.5\times10^2)$ N/m. We estimate k_{cr} (due to plastic deformation around the tip) as $k_{cr}=\kappa k_{el}$, where κ is the stress concentration factor. We assume $\kappa\approx60$ thus $k_{cr}\approx O(1.5\times10^4)$ N/m. We then estimate $\xi_0=k_{el}/F_0=1/\kappa\delta\approx O(4.0\times10^6)$ m^{-1}, the characteristic length $1/\xi_0\approx O(0.25\times10^{-6})$ m, and the value of Γ can be estimated as $\Gamma=E\varepsilon^2\delta/2v_{cr}$; here ε is the strain far from the crack and v_{cr} is the maximum crack propagation velocity [19] that we estimate to be of the same order of magnitude as the sound velocity [$v_c\approx O(10^2$ m/s)]. We also assumed that the elastic energy released is much higher than the energy needed to create a new fracture surface [20]. We assume $\varepsilon\approx2\times10^{-2}$ and $v_{cr}\approx2\times10^2$ m/s, thus $\Gamma\approx2.5\times10^{-4}$ J s/m^2.

We now rewrite Eqs. (2) and (3) in the dimensionless units

$$\dot{\xi}=(\dot{\xi}_0\tau-\xi)-[1-(1+\varphi/\delta_0)e^{-\varphi/\delta_0}], \tag{4}$$

$$\dot{\varphi}=1-\left(\beta+\frac{|\dot{\xi}|}{D}\right)\varphi, \tag{5}$$

where $\xi=\xi_0x$; $\tau=\omega_0t$; $\omega_0=\frac{k_{el}}{\Gamma}$; $\xi_0=\frac{k_{el}}{F_0}$; $\dot{\xi}_0=\frac{\Gamma}{F_0}v_0$; $\varphi=\frac{\omega_0}{v_0}\phi$; $\delta_0=\frac{\omega_0}{v_0}\delta$;

$$\beta=\frac{B}{\omega_0}=\frac{B\Gamma}{k_{el}};\quad D=a\xi_0=\frac{ak_{el}}{F_0};\quad \frac{\dot{\xi}_0}{\beta}=\frac{\xi_0v_0}{B}=\frac{k_{el}}{F_0B}v_0. \tag{6}$$

A typical behavior of the crack tip is demonstrated in Fig. 1.

At large crack velocities, the motion of the tip is smooth (the tip position is linear in time) therefore, the solution for Eqs. (4) and (5) is

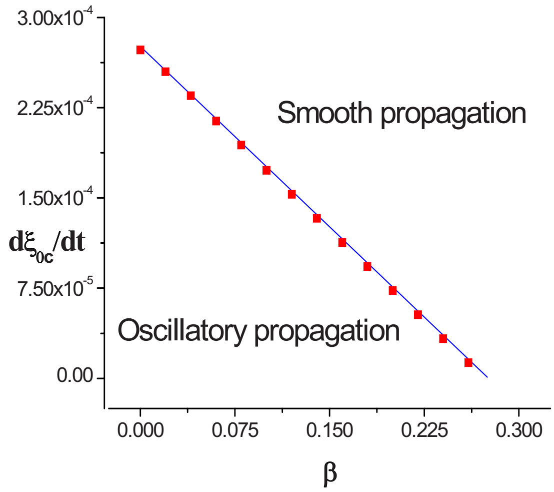

FIG. 2. (Color online) The stability curve β versus $\dot{\xi}_{0c}$ based on the numerical results of Eqs. (4) and (5) and Eq. (14). The parameters are the same as in Fig. 1.

$$\xi = \xi_0 + \dot{\xi}_0\tau, \quad \varphi = \varphi_0 = \frac{1}{\beta + \dfrac{\dot{\xi}_0}{D}},$$

$$\xi_0 = -1 - \dot{\xi}_0 + e^{-\varphi_0/\delta_0}\left(1 + \frac{\varphi_0}{\delta_0}\right). \tag{7}$$

This solution becomes unstable for low velocities. We look at the linear stability of the solution [Eq. (7)] assuming

$$\xi = \xi_0 + \dot{\xi}_0\tau + \varepsilon,$$

$$\varphi = \varphi_0 + \mu. \tag{8}$$

Inserting Eq. (8) and Eq. (7) into Eqs. (4) and (5), after some algebra we obtain

$$\dot{\varepsilon} + \varepsilon = -\frac{\mu\varphi_0}{\delta_0^2}e^{-\varphi_0/\delta_0},$$

$$\dot{\mu} = 1 - \left(\beta + \frac{|\dot{\xi}_0 + \dot{\varepsilon}|}{D}\right)\varphi_0 - \left(\beta + \frac{|\dot{\xi}_0 + \dot{\varepsilon}|}{D}\right)\mu. \tag{9}$$

Assuming $\varepsilon = \varepsilon_0 e^{\kappa\tau}$ and $\mu = \mu_0 e^{\kappa\tau}$ we obtain the following equation for κ:

$$(\kappa + 1)(\kappa + A) - PC\kappa = 0. \tag{10}$$

Here we denoted

$$P \equiv \frac{1}{AD}, \quad C \equiv \frac{1}{A\delta_0^2}e^{-1/A\delta_0}, \quad \text{and } A \equiv \beta + \frac{\dot{\xi}_0}{D}. \tag{11}$$

