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RAPID COMMUNICATIONS

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Model for surface fracture induced by dynamical stress

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We introduce a model where an isotropic, dynamically imposed strain induces fracture in a thin film. Using molecular-dynamics simulations, we study how the integrated fragment distribution function depends on the rate of change and magnitude of the imposed strain, as well as on temperature. A mean-field argument shows that the system becomes unstable for a critical value of the strain. We find a striking invariance of the distribution of fragments for fixed ratio of temperature and rate of change of the strain; the interval over which this invariance holds is determined by the force fluctuations at the critical value of the strain. [S1063-651X(98)50402-3]

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By experience most—if not all—materials will sooner or later develop cracks. Yet, a profound understanding is largely missing of phenomena such as how cracks initiate, the formation of networks of cracks and the resulting distribution of fragments, the dynamics of crack propagation, and the collective behavior of many interacting cracks. In this Rapid Communication we propose a new model that addresses, at least in part, some of these questions. In the model, an isotropic, dynamically imposed strain, caused by material properties changing in time, induces fracture in a surface material. The problem is solved using molecular-dynamics simulations for a set of beads interacting with one another via a continuous potential. This model should be relevant to many phenomena that are known to lead to macroscopic fracture, such as desiccation [1–4] or expansion [5,6], changes in chemical composition [7], changes in temperature [8], or change of phase of the surface layer.

On the basis of a mean-field argument, we demonstrate that the system becomes unstable for a critical value of the strain. We find a striking invariance of the distribution of fragments for a fixed ratio of temperature and rate of change of the strain; the interval over which this invariance holds is determined by the force fluctuations at the critical value of the strain.

Model. We represent the thin film on a coarse-grained scale by beads that mutually interact via a continuous potential that we take to be of the Lennard-Jones form, $4\epsilon[(\sigma/r)^{12}-(\sigma/r)^{6}]$, where $r=|\vec{r}|$ is the distance between two particles. An isotropic strain is imposed by having σ change in time (t), reflecting a change in the range of the interactions on the surface [9]. For simplicity we limit ourselves to the case where the material is initially unstrained and $\sigma(t)$ decreases monotonically with time. This corresponds to a surface where the induced strain makes the material rupture in a state of tension.

The dynamics of the beads obeys Newton's second equation, i.e., the system is simulated using molecular dynamics (MD). We assume the surface layer to be in contact with a heat bath at temperature T; this is done by periodically rescaling the velocities to a fixed kinetic energy [10]. The units are chosen so that the mass $m=\epsilon\equiv 1$. In its initial (strain-free) state, the surface layer consists of a triangular lattice with lattice constant $a_0=2^{1/6}\sigma_0$, where $\sigma_0=\sigma(t_0)$. Periodic boundary conditions are used to eliminate surface effects. The consequence of decreasing $\sigma(t)$ is to put all beads under tensile stress, i.e., each bead feels attracted by its neighbors. We assume $\sigma(t)$ to decrease linearly in time until it attains a final value σ_f at time t_f, whereafter it remains constant. An effective strain parameter of the overlayer is defined by $s(t) \equiv [\sigma_0 - \sigma(t)]/\sigma_0$. The rate of change (''speed'') of σ is denoted $v \equiv \partial\sigma(t)/\partial t$.

We note that the model presented above only contains three parameters $[v, T, s(t_f)]$, and, in particular, no specific assumption or algorithm is introduced to break a bond. In order to describe fracture in real materials, impurities and/or more realistic interactions could be introduced; however, our interest in this Rapid Communication is to keep the model assumptions as simple as possible in order thereby to identify the *basic* mechanisms responsible for the collective behavior of many interacting cracks. We are interested in the fracture pattern at $t=\infty$ which is obtained in practice by choosing a large enough t_f, whose value depends on the three parameters above. In order to calculate the probability $P(f)$ for having a fragment of size f, we discretize the system into cells of size $\sigma(t)$. A fragment is then defined as a cluster of beads that are nearest or next-nearest neighbors to one another.

