Scaling behaviour in the fracture of fibrous materials

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We study the existence of distinct failure regimes in a model for fracture in fibrous materials. We simulate a bundle of parallel fibers under uniaxial static load and observe two different failure regimes: a catastrophic and a slowly shredding. In the catastrophic regime the initial deformation produces a crack which percolates through the bundle. In the slowly shredding regime the initial deformations will produce small cracks which gradually weaken the bundle. The boundary between the catastrophic and the shredding regimes is studied by means of percolation theory and of finite-size scaling theory. In this boundary, the percolation density ρ scales with the system size L, which implies the existence of a second-order phase transition with the same critical exponents as those of usual percolation.

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I. INTRODUCTION

The nature of fracture of non-homogeneous materials is an important problem in material science research. Computer simulation of the fracture phenomenon are very useful since the analytical approachs is very difficult to perform. This difficulty arises from the non-uniform character of the material and their discrete nature, which are fundamental ingredients for understanding the rupture process [1]. Usually, computer simulation in these materials gives interesting results, however the high degree of correlations between the constituents leads to a high computational cost. Bundles of unidirectional fibers form a system with low degree of correlations allowing the fracture process be simulated in a large scale.

The study of fibrous materials is not recent, as one can find in the work of Daniels [2], who in 1941 studied the rupture of a bundle of fibers with a known probability distribution of strength. Recently, Hansen and Hemmer [3] studied the distribution H(S) of the sizes S of burst avalanches, i. e., an instantaneous propagation of a crack. They found a power-law behaviour: $H(S) \sim S^{-\alpha}$ with the exponent α depending on how the load is shared between the fibers. For global load sharing, where the load is shared equally among non breaking fibers, they obtained $\alpha = 2.5$. For local load sharing, when a fiber breaks its load is shared among nearest-neighbours no breaking fibers, they obtained $\alpha = 4.5$. Those results have been obtained for a one-dimensional lattice of fibers, that is, the load sharing is the only correlation between the fibers. Other approaches have been introduced to discuss this problem [4,5]. The role of the homogeneous support matrix on the failure of composite materials has also been discussed by some authors [6–8].

A model of a bundle of unidirectional fibers, which takes into account external parameters like temperature and velocity of traction, has been proposed in 1994 by Bernardes and Moreira [9]. In this model, the correlations between the fibers are present through the probability of rupture of a fiber, which depends on the number of unbroken nearest neighbouring fibers. A cascade mechanism - inspired on models for avalanches - is used to propagate cracks through the material: when a fiber breaks, its neighbours are visited and can break too. In this model, all unbroken fibers have the same deformation, i.e, one has global load sharing. However, the cascade mechanism introduces a local effect. In a subsequent work [10], the dependence of the frequency of cracks with the crack sizes were used to determine the failure regimes. Two basic regimes were discussed: a regime where cracks of the size of the system were present and another one where only small cracks appeared. Those regimes were identified, respectively, with the brittle and ductile failure regimes. The criterion used to distinguish one regime from another was based on self-organized criticality, i.e, in the brittle-ductile transition region, cracks of all sizes were present. However, they did not take into account finite size effects in their analysis, which are very important in this type of process. In fact, a finite-size scaling analysis should be performed, in order to guarantee a better definition of the failure regimes.

The aim of the present paper is to introduce a criterion which defines the failure regimes on fibrous materials. When a fiber bundle breaks, two regimes can be observed: a catastrophic regime, when a sufficiently large number of fibers are simultaneously broken, and a slow process of successive rupture of fibers, here called shredding regime. The first regime occurs at low temperatures and/or high strains and are similar to a brittle fracture. It is characterized by the fact that an initial deformation produces a large crack which percolates through the bundle. The shredding regime occurs for higher temperatures and/or lower strains, and is similar to the ductile regime. In this case, the first deformations produce small cracks which weaken the bundle and thus cause its failure. The criterion is implemented by considering the static failure of a modified version of the model introduced by Bernardes and Moreira [9]. A second order phase boundary between two regimes is found for a given strain. A finite-size scaling analysis is used to determine the critical temperature and exponents.

