Nucleation phenomena in an annealed damage model: Statistics of times to failure

S. G. Abaimov[1,*] and J. P. Cusumano[2,†]

[1]*Department of Theoretical Physics, Moscow Institute of Physics and Technology, Moscow, Russia*

[2]*Department of Engineering Science and Mechanics, Pennsylvania State University, University Park, Pennsylvania, USA*

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In this paper we investigate the statistical behavior of an annealed continuous damage model. For different model variations we study distributions of times to failure and compare these results with the classical case of metastable nucleation in statistical physics. We show that our model has a tuning parameter, related to the degree of damage reversibility, that determines the model's behavior. Depending on the value of this parameter, our model exhibits statistical behavior either similar to classical reversible nucleation phenomena in statistical physics or to an absolutely different type of behavior intrinsic to systems with damage. This comparison allows us to investigate possible similarities and differences between damage phenomena and reversible nucleation.

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I. INTRODUCTION

Damage as a complex phenomenon has been studied by many authors. Studies that have recently appeared in the literature illustrate the similarity between damage phenomena and phenomena of phase transitions [1–3]. This similarity provides an opportunity to apply the well-developed formalism of statistical physics to the occurrence of damage. Indeed, many approaches [2–4] have been developed to apply equilibrium statistical mechanics to damage phenomena. However, this question remains far from being completely resolved since damage phenomena usually exhibit more complex behavior than gas-liquid or magnetic systems [3,5].

The approaches used to model damage can generally be separated into two different categories: quenched or annealed. In the case of quenched damage, the ensemble of systems is represented by the initial distribution of system properties, and fluctuations are attributed to differences in this initial ensemble. This type of behavior can be described by the formalism of statistical physics [3,5]. However, damage growth in this case is governed not by fluctuations occurring in time but by the "frozen," "topological" fluctuations of the initial ensemble. This type of behavior is to be expected in the case of brittle fracture when the dynamical time scale of fracture is much faster than the time scale of material relaxation, so that dissipation processes have no time to attenuate the quenched defects.

On the contrary, in the case of annealed damage the system's behavior is governed by fluctuations occurring during its evolution. These types of phenomena directly inherit their behavior from the formalism of thermal fluctuations in statistical physics. The main representative of the annealed damage model is the Griffith theory, in which a crack that has appeared as the result of a fluctuation can either disappear or grow in size. These types of phenomena usually represent the case of quasistatic load increase when relaxation processes have enough time to provide a "choice" for the crack to either grow or heal.

In this paper we investigate the annealed behavior of a continuous damage model [6]. We consider two major regimes of damage growth: postcritical and precritical. In the case of postcritical (or supercritical) loading we consider the values of initial damage which are much higher than the critical threshold. Due to the presence of nuclei with sizes larger than critical the damage growth is fast, and the role of fluctuations in the ensemble is determined by the quenched disorder of the initial damage.

As the second regime we consider the precritical (subcritical) damage nucleation when the initial values of damage are much lower than the critical threshold (all initial nuclei have sizes much smaller than the critical). The role of fluctuations in this case is played by a noise term we introduce into the mesoscale equation so that the nucleation in the metastable state is performed by means of annealed damage growth.

In Sec. II we introduce the model, while the statistical distributions used in our study are presented in Sec. III. In Sec. IV we investigate postcritical damage growth in the presence of damage nuclei above a critical size. In Sec. V we introduce noise into the system to simulate the irreversible behavior of precritical damage nucleation, for which initially there are no nuclei larger than the critical size. In Sec. VI, to make a correspondence with classical phenomena of nucleation, we investigate what happens if our model becomes reversible. In Sec. VII we introduce a tuning parameter which switches the behavior of the system from the irreversible, "damage" type to the reversible, "classical" type intrinsic to statistical physics.

II. MODEL

In this paper we utilize the continuous damage model developed by Cusumano *et al.* [6]. The model is used to simulate the coupled macroscale-mesoscale physics of elastic media and is based on the principle of stationary action in theoretical mechanics.

The model follows the evolution of longitudinal displacements $u(t, x)$ and damage $\varphi(t, x)$ in the time-space domain until the point of failure when at some location the damage φ reaches unity. In Ref. [6], the damage variable φ is interpreted

*Current address: Advanced Structures, Processes and Engineered Materials Center, Skolkovo Institute of Science and Technology, Moscow, Russia; sgabaimov@gmail.com

†jpc3@psu.edu

as a microcrack or microvoid density, and the nondimensional coupled-field evolution equations are

$$\frac{\partial^2 u}{\partial t^2} - c\nabla^2 \frac{\partial u}{\partial t} - \nabla(1-\varphi)\nabla u = 0, \tag{1}$$

$$\frac{\partial \varphi}{\partial t} = \eta\left\langle \frac{\varphi}{2}(\nabla u)^2 - \alpha\varphi^{2/3} \right\rangle, \tag{2a}$$

$$u|_{x=0} = 0, \quad \{(1-\varphi)\nabla u\}|_{x=1} = F, \tag{3}$$

where angle brackets indicate the positive part (that is, $\langle \Phi \rangle = \Phi$ for $\Phi \geqslant 0$ and zero otherwise), which makes damage growth in our model irreversible (that is, when there is no "healing," the damage can only grow). The parameter c indicates the strength of macroscale damping processes in the system, and parameter η represents the time scale of damage growth.

The term $\alpha\varphi^{2/3}$ is determined using Griffith energy arguments, and represents the critical threshold above which the damage is allowed to grow. The derivation of this term, including the power 2/3, is discussed in detail in Cusumano *et al.* [6].

In our simulations, a continuous model with 128 finite elements is used. Numerical simulations are accomplished with program code based on the Open Source Library deal.II [7]. Further details on the model and its numerical implementations can be found in Ref. [6].

The rate of damage growth, given by Eq. (2a), is proportional to the difference between the tendency for the damage to grow $\frac{\varphi}{2}(\nabla u)^2$ and the critical threshold $\alpha\varphi^{2/3}$. Only damage above the critical value $\varphi_C = [\frac{2\alpha}{(\nabla u)^2}]^3$ is allowed to grow. This works much like a threshold in the Griffith theory for a single crack, or a potential barrier in nucleation. However, in the case of our continuous model [6] we consider not separate cracks but mesoscopic nuclei where each nucleus represents a distribution of microcracks or other defects in a small volume.

The initial values of damage in each simulation must be nonzero since, otherwise, the derivative $\partial\varphi/\partial t$ in Eq. (2a) is zero and does not provide damage growth (the rate of damage growth has a power-law dependence on φ and hence is zero if the damage is zero). Therefore, in all ensembles considered below we choose the initial values of damage to be nonzero with the magnitude and stochastic distribution determined by the ensemble.

One main difference between the model employed by Cusumano *et al.* [6] and that used for our simulations is that we utilize a constant load $F = 3 \times 10^{-4}$ as an external boundary constraint. We choose constant load for this paper for multiple reasons. First, the majority of results in statistical physics are for constant boundary constraints, and since one of the major goals of this study is to compare damage and classical phenomena of nucleation, to develop this comparison we utilize a constant loading here. Second, fatigue behavior of a system under an oscillating load is more complex than the damage arising from a constant load. Therefore, we follow the principle of going from "simple to complex" and postpone the investigation of cyclic fatigue arising from load oscillations to future studies.

Throughout the manuscript we utilize different numerical values for the parameters of Eqs. (1)–(3). These numerical values do not represent specific constants or known properties of particular systems. Instead, they are chosen merely to yield reasonable times for numerical simulations at the Penn State University Unix cluster. Since in the paper we consider very different ensembles, from the postcritical to the precritical with irreversible or reversible damage, simulations of each ensemble generally require their own set of parameters. The time of these numerical simulations is very sensitive to the values of α and η: The values used in this work were chosen to limit computation time to no more than 1 month using 20 CPUs for simulations of each ensemble.

III. STATISTICAL DISTRIBUTIONS

As a convenience to the reader, we here present the probability distributions used in what follows. Throughout, we will use a lowercase p to refer to the probability density function (PDF) of the distribution, whereas a capital P will refer to the cumulative distribution function (CDF).

