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Rate of microcrack nucleation

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We propose a phenomenological model for microcrack nucleation in a solid under constant external stress. We argue that the kinetics of the crack nucleation process is qualitatively different from that occurring in simple metastable states such as supercooled liquids or supersaturated solutions. This difference is caused by irreversible processes such as surface diffusion that restructure microcrack surfaces. This restructuring inhibits microcrack healing and thus yields a microcrack nucleation rate that is much *faster* than that obtained by directly applying nucleation laws appropriate to metastable states in liquids or solutions.

The mechanisms and physical properties of fracture and failure have attracted the attention of many pure and applied researchers over many years.[1-9] However, fundamental aspects of the fracture physics, such as the very *nature* of the state of a stressed solid and the role of thermal fluctuations, were addressed only quite recently.[4-7] Nishioka and Lee,[5] and, more recently, Blumberg Selinger *et al.*[6] treated a stressed solid as a metastable state. Within this approach, the failure threshold corresponds to a metastability limit, or spinodal point, at which the external stress as function of strain reaches its maximum.

A related issue is that of crack *nucleation,* which is, in many respects, analogous to that of the stable phase droplets in a supercooled liquid,[10] as demonstrated in a recent simulation.[6] An inspiration for such a picture of crack nucleation is contained already in the pioneering work of Griffith.[1] He established a criterion for crack growth by estimating the energy cost of creating a crack of length $2L$ in a solid under a uniaxial stress σ perpendicular to the crack (see Fig. 1). Creation of the crack, in a two-dimensional solid ($d=2$), costs an energy of the order

$$E(L)=gL-\sigma^2L^2/2Y\ . \tag{1}$$

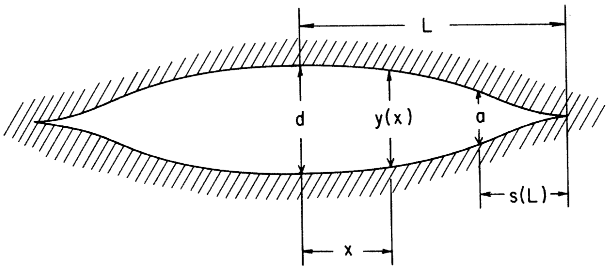

FIG. 1. Crack geometry. $2L$, crack length; d, maximal crack opening displacement; $y(x)$, crack profile; $s(L)$, the distance from the crack tip for which $y[L-s(L)]$ is equal to the atomic size.

The first term in (1) is the energy cost of creating the crack's edges by breaking atomic bonds. Thus ga, with a the atomic size, is of the order of a bond energy. After crack creation, its edges will separate, with maximal opening displacement (see Fig. 1) of the order

$$d=L\sigma/Y\ , \tag{2}$$

with Y the Young modulus. The crack opening relaxes the stress in a domain of size L^2 and lowers the elastic energy by an amount of the order $L^2\sigma^2/2Y$. This yields the second term in (1), which, in contrast to the first one, energetically favors crack growth. [To simplify the discussion, in Eqs. (1) and (2), and in the following, we suppress various numerical factors of order unity.] Energy (1), which can be considered as the potential energy of the crack, reaches its maximum at L equal to the critical Griffith length L_g,

$$L_g=gY/\sigma^2\ , \tag{3}$$

corresponding to the energy

$$E_g=E(L_g)=g^2Y/2\sigma^2\ . \tag{4}$$

The crack state with $L=L_g$ is *unstable*: For $L<L_g$, an increase of L costs a positive amount of energy—this hinders the crack growth for $L<L_g$. For $L>L_g$, the crack growth decreases the potential energy. This leads to a very rapid growth: At L of the order a few L_g the crack tip speed is already of the order of the speed of sound.[2]