II. THE MODEL

The model for the fibrous material here discussed consists of a bundle of $N_0 = L \times L$ parallel fibers with a cross-section forming a triangular lattice. Each fiber has the same elastic constant k, and they are fixed at both ends to parallel plates. One plate is fixed and the other plate can be pulled by an external force. When the bundle is pulled by a force F, all fibers undergo the same linear deformation z = F/Nk, where N is the number of unbroken fibers. We assume that a fiber has a failure probability which increases with the deformation z. When this deformation reaches a critical value z_c , the breaking probability of an isolated fiber is equal to one. When the bundle has a deformation z, a fiber i has a failure probability related to its elastic energy and to the number of unbroken neighbouring fibers n_i , given by

$$P_i(\delta) = \frac{z/z_c}{n_i + 1} \exp\left(\frac{(kz^2/2) - (kz_c^2/2)}{K_B T}\right) , \qquad (1)$$

Defining the strain of the material as $\delta = z/z_c$ and the normalized temperature as $t = K_B T/E_c$, where T is the absolute temperature, $E_c = k z_c^2/2$ is the critical elastic energy and K_B is the Boltzman constant, we can rewrite the failure probability as

$$P_i(\delta) = \frac{\delta}{n_i + 1} \exp\left(\frac{\delta^2 - 1}{t}\right) , \qquad (2)$$

This definition of the failure probability is different from that used by Bernardes and Moreira [9], since now we have introduced δ as a multiplicative factor to impose that, for $\delta = 0$, $P_i(\delta) = 0$.

The static failure of a fiber bundle is produced by applying a constant force F_0 to the bundle, for example, by hanging a weight on the moving plate. The initial strain of the bundle is given by

$$\delta_0 = \frac{z_0}{z_c} = \frac{F_0}{N_0 k z_c} \tag{3}$$

The simulation of the rupture process proceeds as follows. At each time step of the simulation, we randomly choose a set of N_q (= qN_0) unbroken fibers, where the number q represents a percentage of fibers and it allows us to work with any system size. So, differently of an Ising model, where all the sites are "tested" at each time step, in our model only a number N_q of randomly chosen unbroken fibers are tested. It represents the continuous growth of the bundle due to the continuous traction. For each chosen fiber, we evaluate the probability of rupture, using Eq. 1, and compare it with a random number in the interval [0,1). If the random number is less than the failure probability, the fiber breaks. To simulate the load spreading, the same process is repeated for all neighbouring unbroken fibers. The failure probability of these neighbouring fibers increases due to the decreasing of n_i and a cascade of breaking fibers may begin. This procedure describes the propagation of a crack through the fiber bundle, which occurs in all directions perpendicular to the force applied to the system. The cascade process stops when the test of the probability does not allow the rupture of any other fiber on the border of the crack or when the crack meets another already formed crack. This collision leads to the fusion of cracks, and it is the mechanism to explain the rupture of the material in the shredding regime. The same cascade propagation is attempted by choosing another fiber of the set N_q . After all the N_q fibers have been tested, the strain is increased if some fibers have been broken. This new strain is the same for all the remaining unbroken fibers. Since the force is fixed (the weight hung on the bundle), the greater the number of broken fibers, the larger is the strain on the fibers, and the higher is the failure probability. Then, other set of N_q unbroken fibers are chosen and the rupture process restarts. This process stops when all the fibers are broken, i.e. the bundle breaks apart. In this model, a combination of local and global load sharing occurs. That is, after a fiber breaks, a cascade may begin which simulates the local load sharing. When the cascade process stops, the stress is distributed equally between all unbroken fibers which is the global load sharing.

