Test of universality for three-dimensional models of mechanical breakdown in disordered solids

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Two three-dimensional models of mechanical breakdown in disordered solids are investigated by large-scale Monte Carlo simulations. We show that the macroscopic properties of these models, such as the elastic moduli, the external force, and the fractal dimension of the macroscopic cracks, obey universal scaling laws that are independent of the microscopic details of the system. In addition, we show that the predictions of these models are in qualitative agreement with the available experimental data on a variety of materials, including concretes, ceramics, and glasses.

Electrical and mechanical failure in disordered media is of immense technological and economic importance. Microscopic failure plays a fundamental role in many systems of industrial importance ranging from aircraft structures and pressurized nuclear reactors to the propagation of cracks in underground oil reservoirs and in ceramics and fibrous composites. There exists extensive literature on the general problem of electrical and mechanical failure of disordered solids.[1,2] However, most of the models discussed in the classical literature on fracture phenomena incorporate artificial features such as preassigned fracture loci and very complex microscopic laws of fracture. The contribution of such complexities to the phenomenon of failure may not be essential and, therefore, their introduction in the model may only complicate the study of such phenomena.

More recently, several simple models have been introduced for both electrical[3-5] and mechanical[6] failure of disordered solids. These models are based on two-dimensional networks in which each bond of the network is supposed to describe the disordered system on a microscopic level, with elasticity and failure characteristics described by a few control parameters. An external potential, strain or stress, is then applied to the network and gradually increased, as a result of which the individual bonds will break in a certain manner until the system fails macroscopically. The sequence of breaking bonds and the spatial patterns they form are supposed to represent a real breaking process. Various properties of such failure processes have recently been investigated,[7-12] and several important features of their behavior have been discussed.

However, the sequence of breaking bonds depends on the type of disorder and its statistical distribution. It also depends on the microscopic force laws that govern the electrical or elastic behavior of the individual bonds and their interaction with one another. Moreover, these models represent nonequilibrium and highly nonlinear systems, and as such are very different from their linear and static counterparts which are usually represented by percolation networks of resistors or elastic bonds,[13] in which a fraction of the bonds of the network has been cut at random. The macroscopic transport and geometrical properties of percolation networks obey well-defined scaling laws[13,14] which are largely independent of the microscopic details of the system. On the other hand, the geometrical properties of the spatial patterns that are formed in a model of dielectric breakdown[3] may depend on the microscopic details of the system, although no systematic study of this has been reported. So far, no attempts have been made to investigate the universal properties of the models of mechanical breakdown. This is particularly important since, if the macroscopic properties of these models do obey universal laws, then one may employ the simplest model and study whether the available experimental data can be explained with the model. This can also be used as a guide for searching for universal properties in the available data, if any, and for performing more precise experiments. Moreover, no three-dimensional simulations have been reported so far, whereas such simulations may be of direct relevance to real composite solids. The goals of the present paper are to investigate, for the first time, the scaling and universal properties of various *three-dimensional* models of failure phenomena and to test whether they can reproduce any important feature of the available experimental data on failure properties of composite solids. We report the results of extensive Monte Carlo simulations of two three-dimensional models of failure processes which, in special limits, contain almost all previous models[3-6,10] of fracture and failure phenomena.

We consider an $L\times L\times L$ network with periodic boundary conditions in two directions and fixed boundary conditions in the third direction. Every site of the network is characterized by the displacement vector $\mathbf{u}_i=(u_{ix},u_{iy},u_{iz})$, and nearest-neighbor sites are connected by springs. These springs can be stretched and bent. We consider here the case of a brittle material for which a linear approximation is valid up to a threshold (defined below). Thus, the displacement $\mathbf{u}_i$'s are computed by minimizing the elastic Hamiltonian

$$H=\frac{\alpha}{2}\sum_{\langle ij\rangle}g_{ij}[(\mathbf{u}_i-\mathbf{u}_j)\cdot\hat{\mathbf{R}}_{ij}]^2+\frac{\beta}{2}\sum_{\langle jik\rangle}g_{ij}g_{ik}(\delta\theta_{jik})^2 \quad (1)$$

with respect to $\mathbf{u}_i$, where $\hat{\mathbf{R}}_{ij}$ is a unit vector from i to j, and g_{ij} the elastic constant of the bond between i and j (assumed to be unity). Here $\langle jik\rangle$ indicates that the sum is over all triplets in which the bonds $j-i$ and $i-k$ form an angle whose vertex is at i, and α and β denote the stretching and bond-bending (BB) force constants, respec-

tively. $\delta\theta_{jik}$ represents the change of angle between bonds ji and ik. Setting $\beta=0$ yields an elastic network in which only central forces (CF) are present. We used a bcc network to study failure phenomena with CF only, whereas a simple-cubic network was used to study the case in which both the CF and the BB forces are present (a simple-cubic network with only the CF does not have any elastic moduli if any of its bonds are cut). This allows us to test the universality of the scaling laws with respect to both the types of the network and the microscopic force laws that govern the behavior of the springs.