Therefore, the loss of the stability of the smooth (linear) propagation can be found from the following relation:

$$1 + A_c - P_c C_c = 0 \rightarrow A_c^2\delta_0^2 D(1 + A_c) = e^{-1/A_c\delta_0}. \tag{12}$$

If $A\delta \gg 1$, we can approximate $e^{-1/A_c\delta_0} \approx \frac{1}{1+1/A_c\delta_0} = \frac{A_c\delta_0}{1+A_c\delta_0}$ to obtain

$$DA_c\delta_0(A_c + 1)(A_c\delta_0 + 1) = 1 \quad \text{and} \quad A_c \equiv \beta + \dot{\xi}_{oc}/D. \tag{13}$$

Since $A_c < 1$ and $\delta_0 \gg 1$, we can approximate Eq. (12) by a quadratic equation $A_c^2 + \frac{A_c}{\delta_0+1} - \frac{1}{D\delta_0^2} = 0$, thus leading to the following condition for the smooth-to-oscillatory instability to occur:

$$\dot{\xi}_{0c} \approx \frac{\sqrt{D}}{\delta_0} - D\beta. \tag{14}$$

In "real" units, Eq. (15) can be written as

$$v_{0cr} \approx \frac{k_{cr}a}{\Gamma}\frac{1}{\sqrt{4\pi\kappa\delta}} - aB. \tag{15}$$

For the case of $\beta = 0$, we obtain $\dot{\xi}_{0c} \approx \frac{\sqrt{D}}{\delta_0} = \frac{k_{cr}a}{\Gamma}\frac{1}{\sqrt{4\pi\kappa\delta}}$, which puts the limit on the crack opening velocity above which a brittle behavior will be observed. In Fig. 2 we demonstrate the stability curve β versus $\dot{\xi}_{0c}$ based on the numerical results of Eqs. (4) and (5) and Eq. (14). While Eq. (14) is an approximation, we obtain a fair fit.

For small crack velocities, an oscillatory behavior is observed. One can approximate the time period of the oscillation (see Fig. 1) as

$$T = \int_0^{\varphi_{\max}} \frac{1 + \dfrac{\varphi^2}{\delta_0^2 D}e^{-\varphi/\delta_0}}{1 + \left(\dfrac{\dot{\xi}_0}{D} - \beta\right)\varphi}d\varphi. \tag{16}$$

This can be further approximated by

$$T \approx \frac{1}{\dot{\xi}_0 - \beta D}\left[1 - e^{-\varphi_{\max}/\delta_0}\left(1 + \frac{\varphi_{\max}}{\delta_0}\right)\right] \tag{17}$$

and

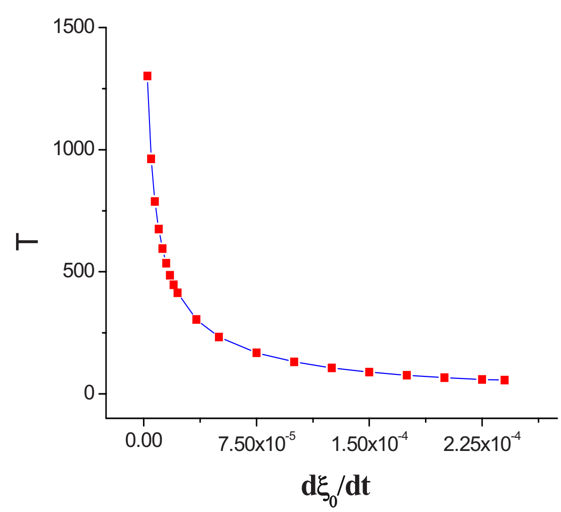

FIG. 3. (Color online) Numerical (red dots) and analytical [Eq. (17), blue line] curve for T as a function of $d\xi_0/dt$. The parameters: $\beta = 0.05$; $\delta_0 = 10^2$; $D = 10^{-3}$.

$$\frac{\varphi_{\max}}{\delta_0} = \ln(1 - \beta\varphi_{\max}) + \ln\left(\frac{\varphi_{\max}}{\delta_0}\right) - \ln(\dot{\xi}_0\delta_0). \qquad (18)$$

A typical feature size for given values of the parameters depends on the value of β and is the maximum for $\beta=0$. We can estimate the feature size as $\Delta x \approx \Delta\xi/\xi_0$. As for $\beta=0$, $\Delta\xi \approx 1$, we estimate $\Delta x_{\max} \approx 1/\xi_0$.

The feature size $\Delta x = Tv_0$ is the maximum for $\beta=0$ which corresponds to the limit of a very high viscosity (low temperature limit). It then decreases with increasing β and discontinuously drops to zero at some value of $\beta=\beta_c$ which corresponds to the high temperature limit. For given values of the parameters, the smallest feature size corresponds approximately to $\Delta x_{\min} \approx \delta/5$.

In Fig. 3 we show the numerical (red dots) and analytical [Eq. (17), blue line] curve for T as a function of $\dot{\xi}_0$ in the logarithmic and linear (the inset) scales. For a given set of parameters, our numerical results show an excellent agreement with the analytical results. An increase in $\dot{\xi}_0$ leads to a decrease in the period T and for a large enough $\dot{\xi}_0$ a transition from the stick slip to a continuous character of the motion of the tip occurs.

In conclusion, we have presented a simple model to demonstrate a transition from the smooth to oscillatory fracture propagation. We believe our model is applicable to the nanoscale fracture propagation in metallic glasses. This model is based upon the nonlinear response of a viscoelastic medium. The results may have wide implications on the fracture behavior of viscoelastic materials in general.

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