

Mechanism of time-delayed fractures

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We use atomistic Monte Carlo simulations to reexamine competing theories of fracture nucleation in solids under weak external stresses. We argue that the energy of the critical Griffith crack is not the actual barrier for thermal fracture nucleation in brittle solids as frequently assumed. The nucleation is dominated by the activation of vacancy clusters and not of microcracks, as assumed in the conventional theory of fracture nucleation.

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I. INTRODUCTION

Fundamental aspects of the fracture physics, such as the very nature of the state of a stressed solid and the role of thermal fluctuations, have been addressed in a number of recent studies [1–5]. There it is posited that a stressed solid can be treated as a metastable state of matter analogous to, say, supercooled liquids. In this picture, the failure threshold corresponds to a metastability limit, or spinodal point, at which the external stress σ as a function of the strain reaches its maximum σ_{\max} [2–4].

If the external tensile stress is smaller than σ_{\max} , the stressed sample will still break, however, with a time-delayed fracture. The sample lifetime depends on the temperature and the applied stress [6]. This phenomenon is believed to be directly related to the process of *microcrack nucleation* and growth [2–5]. Microcrack nucleation is phenomenologically similar to that of the stable phase droplets in a metastable state [7]. The seminal work of Griffith on fracture mechanics [8] already contains all the elements to construct a phenomenological theory of microcrack nucleation. The critical, Griffith crack behaves like a critical droplet: Cracks larger than the Griffith crack grow irreversibly in a rapid fashion [9]. On the other hand, the growth of cracks that are smaller than the Griffith crack size is energetically disfavored. Their size can still change in time, however, in a slow fashion via an activation dynamics [4,5].

In this picture, the energy of the Griffith critical microcrack is naturally identified as the relevant energy barrier for the fracture nucleation. Thus, the rate of nucleation R_N behaves as $R_N \sim \exp(-E_b/k_B T)$, where the energy barrier E_b is identified with the Griffith crack energy E_g . Such a picture of fracture nucleation is frequently accepted as plausible. We shall refer to this picture as the *conventional* theory of fracture nucleation.

Recently, this conventional theory has been challenged by Golubović and Feng (GF) [5]. GF argued that the effective fracture nucleation barrier is much smaller than the Griffith energy E_g . In their phenomenological model, GF include irreversible processes such as the surface diffusion that restructures microcrack surfaces. This restructuring inhibits microcrack healing and thus yields a fracture nucleation rate much faster than the rate given

by the conventional theory.

In this paper we use atomistic Monte Carlo simulations to critically reexamine the fracture nucleation problem. We argue that the Griffith crack energy is not the actual barrier for the fracture nucleation in stressed solids. We find that critical stress-induced defects leading to fracture nucleation have primarily the character of *vacancy clusters* (microcavities), not of Griffith-type critical microcracks. Thus, the relevant energy barrier for thermal fracture nucleation is the energy of a critical vacancy cluster. This energy barrier turns out to be the same as the barrier suggested by Golubović and Feng in Ref. [5].

This paper is organized as follows. In Sec. II we review phenomenological theories of fracture nucleation. In Sec. III we present results of our simulations and interpret them in Sec. IV discussing vacancy clusters. In Sec. V we discuss our results.

II. PHENOMENOLOGICAL THEORIES OF FRACTURE NUCLEATION IN BRITTLE SOLIDS

We begin by reviewing first the conventional theory of fracture nucleation inspired by the pioneering work of Griffith [8]. In this picture microcracks play a role analogous to that of the stable phase droplets in a metastable state. Griffith established a criterion for crack growth by estimating the energy cost of creating a brittle crack of length L in a solid under a uniaxial stress σ perpendicular to the crack. Creation of the crack, for example, in a *two-dimensional solid*, costs an energy of the order