Sample statistical distributions of times to failure for the ensembles considered in the paper were fitted using many different trial distributions. It was found that the closest fits were provided by three distributions: namely, those of exponential, Weibull, and gamma types.

The exponential distribution,

$$p(x) \equiv \frac{1}{\mu}\exp(-x/\mu), \tag{4a}$$

$$P(x) \equiv 1 - \exp(-x/\mu), \tag{4b}$$

is a one-parameter distribution where the parameter μ represents the mean value. If a sample distribution is fitted by the exponential distribution, the results are generally presented in the form of a so-called exponential plot, wherein we plot the dependence of $-\ln[1-P(x)]$ against x so that the exponential CDF transforms into a straight line.

The Weibull distribution,

$$p(x) \equiv \frac{\beta}{x_0}\left(\frac{x}{x_0}\right)^{\beta-1} e^{-(\frac{x}{x_0})^{\beta}}, \tag{5a}$$

$$P(x) \equiv 1 - e^{-(\frac{x}{x_0})^{\beta}}, \tag{5b}$$

is a two-parameter distribution, where the parameter β is called the Weibull exponent (or shape parameter), and x_0 is the scale parameter. This distribution also has its own plot: By plotting $\ln\{-\ln[1-P(x)]\}$ vs $\ln x$ one obtains a straight line for a "pure" Weibull distribution.

Finally, the gamma distribution,

$$p(x) \equiv \frac{x^{k-1}}{\Theta^k \Gamma(k)} e^{-\frac{x}{\Theta}}, \tag{6a}$$

$$P(x) \equiv \int_0^x \frac{y^{k-1}}{\Theta^k \Gamma(k)} e^{-\frac{y}{\Theta}} dy, \tag{6b}$$

is also a two-parameter distribution, where k is the gamma distribution exponent (or shape parameter), and Θ is the scale parameter.

IV. DAMAGE GROWTH WHEN INITIAL DISORDER IS POSTCRITICAL

In this section we consider an ensemble with postcritical (supercritical) damage growth, when the initial disorder in the model is above a threshold so that nuclei larger than the critical size are present.

Using the constant load $F = 3 \times 10^{-4}$ in our simulations, the strain ∇u at early stages of damage growth is constant throughout the model and equals the load F [since Eqs. (1)–(3) are dimensionless]. For reasonable computation times, we set $\alpha = 1.2 \times 10^{-11}$ and $\eta = 1.9 \times 10^{3}$. Note, however, that the resulting statistical distribution of failure times is not sensitive to the precise parameter values.

For this value of α the critical threshold for damage is $\varphi_C \approx 2 \times 10^{-11}$. For c we use a large value, $c = 5$, to damp macroscale oscillations. For the same reason, the initial displacement u was set equal to a static solution of Eq. (1) for the given load.

For the initial values of the damage φ, similar to [6], we utilize a uniform distribution in the range from 0 to 0.01, independently and identically distributed in the spatial variable x. Given the value of the critical threshold, $\varphi_C \approx 2 \times 10^{-11}$, the initial damage at all locations is much higher than φ_C with a probability close to unity. Therefore, simulations with these initial conditions correspond to the case of damage growth well above the critical threshold, and we expect a burst evolution of damage in simulations. Furthermore, because the initial nuclei typically have sizes on the order of $10^{-4} - 10^{-2}$ (as a uniform distribution from 0 to 0.01 among 128 elements), we expect this burst evolution to be so fast and so deterministic that neither changes in irreversibility criterion nor the introduction of possible thermal microfluctuations in the system would have any significant influence on the model's behavior.

For a particular system in the ensemble, the postcritical growth of damage starts from *a priori* defined (quenched) initial values, and since well above the critical threshold annealed fluctuations can be neglected, the system follows a deterministic "trajectory" specified by the particular realization of the initial disorder. To reach material rupture, that is, a point at which the value of damage becomes equal to unity at a particular location, a finite time is required.

The damage variable is present in the equation of "interactions" [Eq. (1)] only via the expression $(1 - \varphi)$, which for small values of damage $\varphi \ll 1$ does not influence the evolution [via Eq. (1)] of u until almost the point of the rupture. Therefore, during almost the whole time prior to rupture, all locations of the model are nearly decoupled and damage in each finite element grows independently from the neighboring locations, so that $\frac{\partial \varphi}{\partial t} \propto \eta \frac{\varphi}{2} (\nabla u)^2 \propto \varphi$. Only at the latest stages of damage evolution does φ approach the value of unity, and so only at that point do the nonlinear effects of interactions between different locations begin to influence the statistics.

Thus, for small levels of damage its evolution at a particular location is nearly independent from the damage state at other locations. Therefore, the site of rupture is determined *a priori* by the location with the maximal value of the initial damage. Since for all simulations this location has the initial value of damage always close to 0.01 (as a maximum of elements of a sample distribution with the upper boundary 0.01), the times to failure are almost deterministic and have similar values for all simulations with a very small variance.

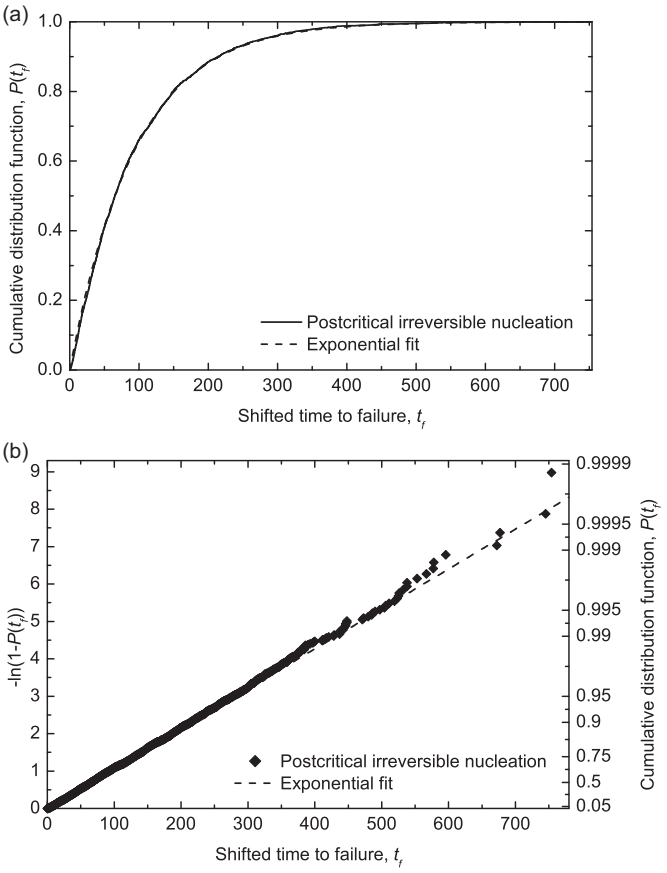

FIG. 1. Cumulative distribution function of shifted times to failure t_f for postcritical irreversible nucleation: (a) CDF plot and (b) exponential plot.

To apply trial distributions, we shift the statistics of times to failure by the minimum time to failure. The cumulative distribution function of shifted times to failure t_f is shown in Fig. 1(a) as a CDF plot, and in Fig. 1(b) as an exponential plot. Also in these figures we plot the maximum likelihood fit of an exponential trial distribution. We see that the statistics of failure times are exponential.

There is a need for experimental studies that specifically investigate postcritical failure time distributions, that is, for the case where initial disorder is above the critical threshold. We hypothesize that the exponential distributions found here are attributed to the structure of Eq. (2a) and will hold for any postcritical system governed by a similar equation.

