

Size effects in fluctuation-based damage mechanics in the semigrand canonical ensemble

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We present results of a fluctuation-based investigation of size effects on damage and fracture of quasibrittle materials and structures. Set within the semigrand canonical ($\Delta\mu VT$) ensemble, we find that size effects of geometrically similar structures are a system property rather than a material property. We reach this conclusion by considering damage and fracture as thermodynamic equilibrium states accessible through Monte Carlo simulations, and develop stress-strain curves and damage isotherms based on ensemble averaging, considering both short-range and long-range bond interactions. We suggest that, to preserve the probability distribution of damage and fracture states for geometrically similar structures, a scaling of the thermodynamic variables of the $\Delta\mu VT$ -ensemble needs to be considered, including a scaling of the bath potential, $\Delta\mu \propto \lambda^{-d} - 1$, for the system's size dilation λ , considering the geometric dimension d of the fracture surface. Derived from mere thermodynamic equilibrium conditions in the fluctuation-based damage approach, we show that such scaling allows the transition between strength theories ($d = 0$) and linear elastic fracture mechanics (LEFM), for which the strength scales as $\sigma_N \propto \lambda^{-1/2}$, for all geometries and types of bond interactions. The rationalization of size effects within the realm of statistical mechanics opens venues toward a large range of engineering applications involving damage-prone materials and structures, from concrete bridges and high-rise buildings to hydraulic fracturing of gas shale and damage of hard and soft biological tissues.

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I. INTRODUCTION

Damage mechanics describes the cumulative effect of defects on the elasticity of materials and structures. Concurrently proposed in the 1950s by Kachanov [1] and Rabotnov [2], it offers a phenomenological extension of Griffith's theory of brittle fracture [3] to the progressive degradation of mechanical properties induced by the formation and coalescence of microscopic cracks. While damage mechanics rapidly diffused throughout the mechanics community [4] from quasibrittle materials like concrete [5,6], ceramics [7] and rocks [8] to soft materials including polymer gels [9] and soft biological tissues [10], the notion of defect homogenization at the mesoscale has sparked considerable debate. Early critics point to inherent instabilities of local damage models, resulting in an imaginary wave speed at the crack front [11] and vanishing energy dissipation in the limit case of Griffith's surface energy dissipation. This realization prompted several enriched damage formulations that diffuse damage by means of a material length scale in nonlocal damage [12], gradient damage [13,14], phase field damage [14,15], peridynamics models [16–18], and more recently displacement curvature

models [19–21]. One limitation of both local and non-local deterministic damage formulations is that none of them explicitly address the existence of intrinsic size effects, which are inherent to all fracture processes [22], and which, therefore, should govern not only brittle fracture phenomena but progressive damage as well. This is precisely the question we address in this study: are size effects a material property or a system property?

While several statistical analogies have addressed fracture and size dependence from the perspective of disorder and fluctuations, they have primarily focused on strength statistics [23,24], localization phenomena [25], avalanche dynamics [26], and critical scaling [27,28]. Statistical extensions of fracture mechanics further combined statistics and energy-based asymptotic arguments to connect crack roughness and size effects [29–31]. In contrast, the present work provides an alternative thermodynamic interpretation of size effect, leveraging ensemble formulations intrinsic to statistical mechanics. Revisiting Griffith's equilibrium theory, where fracture is a surface process connecting nearby equilibrium states independently of the loading path [3], we formulate fracture as a compositional change of the system [32,33] at fixed particle number N (mass conservation), material volume V , and temperature T . This system is naturally cast in the semigrand ensemble ($\Delta\mu, N, V, T$), in direct analogy with binary mixtures [34,35], with potential

$$\Phi_{SG} = F - \Delta\mu N_e, \quad (1)$$

where F is the Helmholtz free energy, N_b and N_e are the numbers of broken and elastic bonds, and $N = N_b + N_e$. For

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a prescribed set of independent variables, fracture states are sampled via a standard Metropolis Monte Carlo scheme with acceptance probability [36]:

$$p_{o \rightarrow n} = \min(1, \exp[-\beta(\Delta U + \delta \Delta \mu)]), \quad (2)$$

where $\delta = -\Delta N_e$ defines the direction of the fracture transition, β is the inverse kinetic temperature, and $\Delta \mu \leq 0$ is the chemical potential difference; whereas $\Delta U = U_n - U_o$ stands for the energy change due to the state transition. The latter comprises (i) the ground state energy additive over all bonds $U_0 = -\sum_{1 \leq i \leq N_b} \epsilon_0^i$, representing the potential energy dissipated at the rupture of bond i ; and (ii) the elastic deformation energy U_λ , accumulated within the bond structure in response to external loading. In this study, we extend this formalism to progressive damage, treated as a sequence of equilibrium states, establish a formal analogy with adsorption, and use it to predict damage propagation via stress-strain curves (Fig. 2) and isosteric heats of adsorption (Fig. 3). Finally, we introduce isotherms of damage (Fig. 5) and derive from them an intrinsic size-effect law for the strength of geometrically similar structures (Fig. 7).

