Model for plastic deformation and fracture in planar disordered materials

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The elastic-plastic behavior and fracture of disordered material under tensile elongation are studied by a computer simulation model. A finite size analysis of the maximum stress shows very significant residue values even for large system sizes and for the maximum disorder in the local density. In the case of ideal plasticity we study various asymptotic behaviors and demonstrate that increasing density disorder and weakening shear stiffness do not contribute to the effective disorder in the same way as in the case of pure elasticity.

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Recently fracture and breakdown phenomena of *disordered materials* have received a considerable amount of interest. This is understandable since mechanical properties of many materials are intimately controlled by disorder. There are two apparently different approaches: one in which these phenomena are studied with analytical tools and the finite element method and the other in which the effects of disorder are studied using simple statistical models [1].

Prime examples of disordered materials are planar or two-dimensional fibrous compounds such as paper, nonwoven textiles, polymers, and fiber reinforced materials. However, an accurate description of these strongly disordered materials by means of the finite element method [2] is computationally expensive to allow statistical considerations of strength and related properties. Furthermore, it is important to understand these phenomena for a wide spectrum of length scales. For example, in fibrous compounds the relevant length scale may range from a microscopic subfiber level to a macroscopic level of large fiber flocs.

Typical statistical models that deal with lattices of bonds or other one-dimensional elements may be applied to fibrous materials at the microscopic level [3]. However, at the level of mesoscopic disorder, these materials are continuous and it is by no means clear how well bond models can describe them. In addition, properties and applicability of these materials depend not only on their elastic but also their plastic behavior. With few exceptions [4], such nonlinear material behavior has been ignored in statistical physics models.

In this paper we present an intermediate approach — a simple statistical model that captures the essence of the elastic-plastic behavior of disordered planar materials under tensile elongation. The model describes disordered planar material at a mesoscopic level by a two-dimensional lattice of adjoined initially square cells whose microscopic structure (e.g., fibers) is averaged out locally. Disorder occurs as a coarse-grained density variation, which modulates the local elastic moduli. As a first approximation the cell densities ρ_{ij} are taken at random from a uniform distribution $[1-d/2, 1+d/2]$, in which d characterizes the degree of density disorder. In reality, for disordered fibrous compounds the density distribution (as measured from, e.g., β radiograms) is Gaussian at large length scales (weak disorder) and Poissonian at small length scales (strong disorder). In reference to the study by Hansen *et al.* [6] on the scale-invariance of the distribution of *breaking* thresholds, we do not expect these differences in the shape of the *density* distribution to be relevant. As will be argued below, a wide density distribution can still give rise to a narrow threshold distribution.

In the model, each cell is defined by the four nodes at its corners, so any pair of neighboring cells share two nodes in common. Thus the deformation of an individual cell inevitably deforms the neighboring cells as well. Then the ease of deforming a cell can be described in terms of the elastic energy of nodal displacements. The sum over all individual cells defines the continuum mechanical energy functional of the system

$$H = \sum \alpha_{ij}\rho_{ij}\{A(+y_1+y_2-y_3-y_4-\pi^2_{A_{ij}} + B(-y_1+y_2+y_3-y_4+\pi_{B1_{ij}}-\pi_{B2_{ij}})^2 + C(+y_1-y_2+y_3-y_4-\pi_{C1_{ij}}+\pi_{C2_{ij}})^2\}\ .$$

Here the variables y_1, y_2, y_3, and y_4 are the longitudinal displacements of nodes defining the cell ij (cf. Fig. 1 for the labeling). The quantity ρ_{ij} is the local density and α_{ij} denotes the *integrity* of the cell ij: $\alpha_{ij}=1$ for intact cells and $\alpha_{ij}=0$ for completely failed cells. The prefactors A, B, and C depend on the Young modulus E and the shear modulus G as $A=\frac{1}{8}E$, $B=\frac{1}{24}(E+G)$, and $C=\frac{1}{8}G$, respectively. It is noted that our model assumes no tranverse deformations, because longitudinal deformations are, on average, much larger. This choice