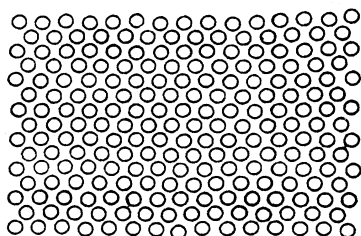
$$E(L) = gL - \frac{\sigma^2 L^2}{2Y} . \quad (1)$$

The first term in (1) is the energy cost of creating 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 of the order

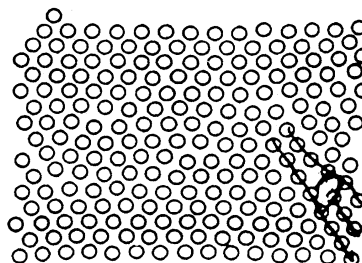
$$d = \frac{\sigma}{Y} L , \quad (2)$$

where Y is the Young modulus. The crack opening relaxes the stress in a domain of size L^2 and lowers the elas-

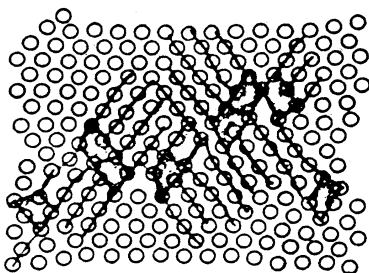
$f=120$, time=400



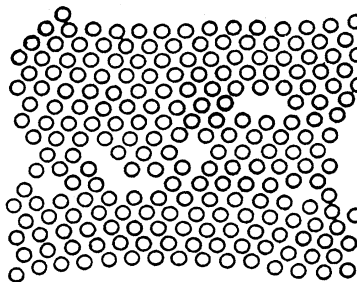
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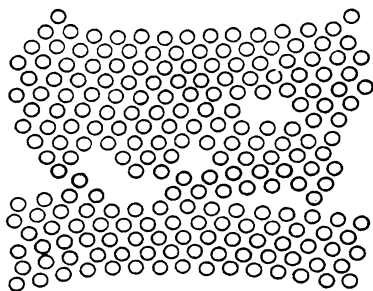
$f=120$, time=900



$f=120$, time=1000



$f=120$, time=1100



$f=120$, time=1400

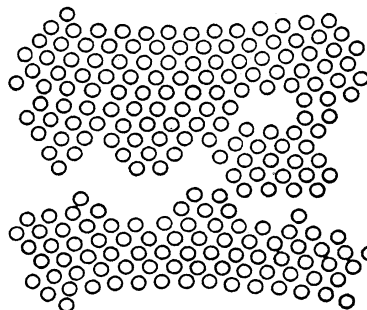


FIG. 1. “Instantaneous” fracture under a strong tensile force $f=120$ at the temperature $k_B T=0.15$ (in units for which the standard parameters of the Lennard-Jones potential are unity, i.e., $\sigma_{LJ}=1$ and $\epsilon_{LJ}=1$).

tic energy of the stressed solid 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. [For simplicity, in (1) and (2), and in the following, we suppress various numerical factors of order unity.] Crack energy (1) reaches its maximum at L equal to the critical Griffith length L_g ,

$$L_g = \frac{gY}{\sigma^2}, \quad (3)$$

corresponding to the energy of the order

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

The crack state with $L=L_g$ is unstable. For $L > L_g$, the crack growth decreases $E(L)$. This leads to the well-known irreversible, very rapid crack growth [9]. For $L < L_g$, an increase of L costs a positive amount of energy (1). This hinders the crack growth for $L < L_g$. This picture resembles that of standard nucleation phenomena [7], with E_g playing the role of the nucleation energy barrier E_b . Thus nucleation rate R_N —or the time needed for the fracture to be nucleated by thermal fluctuations—can be, in general, estimated by the Arrhenius law [7]

