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Threshold diversity and trans-scales sensitivity in a finite nonlinear evolution model of materials failure

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Abstract

We present a slice-sampling method and study the ensemble evolution of a large finite nonlinear system in order to model materials failure. There is a transitional region of failure probability. Its size effect is expressed by a slowly decaying scaling law. In a meso–macroscopic range ($\sim 10^5$) in realistic failure, the diversity cannot be ignored. Sensitivity to mesoscopic details governs the phenomena. © 1997 Published by Elsevier Science B.V.

Brittle fracture manifests an evolution induced catastrophe (EIC) [1]. This is an abrupt transition from the accumulation of damage to a catastrophe. Surprisingly, it shows a great diversity of transition thresholds under the same macroscopic conditions [2,3]. Sometimes this is called sample-specific behavior. Using the slice-sampling method, we show that the above behavior appears in both small and large finite evolution systems, and that there is a scaling law. It is found that some minor mesoscopic differentiation can eventually induce macroscopic failure of materials, owing to the nonlinear evolution far from equilibrium. Thus, sensitivity across meso- and macroscopic scales governs the diversity in macroscopic failure.

Though failure is a complex phenomenon, it is usually supposed that its essential features may be universal. According to its nonlinear and nonequilibrium nature, we present some universal features and laws of this phenomenon, based on a chain model.

We examine a chain with N sites, $X = (x_i, i = 1, 2, \ldots, N)$. There are two options at each site. $x_i = 0$ and $x_i = 1$ denote intact and broken sites, respectively.

The dynamics of damage evolution is assumed to follow a load-sharing principle. That is to say, the load supported by an originally intact but now broken cluster is shared by its two neighboring intact clusters. Therefore, an s-intact cluster (a cluster consisting of s connecting sites) separating a l- and an r-broken cluster will sustain an average stress $\sigma = [1 + (l + r)/2s]\sigma_0$, where σ_0 is the nominal stress. When the stress σ becomes equal to or greater than the site strength σ_c, the s-intact cluster will become broken. This condition can be expressed as [1]

$$L = \frac{2s}{l + r} \leqslant L_c = \frac{\sigma_0}{\sigma_c - \sigma_0}. \tag{1}$$

The nonlinear evolution law results in two kinds of evolution modes of the chain, according to their final states. These are globally stable (GS), that is, dam-

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aged chain but no failure, and evolution induced catastrophic (EIC), i.e., complete failure.

Macroscopically, the system is described by two parameters, the critical ligament L_c and the damage fraction p, where

$$p = \frac{n}{N}. \tag{2}$$

$n = \sum_{i=1}^{N} x_i$ is the total number of broken sites. $p = 1$ represents complete failure. $X = \{x_i\}$ describes the mesoscopic pattern of the chain. We introduce the phase space of the chain to discuss its statistical ensemble evolution and the effects of disorder in a mesoscopic pattern.

The total number of states in phase space can be calculated by Möbius inversion [4],

$$\Omega_N = \sum_{n=1}^{N} \frac{1}{N} \sum_{d|(n,N-n)} \phi(d) \frac{(N/d)!}{(n/d)![(N-n)/d]!}, \tag{3}$$

where ϕ is the Euler function. $(n, N-n)$ is the maximum common divisor of n and $N-n$, and d denotes the prime factors of $(n, N-n)$, and their products are denoted $d|(n, N-n)$, respectively. Ω_N rapidly increases with increasing N. For example, when $N = 20$, $\Omega_N = 52488$ and when $N = 200$, $\Omega_N = 8.03 \times 10^{57}$. Clearly, for small N, one can examine states in the whole phase space. But for large n, this method becomes impossible, owing to the complexity of the computation. The commonly used stochastic sampling method also cannot determine the structure of the phase space. However, this structure is very important to study the sensitivity. Therefore, we developed a stochastic but interrelated sampling method. This method uses two-dimensional slices through phase space [5]. We call it the slice-sampling method.