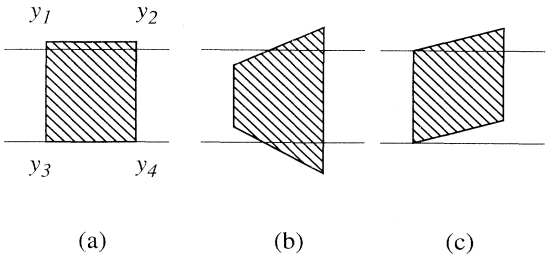

FIG. 1. Three modes of deformation for an individual cell. The external load is applied vertically. The terms with prefactors A, B, and C in the energy functional correspond to (a), (b), and (c).

makes the Poisson ratio $\nu \equiv 0$, but we expect the model to capture the salient features of shearing in fibrous compounds.

Although it might be possible to replace the cell of our model with a group of properly interconnected springs (we have not seen one), we believe that our approach is simpler and computationally more efficient. As a clear difference from simple spring models, our model includes couplings also to next nearest neighbors. The straining of a single weak cell is opposed by all neighboring cells and so as a consequence local stresses are more evenly distributed into its surroundings. On the other hand, electrical analogies (see, e.g., [1]) with conductivity disorder can be equally misleading. Consider a case of a low resistance fuse surrounded by high resistance fuses—the behavior is just the opposite to what happens in a mechanical system. Furthermore, it is not clear how shear stresses can be described with models of scalar nature.

Plasticity is implemented as the irreversible deformation of individual cells. This means that the energy functional has to contain terms ensuring new minimum energy configurations for cells that have been strained beyond the plasticity threshold, i.e., the yield limit. Plastic elongation π is defined separately for each deformation mode in order to make the minimum energy configuration unique. Initially all cells are intact, so that all the π's are zero. External strain is then increased step by step and after every strain step k the lattice energy is minimized by using the conjugate gradient method. This minimization yields the nodal displacement field corresponding to the minimum elastic energy. The possible plastic elongations for each cell are determinend as follows:

$$\pi^k_{A_{ij}} = \max[\pi^{k-1}_{A_{ij}}, (y_1 + y_2 - y_3 - y_4 - 2\theta_A)] ,$$
$$\pi^k_{B1_{ij}} = \max[\pi^{k-1}_{B1_{ij}}, (y_1 - y_3 - \theta_B)] ,$$
$$\pi^k_{B2_{ij}} = \max[\pi^{k-1}_{B2_{ij}}, (y_2 - y_4 - \theta_B)] ,$$
$$\pi^k_{C1_{ij}} = \max[\pi^{k-1}_{C1_{ij}}, (y_1 - y_4 - \theta_C)] ,$$
$$\pi^k_{C2_{ij}} = \max[\pi^{k-1}_{C2_{ij}}, (y_2 - y_3 - \theta_C)] .$$

Here the comparison with previous values (of step number $k-1$) ensures the irreversibility of plastic deformations. Furthermore, we propose a simplification that cuts down the number of independent threshold parameters to one plastic yield limit: $\theta_A = \theta_B = \theta_{\rm pl}$ and $\theta_C = \sqrt{2(1+\theta_{\rm pl})^2 - 1} - 1 \approx 2\theta_{\rm pl}$, where $\theta_{\rm pl}$ is the plastic strain threshold of the isotropic material. The value of θ_C arises from the diagonal strain of the cell. This simplification is assumed to be valid especially in the case of fibrous compounds.

With this framework of the ideally elastic-plastic model it is simple to introduce the failure mechanism by defining the failure limit $\theta_{\rm fr}$ of a cell as a certain amount of plastic deformation. If the failure threshold is set the same as the yield limit, the model describes failure in an elastic material. Note that the entire cell fails if any one of the π terms becomes nonzero. This criterion frees us from defining three different failure criteria for each deformation term — tensile, shear, and combined tensile-shear strain — in the energy functional. An example of another plausible failure criterion would be to use the total energy of a cell. This would probably lead to different fracture paths. It is noted, however, that plastic deformations cannot be defined uniquely by using the energy criterion.