Indeed, neglecting the threshold term in Eq. (2a) and assuming that the evolution of damage at each location is decoupled from other locations ($\nabla u = \text{const}$), we obtain

$$\frac{\partial \varphi}{\partial t} = \eta \frac{\varphi}{2} (\nabla u)^2 \propto \varphi. \tag{2b}$$

The solution of this equation is

$$\varphi(t) = \varphi(t = 0) e^{\frac{\eta (\nabla u)^2}{2} t}. \tag{7}$$

At rupture we have $\varphi(t) = 1$ so that the equation for the time of failure is

$$\varphi(t = 0) = e^{-\frac{\eta(\nabla u)^2}{2} t_f}. \tag{8}$$

From probability theory, we know that if quantity x is distributed in accordance with the PDF $p_x(x)$ and quantity y is a function of x, $y = f(x)$, to keep the probabilities invariant we require $p_y(y)dy = p_x(x)dx$. This provides the connection between two probability distributions as $p_x(x) = p_y[f(x)]\frac{df}{dx}$. Thus, since the initial values $\varphi(t = 0)$ of damage are distributed uniformly, we expect failure times to be well represented by an exponential distribution:

$$p_{t_f}(t_f) = \text{const}\frac{d}{dt_f} e^{-\frac{\eta(\nabla u)^2}{2} t_f} \propto e^{-\frac{\eta(\nabla u)^2}{2} t_f}. \tag{9}$$

On the other hand, if Eq. (2a) had the form

$$\frac{\partial \varphi}{\partial t} = \eta \left\langle \frac{\varphi^{\Theta}}{2}(\nabla u)^2 - \alpha \varphi^{2/3} \right\rangle, \tag{2c}$$

with $\Theta \neq 1$, and again neglecting the threshold term, the solution would be

$$\varphi(t) = \left\{ \varphi^{1-\Theta}(t = 0) + \frac{(1-\Theta)\eta(\nabla u)^2}{2} t \right\}^{\frac{1}{1-\Theta}}, \tag{10}$$

so that the equation for the failure time would transform into

$$\varphi(t = 0) = \left\{ 1 - \frac{(1-\Theta)\eta(\nabla u)^2}{2} t_f \right\}^{\frac{1}{1-\Theta}}, \tag{11}$$

which provides the distribution

$$p(t_f) = \text{const}\frac{d}{dt_f}\left\{ 1 - \frac{(1-\Theta)\eta(\nabla u)^2}{2} t_f \right\}^{\frac{1}{1-\Theta}}$$
$$\propto \left\{ 1 - \frac{(1-\Theta)\eta(\nabla u)^2}{2} t_f \right\}^{\frac{\Theta}{1-\Theta}}. \tag{12}$$

Note that the CDFs of distributions (9) and (12) are linear in t_f for small values of shifted failure times: $P(t_f) \sim t_f$. Therefore, analysis of the statistics extremes, as carried out in Secs. V and VI, returns us to the exponential distribution. Thus, the exponential distribution of shifted failure times is universal for postcritical damage phenomena described by Eq. (2c), for an arbitrary value of the exponent Θ. Summarizing, for the case of postcritical damage growth the observed evolution is deterministic. Above the critical threshold, any stochastic, fluctuating input during the model evolution would be negligible in comparison with the initial quenched disorder, and the evolution of the model follows a deterministic path given by Eq. (2a). For the same reason, the condition of irreversibility imposed on the model does not have any influence on the failure time statistics. Indeed, the system is well above the critical threshold, and therefore the quantity Φ in the structure $\langle \Phi \rangle$ in Eq. (2a) is always positive, so relaxing the irreversibility imposed by the positive part operator would have no effect on the system's behavior.

In the following sections we turn our attention to the precritical case, corresponding to nucleation below the critical threshold. To make this work we will need to switch from deterministic to stochastic evolution. Because only rare fluctuations will be expected to exceed the threshold level, the quantity Φ in the structure $\langle \Phi \rangle$ in Eq. (2a) will take negative values, and we expect the condition of irreversibility to significantly influence the model's behavior.

V. PRECRITICAL IRREVERSIBLE NUCLEATION

In the previous section we investigated the growth of damage for the system with postcritical initial disorder. Since the sizes of nuclei in the model were much higher than the critical value, we neglected annealed fluctuations and observed a burst evolution of damage in which the model was following the deterministic path of Eq. (2a) corresponding to the initial quenched disorder.

In this section we investigate precritical (or subcritical) behavior in which the initial nucleus sizes are much lower than the critical threshold. In contrast to the postcritical burst damage behavior of Sec. IV (where the system "rolls downwards" into a global minimum of a free energy potential), in this section we investigate the slow process of metastable damage nucleation (the system "climbs up" the potential barrier from a local, metastable minimum of the free energy potential).

In the previous section the evolution of each system in the ensemble was deterministic and was determined by the initial quenched distribution of nuclei, which at almost all locations were above the critical value. The same approach cannot be employed here since well below the critical threshold the influence of any initial disorder is negligible in comparison with the long metastable life governed by annealed stochastic fluctuations. Instead, these dynamical thermal fluctuations play the crucial role: only when their size overwhelms the potential barrier will the system rupture. Therefore, from this point on we do not use disorder in the initial conditions.

If we take a closer look at Eqs. (1)–(3), we see that Eq. (1) is macroscopic and determines the evolution of the macrodisplacement u. On the other hand, Eq. (2a) is mesoscopic, determining damage evolution on the level of defects. By using the term "mesoscopic" (instead of "microscopic") we here emphasize that the damage variable φ does not refer to individual cracks or defects, but to a density of microcracks. The microscopic, atomistic level of singular defects is not directly represented in our continuum model.

However, the implementation of microscopic dynamics is crucial for our simulations. Indeed, Eq. (2a) does not contain any possibility for the system below the critical threshold to evolve; for initial damage below this level the growth rate is zero forever.[1] In other words, Eqs. (1)–(3) of our model are deterministic and do not support fluctuating behavior. However, this formulation contradicts damage phenomena we observe in Nature: any solid has a constant process of defect birth and death due to thermal fluctuations. That is, on the microscopic level thermal fluctuations can influence the system's behavior, resulting in complex fluctuating interactions of damage and strain on this scale.

[1] In later sections we will relieve the criterion of irreversibility in order to compare our results with the theory of nucleation. For that case we will see that the threshold returns the system towards the state of zero damage.

Thus, we need to introduce thermal fluctuations into Eq. (2a) to allow for subcritical damage evolution. Each degree of freedom in statistical mechanics has averaged fluctuations of the order of $k_BT/2$ because of the equipartition of energy. If we imagine a piston on a spring as a boundary constraint for a gas in a volume, the piston will have Gaussian micro-oscillations of its position, and its averaged energy will be k_BT due to thermal fluctuations. In the same way, the neighborhood of any defect will have Gaussian microfluctuations of strain. For our model we introduce such fluctuations for the local strain as

$$\nabla u(x \cdot t) \rightarrow \nabla u(x \cdot t) + \Upsilon \xi(x,t), \tag{13}$$

where $\xi(x,t)$ is Gaussian white noise with zero mean and unit standard deviation. A similar approach has been suggested in [8–10]. Substituting Eq. (13) into Eq. (2a), we obtain

$$\frac{\partial \varphi}{\partial t} = \eta \left\langle \frac{\varphi}{2}[\nabla u + \Upsilon \xi(x,t)]^2 - \alpha \varphi^{2/3} \right\rangle. \tag{2d}$$

However, thermal fluctuations are microscopic and do not influence the mesoscopic level of Eq. (2d) directly. And, of course, they do not influence the macroscopic level of Eq. (1). Therefore, we do not include their influence in Eq. (1) for the strain evolution and we should be careful when we are including them in Eq. (2d) for the damage evolution. If, considering only microscopic thermal fluctuations, we directly substituted for ∇u in Eq. (2a) from Eq. (13), the value of Υ would be of the order of k_BT. But, again, this noise would be negligible on the mesoscopic level and would have no influence on the damage evolution.