As σ changes with time, each bead will evolve from a position of global energy minimum to a local minimum state. The local minimum-energy state is stable, however, for $\sigma(t)$ close to σ_0, since the system would need instant cooperative motion of all the beads in order to rearrange into the global minimum-energy state whose lattice parameter is $a = 2^{1/6}\sigma(t)$. Due to the many body nature of the system, each bead will see an energy landscape that changes as the positions of neighboring beads change, and as σ changes in time. The cooperative motion of the beads creates dynamical and spatial barriers between, on the one hand, local metastable minimum-energy states, and, on the other hand, the global minimum-energy state.

For increasing values of σ, the initial configuration eventually becomes unstable. Neglecting fluctuations in the positions of the beads, each will experience a mean-field potential from its nearest neighbors given by

$$V(r,\sigma) = 12\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} + \left(\frac{\sigma}{2a-r}\right)^{12} - \left(\frac{\sigma}{2a-r}\right)^{6}\right].$$

We are interested in the behavior of $V(r,\sigma)$ at the point $r = a + \delta$ with δ small. Expanding the above to fourth order in δ, we find:

$$V(\delta,\sigma) = 12\epsilon\left(\frac{\sigma}{a}\right)^{6}\left\{2\left[\left(\frac{\sigma}{a}\right)^{6} - 1\right] + \left[156\left(\frac{\sigma}{a}\right)^{6} - 42\right]\left(\frac{\delta}{a}\right)^{2} + \left[32760\left(\frac{\sigma}{a}\right)^{6} - 3024\right]\left(\frac{\delta}{a}\right)^{4} + O\left(\left(\frac{\delta}{a}\right)^{6}\right)\right\}.$$

Thus, for δ small, the potential seen by a bead changes from a harmonic single-well to a double-well potential as σ decreases. This happens when $V''(\delta,\sigma)|_{\delta=0}$ changes sign, that is, for $\sigma_c = (7/26)^{1/6} a_0 = (7/13)^{1/6}\sigma_0 \approx 0.90\sigma_0$. In general, the existence of a critical σ_c for an arbitrary interaction $V(r,\sigma)$ is equivalent to $V''(r,\sigma)|_{r=a} = 0$ having a solution. As $\sigma(t)$ approaches σ_c from below, one large fluctuation eventually takes place bringing one of the beads close to its new local minimum-energy position. A cascade of similar events then spreads out from beads adjacent to that which first broke the configurational symmetry. The extent of the propagation of this cascade of events, and the subsequent fracturing of the system, depends, as we will see, on $s(t_f)$, T, and v, as well as on the fluctuations of forces when $\sigma = \sigma_c$.

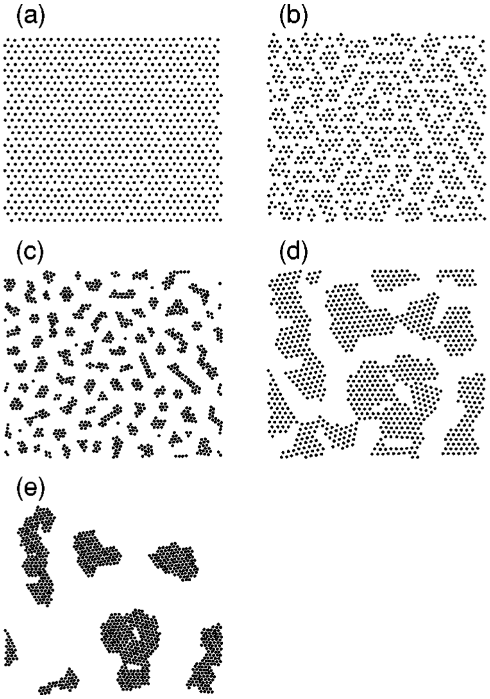

FIG. 1. Snapshots of a $N=1600$ system at different times t, with different change of strain rate v and different final strain $s(t_f)$. The initial configuration is the same, and $T=6.25\times10^{-5}$, in all cases. (a) $s(t)=0.14$, $v=0.0125$, (b) $s(t)=0.25$, $v=0.0125$, (c) $s(t=t_f)=0.5$, $v=0.0125$, (d) $s(t)=0.25$, $v=0.001\,562\,5$, and (e) $s(t=t_f)=0.5$, $v=0.001\,562\,5$.