II. METHOD

A. Fluctuation-based damage mechanics

The extension from the binary bond fracture model to progressive damage is achieved by considering a finite number of N_d admissible damage states $\vec{\omega} \in [0, 1]$ associated with a state vector $\vec{s}_i \in \{0, 1\}^{N_d}$ of unit length:

$$\forall i = 1 \dots N_d; \quad \omega_i = \vec{s}_i \cdot \vec{\omega} = \frac{i-1}{N_d-1}. \quad (3)$$

The damage state transition $\omega_o^{(k)} \rightarrow \omega_n^{(k)}$ is defined by the symmetric random walk transition matrix $\mathbf{P} \in \mathcal{M}_{N_d}([0, 1])$ such that $\omega_n^{(k)} = \vec{s}_n^{(k)} \cdot \vec{\omega} = \vec{s}_o^{(k)} \cdot \mathbf{P} \cdot \vec{\omega}$. In that framework, we can formulate the semigrand damage potential, analogously to Eq. (1) as

$$\Phi_{SG} = F - \sum_{i=1}^{N_d-1} \Delta \mu_i N_i, \quad (4)$$

where $\Delta \mu_i \equiv \mu_i - \mu_1$ and $N = \sum_{i=1}^{N_d} N_i$. Assuming that the ‘compositional’ potential difference between adjacent damage states $\Delta \mu_d := \Delta \mu_i - \Delta \mu_{i-1}$ increases as an arithmetic series, Eq. (4) becomes (for $\mu_1 = 0$)

$$\Phi_{SG} = F - \Delta \mu_\omega N \rho, \quad (5)$$

where $\Delta \mu_\omega = \Delta \mu_d (N_d - 1)$ is the compositional potential difference associated with the change of the (undamaged) bond density ρ , reminiscent of the equivalent monolayer thickness in adsorption physics [37]:

$$\rho = 1 - \sum_{i=1}^{N_d} \omega_i \frac{N_i}{N} = 1 - \frac{1}{N} \sum_{k=1}^N \omega^{(k)}. \quad (6)$$

In this case, a straightforward extension of Eq. (2) entails the acceptance criterion for damage state transition:

$$p_{o \rightarrow n} = \exp[-\beta(\Delta U + \delta_\omega \Delta \mu_\omega)] \leq 1, \quad (7)$$

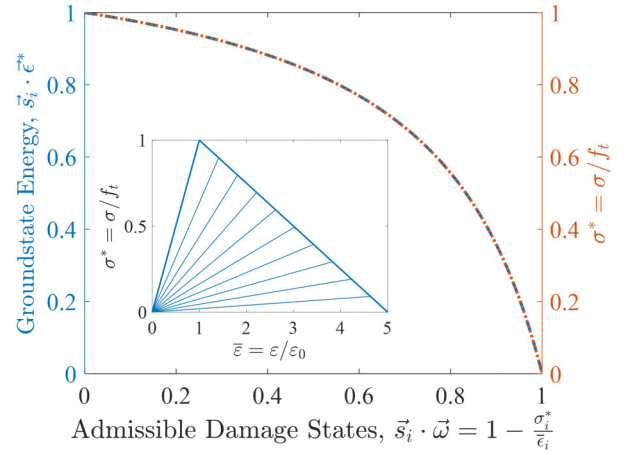


FIG. 1. Ground state energy as a function of damage for a linear stress-strain softening diagram (inset) for $N_d = 516$ damage layers and $\alpha = \epsilon_c / \epsilon_0 = 5$.

where $\delta_\omega = -N \Delta \rho \equiv -\text{sign}(\omega_n^{(k)} - \omega_o^{(k)})$ represents the direction of damage progression. For these N_d damage states, we need to discretize the ground state energy in a vector $\vec{\epsilon}^{(k)}$ corresponding to the admissible damage states $\vec{\omega}$ such that $U_0 = -\sum_{k=1}^N \vec{s}^k \cdot \vec{\epsilon}^{(k)}$, whence an acceptance probability of the form

$$p_{o \rightarrow n} = \exp[-\beta(\Delta U_\lambda + \delta_\omega (\Delta \mu + \Delta \epsilon_0))] \leq 1, \quad (8)$$

where $\Delta \epsilon_0$ is the energy to be dissipated by a damage state transition as exemplified in the inset of Fig. 1.

B. Damage mechanics as a multilayer adsorption process

A formal analogy can be made between our fracture/damage approach and adsorption processes if we recognize that the consideration of ground state energy U_0 and deformation energy U_λ are formally equivalent to solid-fluid interactions and fluid-fluid interactions [38], which are the backbone of the statistical mechanics of adsorption processes [40]. Within this perspective, fracture is viewed as a sequence of admissible configurational states characterized by thermodynamic observables and collective fluctuations in damage. The analogy is therefore intended to capture the statistical organization of damage configurations within a quasiequilibrium framework, while acknowledging that real fracture processes may involve path dependence beyond the scope of the present formulation.

Using classical partition function derivatives (see, for instance, [41]), the binary fracture model gives

$$\beta \text{var}(N_e) = \frac{\partial \langle N_e \rangle}{\partial \Delta \mu} = \left(\frac{\partial \Delta \mu}{\partial \langle N_e \rangle} \right)^{-1}. \quad (9)$$

For the interpretation of such fracture isotherms, it is useful to note that fracture under static conditions, for which $T \rightarrow 0$ (and hence $\beta = 1/k_B T \rightarrow \infty$) entails an infinite slope in the $\Delta \mu - \langle N_e \rangle$ isotherm, is typical of Type I isotherms [42]. Applying a similar derivation for the damage model considering (i) the partition function for N_d damage states with the (ii) $\Delta \mu_d$ arithmetic progression assumption yields $\Delta \mu - \langle \rho \rangle$ isotherms for the undamaged bond density defined

by Eq. (6):

$$N\beta \text{var}(\rho) = \left(\frac{\partial \Delta\mu}{\partial \langle \rho \rangle} \right)^{-1}. \quad (10)$$

That is, for an externally applied potential difference, the damage isotherms thus defined appear as an extension of the monolayer adsorption of the binary fracture model to a multilayer adsorption of N_d damage layers.