This problem is well known in damage mechanics; and experimental studies [11,12] show that the variance of actual fluctuations is much higher than k_BT. Many authors [8,9,12–14] have attributed this behavior to complex interactions of microdisorder in a system (i.e., the presence of microdefects can cause the amplification of fluctuations). Another possibility is to associate this phenomenon with the influence of thermal fluctuations on the unstable, frustrated parts of microdefects (e.g., crack tips) at the microscopic level. Although these fluctuations are spatially and quantitatively microscopic, and influence only microscopic parts of microcracks, their presence causes damage growth on the mesoscopic level. Thus, the "sensitive" crack tip works in this case as an amplifier, causing the microscopic thermally induced fluctuations to influence the mesoscopic growth of damage nuclei. A third possible explanation is provided by considering a phenomenon observed in bubble chambers in particle physics. In that case, radiation of high-energy particles can facilitate nucleation [15] and causes the effective temperature to be higher than the "actual" temperature of a specimen. This effect should be especially noticeable for the materials working in conditions of high radiation. The suggestion that radiation can influence the growth of defects in solids requires experimental verification. However, the counterpart of this effect for gas-liquid systems is well known and widely utilized in bubble chambers.

Following the above discussion, the noise in the mesoscopic Eq. (2d) is supposed to represent not microscopic but effective mesoscopic fluctuations whose amplitude is much higher than the amplitude of thermal fluctuations. Therefore, for our simulations we choose the strain fluctuations to be of the order of the strain itself by setting $\Upsilon = 1$ in Eq. (2d).

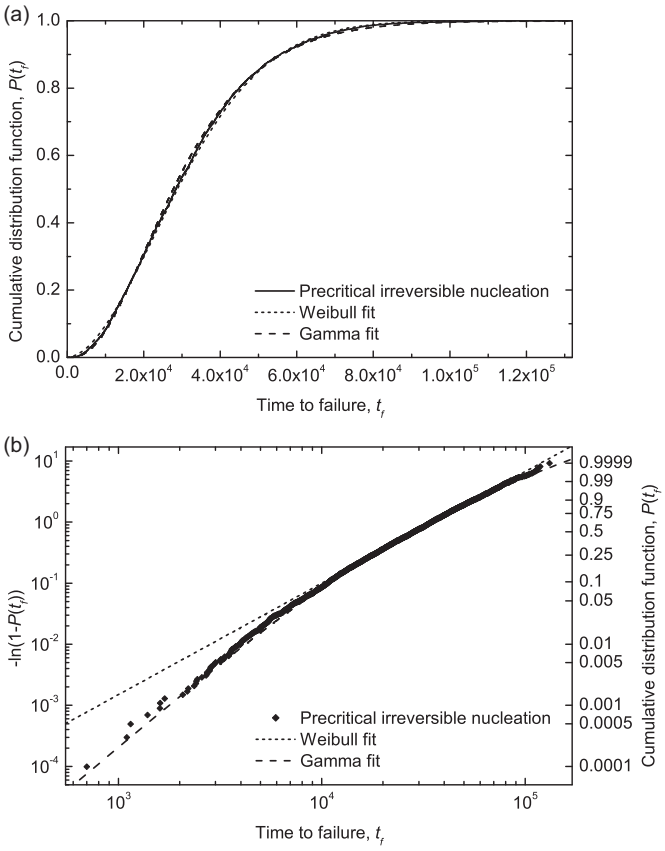

FIG. 2. Cumulative distribution function of times to failure t_f for precritical irreversible nucleation: (a) CDF plot and (b) Weibull plot.

For the damage initial conditions we choose the constant value of 1.5×10^{-6}, all along the length of the model. We do not include any stochastic variability in the initial conditions because after the long precritical evolution of the model due to the presence of noise [Eq. (13)] this "quenched" stochasticity will not influence the final results.

Again, a careful choice of parameters is required to provide a reasonable time for numerical simulations. We utilize $\eta = 10^8$ and $\alpha = 2 \times 10^{-8}$. This value of α, which represents the energy cost of opening additional free surface in a local distribution of microcracks, gives a critical damage level of $\varphi_C = [\frac{2\alpha}{(\nabla u)^2}]^3 \propto 0.01$ for $\nabla u \propto F = 3 \times 10^{-4}$. With this high, macroscopic value of the critical threshold, almost the entire damage evolution, from 1.5×10^{-6} to 0.01, is precritical nucleation. Only after a long metastable time, when the level of damage exceeds the critical threshold 0.01, does the evolution of damage switch from the precritical to postcritical regime, resulting in a sharp transition to burst damage growth. However, the duration of the postcritical burst is very short in comparison with the long, "random walk" time of many "attempts" of the precritical fluctuations to exceed the threshold. Therefore, our statistics of failure times in these simulations are almost purely those of the precritical fluctuating behavior.

The cumulative distribution function of (nonshifted) times to failure t_f is given in Fig. 2(a) as a CDF plot, and in Fig. 2(b) as a Weibull plot. Also in these figures we plot the maximum likelihood fits of the Weibull and gamma trial distributions. We see that the statistics of times to failure are close to the

Weibull distribution with exponent 1.83 ± 0.02. However, Fig. 2(b) shows that although the statistics are close to Weibull, they are, in fact, described by a gamma distribution with exponent 2.85 ± 0.05. This is an interesting result because it appears to contradict the fact that the Weibull distribution has been chosen to be a best-fit distribution in many previous studies of precritical damage nucleation [16]. (However, see also [17,18] and references therein. In particular, in Eq. (3.13) of Ref. [17], the gamma distribution is found to describe the statistics in a special case of a time-dependent fiber-bundle model.) To examine this subtle issue more thoroughly we have to implement additional verifying simulations.

As was discussed above, almost the total evolution time of the model in the metastable state is represented by the fluctuating random walk of many attempts to exceed the threshold, and only a negligible fraction of time is spent by the system in the final, burst, postcritical state before rupture. In Sec. IV, where we specifically studied the postcritical, burst stage of damage growth, we were able to qualitatively explain our results by ignoring the nonlinear coupled interactions of different locations during almost the entire evolution of the system. In the current section, dealing with precritical nucleation, neglecting all possible interactions among different locations is an even better approximation, and we can thus integrate Eq. (2d) as a separate ordinary differential equation for each independent location.

Therefore, we initially construct statistics of "local" failure times by integrating Eq. (2d) separately for each independent location, as if all elements were loaded independently. We will refer to these as "min of 1" statistics, that is, as the statistics of local failure times for one particular model element.

However, we should recall that, from the perspective of damage mechanics, rupture is a "horse race" among different locations, and the global failure time is the time when the "winner crosses the finish line". Therefore, because the system is in a state of uniform macrostrain and model elements are decoupled one from another, we can group N consecutive independent results from simulating Eq. (2d) and choose the minimum time to failure in the group, corresponding to the rupture of a model or a solid built of N independent elements. We say that ensembles of such grouped simulations yield "min of N" statistics. For this study, we used $N = 100$, 500, 1000, and 5000.

The cumulative distribution functions of times to failure t_f are given in Fig. 3(a) as CDF plots, and in Fig. 3(b) as Weibull plots. Also in these figures we plot the maximum likelihood fits of the Weibull and gamma trial distributions for the "min of 1" and "min of 5000" statistics. We see that the "min of 1" statistics, which are the statistics of failure times of a single element, are fit by a gamma distribution with exponent 8.78 ± 0.12. The Weibull distribution for these statistics is clearly not applicable. However, when we increase the number N of elements in the model from 1 to 5000 (i.e., when we move from "min of 1" to "min of 5000" statistics), the sample distribution transforms step by step from the gamma distribution to the Weibull distribution, and for the "min of 5000" statistics we obtain already a good fit to the Weibull distribution with exponent 20.4 ± 0.2.