Crack growth may proceed even for $L<L_g$, for example, due to thermal fluctuations, as was nicely demonstrated in a recent Monte Carlo simulation.[6] This results in the phenomenon of "delayed fracture,"[8] in which the stressed solid remains undamaged, until it eventually breaks, with a lifetime dependent on the temperature and the applied stress. This phenomenon is believed to be directly related to processes of microcrack nucleation and growth. Energy (1) is analogous to that of a stable phase droplet in the phenomenological Zel'dovich theory of nucleation processes in metastable states.[10] We shall refer

to this picture as the *conventional* theory of crack nucleation. In this approach, the energy E_g in Eq. (4) can be interpreted as the energy barrier for the crack nucleation process. The nucleation rate R_N—or the time t_N needed for a crack to be nucleated out of a perfect solid—can be estimated by an Arrhenius law[10]

$$R_N = 1/t_N \sim \exp(-E_g/k_B T) , \tag{5}$$

at temperature $T \ll E_g/k_B$ (k_B is the Boltzmann constant).

Implicit to the activation law (5) is the assumption that the dynamics of the crack size can be described by a Langevin equation of the form

$$\frac{dL}{dt} = -F\frac{dE}{dL} + n(t) , \tag{6}$$

with $E(L)$ as in (1). Here $n(t)$ is a thermal noise contribution to the "velocity" dL/dt with the correlation function $\langle n(t)n(t')\rangle = 2FT\delta(t-t')$; F is a phenomenological "mobility" (inverse friction) constant. With these assumptions, the application of the classical Zel'dovich theory, the overall physical picture of nucleation is identical to that in other nucleation phenomena: The crack size $L(t)$, with $L(0) \ll L_g$, evolves in a diffusive manner until, eventually, it crosses L_g after a typical time of the order t_N, and starts an explosive growth [see Fig. 2(a)]. During the nucleation process $[0 < L(t) < L_g]$, the crack size "velocity" dL/dt can be both positive (growth) and negative (healing). We emphasize that this conventional theory allows also for a *complete* healing of the solid, which occurs if $L(t)$ goes to 0 at some $t > 0$ [see Fig. 2(b)].

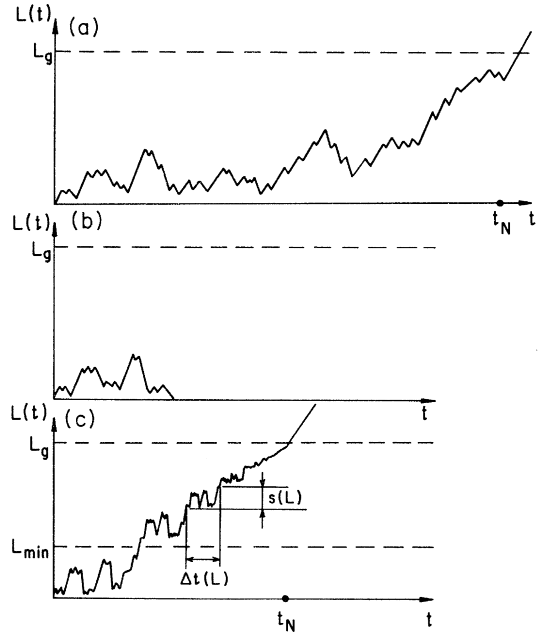

FIG. 2. (a) A typical crack size trajectory $L(t)$ as a function of time t, for the case of the Langevin dynamics uninhibiting crack healing. L_g, Griffith length; t_N, nucleation time. (b) A crack trajectory corresponding to complete crack healing. (c) Crack size dynamics in the presence of surface processes inhibiting its healing. For $L < L_{\min}$ these processes are suppressed and the dynamics is similar to that in (a). For $L_{\min} < L < L_g$, healing is possible at length scales shorter than the length scale $s(L)$, corresponding to the time scale $\Delta t(L)$. At longer scales crack size dynamics has the character of a directed diffusion.