A second parameter of interest within the adsorption analogy is the isosteric heat of adsorption, which is defined as the heat to be released/required when an adsorptive binds to or detaches from the solid surface of an adsorbent. In the fracture-adsorption analogy, it is the heat released when a bond ruptures:

$$q = -\frac{\partial \langle U \rangle}{\partial \langle N_b \rangle} = \frac{\partial \langle U \rangle}{\partial \langle N_e \rangle} = \frac{\text{cov}(U, N_e)}{\text{var}(N_e)}. \quad (11)$$

Recalling that q is a positive quantity within adsorption processes [40], an application of the separation of $U = U_0 + U_\lambda$ into ground state (U_0) and deformation energy (U_λ) yields a fracture criterion analogous to Griffith's criterion [32,39]:

$$q_\lambda = \frac{\text{cov}(U_\lambda, N_e)}{\text{var}(N_e)} \leq -q_0 = -\frac{\text{cov}(U_0, N_e)}{\text{var}(N_e)}, \quad (12)$$

where the left-hand side (q_λ) can be viewed as the statistical analog of Griffith's energy release rate; whereas the right-hand side can be viewed as a bond-fracture energy related to the released ground state energy. The inequality (12), however, is not a strict one when it comes to bond fracture processes, as discussed in [32]: $q_\lambda < -q_0$ means that there is enough bond fracture resistance ($-q_0$) available to dissipate the elastic energy into heat form; while $q > -q_0$ means that the bond fracture resistance of a material or structure is exhausted. The extension to the multilayer damage adsorption is achieved by considering, instead of the number of elastic bonds, the undamaged bond density ρ [i.e., Eq. (6)]:

$$q = \frac{\partial \langle U/N^* \rangle}{\partial \langle \rho \rangle} = \underbrace{\frac{\text{cov}(U_0/N^*, \rho)}{\text{var}(\rho)}}_{q_0} + \underbrace{\frac{\text{cov}(U_\lambda/N^*, \rho)}{\text{var}(\rho)}}_{q_\lambda}, \quad (13)$$

with $N^* = N(N_d - 1)$ the total number of damage layers of all N bonds. That is, in contrast to classical damage approaches, in which rate equations of the form $\dot{\omega}^k = f(u_\lambda^k, \dots)$ define damage evolution [1,4–10], in our statistical approach, local and global damage of the system is by design inherently stochastic, characterized by fluctuations in energy around the equilibrium state. These fluctuations permit evaluating the thermodynamic driving force of damage—by analogy with adsorption processes—from the isosteric heat of adsorption.

C. Reduced units and fracture energy

Our simulation-based investigation is carried out in reduced (Lennard-Jones) units [36], rationalizing all quantities using a set of dimensionally independent quantities: a reference distance between particles D , typically associated with a bond equilibrium distance, and a reference ground state

energy ϵ_0 . We shall therefore investigate the form of our problem in these units, considering a stress-strain softening curve $\sigma = \sigma(\epsilon)$. Using Bažant and Oh's 1983 crack band theory [43], we establish a link between the fracture energy $\mathcal{G}_c = \bar{\epsilon} \cdot \bar{\epsilon}_1/\Gamma$ (with Γ the fracture surface) and the stress-strain softening curve by means of the crack band width w_c :

$$\mathcal{G}_c = w_c \int_0^{\epsilon_c} \sigma(\epsilon) d\epsilon = w_c W, \quad (14)$$

where $\epsilon_c = \alpha \epsilon_0$ is the critical strain where the stress is zero. In reduced units, we note that $\sigma = \sigma^* \epsilon_0 D_R^{-d} D_z^{d-3}$, $w_c = w_c^* D_R$, $W = W^* \epsilon_0 D_R^{-d} D_z^{d-3}$, and $\Gamma = \Gamma^* D_R^{d-1} D_z^{3-d}$. Hence,

$$\forall i = 1 \dots N_d; \begin{cases} \bar{s}_i \cdot \bar{\omega} = 1 - \frac{\sigma^*(\bar{\epsilon}_i)}{\bar{\epsilon}_i}; \quad \bar{\epsilon}_i = \frac{\epsilon_i}{\epsilon_0} \geq 1 \\ \bar{s}_i \cdot \bar{\epsilon}^* = \frac{\int_{\bar{\epsilon}_i}^{\alpha} \sigma^*(\bar{\epsilon}) d\bar{\epsilon}}{\int_0^{\alpha} \sigma^*(\bar{\epsilon}) d\bar{\epsilon}} \end{cases}, \quad (15)$$

for constant $\Gamma^* w_c^*$ throughout damage evolution. By way of illustration, we consider the linear softening damage model (inset of Fig. 1), discretized in intervals:

$$(\bar{s}_i - \bar{s}_{i-1}) \cdot \bar{\epsilon}^* = \frac{1}{2W^*} (\sigma_{i-1}^* \Delta \bar{\epsilon}_i - \Delta \sigma_i^* \bar{\epsilon}_{i-1}), \quad (16)$$

where $\bar{W}^* = \int_0^{\alpha} \sigma^*(\bar{\epsilon}) d\bar{\epsilon} = \alpha/2$. The ground state energy for the i -th layer is thus $\bar{s}_i \cdot \bar{\epsilon}^* = 1 - i \Delta \epsilon^* \equiv \sigma_i^*$, and its evolution as a function of damage is shown in Fig. 1.