What we observe here clearly resembles a crossover effect (that is, a finite-size effect) from one asymptote (the gamma distribution) to another asymptote (the Weibull distribution):

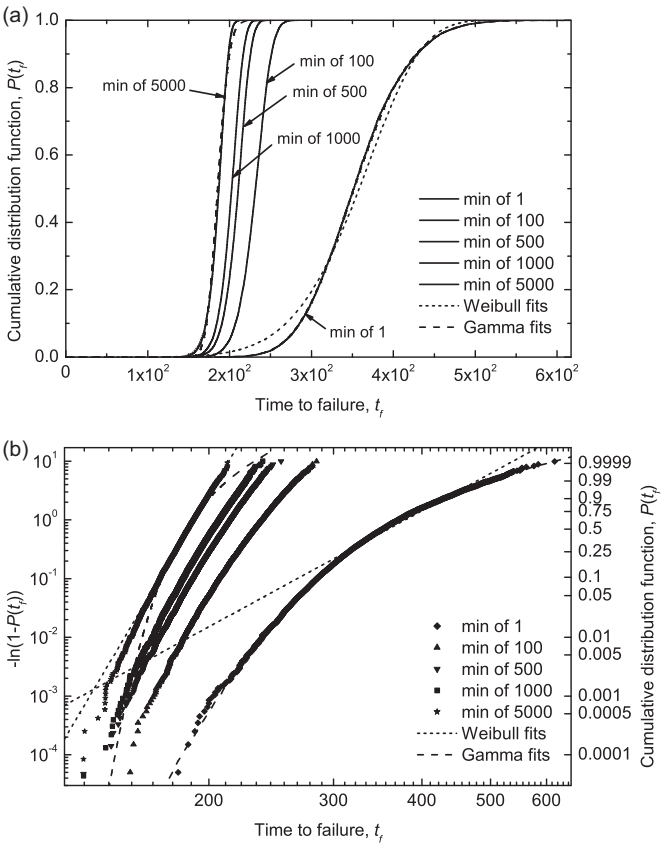

FIG. 3. Cumulative distribution function of times to failure t_f for precritical irreversible nucleation of independent locations: (a) CDF plot and (b) Weibull plot.

The statistics of failure times for one particular, undivided element in our model are determined by the gamma distribution, while in the thermodynamic limit of an infinite number of elements the statistics approach the Weibull distribution. The size N of the system plays the role of a scaling parameter that controls the crossover.

Crossover effects are generally observed when we consider scaling hypotheses in the vicinity of critical or spinodal points [5,19]. The finite-size effect is well known for damage phenomena also (see, e.g., a recent review [20], and studies [17,18] and references therein). In the case of our study, the crossover effect has local damage growth (in one element) up to the value of unity as one asymptotic regime, and rupture at the weakest link as another asymptote.

For the finite element simulation of the continuous model used for Fig. 2 we had 128 elements in the model. These 128 elements represent neither the local nucleation (one element) nor the global nucleation (infinite number of elements). Instead, the 128-element case corresponds to an intermediate value of the scaling parameter when neither of the asymptotic regimes is applicable, but the scaling function forms a "transitional" statistical distribution between the two.

In applications one may expect the results of finite element models to deviate from the thermodynamic limit of the Weibull distribution due to a finite-size effect if the considered number of elements N is too small. Indeed, as we can see from Fig. 2, when $N = 128$, our model is still represented well by the

gamma distribution. However, already with the "min of 500" statistics in Fig. 3 (or, better, the "min of 1000" statistics), the approach to the Weibull distribution asymptote for $N \to \infty$ is apparent. Thus, the crossover number of elements is not expected to be too large. In fact, in many cases it is likely to be comparable to the number of elements normally required for accurate simulations of systems for engineering purposes.

Let us summarize the main aspects of the discussion above. First, in the parameter regime of interest here, damage evolution at each location of our model is effectively decoupled from the adjacent locations, especially in the precritical case which we currently consider. Therefore, there are two different statistics of times to failure in our model. The first statistics describes the distribution of times to failure at a given location, independent from any other location. This statistics we have called "min of 1", and numerical experiments demonstrated that they were well fit by the gamma distribution.

The second statistics corresponds to the failure of the total specimen. We called this type of statistics "min of 5000" because it takes into account "all" (5000 different) locations along the specimen length, each with its own "min of 1" statistics. Therefore, the "min of 5000" statistics is the weakest-link statistics among 5000 elements.

Can we, in a manner consistent with the weakest-link hypothesis, connect these two statistics? Indeed, we can, since it is well known that the Weibull distribution is the consequence of the weakest-link hypothesis when the local distribution has a power-law lower tail [21]. To demonstrate this, let us denote the cumulative distribution function of the "min of 1" statistics as $P_{\text{local}}(t_f)$ because it is responsible for local damage growth, independent of adjacent locations. In contrast, we denote the cumulative distribution of the "min of 5000" statistics as $P_{\text{global}}(t_f)$ because it is responsible for the global specimen failure.

The probability for a particular location along the specimen to have been broken at time t_f is $P_{\text{local}}(t_f)$, by definition. The probability for this location to be still intact is, therefore, $1 - P_{\text{local}}(t_f)$. Then, assuming independent elements, the probability for a whole specimen with N elements to be intact at time t_f is $\{1 - P_{\text{local}}(t_f)\}^N$.

On the other hand, $P_{\text{global}}(t_f)$, by definition, is the probability that the whole specimen will have failed at $\geqslant 1$ location at time t_f. Therefore, we immediately find the connection between these two probabilities to be

$$P_{\text{global}}(t_f) = 1 - \{1 - P_{\text{local}}(t_f)\}^N = 1 - e^{N \ln\{1 - P_{\text{local}}(t_f)\}}. \tag{14}$$

Since we consider the weakest-link hypothesis, and the probability of failure at any one location is very small for sufficiently large N, we can expand the logarithm in Eq. (14) to leading order as

$$P_{\text{global}}(t_f) = 1 - e^{-N P_{\text{local}}(t_f)}. \tag{15}$$

However, our numerical simulations show that $P_{\text{local}}(t_f)$ is given by the gamma distribution, whose probability density function is

$$p_{\text{local}}(t_f) = \frac{t_f^{k-1} e^{-t_f/\Theta}}{\Gamma(k)\Theta^k}. \tag{16}$$

Because weakest-link statistics implies relatively small times to failure ($t_f \ll \Theta$) and we are talking about statistical extremes, we can approximate the lower tail of the local distribution as

$$p_{\text{local}}(t_f) \propto t_f^{k-1}, \tag{17}$$

which, integrated, provides the cumulative distribution function

$$P_{\text{local}}(t_f) \approx \left(\frac{t_f}{t_0}\right)^k, \tag{18}$$

where t_0 is some constant of proportionality.

Substituting expression (18) into (15), we arrive at the Weibull distribution for the failure times of the whole specimen,

$$P_{\text{global}}(t_f) = 1 - e^{-N\left(\frac{t_f}{t_0}\right)^k}, \tag{19}$$

where the gamma exponent plays now the role of the Weibull exponent. Therefore, we see that for sufficiently large N the gamma statistics of times to failure for each particular element transforms into the Weibull distribution for the whole specimen.

As mentioned above, for the Weibull distribution to describe the global failure time it is only required that the lower tail of the local probability distribution be a power law [21]. Since this requirement is satisfied by many statistical distributions, which each represent possible nonuniversal, system-dependent local damage growth phenomena, the finite-size crossover effect is typically expected to result in universal Weibull statistics of times to failure. However, in works [17,18] and references therein, it is demonstrated that in addition to Weibull statistics, other distributions can result from quasi-weakest-link behavior in what are called local load-sharing systems.

Another important fact here is that the found distributions are gamma or Weibull but *not* exponential, and therefore our results do not correspond to classical phenomena of nucleation theory. That is, while the exponential distribution is expected to be universal for the majority of precritical nucleation phenomena, we observe a different result. The appearance of nonexponential distributions in nucleation has been previously found to take place in systems with amorphous disorder, when a free energy potential has multiple minima, and has been suggested for the cases of polymer crystallization [22] and glass-forming materials [23]. For our model, we posit that the primary difference from classical gas-liquid nucleating systems is the irreversibility of damage. In contrast to, say, gas nuclei in a liquid, fluctuations in the system can exceed the threshold of α to grow damage further, but cannot decrease the density of microcracks that are already present in the system. Therefore, it is natural to consider this irreversibility as the reason why our results diverge from the classical theory of nucleation. To test this hypothesis, in the next section we turn our attention to the case of a system with reversible damage.