III. RESULTS

The failure probability (Eq. 2) can be written as

$$P_i(z) = \frac{\Gamma(t, \delta)}{(n_i + 1)} \quad , \tag{4}$$

where we introduce the parameter $\Gamma(t,\delta)$ defined as

$$\Gamma(t,\delta) = \delta \exp\left(\frac{\delta^2 - 1}{t}\right)$$
 (5)

For a triangular lattice (with coordination number 6) and $\Gamma(t,\delta) \geq 6$, the rupture of any fiber induces the rupture of the whole bundle, i.e., the bundle breaks with just one crack. Obviously, this crack forms a cluster which percolates through the entire system.

We can define the density of the percolation crack as

$$\rho = \frac{N_{pc}}{N_0} \quad , \tag{6}$$

where N_{pc} is the number of broken fibers belonging to the percolating crack. Thus, when $\Gamma(t,\delta) \geq 6$, we have $\rho = 1$. On the other hand, as it has been observed in previous works [10,11], for higher temperatures and/or lower strains, the fracture of the bundle is caused by many small cracks, none of then large enough to percolate through the system. Thus, for a fixed temperature, if one starts with a large enough strain δ_0 and one decreases it, the system goes from a regime where $\rho = 1$ to another regime where $\rho \to 0$. This behaviour is the same as the one encountered in the percolation problem.

Figure 1 shows the density of the percolation cluster ρ versus the initial strain δ_0 , for two different temperatures. As one sees, $\rho=1$ for high values of δ_0 , and jumps to zero for low enough value of δ_0 . So, we may assume that, for a fixed temperature, there is a critical value δ_{0c} above which one observes a percolation crack, and below which there is no percolation at all. Another interesting feature that one can observe in Figure 1 is that, if one substitutes into Eq. 5 the values of t and δ_{0c} corresponding to the transition region ($\delta_0 \sim 1.18$ for t=1.0 and $\delta_0 \sim 1.37$ for t=4.0), we get for both instances $\Gamma(t,\delta) \sim 1.73$. The fundamental reason for obtaining this value wil be explained below.

In contrast to that described above, the same behaviour does not occur when we keep δ_0 fixed and change the temperature. Figure 2 shows the results obtained for the density of the percolation cluster ρ versus temperature t, for $\delta_0 = 1.4$. We observe that, initially, ρ decreases as the temperature t increases, and around $t \sim 4.5$, the value of ρ seems to go to zero. However, an additional increase in the temperature will revert the process and a minimum appears. Note that at the point of minimum again ($\Gamma(t = 4.5, \delta = 1.4) \sim 1.73$), which is the same value reported above. For low temperatures (t < 2.0), when a fiber breaks, the probability is so high that this rupture initiates a cascade which breaks the whole bundle. By increasing the temperature, a number of small cracks are formed, inhibiting the formation of a percolating cluster and the density ρ decreases. However, all those processes occur in the first step of the simulation when N_q attempts to break the bundle are performed. Thus, for t < 4.5, the bundle has been broken due to the crack which percolates the system during the first N_q attempts to break it. For t > 4.5, all the first N_q attempts do not succeed to generate a crack which percolates the bundle. However, some fibers have been broken and cracks were formed. In the second step of the simulation, a new value of δ is used (higher than δ_0) and a new set of N_q trials are chosen. But now one has a higher value for $\Gamma(t,\delta)$ therefore it is easier to produce a large crack which percolates the bundle. By increasing the temperature, a smaller number of fibers are broken in the first N_q attempts, and then, in the second step, the are more unbroken fibers and therefore the density ρ increases, thus forming a minimum in the graph of Figure 2.