In addition to these closed-form relationships, we can further simplify our problem by expressing the transition probability from Eq. (8) in reduced units:

$$p_{o \rightarrow n} = \exp \left[-\frac{\Delta U_\lambda^* + \delta_\omega (\Delta \mu^* + \Delta \epsilon_0^*)}{T^*} \right], \quad (17)$$

with $\delta_\omega = \text{sign}(\omega_n - \omega_o)$, and

$$T^* = \frac{k_B T}{\epsilon_0}; \quad \Delta U_\lambda^* = \frac{\Delta U}{\epsilon_0}, \quad (18)$$

$$\Delta \mu^* = \frac{\Delta \mu}{\epsilon_0}; \quad \Delta \epsilon_0^* = \frac{\Delta \epsilon_0}{\epsilon_0}. \quad (19)$$

From Eq. (17), we note that $\Delta \mu^* \in [-1, 0]$. The compositional change that occurs at $\Delta \mu^* = -1$ corresponds to the limit state of a gas, when the chemical potential annihilates the change in ground state energy $\Delta \mu^* = \mathcal{O}(\Delta \epsilon_0^*)$: the material is thus effectively without a potential well, to which to return as an equilibrium state.

III. DAMAGE PROPAGATION

We illustrate the presented method with a first application: a three-point beam bending test with and without notches (Fig. 2). This test, widely considered as the backbone engineering test for fracture properties determination [44,45], lends itself readily to our simulation-based investigation into the effects of short-range and long-range interactions on equilibrium-based damage propagation. Bond interactions are hereby understood in a generalized sense as a representation of the elastic energy stored in a material or structural system due to particle positions. While earlier approaches focused on

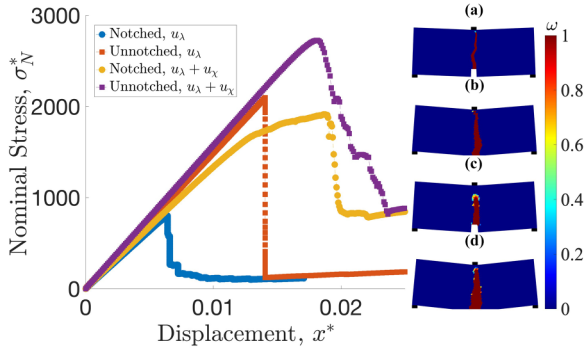


FIG. 2. Nominal stress-displacement curves for three-point bending beam tests with (a)–(c) and without (b)–(d) notches, considering (a),(b) short-range interactions and (c),(d) long-range, curvature-enriched interactions. Results obtained with a linear softening model.

two-point interactions in regular lattice representations of homogeneous [32] and heterogeneous materials [33], we herein choose a finite element representation of bond energies. In such a continuum-based formulation, two-point interactions are represented by the strain energy as a function of the displacement gradient $\xi = \nabla \bar{x}$ contained in the finite ‘bond’ volume V_k ; that is, in the harmonic limit case of an isotropic elastic material ‘bond’:

$$u_\lambda^k = \frac{(1 - \omega^k)}{2} \int_{V_k} \left[K \varepsilon_v^2 + 2G \left(\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} - \frac{1}{3} \varepsilon_v^2 \right) \right] dV, \quad (20)$$

with K, G the bulk and shear modulus, $\boldsymbol{\varepsilon} = \frac{1}{2}[\xi + \xi^T]$ the strain tensor, and $\varepsilon_v = \text{tr} \xi$ the volume strain. In turn, the continuum counterpart of three-point interactions is a restoring energy due to the displacement curvature $\nabla \xi = \nabla(\nabla \bar{x})$, which acts over a finite material length scale ℓ_0 (related to the fracture process zone), akin to a cutoff radius [19–21]:

$$u_\chi^k = \frac{1}{2} \int_{V_k} \kappa (\ell_0 \nabla \xi)^2 dV, \quad (21)$$

with κ the curvature modulus; we’ll set $\kappa^* = \frac{E^*}{15}$ for the rest of the study as suggested in [20]. Figure 2 represents, in reduced units, the nominal stress–displacement curves on the bottom fiber of the beam section in midspan, the so-called modulus of rupture $\sigma_N^* = 6M^*/(b^*h^{*2})$ (with $M^* = M/\epsilon^0$ the bending moment in midspan, and b^* and h^* the section’s width and height in reduced units, respectively). Simulations are carried out under ‘static’ conditions, i.e., for a kinetic temperature of $T^* \rightarrow 0$ (here, $T^* = 10^{-5}$), and at a system potential of reference $\Delta\mu^* = \Delta\mu/\epsilon_0 = 0$. The following observations deserve attention: In the absence of long-range interactions [Figs. 2(a) and 2(b)], there are only two damage microstates accessible at equilibrium $\omega^k = 0$ and $\omega^k = 1$, irrespective of the chosen softening behavior represented by N_d admissible damage states (here, $N_d > 500$, see Fig. 1). In a continuum representation of the bond energies [i.e., Eq. (20)], the local damage model suffers the well-known localization of damage into a single band, with damage transitioning $\omega^k = 0 \rightarrow 1$ in a single element situated at the damage front [Figs. 2(a) and 2(b)]. That is, the local damage model degenerates at