Results. Figures 1(a)–1(c) show snapshots of one system for different values of strain but fixed temperature and strain rate. Figure 1(a) corresponds to $\sigma(t)$ slightly larger than σ_c. The very first cracks have appeared and shortly after the system completely disintegrates into many pieces, characterized by a macroscopic Young's modulus that goes to 0 [6,11]. This has happened in Fig. 1(b). In Fig. 1(c), we have the final state of the system when the strain no longer varies in time. The effect of varying the speed v can be seen in Figs. 1(d) and 1(e): here, the initial conditions are the same as in Figs. 1(a)–1(c), but v is eight times smaller. The strain in Fig. 1(d) is the same as in Fig. 1(b); clearly, a smaller strain rate gives the system a longer time to respond so that the positions of the beads are correlated over a longer distance and the cracks are straighter. As a result, the fragments in the final configuration, Fig. 1(e), are larger than they are under a rapidly varying strain [compare Fig. 1(c)].

If $T\equiv0$ the absence of thermal fluctuations would mean that the system remains in its initial state and never breaks, despite the fact that the energy difference between initial and stressed states increases as $\sigma(t)$ decreases. For $T\neq0$ [12] and $v\rightarrow\infty$, on the other hand, the rupture of the system is completely dominated by fluctuations, in which case the probability density $P(f)$ for having a fragment of given size f is given by a binomial distribution $P(f) = K_{(6,f)}(1/6)^f(5/6)^{6-f}$, since each of the six neighbors of a

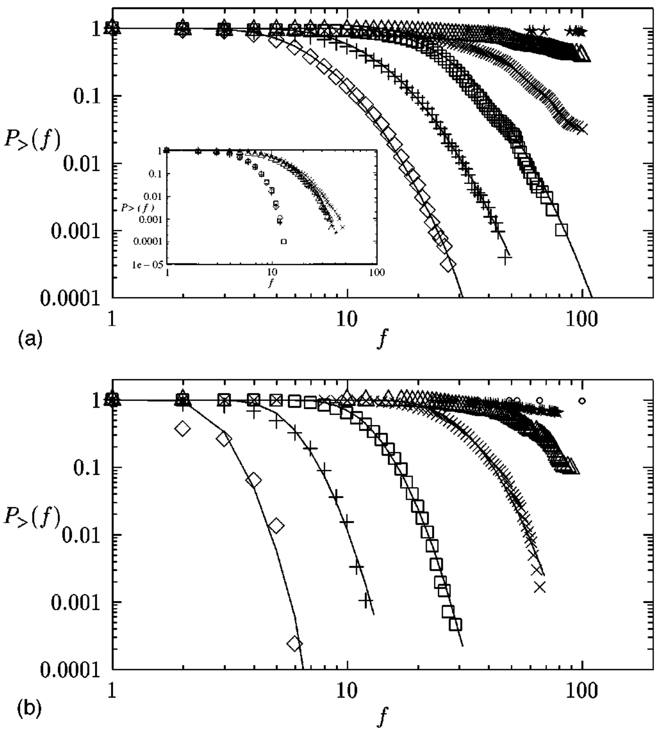

FIG. 2. Cumulative probability distribution $P_>(f)$ for finding a given fragment of area larger than f, and $T=6.25\times10^{-5}$ (a) $s(t_f)=0.5$; $v=0.025$ (◇), 0.0125 (+), 0.006 25 (□), 0.0042 (×), 0.003 125 (△) and 0.001 562 5 (*). The lines are fits to a log-normal distribution. Inset: finite-size scaling with $s(t_f)=0.5$, $v=0.0125$; $N=$ 100 (×), 400 (△) and 900 (*); $s(t_f)=0.75$, $v=0.0125$; $N=100$ (◇), 400 (+) and 900 (□). (b) $s(t_f)=0.75$; $v=0.0375$ (◇), 0.018 75 (+), 0.009 375 (□), 0.004 687 5 (×), 0.003 125 (△), 0.002 679 (*) and 0.002 344 (small white circle). The lines are fits to a log-normal distribution.