Recent numerical simulation[6] of a thermal equilibrium model defined in such a way to allow complete healing of the solid yields results that are in agreement with the above picture of crack nucleation. By using the estimate $g \cong aY$,[1] Eqs. (3), (4), and (5) yield

$$L_g = a(Y/\sigma)^2, \tag{7a}$$

and

$$R_N = 1/t_N \sim \exp[-gL_g/k_B T] = \exp[-(Y/\sigma)^2(T_m/T)] \quad (d=2) , \tag{7b}$$

where $T_m = ga/k_B$ is a characteristic temperature comparable to, but typically bigger than, the solid's melting temperature. Note that for a realistic temperature $T < T_m$ or $T \ll T_m$, and small strains σ/Y, R_N as given by (7b) is extremely small. Moreover, even for a relatively large strain, say σ/Y of the order 10%, and an unrealistically high T of the order T_m, Eq. (7b) would still predict that the nucleation time t_N is proportional to a number exceeding the number of atoms in any realistic solid. Thus the estimates based on the conventional theory suggest that the crack nucleation is physically totally irrelevant. If so, most realistic solids would break only in the vicinity of the spinodal point[5,6] where stress as a function of strain reaches its maximum and the solid loses its mechanical stability. In practice, however, many brittle materials fracture in the regime in which the stress-strain relationship is still linear to a good approximation and the strain is of the order 10%. In these cases the crack nucleation and growth processes are believed to play an important role in the mechanism of fracture.[8] However, the estimate equation (7b), derived from the conventional nucleation theory, seems to give much too small a nucleation rate to explain these observations.

In this paper we shall argue that the kinetics of the crack nucleation is in fact much faster than that of the conventional diffusive dynamics equation (6), which yielded, for a two-dimensional (2D) solid, the estimate (7b) for the nucleation rate. We will argue in particular that, for a 2D solid,

$$R_N = 1/t_N \sim \exp[-(Y/\sigma)(T_m/T)] \quad (d=2) , \tag{8}$$

instead of Eq. (7b). While the temperature dependence of the nucleation rate (8) is the same as in Eq. (7b), the dependence on the stress is significantly different. Note that, for a weak strain $\sigma/Y \ll 1$, the rate in Eq. (8) is much bigger than that in Eq. (7b). The difference between these two results arises from *surface processes* such as *surface diffusion,*[11] which restructure crack edges and *inhibit* microcrack healing.

These processes are ignored in the conventional crack nucleation model (6) [and thus in Eq. (7b)], which allows for *uninhibited* microcrack healing. We assert instead that a microcrack is a long-lived object whose size L grows via some kind of *directed* diffusion in the range of microcrack sizes

$$L_{\min}=a(Y/\sigma)<L<L_g=a(Y/\sigma)^2 , \tag{9}$$

as depicted in Fig. 2(c). Here, in addition to the Griffith length L_g, a new length scale $L_{\min}$ emerges: Cracks with $L<L_{\min}$ evolve according to Eq. (6) and may heal completely—these microcracks are, like vacancies, *annealed* defects of a solid. On the other hand, cracks in the size range (9) may never heal completely. Their size evolves according to a *directed diffusion* process for which dL/dt is, on average, *positive* [see Fig. 2(c)]. This is in sharp contrast to the Langevin dynamics (6) [compare Figs. 2(c) and 2(a)]. Note that, at weak strains $\sigma/E \ll 1$, $a/L_{\min}=L_{\min}/L_g=\sigma/Y \ll 1$. Thus, in a brittle solid, where fracture occurs at strains σ/Y of order 5–10%, the size range for L in Eq. (9), which corresponds to the regime with the directed diffusion in Fig. 2(c), can be very large. As $gL_{\min}/k_BT=gaY/\sigma k_BT=T_mY/\sigma T$, Eq. (8) can be rewritten in the form

$$R_N \sim \exp(-gL_{\min}/k_BT) \quad (d=2) , \tag{8$'$}$$

which is similar to the first line of Eq. (7b) with L_g, however, replaced by $L_{\min}$. Note that the ratio $L_g/L_{\min}=Y/\sigma$ is large for weak strains σ/Y. In this case the rate predicted by Eq. (8′) is enormously larger than that predicted by the conventional nucleation theory, Eq. (7b).