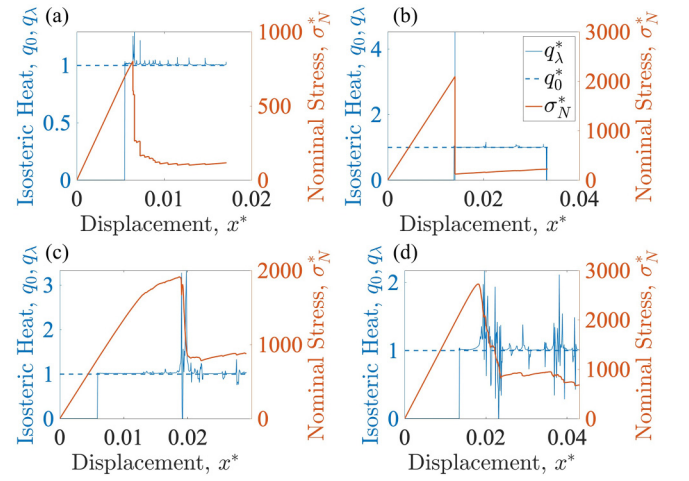


FIG. 3. Isothermic heat development in three-point bending: (a),(b) with short-range and (c),(d) long-range interaction; with (a),(c) and without (b),(d) notches. Results obtained with the linear softening model presented in Fig. 1.

thermodynamic equilibrium into a brittle fracture model with and without notches. The σ_N^* discontinuity is reminiscent of a first-order phase transition, confirming earlier observations made for brittle fracture phenomena [32]. In contrast, when additional long-range interactions redistribute deformation energy over a material length scale ℓ_0^* , the SGC MC approach permits access, at thermodynamic equilibrium, to the entire range of admissible damage states $\omega^k \in [0, 1]$ in the form of a damage process zone ahead of the fracture front where $\omega = 1$ [Figs. 2(c) and 2(d)], consistent with Barenblatt’s suggestion of equilibrium-based quasibrittle fracture [46].

An interesting observation is the competition between short-range and long-range interactions, which can be derived from the isothermic heat of adsorption (Fig. 3): in the absence of long-range interactions [Figs. 3(a) and 3(b)], the lack of nonlocal energy redistribution induces a global instability: damage initiation, marked by the threshold $q_\lambda^* = -q_0^*$ coincides with immediate macroscopic failure, as evidenced by the σ_N^* discontinuity. By contrast, when long-range interactions are present [Figs. 3(c) and 3(d)], this global instability is delayed beyond the onset of damage, as bond-fracture exhaustion is progressively distributed over the fracture process zone.

IV. DAMAGE ISOTHERMS

We now explore our statistical approach, leveraging the semigrand ensemble and the associated damage isotherms. By analogy with adsorption processes [37,42], such damage isotherms in the $\Delta\mu VT$ ensemble represent the system’s residual bond density as a function of the bond potential $\Delta\mu^* = [\Delta\mu/\epsilon_0] - 1, 0$, at a prescribed generalized volume x^* and temperature T^* . At the reference bond potential $\Delta\mu^* = 0$, the displacement x^* is first applied. The bond potential is then incrementally reduced to $\Delta\mu^* = -1$, which defines the (fractured) solid–gas phase transition [32]. Subject to a reduced bond potential $\Delta\mu^* = -1 \leftarrow 0$, the system—in the reduced unit state space $(\Delta\mu^*, V^*, T^*)$ —transitions sequentially from

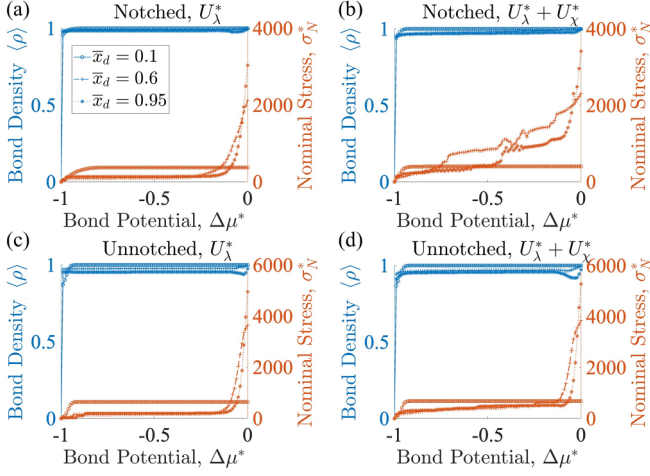


FIG. 4. Damage isotherms of a notched beam: ‘Bond-mass’ density $\langle \rho \rangle$ and nominal stress σ_N^* , vs bond potential $\Delta\mu^*$ at a low temperature $T^* = 10^{-5}$. The damage isotherms are not affected by the applied load $\bar{x}_d^*$ for both (a),(c) short-range and (b),(d) long-range interactions, regardless of the geometry.

an elastic solid to a damaged solid to a gas, for which $\langle \rho \rangle \rightarrow 0$.