given bead has probability 1/6 of forming a cluster with that bead. For finite (T,v), finally, the fracturing is determined by the coherent motion of the N beads. In Figs. 2(a) and 2(b) we show the cumulative probability distribution $P_>(f)$ for a given T and different v; as we have seen above, the smaller the value of v, the larger the fragments. In Fig. 2(a), $s(t_f)=0.5$, whereas $s(t_f)=0.75$ in Fig. 2(b). In order to calculate $P_>(f)$, we have averaged over 200–500 $N=100$ systems with different initial configurations, all at the same temperature T. (We chose to use many small systems rather than a few large ones in order to get better statistics). Finite-size scaling of $P_>(f)$ is shown in the inset of Fig. 2(a), which allows us to extend our results [for the given (T,v)] to the case $N\rightarrow\infty$. The lines are fits to a log-normal distribution; clearly, the data suggest this form of $P_>(f)$ for large v. This is the signature of a fracturing process that happens in a multiplicative manner [13], where a given piece at a random point breaks into two pieces, which themselves randomly break into two other pieces, etc. For very small v, $P_>(f)$ crosses over to a Heaviside θ function, since in this case breakdown happens due to one large crack spanning the whole system. The speed for which $P_>(f)$ can no longer be described by a log-normal distribution depends on T and N, and is due to finite-size effects.

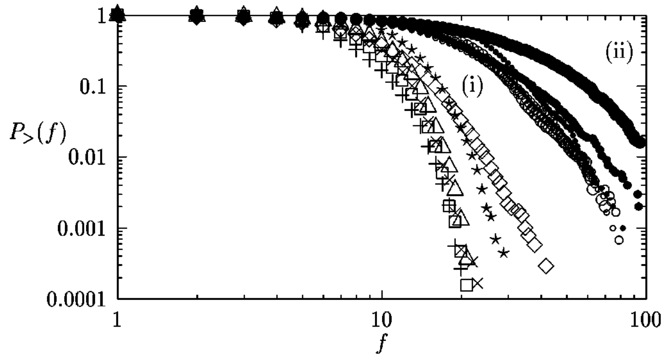

FIG. 3. $P_>(f)$ vs f for fixed value of $\kappa\equiv E_k^{1/2}/v$ and $s(t_f)$ for a $N=100$ system. (i) $\kappa=1.03$, $s(t_f)=0.75$, and $(T,v)=(6.4\times10^{-2},0.30)$ (◇), $(1.6\times10^{-2},0.15)$ (+), $(4\times10^{-3},0.075)$ (□), $(10^{-3},0.0375)$ (×), $(2.5\times10^{-4},0.018\,75)$ (△) and $(6.25\times10^{-5},0.009\,375)$ (*). (ii) $\kappa=1.55$, $s(t_f)=0.5$, and $(T,v)=(6.4\times10^{-2},0.20)$ (large black circle), $(1.6\times10^{-2},0.10)$ (black circle), $(4\times10^{-3},0.05)$ (small white circle), $(10^{-3},0.025)$ (white circle), $(2.5\times10^{-4},0.0125)$ (large white circle) and $(6.25\times10^{-5},0.006\,25)$ (small black circle).

An instantaneous change in σ means a change in both the magnitude and the fluctuations of the forces. We find the system to respond in a *qualitatively* different manner to changes in σ depending if it is $<\sigma_c$ or $>\sigma_c$. For a broad range of speeds v, we find the average magnitude of the force on the beads, $F\equiv\Sigma_i^N|f_i|/N$, and its fluctuation, $\delta F\equiv\Sigma_i^N\sqrt{f_i^2-F^2}/N$, to be *independent* of v for $\sigma(t)<\sigma_c$. We have also calculated the characteristic length $\xi(t)$ of the stress field $F([\vec{r}(t)])$ by taking the first moment of the radial averaged structure factor $S(k,t)$. In [4], a coarsening phenomenon of $F[\vec{r}(t)]$ prior to the first fracture was found to be crucial for the subsequent rupture of the system; in the present model, we observe no time evolution of $\xi(t)$ for $\sigma(t)<\sigma_c$, and $\xi(t)\simeq a$. (However, when the first macro cracks appear, $\xi(t)$ increases dramatically]. Therefore, the observed dependence of $P_>(f)$ on v must be due to the way the system responds to changes in σ *after* the σ_c point has been passed.