$$R_N = \frac{1}{t_N} \sim \exp\left[-\frac{E_b}{k_B T}\right]. \quad (5)$$

Within the conventional fracture nucleation picture E_b is identified with E_g ,

$$E_b = E_g = \frac{g^2Y}{\sigma^2}. \quad (6)$$

This conventional theory was criticized by Golubović and Feng (GF) [5]. They consider *surface processes* such as *surface diffusion* [10], which restructure crack edges and may *inhibit* healing of microcracks shorter than the Griffith length (3). These processes become active as soon as the crack opening displacement in Eq. (2) becomes larger than the atomic size a . By (2), this happens for $L > L_{\min}$ with

$$L_{\min} = \frac{aY}{\sigma}, \quad (7)$$

or, as $g \approx aY$,

$$L_{\min} = \frac{g}{Y}. \quad (8)$$

By considering surface processes inhibiting crack healing, GF argued that the effective energy barrier for the fracture nucleation is of the order $E(L_{\min})$. Thus, by (8) and (1),

$$E_b = E(L_{\min}) = gL_{\min} = \frac{g^2}{\sigma}, \quad (9)$$

in the phenomenological theory of fracture nucleation proposed by GF.

By (3), (4), (8), and (9),

$$\frac{E_g}{E(L_{\min})} = \frac{L_g}{L_{\min}} = \frac{Y}{\sigma}. \quad (10)$$

Thus, for weak strains σ/Y , the nucleation rate predicted by GF is enormously larger than that of the conventional theory.

III. NUMERICAL SIMULATIONS

To clarify the nature of fracture nucleation we performed atomistic Monte Carlo simulations of a two-dimensional (2D) Lennard-Jones solid under a tensile stress. Our simulation is similar to a recent simulation of Selinger, Wang, and Gelbart [4]. Their main objective was to obtain the temperature dependence of the fracture stress σ_{\max} under which the solid breaks instantaneously, i.e., with no significant time delay. σ_{\max} corresponds to the spinodal point, i.e., to the maximum of the σ versus strain curve [4].

Our main concern here is fracture nucleation phenomena in a time-delayed fracture. Let us first illustrate the difference between the “instantaneous” fracture, occurring for $\sigma > \sigma_{\max}$, and the time-delayed fracture, occurring for $\sigma < \sigma_{\max}$. In Fig. 1 we give the time evolution of the solid under a *strong* external tensile force f along the vertical direction. We see a rapid nucleation of numerous dislocation dipoles that *cooperatively* generate a fracture going across the sample at the time $t \sim 1200$ MCC [one Monte-Carlo Cycle (MCC) involves updates of *all* particles’ positions via the standard Metropolis algorithm].

With decreasing tensile force, one crosses over from this instantaneous fracture to a time-delayed fracture. This is illustrated in Fig. 2, giving the time evolution of the sample’s vertical size for various values of the tensile force f . At a *weak* tensile stress, the sample’s vertical size vs time has a plateau ending at the instant of fracture, at the time scale $t \sim 1/R_N$. Thus the fracture is delayed in time.

Figure 3 illustrates the time evolution of a sample under a weak tensile force yielding a long metastable plateau, i.e., a long sample lifetime of the order 10^5 MCC. Up to $t \sim 5000$ MCC, we observe in Fig. 3 only rare dislocation dipoles or isolate dislocations generated from the

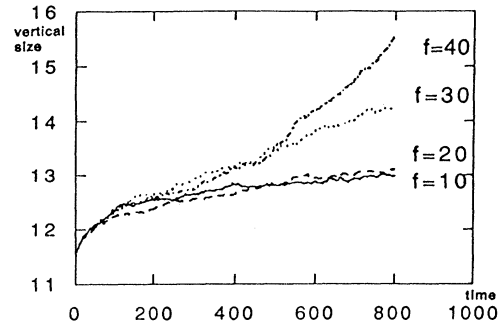


FIG. 2. Time evolution of the sample’s vertical size for various values of the tensile force f .

