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Elastic percolation models for cohesive mechanical failure in heterogeneous systems

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We introduce a class of models for microstructural damage and cohesive macromechanical failure in heterogeneous systems. Our models are based on random networks of Hooke-type springs with load limit, such that a spring breaks irreversibly if stretched beyond a critical length u_c. We consider several special cases in which both the spring constant k and u_c are distributed quantities, and we show that the macroscopic response of the system depends crucially on the form of the probability distribution functions (PDF's) for k and u_c. If the first inverse moment of the PDF is finite, it appears that macromechanical failure occurs by means of a sharp transition, in which a single crack spans the entire system ("brittle failure"). By contrast, if the first inverse moment is infinite, many cracks appear in the system. Then, at a certain microdamage level, as defined by the fraction of broken springs, all moduli of the system vanish ("pseudobrittle failure") and the system undergoes a percolationlike transition.

The technological and economic importance of mechanical failure in disordered systems is sufficient to explain the widespread interest in this classical field of research. The integrity of aircraft structures and pressurized nuclear reactors, the tearing of woven textiles, the propagation of cracks in solids such as underground petroleum reservoirs, and the fracture of brittle solids provide but a few examples where microscopic failure plays a fundamental role. Although there exists extensive literature on the general problem of mechanical failure and fracture phenomena,[1-7] most of the models employed previously incorporate artificial features such as noncentral forces, preassigned fracture loci, and very complex force laws. Before introducing complexities such as these, whose contributions to the phenomena may not be essential, it may be useful to study simpler models, which contain some of the essential physics of the phenomena, in order to gain insights into the processes.

In this paper we introduce a class of models for cohesive failure in disordered solids, based on networks of Hooke-type springs with load limit. Thus, if a given spring is stretched beyond some critical displacement u_c, it breaks irreversibly. We consider networks of such springs in which both u_c and the spring constant k are randomly distributed quantities. The irreversibility and nonlocalized nature of the failure processes occurring in our models give rise to a much richer variety of behavior than exhibited by the transport[8-10] and mechanical properties[11-13] of linear percolation networks which have been studied extensively in the past. Although certain models have been proposed recently[14,15] for macroscopic failure in disordered solids, they are more appropriate for scalar-transport problems, such as electrical breakdown, than for phenomena such as fracture propagation, which are inherently vector-transport processes.

For simplicity, we consider here the case of a two-dimensional triangular network, a system which bears a close resemblance to various finite-element models employed in macroscopic stress analysis. It can be constructed by a finite-element discretization of the Navier equations[16] in which one employs bilinear basis functions defined on an equilateral triangle and a Poisson's ratio equal to $\frac{1}{3}$. Hence, our model may be considered an analog of a three-dimensional solid in planar strain, pierced by cylindrical holes normal to the plane of strain, or else a hypothetical two-dimensional solid, with Poisson's ratio defined in terms of the contractile strain and tensile strain in pure tension. Finally, we assume that only bond- or spring-stretching forces are present in the network and neglect all bending forces. Although networks with both stretching and bending might appear more realistic,[11,12] we are not aware of any set of elastic-continuum equations whose finite-element or finite-difference discretization corresponds to elastic networks with both central and bending forces. While the latter have been introduced in other contexts as plausible and properly invariant elastic systems, their relation to real systems is not clear to us.

Our approach is quite different from previous studies[1,5] of macroscopic fracture mechanics which use triangular networks of Hooke-type springs. With a view towards the dynamics of fractures, Ashurst and Hoover[1] and Paskin and co-workers[5] have performed *molecular-dynamics* (MD) *simulations* based on Newtonian dynamics and a Lennard-Jones potential. Their network is initially uniform everywhere except in the vicinity of a single microcrack. Hence, one would expect their simulations to describe fracture dynamics in a hypothetical uniform material. However, the microscopic disorder, present in most real materials, in the form of atomic vacancies and interstitials, provides flaws of different shapes, sizes, and orientations, which will give rise to a large scatter of fracture strengths in nominally identical small-scale specimens. What interests us here is precisely the effect of such disorder on the system properties. Ray and Chakrabarti[4] have performed MD simulations in a disordered system, but their simulations have been carried out near the percolation threshold where the system is already highly flawed, which obscures important phenomena (see below).

