Patterns and scaling in surface fragmentation processes

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We consider a finite-element model for the fragmentation of a coating covering a bulk material. The coating breaks under a quasistatical, slowly increasing strain (induced, e.g., by temperature changes, by desiccation, or by mechanical deformations). We model the coating through an array of springs and account for its statistical inhomogeneities by assigning each spring a breakdown threshold taken from a given probability distribution (PD). The adhesion to the bulk is modeled through other springs, which connect the coating to the substratum. We consider the dependence on the strain of the mean fragment size and also the ensuing pattern of cracks. We find that the mean fragment size obeys a power-law dependence on the strain; the exponent of the power law is related to the strength of disorder (i.e., the behavior of the assumed PD for breakdown thresholds in the vicinity of zero). Moreover, the mode of fragmentation also depends on the disorder's strengths: for small disorder (narrow PDs) the system fragments through crack propagation, for strong disorder (wide PD, starting from zero) the cracks are formed by the coalescence of initially independent point defects. [S1063-651X(96)09509-8]

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I. INTRODUCTION

The statistical description of failure phenomena in disordered, complex systems has drawn much attention in the past decade; since then the understanding for the basic mechanisms leading to failure has grown and the important role played by the local inhomogeneities on the global fracture patterns was clearly stressed [1–4]. Apart from the technologically motivated interest in the mechanics of coatings, failure phenomena are part of the large framework of irreversible pattern formation. The mechanical description of fracture often starts from a mesoscopic picture based on finite elements; their mechanical properties vary through the sample, but are, once assigned, fixed (quenched) for a given realization. Some recent works in the field are Refs. [5–9]. Now the failure pattern depends strongly on the geometry of the system and on the particular features of the disorder. The analytical models considered so far tend to oversimplify the topology of the system by taking as building blocks bundles of fibers or some other hierarchically arranged subsystems. We note that failure phenomena depend very strongly on the properties of the disorder and thus cannot be treated in the framework of a perturbation theory; see Ref. [8].

Here we consider a coating that breaks under a quasistatical, slowly increasing strain (induced, e.g., by temperature changes, by desiccation, or by mechanical deformations); this situation is of common occurrence (see Ref. [9] for a general survey). The coating is represented by an array of springs; we account for its local randomness by assigning to each spring a breakdown threshold taken from a given probability distribution. The adhesion to the bulk is modeled through other springs, which connect the coating to a substratum. The stretching or bending of the substratum corresponds then to a gradual, homogeneous change of coordinates. Of interest are the ensuing pattern of cracks and the dependence of the fragment-size distribution on the strain.

The problem of surface fragmentation is in general different from such fractal growth phenomena as diffusion-limited aggregation or Laplacian growth. From everyday life one knows that in not too disordered systems fragmentation produces (roughly) hexagonal or tetragonal patterns. On the other hand, fractal crack patterns can emerge if the degree of disorder is very high. Reviews of surface fragmentation studies, both experimentally and numerically, are given in Refs. [2,3]. The investigations reported there show the basic similarity between the observed and the numerically obtained crack patterns.

A scalar model for surface fragmentation (i.e., the electrical analog of the mechanical failure problem considered) was numerically investigated in Ref. [10]. In Refs. [11–13] the same model was treated analytically in one dimension. The main result of these works is that the breaking process displays different regimes, depending on the local distribution of breakdown thresholds; this shows up, for instance, in the dependence of the mean fragment size on the sublayer's elongation. A two-dimensional model for a thin film is more realistic and much more rich, since many of its geometrical aspects (patterns) do not exist in one dimension. In the present work we will investigate the dependence of the fragments' sizes and patterns on the applied strains and on the probability distribution (PD) of local breakdown thresholds. We find that the mean fragment size obeys a power-law dependence on the strain, where the exponent of the power law is related to the assumed PD. Furthermore, both the fragment size distribution and the crack patterns depend strongly on this PD. On the other hand, although the patterns of cracks that appear during fragmentation can be very complex, elongated strips in two dimensions show an overall scaling be-