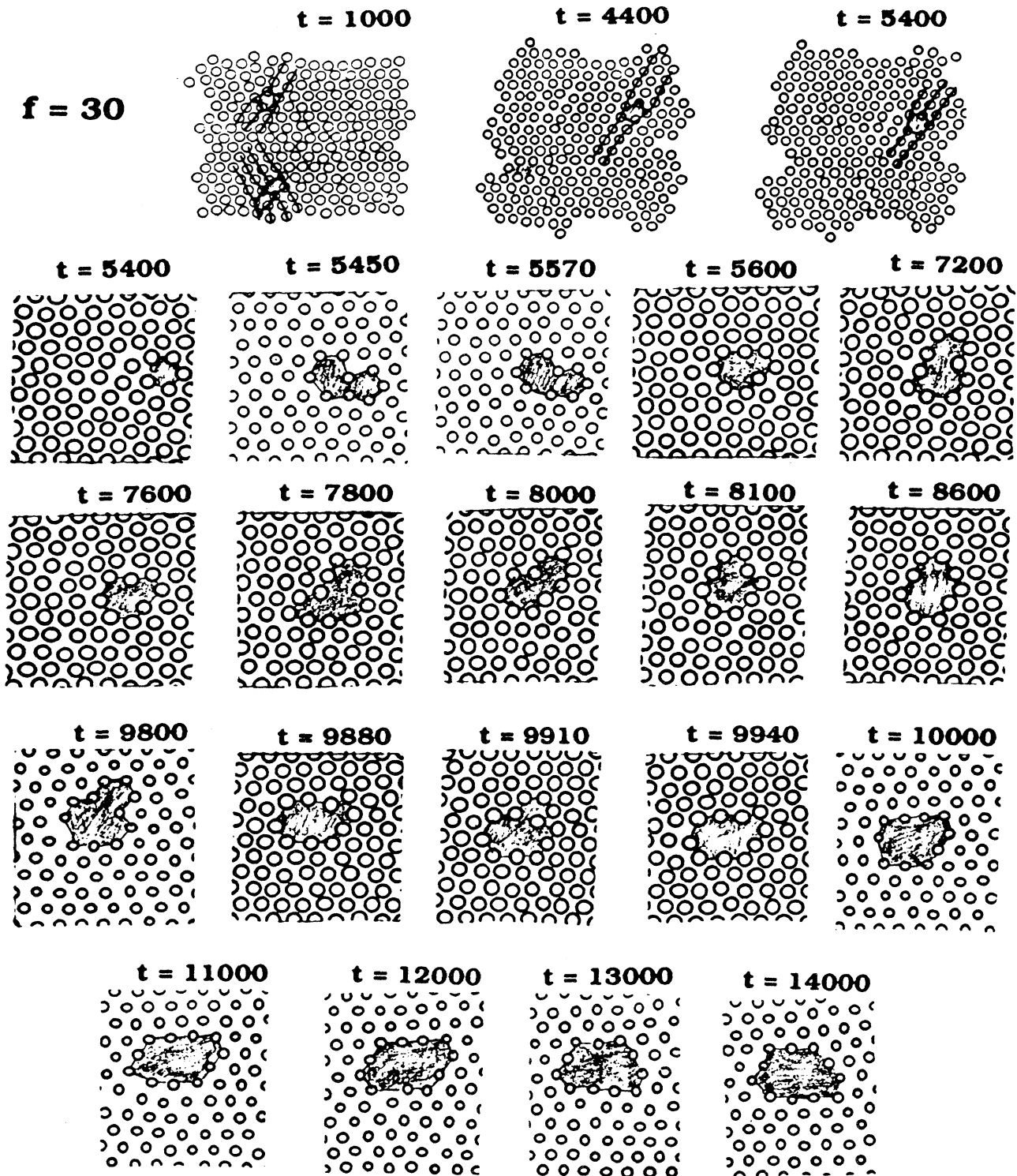


FIG. 3. Vacancy cluster nucleation in a time-delayed fracture under a weak external force $f=30$. Note that in most of the figures we give only a portion of the sample around the microcavity. (The size of the circles representing the atoms is of no significance. In some figures we use smaller circles to make atomic configurations more clear.)