We proceed to detail our arguments. Once again, for simplicity, we will first consider a 2D solid under a constant uniaxial stress σ ($\sigma \ll Y$), with a crack of size $2L$. In the absence of interactions between the opposing crack edges, the crack opening displacement d is given by Eq. (2). In reality, the attractive short-range interactions will try to close the crack, i.e., to heal the solid. Let the range of these interactions be of the order of the atomic size a. By demanding that $d<a$, one obtains from Eq. (2) that $L<L_{\min}=a(Y/\sigma)$. For cracks with $L<L_{\min}$ the attractive forces between the crack edges are important. Moreover, since $d<a$ for $L<L_{\min}$, various irreversible, processes restructuring the profile of the crack edges, such as atomic migrations via surface diffusion,[11] or surface reconstruction, are suppressed. Such processes might create a mismatch between the upper and lower crack edges and prevent microcrack healing even when the external stress is released. However, for a fresh crack with $L<L_{\min}$, i.e., $d<a$, surface processes which restructure the crack edges are suppressed and the kinetics of its size can still be well described by a standard Langevin dynamics, Eq. (6), with $E(L)\cong gL$. Then the typical time scale for activating a crack of size $L_{\min}$, t_1, behaves as $t_1 \sim \exp(E_{\min}/k_BT)$, with

$$E_{\min}=E(L_{\min})\cong gL_{\min}=gaY/\sigma=k_BT_mY/\sigma .$$

Thus we have

$$t_1 \sim \exp(gL_{\min}/k_BT)=\exp[(Y/\sigma)(T_m/T)] . \tag{10}$$

A crack of size $L_{\min}$ will grow until, after another time scale t_2, its size reaches the Griffith length L_g. At time scales $t>t_N=t_1+t_2$ the nucleation process is over and the crack size will start to increase rapidly. In the following we will argue that, like t_1,

$$t_2 \sim \exp(gL_{\min}/k_BT) . \tag{11}$$

Equations (10) and (11) imply our main result, Eq. (8), for the crack nucleation rate $R_N=1/t_N=1/(t_1+t_2)$ in a 2D solid.

It remains to justify Eq. (11). To this end, we note that the distance between the crack edges $y(x)$ as a function of the distance from the crack center, x (see Fig. 1) is[12]

$$y=d[1-(x/L)^2]^{1/2} , \tag{12}$$

with d as in Eq. (2). Equation (12) is derived by ignoring the short-range attractive interactions between the crack edges, which have a range of the order of atomic size a. So, the crack profile deviates from (12) in the vicinity of crack tips, only when $y(x)<a$ (see Fig. 1). Let $s(L)$ denote the distance from the crack tip for which the distance between the crack edges is equal to the atomic size a (Fig. 1). It is then straightforward to show from Eqs. (2) and (12) that

$$s(L)=a^2Y^2/L\sigma^2 . \tag{13}$$

We will term the interval $[L-s(L)]<x<L$ as the *tip zone*. Thus, within the tip zone the distance between the crack edges is smaller than the atomic size. Note that, by (13) and (9), as L increases from $L_{\min}$ to L_g, the length of the tip zone $s(L)$ decreases from $s(L_{\min})=L_{\min} \gg a$ to $s(L_g)=a$.