A first observation comes from Fig. 4 displaying the isotherm variations with respect to the (relative) applied loading $\bar{x}_d^*$ for a notched geometry. Given the surface nature of fracture, the isotherms are mostly independent of the imposed loading for both short Figs. 4(a) and 4(c) and long Figs. 4(b) and 4(d) range interactions entailing a functional relationship of the form $\rho = \mathcal{F}(\Delta\mu^*, T^*)$ reminiscent of adsorption processes [37]. More generally, damage isotherms are not sensitive to pre-existing discontinuities, nor to the presence of long-range interactions, as illustrated by Fig. 5.

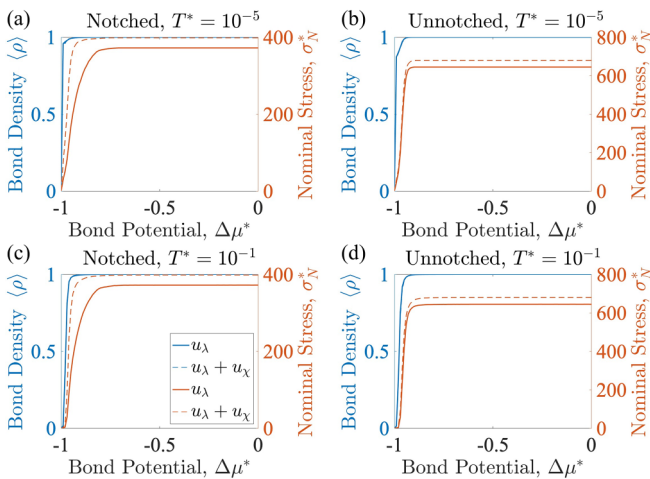


FIG. 5. Damage isotherms and nominal stress σ_N^* vs bond potential $\Delta\mu^*$ at constant prescribed displacement x^* ; for different temperatures T^* . A sequential phase transition from intact solid to damaged solid and to gas is observed for (a),(c) notched and (b),(d) unnotched beams, considering short-range [u_λ , Eq. (20)] and long-range [u_χ , Eq. (21)] interactions, at two different kinetic temperatures.

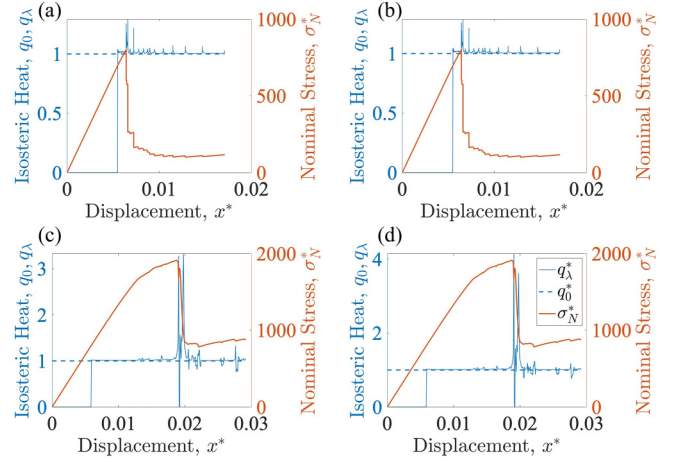


FIG. 6. Nominal stress-displacement curves for notched three-point bending beam tests with short-range interactions (a),(b) and long-range interactions (c),(d) for $\lambda = 1$ (a),(c) and $\lambda = 2$ (b),(d) mesh dilation. Results obtained with the linear softening model are presented in Fig. 1.

They exhibit a sharp solid-fracture phase transition at a critical bond potential that depends only on temperature. In contrast, the corresponding bond-cohesion curves $[(\Delta\mu^*, \sigma_N^*)]$, Fig. 5] depend on both (notched or unnotched) geometry and the activation of short- and long-range interactions. In fact, the bond-cohesion curves for notched specimens [Figs. 5(a) and 5(c)] are smooth, indicative of a smooth solid-fracture phase transition modulated by damage. In turn, in the absence of geometric discontinuities for fracture initiation, this solid-fracture-gas transition is steeper [Figs. 5(b) and 5(d)]—akin to a first-order phase transition characteristic of brittle fracture phenomena [32]. Otherwise said, from an adsorption perspective, damage serves as an intermediate state between intact solid and gas, triggered by the desorption of bonds.

V. SIZE EFFECT

We can now investigate damage size effects by comparing the nominal strength $\max_{x^*} \sigma_N^*$ of geometrically similar structures [47], in an affine dilation of the system $D(\lambda) = \lambda D_{\text{ref}}$. In the phase space of the semigrand canonical ensemble, the imposed Lennard-Jones system of units prevents any apparent size effect under a constant $\Delta\mu^*$ (see Fig. 6). We will demonstrate that size effects can, in fact, be derived from statistical–thermodynamic principles intrinsic to the semigrand ensemble—rather than from the geometric arguments conventionally used in fracture mechanics.