Take two-dimensional coordinates (α, β), with $0 \leqslant \alpha \leqslant N_1$ and $0 \leqslant \beta \leqslant N - N_1$, where N_1 is an arbitrary integer in the range $1 < N_1 < N$. Let the integers $\alpha = 1, 2, \ldots, N_1$ and $\beta = 1, 2, \ldots, N - N_1$ correspond to the N sites of a chain randomly chosen one by one. Then, a point with integer coordinates (α_1, β_1) represents an initial state with $\alpha_1 + \beta_1$ broken sites. These broken sites are located in the chain, according to the one by one randomly chosen rule in the integer range $1 \leqslant \alpha \leqslant \alpha_1$ and $1 \leqslant \beta \leqslant \beta_1$; see Fig. 1. In this way, we construct a two-dimensional

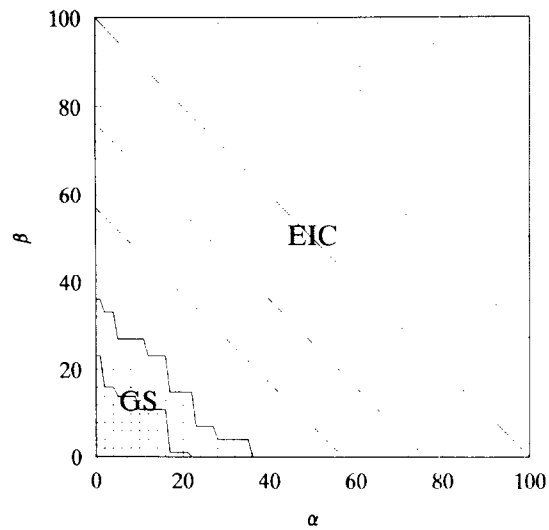

Fig. 1. An example of a slice. $N = 200$, $N_1 = 100$, $L_c = 1.0$. (—) EIC–GS boundary based on mean field theory, (- - -) p-set, dotted area: nonsensitive zone of GS; lightly dotted area: sensitive zone of GS.

slice through phase space, which represents a number of interrelated states. The Hamming distance between two states (α_1, β_1) and (α_2, β_2) should be defined by

$$H = |\alpha_2 - \alpha_1| + |\beta_2 - \beta_1|. \tag{4}$$

For example, the Hamming distance between two states due to a site break in a chain is $H = 1$. The diagonal in the coordinates

$$\alpha + \beta = pN \tag{5}$$

is a p-set of states, i.e., all states with the same initial damage fraction p in the slice.

In order to investigate the statistical ensemble evolution, we take a large number of slices at random and examine the evolution of every state on the slices for a given L_c. The number of slices is selected according to the required precision.

Before considering our results in detail, we briefly look at the prediction of the mean field approximation and percolation theory. According to these theories, there is a clear-cut transitional threshold from GS to EIC modes,

$$p_c = 1/(1 + L_c). \tag{6}$$

Obviously, the transition is uniquely determined by the macroscopic parameter L_c or p_c, and the chain

shows no sample-specific behavior. This is due to the mean field approximation in the theory. On the contrary, stress fluctuations can always exist, because of mesoscopic disorder in the materials. The assumed load-sharing rule (1) is a modeling description of the fluctuations.

Now, let us examine the results of the present model. Fig. 1 shows an example of a slice, $N = 200$, $N_1 = 100$, and $L_c = 1$. For reference, the result of percolation theory is also shown in the figure. One can see that the boundary between GS and EIC modes does not coincide with the p-set lines. This means that the system is sample specific. That is, the macroscopic parameters p and L_c are not sufficient to determine macroscopic failure (GS to EIC). After giving these macroscopic parameters, one can only determine the failure probability $\Phi(p, L_c)$. Numerical results, based on the statistics of a large number of slices, are shown in Fig. 2. A distinct feature is the existence of a transitional region $p_L < p < p_U$, where $0 < \Phi < 1$. In this transitional region, GS and EIC modes coexist. The thermodynamical limits of the two bounds p_L and p_U can be derived as

$$\lim_{N\to\infty} p_L = 0, \tag{7}$$

$$\lim_{N\to\infty} p_U = \frac{1}{1+L_c}, \tag{8}$$

respectively. Additionally, the results obtained by both slice-sampling and all-over methods are consistent with each other for the cases with $N = 20$ and 30; see Fig. 2.