In fact, we can assume that there is a critical value for $\Gamma(t,\delta)\sim 1.73$ that defines the transition between two regimes. In the first one, a catastrophic fracture occurs due to the first attempt to break the bundle, while in the second case the rupture of the bundle occurs due to the formation of small cracks, which weaken the bundle. A percolating crack may also occur in the second case, however the fracture dynamics is given by the weakening of the bundle not by the catastrophic propagation of a crack

In order to consider the present model in the context of percolation theory, we shall use the parameter Γ as an arbitrary parameter without regarding it as a function of the strain δ and temperature t. Within the percolation point of view, we map the original model into a triangular lattice where the empty sites corresponds to the unbroken fibers. The parameter Γ is the analog to the percolation probability. The algorithm for the mechanism of fracture is mapped into the following algorithm for the percolation problem. An empty site (unbroken fiber) i is chosen at random; Its occupation (failure) probability P_i is calculated by dividing Γ by the number of its neighbouring empty sites (unbroken fibers) plus one. This probability P_i is compared with a random number $r \in [0,1)$; If $P_i > r$, the site is occupied (the fiber is broken) and a cluster (crack) can be formed, i.e, an empty neighbouring site (an unbroken neighbouring fiber) is randomly chosen and the process are repeated; Otherwise, another site, on N_q in total, is chosen.

When a cluster is formed, we test if it percolated through the system. If it does, we calculate the density ρ of the percolating cluster. Figure 3a shows the results obtained for several system sizes. Two regions are separated by the transition point Γ_c . The larger the system size, more clearly is the transition between those two regions. Observe in the detail, shown in Figure 3b, that a second order phase transition takes place at $\Gamma_c = 1.733(1)$. This implies that, at that point, clusters of all sizes should be present, as confirmed by the results shown in Figure 4. In this figure, the results have been obtained for a system size $L = 5000 \ (2.5 \times 10^7 \ \text{fibers})$ and averaged over 1000 samples (it took nearly 24h on a Sun Enterprise 8GB computer) which gives the following power law

$$H(S) \sim S^{-\tau}$$
 , (7)

where $\tau = 2.037 \pm 0.007$. A finite size analysis can be performed by plotting $\tau(L)$ as a function of $L^{-1/\nu}$, where ν

is the exponent related to the divergence of the correlation length at the transition. We tested several value of ν and the best linear fitting were obtained for $\nu=4/3$, as shown in Figure 5. This value corresponds to the exact exponent ν for percolation at d=2. The value of the exponent τ for an infinite lattice is, then, evaluated to be $\tau(\infty)=2.05\pm0.01$, in an excellent agreement with the theoretical value, $\tau_{\infty}=2.055$ [12].

In order to check if our problem belongs to the same universality as the percolation problem, we have done a finite-size scaling analysis by assuming the scaling law [12]

$$\rho(\Gamma, L) = L^{-\beta/\nu} \psi\left(\epsilon L^{1/\nu}\right) \quad , \tag{8}$$

where

$$\epsilon = \left| 1 - \frac{\Gamma}{\Gamma_c} \right| , \qquad (9)$$

 ψ is a universal function of $\epsilon L^{1/\nu}$ only, and β and ν are the critical exponents for the infinite lattice. Figure 6 shows the finize-size scaling plot $\rho L^{\beta/\nu}$ versus $\epsilon L^{1/\nu}$ for nine sizes of L. We have used $\Gamma_c=1.733,\ \nu=4/3$ and the best value of β which validates Eq. 8 is $\beta=0.14$. This value is also in an excellent agreement with the known value for the usual percolation.

Now, returning to the original fracture model, we use Eq. 5 to obtain the critical temperature t_c in terms of the critical parameter Γ_c and of the initial strain δ_0

$$t_c = \frac{\delta_0^2 - 1}{\ln(\Gamma_c) - \ln(\delta_0)}.$$
 (10)

Using this expression we plot the fracture regimes diagram, in the temperature t versus the initial strain δ_0 plane, depicted in Figure 7. Two fracture regimes are separated by a second order transition line. In region \mathbf{C} the fracture is catastrophic and in region \mathbf{S} we have the shredding regime. Note that the catastrophic regime only occurs for $\delta_0 > 1$ and for low temperatures. In this figure, the solid line corresponds to the analytical results, and the points were obtained by simulations.