Most of our calculations were performed with networks of linear dimension $L=40$, subject to periodic boundary conditions in one direction and specified macroscopic strain in the other direction, and we typically made 20 realizations of each network. In what follows we describe our models and report our preliminary results. A more detailed account of our work will be reported in a future paper.

Model I. Here we assign the same spring constant $k=1$ to a randomly chosen fraction p of the springs, the rest having $k=0$. If a spring is stretched beyond a critical value u_c, it breaks irreversibly, thereby initiating a microcrack in the solid. As such, the model is somewhat similar to that of de Arcangelis, Redner, and Herrmann[15] and Takayasu[14] for scalar-transport problems. However, our model is more general and has a much richer range of behavior as discussed below. A macroscopic strain S is then imposed on the system and the displacements of the nodes are calculated. These displacements are then examined to see if any has exceeded u_c (assumed the same for all); S is adjusted such that at least one spring will break. We then adjust S and repeat the computations such that further springs break, and so forth. Given such a history of progressive, irreversible failure we can then identify a *damage level* $\hat{q}$ as the fraction of *originally intact springs* which have broken. Alternatively, we can speak of the probability $\hat{p}=1-\hat{q}$ of finding an *originally intact spring still unbroken,* which is of course to be distinguished from p. If $p\simeq 1$, the system is almost homogeneous and one expects that if a spring is broken, the subsequent breaks will occur in the neighbors of the first such that a single crack will propagate throughout the system. Typical of "brittle failure" in solids,[1,4,5,7] this is indeed what we find in our simulations, although the location of the initial microcrack and the length of the subsequent crack in the network vary among the realizations. However, if $p\simeq p_{ce}$, the elastic threshold of the network ($p_{ce}\simeq 0.65$ for the triangular network[13]), one already has a highly flawed system, for which we expect the behavior and the propagation of the cracks to be very different from that of a network with $p\simeq 1$; again, this is what we actually find, and in the flawed system cracks are generated at several locations and propagate throughout. This contrasting behavior serves, in effect, to distinguish intrinsically flawed systems from damaged systems.

Of particular interest here is the scaling behavior of moduli of the system. We determined two moduli: One of these, G_1 say, is the effective shear modulus of the system for $p\simeq p_{ce}$, but before any failure has occurred. One may expect that $G_1 \sim (p-p_{ce})^{f_1}$, where f_1 is the elastic exponent first introduced by Feng and Sen[11] and later estimated carefully by Lemieux, Breton, and Tremblay[17] by means of the transfer-matrix method. We have found $f_1\simeq 1.5\pm 0.2$, in agreement with their estimate, $f_1\simeq 1.4\pm 0.2$. The second modulus, G_2 say, is that prevailing at a damage level $\hat{q}$ just above the point of incipient global failure (normalized by the length of the network), where the moduli of the network vanish as a result of crack propagation. In Fig. 1 we present the behavior of G_2 with $p-p_{ce}$ (the error bars represent one standard deviation). A fit of the data gives $G_2\sim (p-p_{ce})^{f_2}$, with $f_2\simeq 0.8\pm 0.15$. Therefore, f_2 does not appear to be related to f_1, and if we identify f_1 with "flawed" systems and f_2 with "damaged" systems, the difference f_1-f_2 is a measure of the difference between the two systems. While our estimate of f_2 might be significantly affected by the network size, the relatively small number of realizations, and the point at which G_2 is computed, we believe that $f_1\neq f_2$.