An attractive problem is the size effect of the transitional region. Define the central position and the width of the transitional region as follows,

$$p_t = \int_0^1 p \frac{\partial \Phi}{\partial p} \mathrm{d}p \tag{9}$$

$$\Delta = \left(\int_0^1 (p - p_1)^2 \frac{\partial \Phi}{\partial p} \mathrm{d}p \right)^{1/2}. \tag{10}$$

It is found that p_t and Δ show similar behavior for different values of L_c. Fig. 3 shows p_t and Δ as functions of the chain size N, when $L_c = 1$. Approximately, we can write such scaling laws as

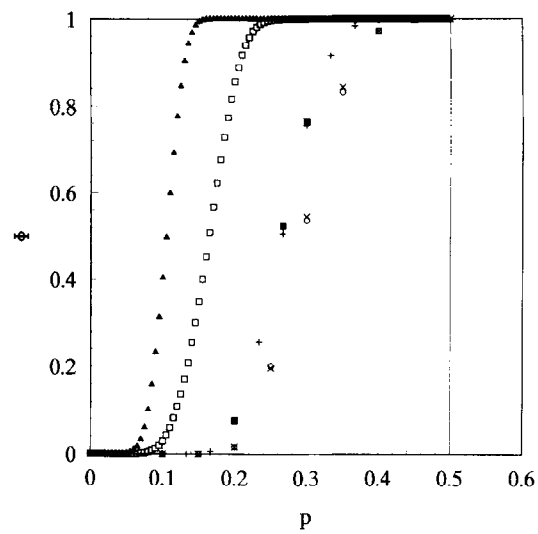

Fig. 2. Failure probability Φ. $L_c = 1.0$. Slice method: (○) $N = 20$; (+) $N = 30$; (□) $N = 200$; (▲) $N = 2000$. Exact method: (x) $N = 20$; (■) $N = 30$. (—) Mean field theory.

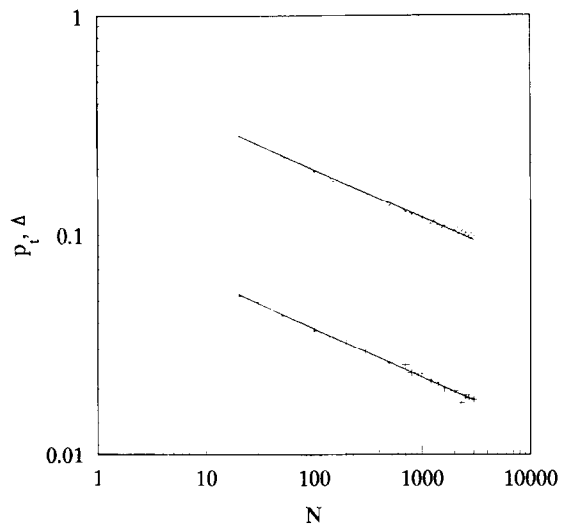

Fig. 3. Size effect of central position p_t and width Δ of the transitional region. $L_c = 1.0$. (+) p_t, (x) Δ, (—) scaling law.

$$p_t = aN^{-\alpha}, \tag{11}$$

$$\Delta = bN^{-\beta}, \tag{12}$$

where a, b, α and β are all dependent on the parameter L_c. For $L_c = 1.0$, we have $a = 0.5454$, $\alpha = 0.2199$, $b = 0.1038$, and $\beta = 0.2205$. For example, when $N = 10$, $\Delta_{10} \sim 0.06$. Because $\alpha \simeq \beta$, Δ/p_t is approximately independent of the size N.

Looking at realistic failure of materials, one may notice that the size range between macroscopic failure (m–cm) and mesoscopic structures (μm) is in the order of $10^6 - 10^4$. So, according to the scaling law (12), $\Delta \sim (0.005\text{–}0.014) \sim 0.1\Delta_{10}$. Compared to the huge size span, the variation of the width of the transitional region appears rather insensitive to the size. Moreover, in accordance with the scaling laws (formulas (11) and (12)), $\Delta p \to 0$ and $p_t \to 0$, when $N \to \infty$. At this extreme, sample-specific behavior of this model vanishes, whereas realistic failure never shows features like $p_t \to 0$. This is clearly due to the finite meso–macroscopic size span involved in materials failure.

The underlying mechanism of the threshold diversity is the sensitivity of macroscopic failure to the details of the mesoscopic pattern. In phase space, there is a sensitive zone, where a slight mesoscopic change in a state may lead to a significant macroscopic consequence, the transition from GS to EIC. Actually, the sensitive zone is always located in the vicinity of the boundary between GS and EIC, see Fig. 1. Comparing Figs. 1 and 2, one finds that the sensitivity appears over the whole transitional region.