Whether or not the system has time to counteract the imposed strain passed σ_c depends on the time scale over which changes in σ take place compared to the response time of the system; the latter is determined by the random thermal motion, i.e., kinetic energy E_k, of the beads. The ratio of these

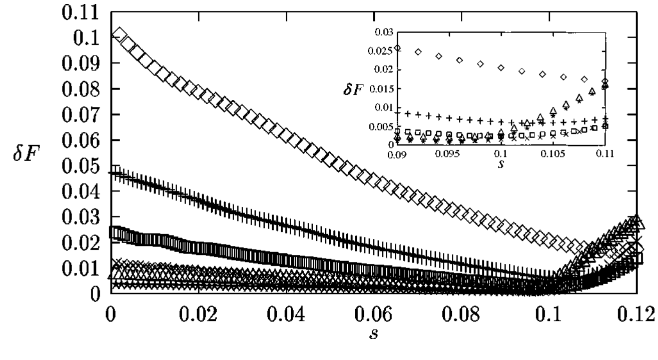

FIG. 4. δF vs s for $\kappa=1.55$ and $(T,v)=(6.4\times10^{-3},0.20)$ (◇), $(1.6\times10^{-2},0.10)$ (+), $(4\times10^{-3},0.05)$ (□), $(10^{-3},0.025)$ (×), $(2.5\times10^{-4},0.0125)$ (△) and $(6.25\times10^{-5},0.006\,25)$ (*).

two time scales is thus given by $\kappa \equiv \sigma v^{-1}/(m^{1/2}\sigma/E_k^{1/2}) = \sqrt{E_k}/v$. One therefore expects systems with the same value of κ to fracture in the same way. The fracture is expected to be dominated by fluctuations for $\kappa \ll 1$, whereas for $\kappa \gg 1$ it will have time to respond to the changing strain in a correlated manner. This is in fact verified in Fig. 3 which shows a remarkable invariance of $P_>(f)$ over almost 3 decades in temperature for systems with two different values of κ. The lowest and highest temperature in Fig. 3 for which the invariance of $P_>(f)$ no longer holds, and the subtle temperature dependence at intermediate values, can be understood from the dependence on strain of the force fluctuations δF, shown in Fig. 4 for the same values of T as in Fig. 3. Because of the fluctuations, different temperatures lead to a critical s_c (defined as the s for which δF has its minimum) slightly different from the mean-field value of $s_c = (\sigma_0 - \sigma_c)/\sigma_0 = 0.10$. The small temperature dependence of $P_>(f)$ at intermediate temperatures can then be understood in terms of a slight increase of $\delta F(s_c)$ with T, since one would expect larger force fluctuations at s_c to lead to smaller fragments. As seen in Fig. 4, the only exception to this is the case of the highest T where, on the contrary, a large $\delta F(s_c)$ leads to a large-fragment tail in $P_>(f)$. The reason for this is that T is so high that coalescence of already-formed fragments takes place; coalescence is not observed for lower T. Finally one also notes from Fig. 3 that deviations in $P_>(f)$ occur for very low temperatures, where the simple scaling argument leading to invariance of $P_>(f)$ under a given κ apparently no longer holds.

Conclusion. We have introduced a model where a dynamically imposed strain induces fracture in a thin film. Using molecular-dynamics simulations, we have shown the accumulated fragment distribution function to obey a log-normal distribution characteristic of fracturing processes that happen in a random multiplicative manner. A mean-field argument shows how the system undergoes an instability for a critical value of the imposed strain. We find a striking invariance of the fragment distribution function for a given ratio of temperature and speed of strain; the interval over which this invariance holds is determined by the force fluctuations at the critical value of the strain.

Recently many experiments have focused on the dependence of the fragment distribution function on the dimensionality and shape of the fractured object as well as on the impact energy [14]. In all these cases fragmentation resulted because of the propagation of a shock wave from the point of impact. Our findings suggest it could be interesting to look at other variables, such as temperature and change of strain rate, in experiments where a coating breaks due to desiccation or expansion. Recently we learned of a new interesting two-dimensional MD simulation study of the fracture of membranes [15]. As in the present paper the authors studied the effect of temperature on fracture under an expansion, but in a quasistatic state, in contrast to the dynamical dependence studied in this paper.

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