Model II. In this model u_c is still uniform, but the spring constants k are randomly distributed quantities. One motivation for investigating this model is the recent analysis of Halperin, Feng, and Sen[18] of the random-void model of continuum percolation systems. In this model, spherical holes are randomly placed in a medium having otherwise uniform transport properties. A distribution of effective

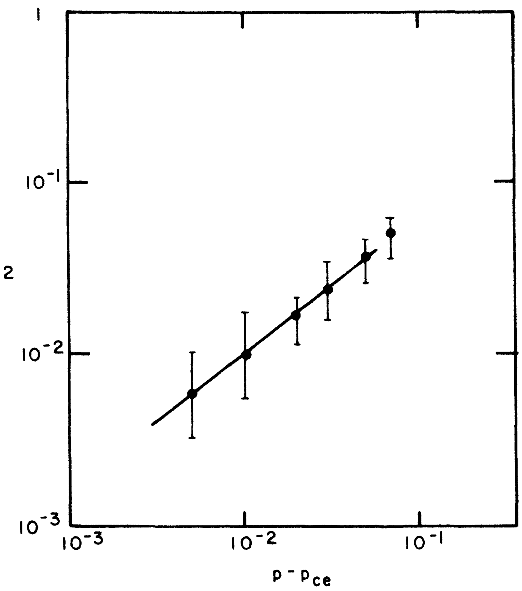

FIG. 1. Double logarithmic plot of the modulus G_2 of the network in model I as a function of $p-p_{ce}$. The error bars indicate the statistical uncertainties.

spring constants is then derived from geometrical analysis of the channels between nonoverlapping holes. In this way, a network with distributed spring constants may provide a realization of certain continua. We have used several different distributions, in the first case distributing the spring constants uniformly in the interval [0,1], and repeating the computations as in model I. We find that, unless a large fraction of springs have $k=0$, only a single crack is formed which propagates throughout the system, eventually splitting it into two pieces. However, the location of the initial microcrack and the length of the crack vary among the different realizations of the network. That only a single crack should propagate throughout the system is not altogether surprising. Since the spring constants have been uniformly distributed, the tip of the crack once formed will seek the easiest path. Although side branches do sometimes form, they appear to be so short as to have no statistical significance. Similar results were obtained with a log-normal distribution of spring constants.

In his modeling of electrical breakdown, Takayasu[14] employed a resistor network somewhat analogous to model II discussed above. In particular, if the voltage drop along a given resistor exceeds a preassigned value, its resistance R is reduced by a factor ϵ, where ϵ is a small number. Such damaged resistors are not subsequently altered in the calculation, so that the network remains connected at all times. Initially, the resistances R are uniformly distributed, as with our distribution of the spring constants in model II discussed above. However, Takayasu[14] finds that the cluster of damaged resistors at the percolation threshold is highly ramified and possesses an apparently well-defined fractal dimensionality, larger than unity; this differs from the present findings. It is possible that the difference between model II discussed above and the system of Takayasu[14] arises from the incomplete burnout of damaged resistors in his model, which maintain a reduced resistance during the remainder of the overall failure process and thus make it easier for the crack to sidebranch.

As a third type of k distribution, we have employed the power-law form:

$$f(k)=(1-\alpha)k^{-\alpha},\quad 0<\alpha<1\ , \tag{1}$$

which is of the same type as that derived by Halperin *et al.*[18] from their random-void model. Most of the calculations were carried out with $\alpha=\frac{1}{2}$ and $\frac{3}{4}$, and they resulted in drastically different results. If $\alpha\simeq 0$, then the fracture process is almost of the brittle type, in which one long crack and several very short side branches appear. As α increases, the side branches become longer and many cracks are formed and propagate throughout the system, so that a fractal-like cluster of broken springs is formed as we approach the point of global disintegration of the system. We call this more gradual type of fracture process "pseudobrittle." Although our numerical results exhibit large statistical fluctuations, we estimated an approximate fractal dimension D of the cluster to be $D\simeq 1.55\pm 0.25$. We have also calculated the shear modulus G of the system, the behavior with $\hat{p}-\hat{p}_{ce}$ of which is presented in Fig. 2. This figure indicates that $G\sim(\hat{p}-\hat{p}_{ce})^{f_3}$, with $f_3\simeq 2.0\pm 0.6$, quite different from f_1 or f_2 defined above. Again, however, our estimate of f_3 may not be very accurate. Moreover, the value of $\hat{p}_{ce}$ and the shape of the cracks appear to be dependent on α. For $\alpha \ll 1$, we always found $\hat{p}_{ce}$ to be larger than p_{ce}. As $\alpha\rightarrow 1$, the value of $\hat{p}_{ce}$ also appeared to approach p_{ce}. It remains to be seen whether the exponent f_3 (if it is indeed well defined) also depends on α. We also observed fairly large variations among different realizations of the network.