We now introduce a threshold value l_c for the length of a bond,[6] which is selected according to the probability density function

$$P(l_c)=(1-\gamma)l_c^{-\gamma}, \tag{2}$$

where we use two values of γ, $\gamma=0.80$ and 0 [a uniform distribution in (0,1)]. These two values of γ allow us to investigate the effect of the statistical distribution of l_c on the universal properties of the failure phenomena. We use this power-law distribution because, unlike a uniform distribution (the limit $\gamma=0$), such distributions have given rise to unusual properties for percolation networks and have affected their universal properties[15,16] and, therefore, we would like to see to what extent such extreme distributions can affect failure phenomena studied here. We then initiate the failure process by applying a fixed external strain on a fully connected network in a given direction. We then determine the nodal displacements $\mathbf{u}_i$ by minimizing H with respect to $\mathbf{u}_i$ for all nodes i of the network. The resulting set of linear equations for the nodal displacements are solved by the adaptive accelerated Jacobi-conjugate gradient method, which uses an acceleration parameter optimized for each iteration. Two different methods have been used to initiate the failure process. In the first method, we select that spring for which the ratio $\rho=l_m l/l_c$ is maximum, where l is the current length of the spring in the strained network and l_m is the maximum microscopic length of a bond in the network, and remove the spring from the system (break it). In the second method, we select that bond for which the ratio $\lambda=f_m l_c/f$ is minimum, where f is the total microscopic force that the spring suffers, and f_m is the maximum microscopic force on a bond of the network, and remove the spring (in the case of the BB model, both f_m and f include the BB or angle-changing forces). This second method of breaking a bond is somewhat similar to Tresca's or von Mises's classical yielding criterion for an elastic beam or spring. Breaking one bond at a time is equivalent to the assumption that the rate at which the elastic forces relax through the network is much faster than the breaking of a spring. These two methods allow us to investigate the effect of yielding criterion on the universal properties of the failure process. One can also remove all the bonds whose lengths have exceeded their threshold.[6] This would give rise to a percolationlike behavior for the fracture process,[6] but we will not pursue this here and leave it to a future study.

After a spring is broken, we recalculate the nodal displacements $\mathbf{u}_i$ for the new configuration of the network, select the next spring that is to be broken, and so on. This process continues until the network finally becomes macroscopically disconnected. As can be seen, the process of breaking the springs to reach the macroscopic failure of the network is very time consuming. We used system sizes ranging from $L=4$ to 12 and have averaged our results over many independent realizations of the network. Up to 600 independent realizations were used, and all computations were carried out with the Cray X-MP of the San Diego Supercomputer Center. Use of larger networks is currently not possible because it would require an enormous amount of computer time.

One of the most interesting bits of information, which is also experimentally accessible, is the behavior of the elastic moduli of the system as the breaking process proceeds. In Fig. 1 we present the Young's modulus Y of the microcracked CF and BB models as a function of the fraction p of the unbroken bonds (these results were obtained with the second method of bond breaking, but similar results were also obtained with the first method). Also shown is the Young's modulus of a percolating simple-cubic network with the BB forces in which a fraction p of the bonds has been removed at random. Clearly, the breaking process weakens the system much faster than a random percolation process and, as a result, the system fails much sooner. This is because of the fact that during the breaking process a sample-spanning cluster of broken bonds is formed much faster than in random percolation, since the stress and strain distributions in the network cause the