VI. REVERSIBLE NUCLEATION

In Sec. V we followed [6] in considering only irreversible damage growth. This was represented in Eq. (2d) by the positive part operator, denoted by angle brackets ($\langle \Phi \rangle = \Phi$ for

$\Phi \geqslant 0$ and zero otherwise). However, the majority of studies in the theory of nucleation investigate reversible systems. Indeed, in the theory of gas-liquid systems, if a small bubble of another phase appears in a metastable state, there is no constraint on these systems that would prohibit the bubble from disappearing. The same is true for magnetic systems where nothing prohibits a small domain of another phase from disappearing. Thus, to compare our results with previous studies in nucleation theory, in this section we remove the condition of irreversibility and allow defects to disappear.

To consider reversible phenomena that allow material healing we remove the angle brackets from Eq. (2d):

$$\frac{\partial \varphi}{\partial t} = \eta \left\{ \frac{\varphi}{2} [\nabla u + \Upsilon \xi(x,t)]^2 - \alpha \varphi^{2/3} \right\}. \tag{2e}$$

However, if we simulate the system below the critical threshold, the probability of successful attempts to grow damage is expected to be small. Thus, the derivative $\partial\varphi/\partial t$ is generally negative, which attenuates damage to zero. However, at zero damage, $\partial\varphi/\partial t$, which has a power-law dependence on φ, is also zero, and so Eq. (2e) does not allow the system to evolve away from zero.

Contrary to this, in Nature there is always a nonzero level of microdamage, as a result of fluctuations. Therefore, we introduce a small, nonzero level of damage φ_0 below which the system cannot go: $\varphi = \max(\varphi, \varphi_0)$. In other words, we allow the model to heal but at each time step of our simulations we check whether the damage has fallen below the minimum level and, if it has, we restore the damage back to φ_0:

$$\frac{\partial \varphi}{\partial t} = \eta \left\{ \frac{\varphi}{2} [\nabla u + \Upsilon \xi(x,t)]^2 - \alpha \varphi^{2/3} \right\}, \quad \text{where}$$
$$\varphi \geqslant \varphi_0 \ \text{ always}, \tag{2f}$$

which for the damage evolution provides

$$\varphi_{t+dt} = \begin{cases} \varphi_t + \frac{\partial \varphi}{\partial t} dt & \text{if } \left(\varphi_t + \frac{\partial \varphi}{\partial t} dt\right) \geqslant \varphi_0 \\ \varphi_0 & \text{if } \left(\varphi_t + \frac{\partial \varphi}{\partial t} dt\right) < \varphi_0 \end{cases}. \tag{20}$$

The initial values of damage are set to the same level φ_0 without any variability since any influence on the final results of such quenched stochasticity will be lost during the long precritical evolution.

To provide a reasonable time for numerical simulations, we utilize in this section a high value of the damage base level, $\varphi_0 = 0.0003$, which is still well below the critical value $\varphi_C = [\frac{2\alpha}{(\nabla u)^2}]^3 \propto 0.01$. Other parameters we keep unchanged. Again, damage nucleation dynamics from 0.0003 to 0.01 dominates the duration of the simulations up to failure, and our statistics of times to failure are almost purely the consequence of the precritical fluctuating behavior.

The cumulative distribution function of (nonshifted) times to failure t_f for this case is given in Fig. 4(a) as a CDF plot, and in Fig. 4(b) as an exponential plot. Also in these figures we plot the maximum likelihood fit of the exponential trial distribution. We see that the failure time statistics are exponential. This result is similar to the result obtained by Bonn *et al.* [24] and also to the results of nucleation theory [15,25].

As in the previous section, we verify our results with spatially decoupled numerical simulations. The cumulative

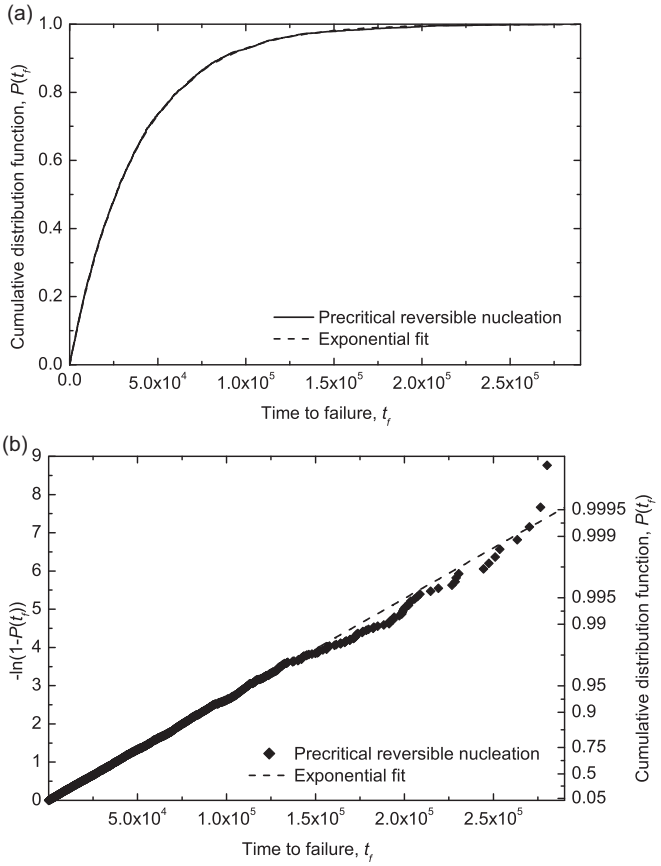

FIG. 4. Cumulative distribution function of times to failure t_f for precritical reversible nucleation: (a) CDF plot and (b) exponential plot.

distribution functions of times to failure t_f are given in Fig. 5(a) as CDF plots and in Fig. 5(b) as Weibull plots for "min of 1", "min of 100", "min of 500", "min of 1000", and "min of 5000" statistics. In these figures we also plot the maximum likelihood fits of the exponential trial distributions. In Fig. 5(a), to exhibit all data on a single plot, we have rescaled failure times by factors of 80, 320, 510, and 1600 for "min of 100", "min of 500", "min of 1000", and "min of 5000" statistics, respectively. For the same reason—to be able to plot on the same figure a very wide range of failure times—we have utilized in Fig. 5(b) the Weibull plot with a logarithmic abscissa axis instead of the more appropriate exponential plot whose abscissa axis is linear. We see that the statistics of times to failure are exponential.

The exponential statistics of times to failure in this case are as expected. A brittle solid ruptures just as a liquid nucleates, that is, when the size of fluctuations overwhelms the critical activation energy. For our model the specific activation energy is

$$E_C = \alpha {\varphi_C}^{2/3} = \varphi_C (\nabla u)^2/2 = \frac{4\alpha^3}{(\nabla u)^4}. \tag{21}$$

The probability for a fluctuation to reach energy level E is

$$p(E) \propto \exp(-\text{const} \cdot E/\Upsilon^2), \tag{22}$$

where Υ^2 represents the temperature. Therefore, failure times are distributed exponentially and the average time to failure

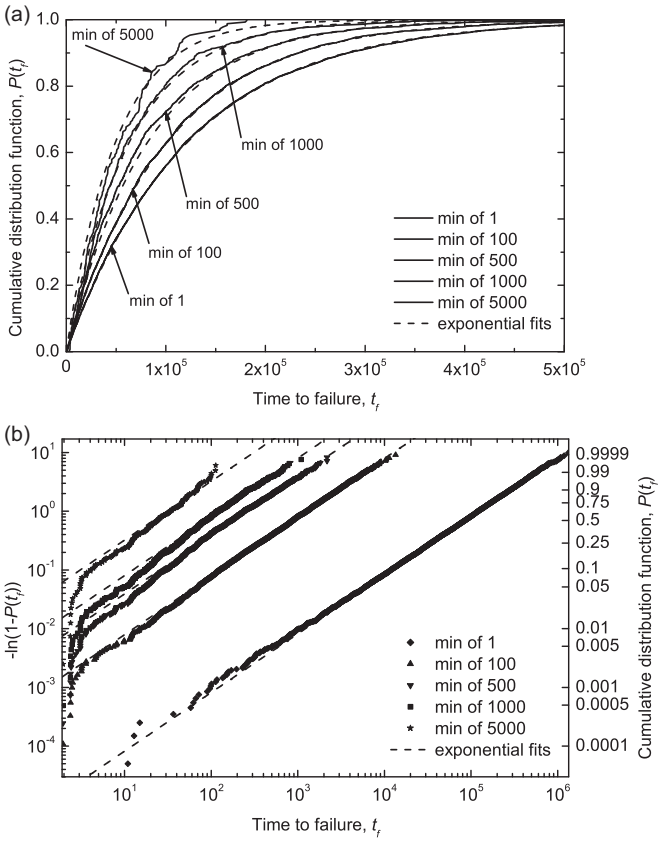

FIG. 5. Cumulative distribution function of times to failure t_f for precritical reversible nucleation of independent locations: (a) CDF plot and (b) Weibull plot. In (a) we rescaled failure times by factors of 80, 320, 510, and 1600 times for the "min of 100", "min of 500", "min of 1000", and "min of 5000" statistics, respectively.