For the purpose of studying the scaling behavior of an elastic-plastic system we varied the linear size L over two orders of magnitude up to $L = 400$. In the transverse direction we used either free or periodic boundary conditions, but saw no significant effect on the finite size scaling. First we investigate the elastic case and show the scaling results of the stress-strain behavior in Fig. 2. The scaling agrees with previous works [7,8] in which the stress (i.e., external force over L) in the Hookean regime is independent of the system size L. As is clear from this figure, the data collapse is complete. However, for the studied system sizes we do not see evidence for the subtle $\ln(L)$ correction [7], which would suggest the elastic modulus to be independent of L. As a further test of the finite size scaling behavior we determined the number of failed cells N_f at the maximum stress and found $N_f \sim L^{1.72}$ when $L \to \infty$, in very good agreement with previous studies [5,8].

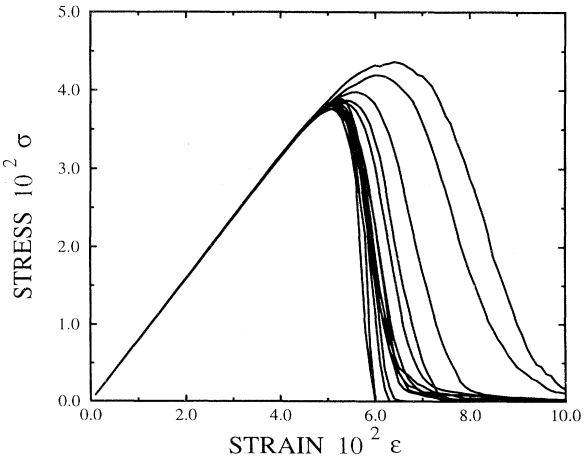

FIG. 2. Stress-strain curves of the elastic fracture system with $G/E = 0.25$, $E = 1$, and $d = 2$ for system sizes $L = 12$–400 averaged over 500–5 samples, respectively. The breakdown strain threshold of cells is set to $\theta_{\rm fr} = 0.2$.

An important difference between the results of elastic bond model studies of averaged stress-strain curves [5–8] and Fig. 2 for strong disorder and a small shear modulus is that the former models depart from linearity well before the maximum stress. However, our model exhibits Hookean behavior nearly all the way to the maximum stress. Recently it has been shown that the widely used "bond" averaging procedure leads to errors in the averaged stress-strain curves [9], which in turn can enhance apparent nonlinearities. However, even a single stress-strain test on a bond model may easily depart from linearity [9]. To understand this difference we again note that in our model nodes are more effectively coupled than in bond models, including couplings to next nearest neighbors as is likely in continuum materials. Therefore, the local stress is more evenly distributed corresponding to "weaker" disorder in terms of the breaking thresholds. Furthermore, increasing the shear coupling G/E made the Hookean regime of the stress-strain curve longer. An analogous effect was observed by Karttunen *et al.* [8] in a simpler cell model. Thus we conclude that *disordered continuum materials*, which show clear deviations from linear behavior in the stress-strain curve, cannot be modeled as a purely elastic system with a brittle fracture mechanism.