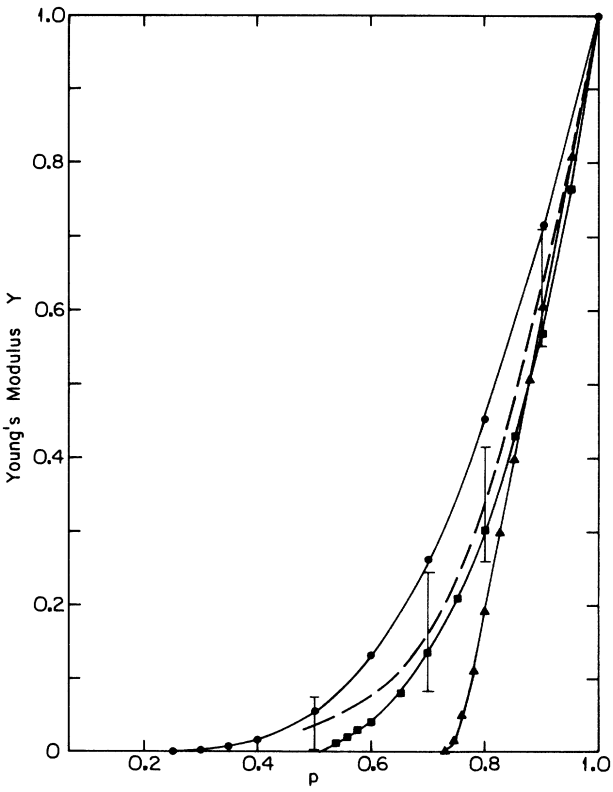

FIG. 1. Young's modulus of the microcracked CF (▲) and BB (■) models (with $\beta/\alpha=0.04$) vs the fraction of unbroken springs p. Also shown are the moduli of the percolating BB model (●) and the experimental data (dashed line). Error bars are one standard deviation.

broken bonds to be in the vicinity of one another, and the location of any broken bond may be correlated with the position of other broken bonds, whereas such effects are totally absent in random percolation. We also show in Fig. 1 some experimental data on the Young's modulus of ceramics and glasses reported by Rice.[17] The data represent the average of 50 sets of ceramics and glasses (the error bars shown in Fig. 1 are those of the experimental data, and those of the simulations are much smaller). As can be seen, the predictions with the microcracked BB model are well within the range of experimental data. Moreover, except for $p \simeq 1$, the results with the microcracked CF model do not agree well with the experimental data because such systems fail at high values of p. For $p \geq 0.5$, the results with the random percolation model with BB forces do not agree with the data as well as the microcracked BB model, presumably because the percolation threshold of such systems is somewhat low and, as a result, the predicted modulus is somewhat large. By changing the value of β/α one can shift the curves, which means that the microcracked BB model would fail at lower values of p.

Next, we address the question of universality in these models. If at each step of the simulations we had broken many bonds (e.g., those which had exceeded their threshold l_c), then, near the failure point p_c, the elastic modulus would obey well-defined universal power laws, $Y \sim (p - p_c)^{\tau}$, where τ is a critical exponent. But, in the present case the point at which the system fails macroscopically resembles a first-order phase transition (although the results in Fig. 1 give the impression that the phase transition is second order). In any event, τ is difficult to measure experimentally because the value of p_c can fluctuate widely. Here, we are interested in the scaling behavior of the external stress or force and its variations with the size of the system since this can be easily measured. To study this, we calculate the external force F that must be applied to break a bond. This force is proportional to ρY and λY in the first and second method of bond breaking, respectively. Thus, a plot of F vs ρ or λ would be similar to the traditional stress-strain curves that have been measured experimentally for many composite systems.[1,2] Instead of showing the results for each model and network size L separately, we collapse[10] the data for all values of L. Figures 2 and 3 represent the results for the microcracked CF and BB models, respectively, if the bonds are broken according to the second method of bond breaking (with similar results for the first method). However, the data collapsing is not complete and, as can be seen, there are three distinct regimes. In the first regime, which is before the maximum has been reached, and is far from it, microcracking takes place which propagates at a relatively slow rate (this is the regime of linear elasticity). As microcracking proceeds, one arrives in the second regime, which is in the vicinity of the maximum, in which intense microcracking takes place and the system is close to macroscopic failure. Beyond the maximum, the system is in the so-called post-failure regime,[18,19] and is highly sensitive to small variations in λ (or ρ). These qualitative features are in agreement with direct experimental mea-

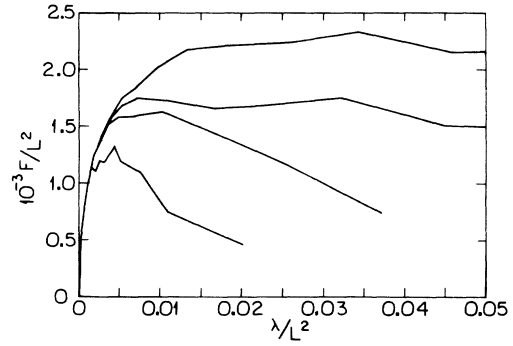

FIG. 2. F/L^2 vs λ/L^2 for the microcracked BB model with $\gamma = 0.8$.