Model III. In this model we assign the same spring constant $k=1$ to all of the springs, but the strain u_c is assumed to be a distributed quantity. This is motivated by the idea that a solid system made up intrinsically of the same material (same k), may contain regions having different resistances to breakage under an imposed external stress, as reflected in different u_c, e.g., because of defects in a manufacturing process. As for model II, we have used both a uniform and a power-law distribution for u_c. With the uniform distribution we found that failure of the system occurred by means of a single crack spanning the entire system, i.e., brittle failure occurred. The crack was sometimes accompanied by tiny side branches whose locations varied widely among different realizations. However, with the power-law distribution the systems showed a pseudobrittle failure, i.e., many cracks appeared in the system, although the value of $\hat{p}_{ce}$ at which the system failed appeared to be somewhat uncertain and dependent upon α. The emergence of pseudobrittle failure can be understood by realizing that, according to Eq. (1), many springs will break if stretched beyond a small length u_c. Therefore, the system readily initiates cracks at numerous widespread locations. Our simulations also showed that sometimes the growth of a crack halted, as the crack encountered a relatively strong region. This phenomenon was also observed for model II.

A quantity of fundamental interest in the models discussed so far is the macroscopic strain S imposed on the system. For pseudobrittle behavior our simulations show that as the fraction of broken springs increases, S should also be increased in order to continue the breaking process. As the percolation threshold is approached, S appears to increase without bound. Thus, if we postulate a scaling law such as $S\sim(\hat{p}-\hat{p}_{ce})^{-z}$, we find that $z\simeq 1.05\pm 0.20$, and the exponent z appears to be distinct from other exponents such as f_1, f_2, f_3, or ν, the exponent of the correlation length. This scaling law for S would imply that $G\sim S^{-\delta}$, where $\delta=f_3/z$. Thus, a plot of $\log G$ vs $\log S$ may be used to characterize the cohesive mechanical failure. For ductile failure, the corresponding slope δ is zero (since an increase in S causes no change in G), whereas $\delta=\infty$ for brittle behavior, which occurs at a finite and nearly constant S. On the other hand, for pseudobrittle failure the value of δ appears to be finite. These qualitative considerations are represented in Fig. 3. If the exponent δ proved to be well

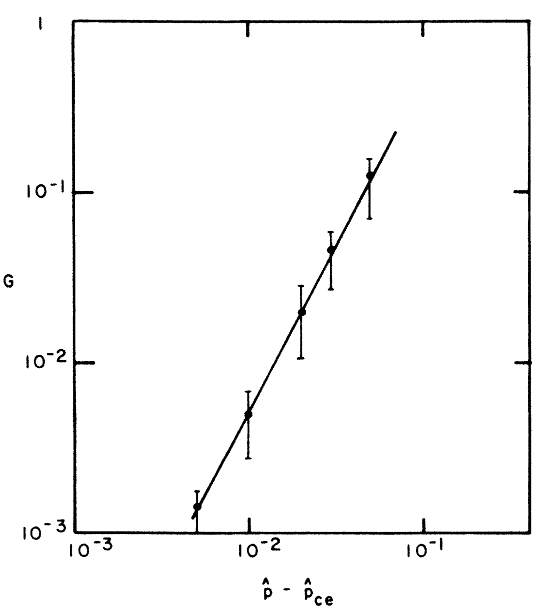

FIG. 2. Double logarithmic plot of the modulus G of the network in model III as a function of $\hat{p}-\hat{p}_{ce}$. The error bars indicate the statistical uncertainties. The results are for $\alpha=\frac{3}{4}$.