Introduction of the tip zone length $s(L)$ allows us to discuss qualitatively the influence of various irreversible surface processes, such as surface reconstruction or surface diffusion,[11] on the kinetics of a crack with size in the range $L_{\min}<L<L_g$. For such a crack, the maximal crack opening displacement, Eq. (2), is bigger than the atomic size a. This, for example, allows atoms to migrate freely along the crack edges via the process of surface diffusion.[11] This process might create a mismatch between the upper and lower crack edge and thereby prevent crack healing, even when the external stress is released completely. This suppression of the solid's healing, by the restructuring of crack edges, is obviously even stronger if the external stress is held constant, as presumed here. Thus, in contrast to microcracks with $L<L_{\min}$, a microcrack with size L in the interval $L_{\min}<L<L_g$ behaves more like a *quenched* defect of the solid. Nevertheless, some healing of the solid is still possible within the crack tip zone: Atoms diffusing along crack edges and restructuring them cannot enter the tip zone in which the distance between crack edges is smaller than the atomic size a (see Fig. 1). This implies that the evolution from the size L to the size L', with $L'-L$ *smaller* than the tip zone length $s(L)$, can still be described by the Langevin dynamics, Eq. (6), which neglects the restructuring of crack edges inhibiting crack healing. Thus, the dynamics of the crack size, growing from L to $L+s(L)$, can be described by the Langevin equation (6) with the *constraint* $L(t)>L$, imposed by the surface processes that create mismatch between crack edges and inhibit crack healing. So, the time $\Delta t(L)$ needed for the crack size to grow from L to $L+s(L)$ can be estimated from the Arrhenius law $\Delta t(L) \sim \exp(\Delta E/k_B T)$, with $\Delta E = E[L+s(L)]-E(L)$ and $E(L) \cong gL$. Thus $\Delta E \cong gs(L)$, and

$$\Delta t(L) \sim \exp[gs(L)/k_B T] \ . \tag{14}$$

Once the crack size has reached $L+s(L)$, the crack will continue to grow to the size $L+s(L)+s(L+s(L))$ governed by the Langevin dynamics Equation (6) with the directed growth constraint $L(t) > L+s(L)$, which will take a time of the order

$$\Delta t(L+s(L)) \sim \exp[gs(L+s(L))/k_B T] \ ,$$

according to Eq. (14). This process continues until $L(t)$ reaches the Griffith length L_g when the nucleation process is over and rapid fracturing process takes over.

As time scales longer than $\Delta t(L)$, the crack size evolution has a directed character, since $L(t+\Delta t) = L(t)+s(L(t))$ is bigger than $L(t)$. This is illustrated in Fig. 2(c) [note that the crack healing, $dL/dt < 0$, is possible *only* on time scales shorter than $\Delta t(L)$, corresponding to the length scale $s(L)$]. One can characterize this directed evolution by introducing the mean crack size velocity which characterizes its growth from L to $L+s(L)$ during the time $\Delta t(L)$ estimated by Eq. (14):

$$v(L) = s(L)/\Delta t(L) \sim s(L)\exp[-gs(L)/k_B T] \ . \tag{15}$$

Now we can estimate the time t_2 needed for a microcrack size to grow from $L_{\min}$ to L_g:

$$t_2 = \int_{L_{\min}}^{L_g} \frac{dL}{v(L)} \sim \int_{L_{\min}}^{L_g} \frac{dL}{s(L)} \exp[gs(L)/k_B T] \ . \tag{16}$$

At low T, this integral is dominated by its lower bound at $L = L_{\min}$, where $s(L)$ attains its maximal value $s(L_{\min}) = L_{\min}$. Thus $t_2 \sim \exp(gL_{\min}/k_B T)$. This justifies Eq. (11) and completes the derivation of our main result stated in Eqs. (8′) and (8). Note that the corresponding nucleation rate

$$R_N \sim 1/t_1 \sim 1/t_2 \sim \exp[-gL_{\min}/k_B T] \ ,$$

Eq. (8′), depends crucially on the length scale $L_{\min}$, while being practically *independent* of the Griffith length L_g [see, for example, the integral (16) which is, at low T, dominated by its lower bound $L_{\min}$ rather than by its upper bound L_g]. In the *absence* of surface restructuring processes, on the other hand, the rate depends dominantly on L_g via $R_N \sim \exp(-gL_g/k_B T)$, Eq. (7b). Since $L_{\min}/L_g = \sigma/Y$, the rate estimate in (8′) is, at weak strains σ/Y, enormously larger than that in Eq. (7b).

Let us emphasize some important consequences of our new picture of microcrack nucleation.