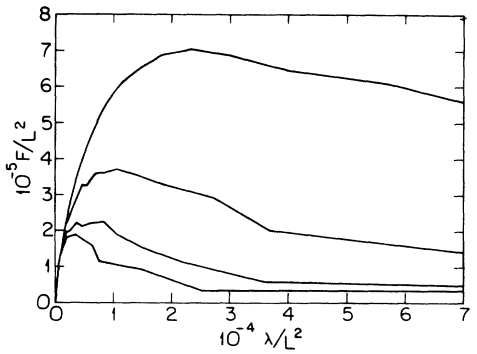

FIG. 3. F/L^2 vs λ/L^2 for the microcracked CF model with $\gamma = 0.8$.

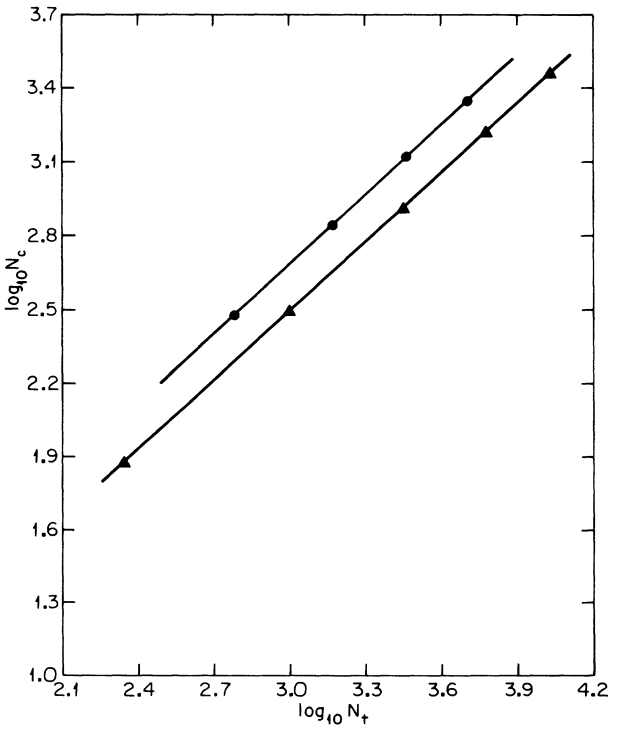

FIG. 4. Number of broken bonds N_c at failure vs total number of bonds N_t for the microcracked CF (▲) and BB (●) models.

surements and observations.[18,19] The shapes of the curves in Figs. 2 and 3 are also in excellent agreement with the stress-strain curves measured by van Mier[20] for various kinds of concrete, which indicates the usefulness of these models for investigating real systems. Moreover, as Figs. 2 and 3 indicate, the regimes before the maximum can be described well by the scaling law

$$F \sim L^{\delta} h(\lambda / L^{\delta}) , \tag{3}$$

where, $h(x)$ is a scaling function and $\delta \simeq 2 \pm 0.1$. This equation is written in analogy with the finite-size scaling hypothesis for equilibrium and static systems.[21] The estimated errors are only statistical, and systematic errors due to the finite size of the lattices may be significantly higher. Although the size of the networks used are relatively small, we believe that the estimated value of δ is reliable. We find the value of δ to be insensitive to γ, network type (bcc or simple cubic), the microscopic force law (with or without BB forces), or the bond-breaking method. Similar simulations with two-dimensional networks yield $\delta \simeq 1$ (the details will be given elsewhere). We thus propose that, $\delta = d - 1$ for a d-dimensional system. On the other hand, if, as the boundary condition, we impose an external stress on the network (which has to be gradually increased as microcracking proceeds), the post-failure regime would completely disappear and the behavior of the system is well described by a single curve given by Eq. (3), i.e., the data collapsing would be complete (the details will be given elsewhere).

As a further test of universality, we looked at the shape of the macroscopic cracks and measured their fractal dimension D. Figure 4 represents the number of broken bonds N_c, at macroscopic failure, versus the total number of bonds N_t (or, equivalently, L) for both the microcracked CF and BB models. One must have, $N_c \sim N_t^{\eta}$, where $\eta = D/3$. We find $D \simeq 2.65 \pm 0.20$, irrespective of any details of the system. Although, in addition to the macroscopic crack, there are also disconnected microcracks, they do not alter significantly the value of D.

Our results suggest that the models we have studied here may possess universal properties, and can reproduce some features of the experimental data. Therefore, the next logical step would be to use such models for a quantitative explanation of the experimental data, and to search for possible universal features in the data.

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