As can be observed from Fig. 2, the decay of the maximum or fracture stress σ_f as a function of L seems to slow down significantly and even stop for large values of L. This tempted us to try a nonlinear least-squares fit of the form $\sigma_f \sim a + bL^c$. Of the fitting parameters (a, b, and c) a could be interpreted as the remaining fracture stress in the thermodynamic limit (should it be nonzero) and c as the effective scaling exponent. As seen in Fig. 3, the fitting, with the exponent $c \approx -0.94$, is accurate over two orders of magnitude in L. The nonzero limiting value ($\sigma_f \to 0.037$ when $L \to \infty$ and $G/E = 0.25$, $E = 1$, $\theta_{\rm fr} = 0.2$, and $d = 2$) indicated by this power-law fit is consistent with our previous work [8], in which $\sigma_f \to 0$ only when the "shear" coupling between cells was zero. On the other hand, for percolation systems it has been suggested [10] that the fracture stress σ_f should vanish logarithmically as $\sigma_f \sim 1/[a+b(\ln L)^c]$, with $1/2 \le c \le 1$ in two dimensions. An attempt to do this kind of fit by demanding $c \ge 0$ and omitting data points $L \le 20$ is shown in Fig. 3 by the dashed line. Although this fit falls within the error bars, it is not as good as the power-law fit. It is noted, however, that our present model differs from the percolation model in that the probability of a cell to have zero density is extremely small (in fact of zero measure), while in the percolation case it is not. In addition, as indicated above, our model has a greater tendency to distribute stress to the wider neighborhood of a cell than bond models. Whether these differences are sufficient to cause different scaling behaviors is beyond the studied system sizes. Nevertheless, since our model of mesoscopic or macroscopic cells corresponds to realistic system sizes, the large residue failure stress (almost one-fifth of the ideal maximum strength of $E\theta_{\rm fr}$ for $d = 0$) is a finding of experimental and technological significance.

In Fig. 4 we show the effect of disorder on the elastic-plastic system, where the cells never break. Thick lines

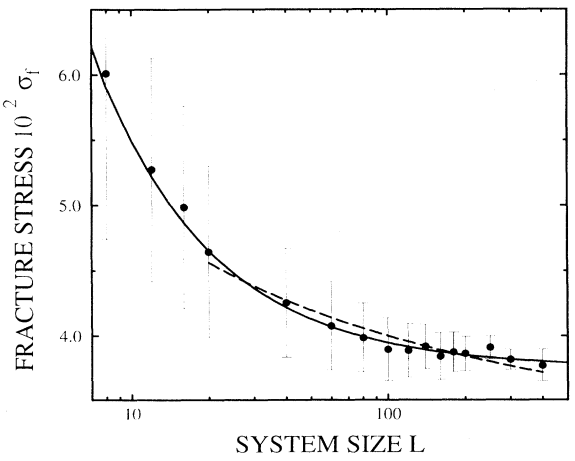

FIG. 3. Finite size scaling of fracture stress σ_f of an elastic system with $G/E = 0.25$, $E = 1$, $\theta_{\rm fr} = 0.2$, and $d = 2$. Dots present the simulation data and error bars indicate standard deviations. The solid line presents the exponential scaling relation with $c = -0.94$ and the dashed line is the logarithmic form with $c = 0.04$.