(i) The crack nucleation rate, at low T and σ, is much bigger than that predicted by naively applying the conventional nucleation theory, i.e., Eq. (5), appropriate for the nucleation processes in supercooled liquids, supersaturated solutions, and other simple metastable states. The causes of this are irreversible processes, such as surface diffusion, which restructure crack edges. We assume that these processes are sufficiently rapid to hinder crack healing. To justify this assumption we note that the typical time scale for surface diffusion behaves at low T as $\exp(ga/k_B T)$.[11] This time scale is much smaller than the typical crack growth time scale, which, by Eq. (14), behaves as $\exp[gs(L)/k_B T]$. We recall that $s(L)$, Eq. (13), varies from $L_{\min} \gg a$ to a, as L increases from $L_{\min}$ to L_g.

(ii) Our picture indicates that a solid under a stress is not a simple metastable state with microcracks being direct analogs of, say, the subcritical stable phase droplets in a supercooled liquid. There a subcritical droplet has a single metastable state that is analogous to cracks of sizes $L < L_g$. In contrast to this naive analogy, we propose a picture of the nucleation process that can be qualitatively interpreted as a passage of a given crack through a sequence of quasimetastable states: a crack spends within each of these states a time of the order $\Delta t(L)$, Eq. (14), during which its length increases from L to $L+s(L)$, with $s(L)$ given by Eq. (13) [see Fig. 2(c)]. At times scales shorter than $\Delta t(L)$, the crack state is like a metastable state in which crack healing is allowed, as depicted in Fig. 2(c), and $L(t)$ evolves according to the standard Langevin dynamics equation (6). As the crack size grows from 0 to L_g, it passes through N quasimetastable states, where

$$N = \int_0^{L_g} \frac{dL}{s(L)} = (L_g/L_{\min})^2 \cong (Y/\sigma)^2 \gg 1 \ .$$

We stress that these states are not *true* metastable states that occur, for example, if the crack potential energy $E(L)$ in Eq. (6) has multiple minima. In this case one may have returns from a state corresponding to a bigger L to one corresponding to a smaller L. On the other hand, for the quasimetastable states, these returns are forbidden by the surface restructuring processes.

(iii) Our discussion can be extended to microcracks in a three-dimensional solid. For a penny-shaped crack of radius L, Eq. (1) is replaced by $E(L) = gL^2 - \sigma^2 L^3/Y$ yielding L_g as in Eq. (3) and, within the conventional crack nucleation theory, the estimate

$$\begin{aligned} R_N &\sim \exp[-E(L_g)/k_B T] \\ &= \exp[-g(L_g)^2/k_B T] \\ &= \exp[-(Y/\sigma)^4 (T_m/T)] \quad (d=3) \ . \end{aligned} \tag{17}$$

Here $T_m = ga^2/k_B$ is a characteristic temperature comparable to the melting temperature of the 3D solid, and $g = aY$. On the other hand, our new picture of the crack nucleation process yields, in analogy to Eqs. (8) and (8′), the nucleation rate $R_N \sim \exp[-g(L_{\min})^2/k_B T]$, where $L_{\min}$ is, as before, the crack size for which the maximal crack opening displacement d equals the atomic size a. $L_{\min}$ can be estimated from Eq. (2), which is valid also for penny-shaped cracks in 3D. This yields the same estimates for $L_{\min}$ as in 2D, Eq. (9). Thus

$$R_N \sim \exp[-(Y/\sigma)^2 (T_m/T)] \quad (d=3) \ . \tag{18}$$

Note that the difference between the estimates (17) and (18) is significantly larger than that between the corresponding results in 2D, Eqs. (7b) and (8).

(iv) Our theory ignores some potentially interesting aspects of the fracture physics; for example, plastic deformations in the vicinity of crack tips (which, however, can be weak in a brittle solid, as appears to be the case for iron whiskers[8,9]).

In conclusion, in the present work we propose a simple phenomenological theory of microcrack nucleation in stressed solids, which accounts for the effects of irreversible processes restructuring crack surfaces. These processes, by inhibiting crack healing, significantly enhance the microcrack nucleation rate.

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