[26] is proportional to

$$t_f \propto \exp(\text{const} \cdot E_C/\Upsilon^2) \propto \exp(\text{const}/(\nabla u)^4), \tag{23a}$$

where in the last proportionality we put $\Upsilon = 1$, as in our simulations.

However, almost the entire duration of the precritical damage nucleation takes place when the damage is very small (that is, for the simulations in this section, for fluctuations near $\varphi_0 = 0.0003$), and so does not couple to Eq. (1) for stress redistribution. Therefore, precritical nucleation does not distinguish between constant stress and constant strain as possible boundary constraints, and we can use the external force F instead of the strain ∇u in Eq. (23a):

$$t_f \propto \exp(\text{const}/F^4). \tag{23b}$$

We see that the logarithm of the average time to failure is inversely proportional to the fourth power of the constant external strain or constant external stress as a boundary constraint. This is a direct consequence of the Griffith theory [27,28]. Similar results of load dependence were obtained experimentally by Guarino *et al.* [12,14,29] for the irreversible damage of wood and fiberglass. Pauchard and Meunier [11] obtained similar dependence for two-dimensional solids with the inverse proportionality to the second power of strain/stress,

$$t_f \propto \exp(\text{const}/F^2). \tag{24}$$

Dependence (24) was also found in numerical investigations of a fiber-bundle model with noise [8]. As discussed by Bonn *et al.* [24], the general dependence for the average time to failure is

$$t_f \propto \exp(\text{const}/(\nabla u)^\tau) \propto \exp(\text{const}/F^\tau), \tag{25}$$

where the exponent τ is determined by the dimensionality of the system and by the fractal structure of the microdisorder. Our model, based on Griffith theory, provides $\tau = 4$; however, by changing exponents in Eq. (2f), $\frac{\partial\varphi}{\partial t} = \eta\{\frac{\varphi^\chi}{2}[\nabla u + \Upsilon\xi(x,t)]^2 - \alpha\varphi^\kappa\}$, we can easily achieve other values of $\tau = \frac{2\kappa}{\chi-\kappa}$.

But what would happen if for the case of reversible damage we again considered two statistics, local and global, similar to the formulae of Eqs. (14)–(19)? If $P_{\text{local}}(t_f)$ is the exponential distribution,

$$P_{\text{local}}(t_f) = 1 - e^{-t_f/t_0}, \tag{26}$$

and, again, a weakest-link argument provides small values of times to failure, we can expand (26) as

$$P_{\text{local}}(t_f) \approx \frac{t_f}{t_0}. \tag{27}$$

Substituting this expression into (15),

$$P_{\text{global}}(t_f) = 1 - e^{-Nt_f/t_0}, \tag{28}$$

we return to the exponential distribution. In other words, a local exponential distribution of failure times provides a global exponential distribution of failure times for the whole specimen, which was confirmed by numerical simulations.

VII. PARTIAL REVERSIBILITY

In previous sections we investigated two extreme cases of nucleation: that of complete irreversibility, intrinsic for brittle materials; and that of complete reversibility, intrinsic to liquids and gels. In this section we consider the intermediate case of partial reversibility.

As was suggested by Golubovic and Feng [28] and Golubovic and Peredera [30], processes of surface and body diffusion can relieve the stress in a crack's neighborhood that was caused by its formation. This suggests that the longer a particular part of a crack exists, the less it becomes reversible. To provide a simple modification to our model representing the effect of reversibility, we assume that a given fraction D of damage is reversible. In other words, if $\varphi_{\max}$ is the maximum value of damage that has occurred up to a given time at a given location, we assume that, for this location, damage is reversible in the range $[(1–D)\varphi_{\max}, \varphi_{\max}]$ and irreversible in the range $[0,(1–D)\varphi_{\max}]$. This choice seems to be reasonable: for a circular crack, the condition that a fraction D of damage is reversible is equivalent to the condition that the fraction $R = 1 - \sqrt{1-D}$ of the crack radius is reversible while the fraction $1 - R = \sqrt{1-D}$ of the crack radius is irreversible. The same characterization of reversibility as a fraction of crack radius was originally used by Golubovic and Feng [28] and Golubovic and Peredera [30].