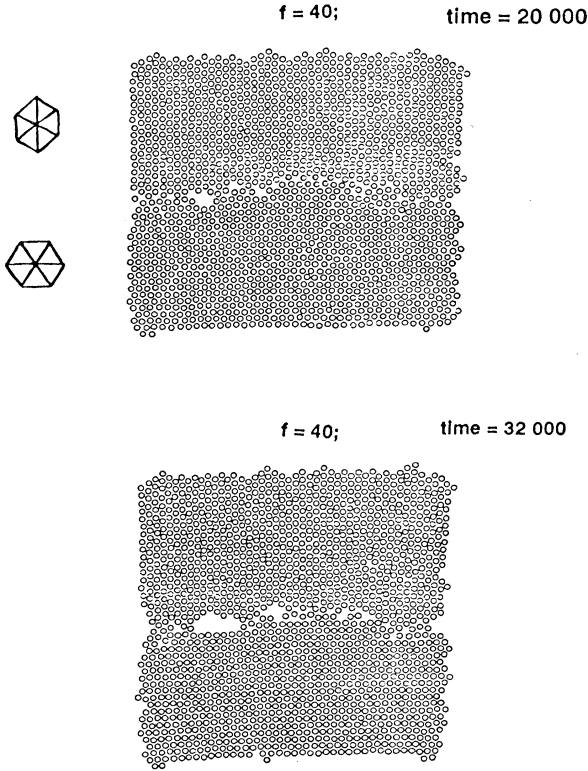


FIG. 4. Intergranular microcavities nucleated in a polycrystalline sample under a weak tensile force $f=40$. (Note that, due to a larger size of this sample, the stress here is smaller than in the monocrystal in Fig. 3.)

surface of the sample. Their number is not increasing with time indicating that the system is in a local, metastable equilibrium. This is in contrast to the instantaneous fracture in Fig. 1, where a metastable equilibrium is absent and the solid is actually unstable.

However, between $t=5400$ and 5600 MCC, a crucial event occurs in Fig. 3. During this time interval one of the dislocations evolves into a small *microcavity* having the same Burgers vector as the original mother dislocation. In the evolution that follows, the microcavity increases in size, whereas its Burgers vector remains constant up to $t \approx 12\,500$ MCC, when the microcavity “neutralizes” by a slip becoming an ordinary *vacancy cluster* with zero Burgers vector (see Fig. 3 at $t=13\,000$ MCC).

As another example, in Fig. 4 we illustrate the behavior of a larger *polycrystalline* sample containing a *grain boundary*. Again, the dominant defects that are thermally nucleated in a weak external stress are vacancy clusters, now in the form of *intergranular* microcavities.

IV. NUCLEATION OF VACANCY CLUSTERS (MICROCAVITIES)

The message of the simulations of Sec. III, is that microcavities (i.e., clusters of vacant sites) rather than microcracks (i.e., lines or surfaces of “broken bonds”) are major nucleated defects in the delayed fracture regime. Thus, the major kinetic process in the time-delayed frac-

ture is the nucleation of vacancy clusters or microcavities (possibly having some nonzero Burgers vector), *not* of critical Griffith-type microcracks. The energetics of a vacancy cluster nucleation is rather different from that of the Griffith crack (Sec. II). For comparison with Sec. II, let us consider a vacancy cluster in a 2D solid. If R is its linear size, the cluster involves $\approx (R/a)^2$ vacant sites. Its size-dependent energy is of the form

$$E_{\text{vac}}(R) = gR - \sigma R^2. \quad (11)$$

The first term in (11) is, as in Eq. (1), the surface energy contribution (\sim perimeter $\sim R$ in 2D). The second term in (11) is a stress-induced volume contribution (\sim area $\sim R^2$ in 2B) [11]. This volume term can be rationalized as follows. Consider a solid under a tensile stress σ with no vacancy cluster initially present. As the number of atoms is conserved, the creation of the cluster induces an increase of the sample’s linear size preferentially along the direction of the applied stress [11]. This lowers the energy by $\delta E = \text{stress} \times \text{cluster volume} \sim \sigma R^2$ yielding the second term of Eq. (11).