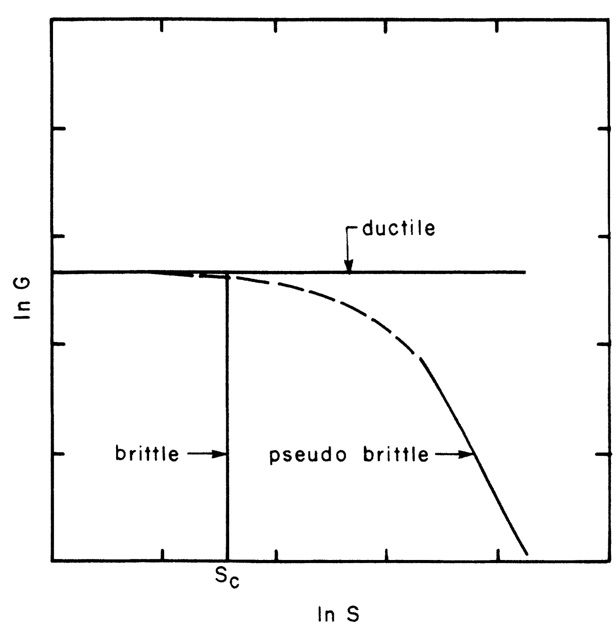

FIG. 3. The expected behavior of logarithm of the modulus G of the network as a function of logarithm of the macroscopic strain S.

defined and universal, it would serve to characterize a broad range of failure modes in disordered solids. The question of universality of δ is therefore quite important and should be addressed by more accurate numerical simulations and by theoretical methods, such as renormalization-group techniques.

In summary, we have introduced a class of models for microstructural damage and macromechanical cohesive failure in heterogeneous systems based on random networks of Hooke-type springs with load limit, in which both the spring constant and critical strain are stochastic quantities. We have considered various probability density functions (PDF's) for these quantities, and we have shown that the macroscopic response of the system depends crucially on the form of these PDF's. From our investigations on models II and III we propose that if

$$f_{-1}=\int_0^\infty \frac{f(y)}{y}dy \tag{2}$$

is finite, where f is the PDF of either k or u_c, then the system should exhibit brittle behavior. If, on the other hand, f_{-1} is divergent, one will observe pseudobrittle failure characterized by a percolationlike transition with apparently well-defined exponents. The latter, however, seem not to be related to those of linear systems. Thus, in agreement with the previous molecular-dynamics simulations[1,5] and in analogy with conduction[18-20] and diffusion[21] in random percolating systems, brittle failure corresponds to universal behavior (i.e., f_{-1} is finite) of weakly disordered systems. On the other hand, pseudobrittle failure is nonuniversal (i.e., f_{-1} is infinite and the critical exponents may depend on the parameters of the distribution) and will be observed only with certain special types of systems. Clearly, many other models may be developed and studied. For example, a more realistic model might be one in which k and u_c are correlated, according to a joint statistical distribution. It would also be interesting to investigate whether the inclusion of more microscopic detail about the behavior of the system (e.g., bond-bending forces), would significantly alter our results. The question of the existence of well-defined scaling laws for pseudobrittle behavior and the universality of the associated critical exponents are of particular importance. These matters will be taken up in a future work.[22]

After this paper was submitted we became aware of a paper[23] in which a phenomenological continuum theory of mechanical failure in disordered solids is proposed. The theory is based on a rate-independent model of distributed damage and the application of a mixture theory to account for the composite nature of the system. The predictions of the theory are in qualitative agreement with the results of our simulations.

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