Our starting point for a size effect analysis is the realization that at thermodynamic equilibrium the probability to delete or insert a bond is on average the same. Following earlier work [32], we approximate the change in energy due to the addition or deletion of a bond by expression (11)

$$\Delta U_{N_e \pm 1}^* \approx \frac{\partial \langle U^* \rangle}{\partial \langle N_e \rangle} \Delta N_e = \pm q^*. \quad (22)$$

The equality of probability thus entails

$$\begin{aligned} P_{N_e \rightarrow N_e+1} &\equiv P_{N_e \rightarrow N_e-1} \\ &\Downarrow \\ \exp \left[\frac{1}{T^*} (-\Delta\mu^* + q^*) \right] &\equiv \exp \left[\frac{1}{T^*} (\Delta\mu^* - q^*) \right]. \end{aligned} \quad (23)$$

It follows that at thermodynamic equilibrium, we have

$$\Delta\mu^* \equiv q^* = q_0^* + q_\lambda^*, \quad (24)$$

with

$$q_0^* = -\frac{\partial \langle U_0^* \rangle}{\partial \langle N_b \rangle} = \frac{\partial \langle U_0^* \rangle}{\partial \langle N_e \rangle}; \quad q_\lambda^* = -\frac{\partial \langle U_\lambda^* \rangle}{\partial \langle N_b \rangle} = \frac{\partial \langle U_\lambda^* \rangle}{\partial \langle N_e \rangle}. \quad (25)$$

The equilibrium condition, Eq. (24), includes for $\Delta\mu^* = 0$ the Griffith fracture criterion $q_\lambda^* = -q_0^*$, whereas $q_\lambda^* = -q_0^* + \Delta\mu^*$ for $\Delta\mu \in [-1, 0]$. Otherwise said, the admissible bond-energy release rate q_λ^* decreases below the bond fracture energy $-q_0^*$ when the chemical potential difference targets all bonds in the system. This suggests that size effects on the structural strength originate as a system property monitored through the chemical potential difference $\Delta\mu^*$.

We therefore consider an affine dilation $D(\lambda) = \lambda D_{\text{ref}}$ of all reference geometric dimensions. As previously shown, when $\Delta\mu^* = 0$, such dilation has no effect—expressed in reduced units—on the nominal strength (Fig. 6). On the other hand, such a dilation will increase the fracture surface Γ^* , as well as the number of (broken) bonds crossing this (dilated) surface:

$$\frac{\partial \langle \Gamma^* \rangle}{\partial \langle N_b \rangle}(\lambda) = \lambda^{-d} \frac{\partial \langle \Gamma^* \rangle}{\partial \langle N_b \rangle}(\lambda = 1), \quad (26)$$

where d is the Euclidean dimension of the surface ($d = 1$ for 2D, $d = 2$ for 3D systems). The bond size-scaling originates here from the material microstructure itself: the existence of an intrinsic interatomic spacing implies a finite bond size and therefore a finite bond density per unit fracture surface. Geometrically similar structures consequently contain an extensive number of admissible fracture states scaling naturally with the fracture surface. Then recall that the elastic energy $\langle U_\lambda^* \rangle$ —in reduced units—is unaffected by the dilation. The bond energy release, q_λ^* , thus scales as

$$\begin{aligned} q_\lambda^*(\lambda) &= -\frac{\partial \langle U_\lambda^*(\lambda) \rangle}{\partial \langle N_b(\lambda) \rangle} = -\frac{\partial \langle U_\lambda^*(\lambda = 1) \rangle}{\partial \langle \Gamma^* \rangle} \frac{\partial \langle \Gamma^* \rangle}{\partial \langle N_b \rangle}(\lambda) \\ &= \lambda^{-d} q_\lambda^*(\lambda = 1), \end{aligned} \quad (27)$$

where we recognize Griffith's energy release rate $\partial \langle U_\lambda^* \rangle / \partial \langle \Gamma^* \rangle$. In contrast to the deformation energy, the ground state energy increases with the number of bonds. Specifically, for a statistically homogeneous material $U_0^*(\lambda) = \lambda^d U_0^*(\lambda = 1)$. Whence,

$$-q_0^*(\lambda) = \frac{\partial \langle U_0^*(\lambda) \rangle}{\partial \langle N_b(\lambda) \rangle} \equiv \frac{\partial \langle U_0^*(\lambda = 1) \rangle}{\partial \langle N_b(\lambda = 1) \rangle} = -q_0^*(\lambda = 1). \quad (28)$$

Therefore, using Eqs. (27) and (28) in the thermodynamic equilibrium condition, Eq. (24), we find the link between the chemical potential difference and the dilation parameter,

$$\Delta\mu^*(\lambda) = q_0^*(1 - \lambda^{-d}). \quad (29)$$

The size effect law, Eq. (29), can be interpreted as an extension of Griffith's criterion $q_\lambda^*(\lambda = 1) = -q_0^*$, applied to a consistent, self-similar scaling of the ensemble parameters $(\Delta\mu, V, T)$ in the semigrand canonical ensemble. This self-similarity of the first kind implies the absence of an intrinsic material length scale governing fracture, and justifies using $\lambda = 1$ as a reference dilation [48]. It equally holds for homogeneous ($-q_0^* = 1$) and heterogeneous materials, for which $0 < -q_0^* < 1$ [33], provided that the bonds broken on a fracture surface are statistically representative of the bulk bond heterogeneity. That is, for Eq. (28) to hold, the fracture surface must be sufficiently large compared to the characteristic length scale delineating the bond heterogeneity. The case of statistical inhomogeneity is beyond the purpose of our investigation.

In return, the introduction of a finite fracture process zone implies that the system reference configuration must be defined relative to an intrinsic material length, relating the chemical potential difference $\Delta\mu^* = 0$ to the internal dynamics of the system. This requires the additive renormalization $\lambda \rightarrow \lambda - 1$, redefining the system dilation as a ratio between the structural size and the fracture process zone scale, enforcing $\lambda = 0$ as the physically meaningful state where no separation of scales exists [47]. Upon renormalization, the thermodynamic relation derived in Eq. (29) remains formally unchanged, while the damage process transitions from a self-similar process of the first kind (embedded in linear elastic fracture mechanics) to one of the second kind following Barenblatt's classification [48], naturally capturing the asymptotic matching between strength and fracture theories in quasibrittle fracture.