By Eq. (11), the size of the critical vacancy cluster, maximizing $E_{\text{vac}}(R)$, is of the order

$$R_c = \frac{g}{\sigma}, \quad (12)$$

whereas the energy barrier for the vacancy cluster nucleation is of the order

$$E_b = E_{\text{vac}} = \frac{g^2}{\sigma}. \quad (13)$$

This energy-barrier scale for fracture nucleation coincides with that in Eq. (9) obtained by Golubović and Feng [5], however, from seemingly different arguments.

V. DISCUSSION

Our results indicate that the kinetic mechanism dominating time-delayed fractures, i.e., fracture nucleation, is the nucleation of vacancy clusters (microcavities), not of critical Griffith microcracks as assumed in the conventional fracture nucleation picture. In particular, this implies fracture nucleation rates much faster than those obtained with the conventional theory. Thus, for a 2D solid, within the microcavity nucleation picture we obtain, by using (5), (13), and $g \approx aY$,

$$R_N \sim \exp \left[-\frac{Y}{\sigma} \frac{T_m}{T} \right] \quad (d=2), \quad (14)$$

with $T_m = ga/k_B$, whereas from the conventional theory one obtains, by (6) and (7),

$$R_N \sim \exp \left[-\left(\frac{Y}{\sigma} \right)^2 \frac{T_m}{T} \right] \quad (d=2). \quad (15)$$

For weak strains $\varepsilon = \sigma/Y$ this conventional theory nucleation rate is enormously smaller than that in Eq. (14).

These conclusions apply also to a three-dimensional (3D) solid. Discussions of Secs. II and IV can be easily extended to a d -dimensional solid. For example, the en-

ergy of a vacancy cluster of the linear size R has the form

$$E_{\text{vac}}(R) = gR^{d-1} - \sigma R^d, \quad (11')$$

whereas the energy of a microcrack of the linear size L has the form

$$E(L) = gL^{d-1} - \frac{\sigma^2 L^d}{2Y}, \quad (1')$$

and $g \approx aY$. Within the microcavity picture one thus obtains

$$R_N \sim \exp \left[- \left[\frac{Y}{\sigma} \right]^{d-1} \frac{T_m}{T} \right], \quad (16)$$

with $T_m = ga^{d-1}/k_B$, whereas the conventional nucleation theory would yield a much smaller rate:

$$R_N \sim \exp \left[- \left[\frac{Y}{\sigma} \right]^{2(d-1)} \frac{T_m}{T} \right]. \quad (17)$$

Microcavity nucleation yields fracture nucleation barriers and corresponding rates identical to those proposed before, in a different manner, by Golubović and Feng [5].

This agreement is *not* accidental. These authors invoke in their discussion diffusion processes that start to restructure microcrack edges as soon as the microcrack size reaches the lengthscale L_{\min} in Eq. (8). This lengthscale coincides with the size of the critical vacancy cluster R_c in Eq. (12). As $R_c = L_{\min}$, one may argue that the processes restructuring microcrack edges would transform the microcrack of the size L_{\min} into a microcavity of the size R_c , which then continues to grow irreversibly. In this way one can rationalize the suggestion of Golubović and Feng that a crack with $L = L_{\min}$ never heals and continues to grow irreversibly. Thus, L_{\min} , rather than the Griffith length L_g in Eq. (3), is the critical size of defects in solids under weak tensile stresses.

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