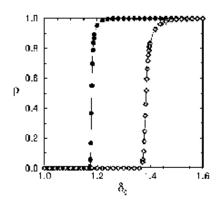
IV. CONCLUSIONS

In conclusion, we have studied a model for fracture in fibrous materials in (2+1)-dimensions and shown the existence of two failure regimes: the catastrophic regime, where the initial deformation produces a single crack which percolates through the bundle; and the slowly shredding regime, where the initial deformation produces small cracks which gradually weaken the bundle. By using percolation theory and finize-size scaling arguments, we were able of finding the transition line between these regimes. Our results indicate that this transition is of

second order. Finally, we have shown that this model belongs to the same universality class as the percolation problem.

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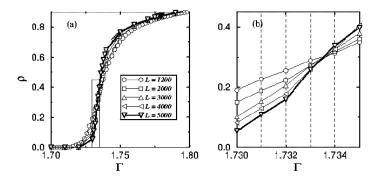
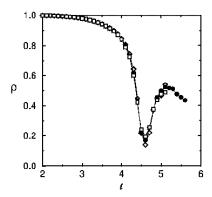


FIG. 1. Density of the percolating cluster ρ versus the initial strain δ_0 for two different temperatures: t=1.0 (filled circles) and t=4.0 (open diamonds). The system size is L=1000 and the data were averaged over 1000 statistically independent samples.

FIG. 3. (a) Density of the percolating cluster ρ versus Γ for five different system sizes; (b) Zoom of the region corresponding to the small box drawn in the left plot, showing more clearly the crossing of the curves. The data were averaged over 1000 statistically independent samples.



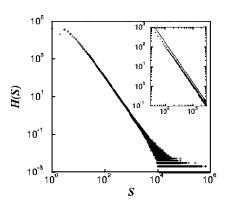


FIG. 2. Density of the percolating cluster ρ versus temperature for an initial strain $\delta_0=1.4$ and three different system sizes: L=800 (open squares); L=900 (filled circles) and L=1000 (open diamonds). The data were averaged over 1000 statistically independent samples.

FIG. 4. Log-log plot of the averaged number of cracks H(S) versus the crack size S for L=5000 at $\Gamma_c=1.733$. The points have been obtained by averaging over 1000 statistically independent samples. The data show a power law behaviour (expected at the criticality) with exponent $\tau=2.037\pm0.007$. The insert shows a detail of the whole set. The solid line in this insert has exponent 2.037.

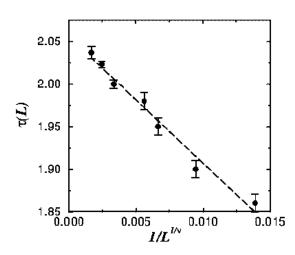


FIG. 5. Estimate of the value of τ_{∞} . We plot the value $\tau(L)$ versus $L^{-1/\nu}$ with $\nu=4/3$. A linear regression has t performed, giving $\tau_{\infty}=2.05\pm0.01$.

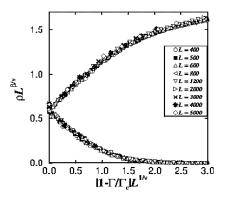


FIG. 6. Plot of the scaling relation $\rho L^{\beta/\nu}$ versus $\epsilon L^{1/\nu}$ for nine system sizes (provided in the legend) with $\Gamma_c=1.733,~\beta=0.14$ and $\nu=4/3$.

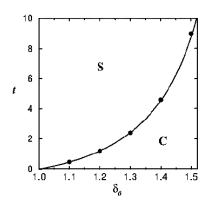


FIG. 7. Fracture regimes diagram of the temperature t in function of the initial strain δ_0 , where **C** represents the catastrophic regime and **S** represents the shredding regime. Solid line represents the theoretical curve and filled circles represent the data obtained in our simulations.