Derived here from mere thermodynamic equilibrium conditions, we corroborate our scaling proposition, Eq. (29), in Fig. 7 in the form of simulation results to be compared with Bažant's size-effect law in Lennard-Jones units [22]:

$$\sigma_N^* = \sigma_p^* [1 + (\lambda D_0^*)^r]^{-1/2r}, \quad (30)$$

where r is a shape parameter, typically chosen to be $r = 1$, σ_p^* is the material strength limit, and D_0^* is the transitional length

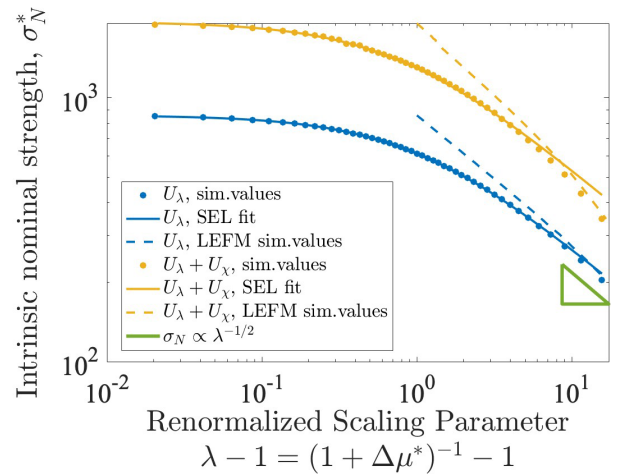


FIG. 7. Intrinsic damage size effects: normalized strength as a function of the renormalized scaling parameter $\lambda - 1 = D/D_{\text{ref}} - 1$ for a notched beam.

between the plastic and fracture asymptotes [47] (related to the internal material length). Upon calibration of the (σ_p^*, D_0^*) parameters through Levenberg-Marquardt regression, we obtain nominal strength scaling relations $\sigma_N^*(\lambda)$ as a function of the renormalized scaling parameter $\lambda = D/D_{\text{ref}} - 1$ for a notched beam. Specifically, in the absence of an intrinsic material length, the simulation results converge to the classical scaling relation of linear elastic fracture mechanics $\sigma_N^*(\gamma) \propto \lambda^{-1/2}$, regardless of the consideration of long-range interactions (Fig. 7). Similarly, considering the existence of such a material length through renormalization allows us to capture the two-asymptote nature of quasibrittle fracture together with the intermediate transitional region regardless of long-range interactions [47]. We obtain $D_0^* = 0.94$ for short-range interactions and $D_0^* = 1.24$ for long-range interactions, demonstrating that nonlocal elastic redistribution delays the system transition toward the brittle asymptote. These values are consistent with the interpretation of D_0^* as the intrinsic length governing the incomplete similarity of the fracture process.

VI. CONCLUSION

In summary, considering a fundamental question of damage and fracture mechanics [49,50], our statistical mechanics investigation suggests that damage and fracture size effects are a system property—not a material property. That is, in contrast to classical Griffith-type fracture mechanics, in which size effects result from the dimensional mismatch between volumetric strain energy and surface dissipation of this energy during the creation of the fracture surface, our fluctuation-based fracture mechanics approach attributes size effects to the impact of an external source, the chemical potential difference $\Delta\mu^*$. Our study shows that the rescaling of the bath pressure for the system's size dilation $\Delta\mu^* = q_0^*(1 - \lambda^{-d})$ ensures the same probability of damage and fracture for geometrically similar structures. This allows us to consider the geometry of the fracture surface in order to bridge the strength limit $\sigma_N^* = \text{const}$ for $d = 0$ and the classical fracture strength size effect $\sigma_N^* \propto 1/\sqrt{\lambda}$ for well-developed fracture surfaces. As a system property, this size effect holds for both notched and unnotched geometries, with and without the consideration of long-range bond interactions. Central to this finding is the consideration of damage and fracture as

thermodynamic equilibrium states in the semigrand canonical ensemble as an intrinsically stochastic process that permits ensemble averaging. While the present work focuses primarily on establishing a statistical-thermodynamic framework for quasibrittle fracture, future developments will investigate the direct engineering interpretation of the thermodynamic variables introduced here, particularly the role of the kinetic temperature T^* as a measure of material heterogeneity (akin to the Weibull distribution in deterministic damage mechanics [24]), and the relationship between the chemical potential difference $\Delta\mu^*$ and fracture-related quantities such as the fracture energy $\mathcal{G}_f$. In addition, although the present formulation treats fracture as a sequence of quasiequilibrium states, extending the framework toward nonequilibrium path ensembles ([51,52]) could provide a natural route to incorporate path dependency and hysteresis within this quasiequilibrium approach. Of course, while other irreversible deformation states than damage and fracture—not considered in our study—will affect the size effect law (see, e.g., [47,49,50]), the rationalization of size effects within the realm of statistical mechanics opens venues toward the safe design and operation of damage-prone materials and structures ranging from concrete bridges and high-rise buildings to hydraulic fracturing of gas shale and the fracture risk evaluation of hard and soft biological tissues.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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