To illustrate the sensitivity, let us look at a simple example. According to the dynamics of the evolution (1), one can construct a marginal EIC pattern, such as $s_j = \mathrm{Int}[(L_c/2)(j + 1 + \sum_{j'=1}^{j-1} s_{j'})]$ for an s_j-intact cluster by assuming $s_1 = \mathrm{Int}(L_c)$ and $r_j = l_j = 1$. So, $s_j = 1, 2, 3, 5, 8, 13, 20, 30, 46, \ldots$, when $L_c = 1.0$ and $N \to \infty$. This is quite similar to the Fibonacci series. As $N \to \infty$, we construct infinite marginal EIC states of such a kind. Then we can inversely construct infinite marginal GS states, by changing only one broken site in such a marginal EIC state to an intact one. Apparently, the distinction between GS and EIC is deeply rooted in such a subtle differentiation in the chain.

In order to elaborate this sensitivity, we define a transitional probability $\Psi(p, L_c)$. It is the probability of jumps from GS to EIC, merely owing to a stochastical increment $\Delta p = 1/n$ (the Hamming distance is $H = 1$). This gives a measure of the sensitive zone in phase space. Similar to the probability of all jumps to EIC owing to $\Delta n = 1$ in Ref. [6], there is a relationship between the transitional probability Ψ and the failure probability Φ,

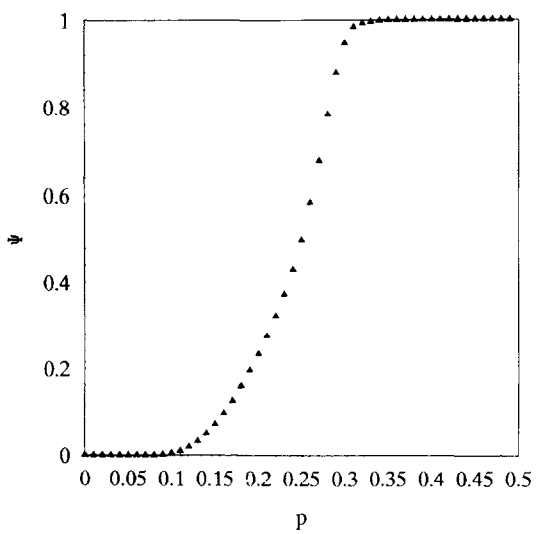

Fig. 4. Transitional probability Ψ. $N = 100$, $L_c = 1.0$.

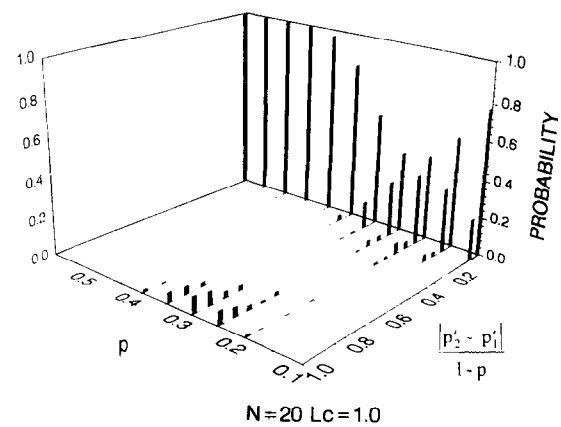

Fig. 5. The probability of the difference of the final damage fraction for pairs of samples with the same initial p and $H = 2$. $N = 20$, $L_c = 1.0$.

$$\Psi(p, L_c) = \frac{\partial \Phi / \partial p}{N(1 - \Phi)}. \tag{13}$$

Fig. 4 shows the numerical results for Ψ from a great number of slices. It has the same scaling law as (11) or (12).

Furthermore, we have also investigated the difference of the macroscopic behavior of a pair of samples with the same initial damage fraction p but the slightest mesoscopic difference. That is to say, there is only a pair of neighboring sites with different options (Hamming distance $H = 2$). Fig. 5 shows the probability of the differences of their final damage fractions

for the case with $N = 20$ and for $L_c = 1.0$. In this figure, the peak of the probability distribution at the extreme difference $|p_2' - p_1'|/(1 - p) = 1$ is a measure of the probability of this sensitivity [7]. Obviously, it should not be neglected.

The threshold diversity and the trans-scales sensitivity seem to be a fundamental feature in the nonlinear evolution of disordered finite systems with multi-scales. A full investigation of this feature can contribute to the understanding of materials failure and similar phenomena.

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