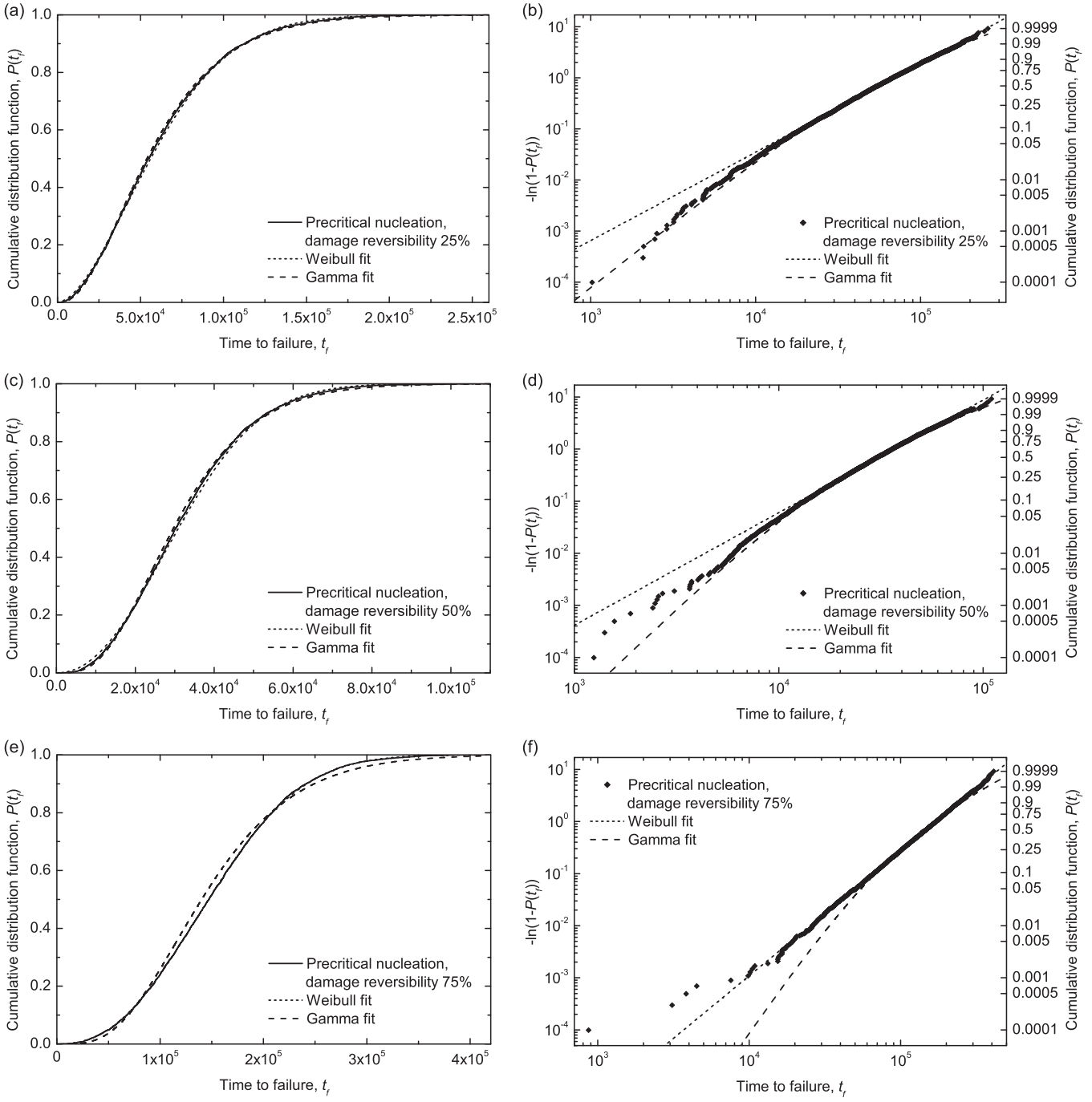

FIG. 6. Cumulative distribution function of times to failure t_f for precritical nucleation with damage reversibility: $D = 25\%$: (a) CDF plot and (b) Weibull plot; $D = 50\%$: (c) CDF plot and (d) Weibull plot; $D = 75\%$: (e) CDF plot and (f) Weibull plot.

As examples we consider the cases of partial reversibility: $D = 25\%$, $D = 50\%$, and $D = 75\%$. First, we carry out simulations using the continuous, fully coupled, $N = 128$, finite element model. The cumulative distribution functions of times to failure t_f are given in Figs. 6(a), 6(c), and 6(e) as CDF plots, and in Figs. 6(b), 6(d), and 6(f) as Weibull plots. In these figures we also plot the maximum likelihood fits of Weibull and gamma trial distributions. We see again the crossover of the statistics of failure times from the gamma to Weibull distributions, as previously described for Fig. 3.

To examine the crossover effect in the system's failure time statistics more carefully, we compare the above results with the spatially decoupled model. As an example we consider the case $D = 50\%$. The cumulative distribution functions of times to failure t_f for the decoupled model are given in Fig. 7(a) as CDF plots, and in Fig. 7(b) as Weibull plots, and we also plot the maximum likelihood fits of the Weibull and gamma trial distributions for the "min of 1" and "min of 5000" statistics. We see that for the "min of 1" statistics, which are for failure times of a single element, the distribution of failure times is gamma with exponent 7.11 ± 0.12. The Weibull

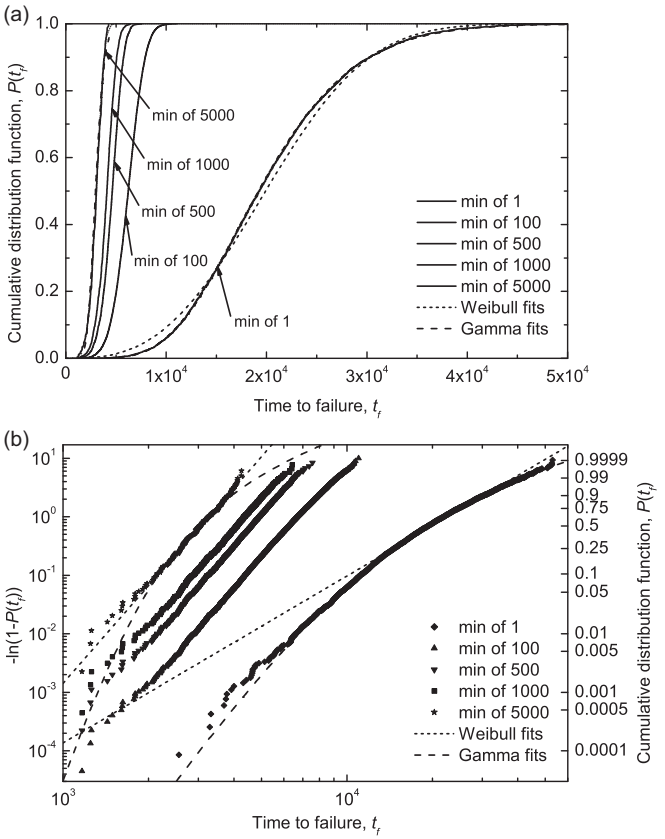

FIG. 7. Cumulative distribution function of times to failure t_f for precritical nucleation of independent locations with damage reversibility $D = 50\%$: (a) CDF plot and (b) Weibull plot.

distribution for this case is clearly not applicable. However, when we increase the number of elements in the model from $N = 1$ to $N = 5000$, the sample distribution transforms step by step from the gamma distribution asymptote to the Weibull distribution asymptote: Already for the "min of 5000" statistics we obtain a good fit of the Weibull distribution with exponent 2.85 ± 0.03.

We see that the behavior for 50% reversibility is more similar to the completely irreversible case than to the completely reversible, with, however, a much lower Weibull exponent. Therefore, for systems with restricted reversibility we expect the behavior to be different from nucleation in completely reversible systems. For the general case of partial reversibility we can conclude that the statistics of failure times for one particular, undivided element in our model is represented by the gamma distribution, while in the thermodynamic limit of an infinite number of elements the statistics approach the Weibull distribution. The transition from Weibull to exponential global failure time distributions is expected to occur near the point where complete reversibility switches to partial irreversibility. This behavior will be investigated in further studies: We may find a bifurcation or a phase transition in the vicinity of $D = 100\%$.

VIII. CONCLUSIONS

In this study we have investigated the behavior of damage nucleation, particularly concentrating on the statistics of times to failure. We consider two distinct cases: postcritical, burst damage growth, when the system has already overwhelmed the potential barrier; and precritical, metastable nucleation, when the system climbs up the potential barrier by means of large fluctuations.

For the first case, the growth of damage is deterministic—well above the critical threshold, when any stochastic input in Eq. (2d) becomes negligible in comparison with the initial disorder, and so deterministic, nonlinear damage growth occurs. While the evolution of a particular system in the ensemble is deterministic, the variability of the quenched disorder in the ensemble leads in our case to the appearance of exponential failure time statistics. The exponential dependence seems to be universal when the derivative of damage with respect to time is proportional to a power law in the damage itself. Furthermore, since the system is considered to be well above the critical threshold, its evolution does not distinguish irreversible and reversible damage formulations.

For the second case, subcritical nucleation, the behavior of the system is significantly different. We introduce the tuning parameter D as a measure of the reversibility of damage and discover that this parameter affects the failure time statistics. That is, for the completely reversible $D = 100\%$ case we obtain results analogous to nucleation theory in gas-liquid systems, when the statistics of failure times are exponential (equivalent to the Weibull distribution with exponent 1). So, in the case of complete reversibility our system falls into the universal class of systems exhibiting Poissonian nucleation. However, for the irreversible or partially reversible cases we obtain the Weibull distribution for failure times. The more irreversible the damage is, the higher the Weibull exponent: 1 for $D = 100\%$ (completely reversible fluctuations), 2.85 ± 0.03 for $D = 50\%$ (half of the damage is reversible), and 20.4 ± 0.2 for $D = 0\%$ (the irreversible, subcritical case).

Thus, we find that the introduction of irreversibility significantly modifies the behavior of the system and pushes it away from the universality class of classical nucleation phenomena. On the other hand, since the exponential distribution is just the Weibull distribution with exponent 1, one could say that the common universality class of nucleation phenomena that follow Weibull statistics includes completely reversible phenomena with exponential statistics as a subclass.

In this study we found that the failure time statistics were described by a Weibull distribution for the cases of 0%, 25%, 50%, and 75% reversibility. Therefore, we expect the transition from exponential to Weibull failure time statistics to take place in the vicinity of the point where the system changes from completely reversible to partially irreversible phenomena. We hypothesize that this behavior may arise from a bifurcation or, possibly, a phase transition in the system that moves the failure time distribution's Weibull exponent away from unity. The case of low rates of irreversibility will be investigated in future studies.

These results indicate that damage phenomena represent a specific type of nucleation with its own intrinsic features, and so caution should be exercised when nucleation theory is applied to their study.

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