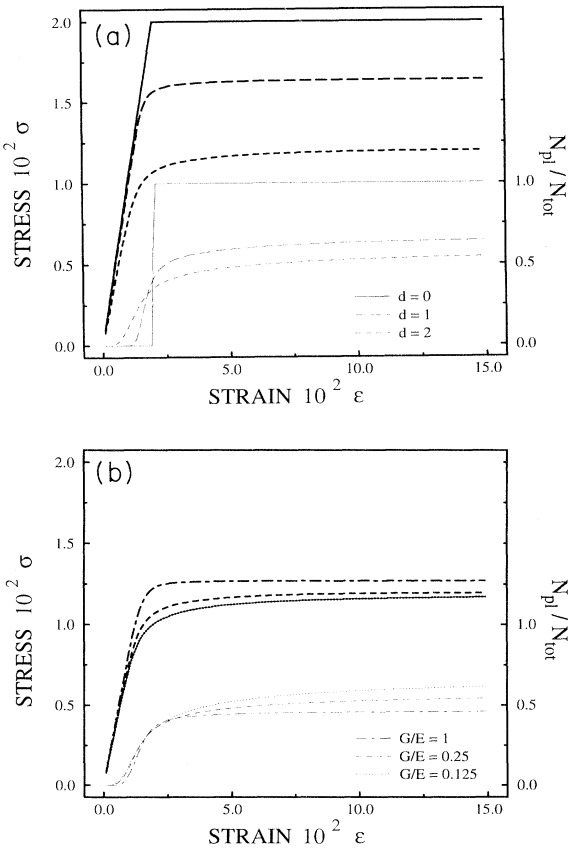

FIG. 4. Stress (thick lines) and number of plastic cells (thin lines) against external strain for (a) $d = 0, 1, 2$ and $G/E = 0.25$ and (b) $d = 2$ and $G/E = 0.125, 0.25, 1$. The system size $L = 50$, the yield strain $\theta_{\rm pl} = 0.01$, and the modulus $E = 1$.

present the stress σ and thin lines the number of plastic cells $N_{\rm pl}$ against the external strain. The degree of disorder d [Fig. 4(a)] and the relative shear modulus G/E are varied [Fig. 4(b)]. For the homogeneous system (no disorder $d = 0$) the stress-strain curve is piecewise linear, divided into a pure Hookean regime and ideally plastic regime. In this case all the cells of the system become plastic simultaneously at the yield limit. For disordered systems, however, the plastization occurs gradually. The deviation from the piecewise linear behavior is larger, for either larger d values or smaller G/E ratios. In addition, increasing the degree of disorder d decreases the asymptotic total number of plastic cells $N_{\rm pl}$ at large strains. This is because the plastic cells tend to form bands across the system. Increasing disorder makes the system statistically weaker and hence one band begins to dominate at smaller value of external strain. On the other hand, when G/E decreases (i.e., shear deformations become more likely), the asymptotic stress value decreases. At the same time $N_{\rm pl}$ increases. This happens because easier shearing makes the plastic bands across the system more complex, but easier to find. We conclude that increasing density disorder and weakening shear stiffness do not contribute to effective disorder the same way as in the case of pure elasticity [8].

We have also studied the size dependence of ideal plasticity. To our knowledge, the only statistical account for a disordered plastic system is the electrical random resistor-network analogy of Roux and Hansen [4]. It was predicted that in the case corresponding to $d = 2$, the asymptotic total number of plastic cells should become constant ($N_{\rm pl}^{\infty}/L^2 = 0.27$) as the system size L increases. In agreement with that, we found that the concentration of plastic cells did not change significantly. However, from Fig. 4 it is evident that in our case the asymptotic values of $N_{\rm pl}$ are much larger than those predicted by Roux and Hansen. In the limit of a homogeneous system $d = 0$, all the cells become plastic or $N_{\rm pl}^{\infty}/L^2 = 1$. Also, our work on the effective medium approximation [11] implies that $N_{\rm pl}^{\infty}/L^2 \geq 0.375 - 0.4$, depending on the elastic moduli ratio G/E. However, our findings are consistent with those of Roux and Hansen if the relative "weakness" of disorder in our continuum model is taken into account.

Our results also suggest that in a continuum material with disorder, $N_{\rm pl}$ becomes constant only at asymptotically large strain $\epsilon \to \infty$. It is only in this limit that all further elongation of the system occurs in a plastic band. In order to see this, suppose that at some point a path of plasticized cells is formed across the system. As the external strain increases, the elongation of the plastic cells increases. If there are any kinks in the plastic band, the elastic cells next to plastic ones will eventually be taken beyond the yield limit. Then, as the external strain increases, kinks in the plastic band travel across the system so long that they all annihilate each other or disappear at the boundaries. Thus the plastic band will "swell" in width [12]. It seems that in the thermodynamic limit $L \to \infty$ this swelling process stops perhaps only at $\epsilon \to \infty$. The precise strain dependence of $N_{\rm pl}$ would hence be needed for determining the size dependence of the asymptotic value $N_{\rm pl}^{\infty}$. In reality the system would of course fail well before this. Studies on localization of plastic deformations as well as the interplay of plasticity and fracture will be reported in the future [11].

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