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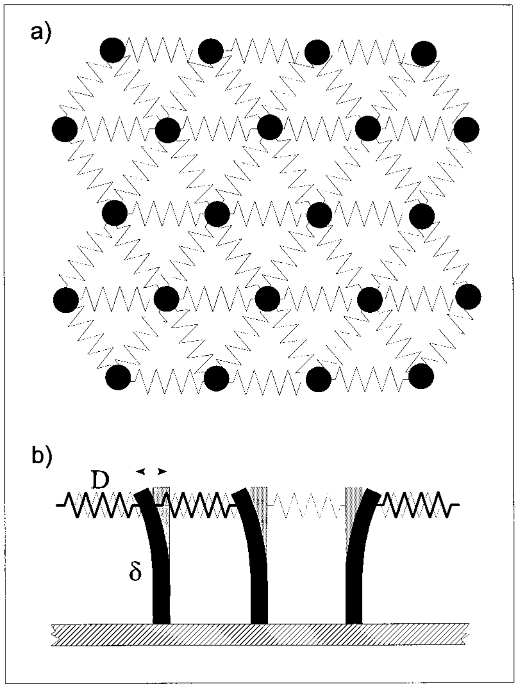

FIG. 1. Model used in the simulations: (a) view of the surface layer and (b) view from the side (vertical cross section).

havior closely related to fragmentation in one dimension; thus, in this case no new length scales enter into the problem.

II. THE THIN-FILM MODEL

In our study of thin films we start from a model put forth in Ref. [3]. The coating is viewed as being an array of springs with elastic constants D, forming a triangular lattice; see Fig. 1. The lattice constant (side length of each triangle) is taken to be unity. The film is attached to the substrate elastically, so that the surface layer can move relatively to the bulk; this motional freedom is accounted for by connecting the nodes of the coating and the corresponding sites of the substrate through leaf springs of elastic constant δ; see Fig. 1. The surface layer is brittle, so that each spring can break under stress. The value at which a particular spring breaks is random, but fixed at the start of the fragmentation process (i.e., the disorder is quenched). The PD of breakdown thresholds is a material property and is known from the start. As systems we consider (i) a plate under homogeneous stress and (ii) an elongated strip undergoing stretching.

We describe first our numerical approach to the problem. One step of the calculation involves the computation of the forces acting on the springs and the removal of those springs that break (because their breakdown threshold is smaller than the acting force). Iterating the procedure leads to crack propagation. Under a quasistatically increasing stress the forces acting on the springs are given by the solution of the equations for mechanical equilibrium at each node i; as a projection on the (x,y) plane parallel to the substrate one has

$$\sum_j D_{i,j}(|\mathbf{r}_j-\mathbf{r}_i|-r_0)\mathbf{e}_{ji}+\delta|\mathbf{r}_i-\mathbf{R}_i|=0, \qquad (1)$$

where the sum runs over the nearest neighbors of the ith node, $\mathbf{r}_j$ is the position of the jth node, $\mathbf{R}_j$ that of the corresponding substratum site, and r_0 is the equilibrium length of a spring in the absence of stress and $\mathbf{e}_{ij}=(\mathbf{r}_i-\mathbf{r}_j)/(|\mathbf{r}_i-\mathbf{r}_j|)$ is a unit vector in the spring's direction. The elastic constants $D_{i,j}$ are $D_{i,j}=D$ for intact and $D_{i,j}=0$ for broken springs. At the beginning of the process the surface layer is in equilibrium and no forces act on it.

The system of equations (1) involves absolute values of vectors and is therefore essentially nonlinear. We use a simple relaxation algorithm to solve it; we obtain, namely, the $\mathbf{r}_j$ by numerical integration of the overdamped equations of motion

$$\dot{\mathbf{r}}_i=-\alpha\left[\sum_j D_{i,j}(|\mathbf{r}_j-\mathbf{r}_i|-r_0)\mathbf{e}_{ji}+\delta|\mathbf{r}_i-\mathbf{R}_i|\right]. \qquad (2)$$

Here the constant $\alpha>0$ is chosen in such a way as to guarantee the stability and fast convergence of the overall scheme of computations.

The deformation of the substrate is modeled by gradual changes in the coordinates $\mathbf{R}_j=(X_j,Y_j)$ of the substrate's sites: the corresponding coordinates grow with ''time'' (procedure step) t as

$$X_j=(1+a_x t)X_{j,0}$$

and

$$Y_j=(1+a_y t)Y_{j,0} \qquad (3)$$

We consider here both isotropic and anisotropic homogeneous changes; for these $a_x=a_y$ and $a_x\neq a_y$, respectively. If the elastic force acting on a spring, $f=D_{i,j}(|\mathbf{r}_j-\mathbf{r}_i|-r_0)$ attains its prescribed breakdown value $f^b_{i,j}$, the spring breaks irreversibly, and its elastic constant is set to zero. This is followed by additional relaxation steps, in which the new equilibrium positions are calculated; these steps may lead (for a brittle regime of fracture propagation) to the breaking of additional springs. If at a given strain no further springs break, the whole procedure is iterated by increasing the time from t to $t+\Delta t$. By this, through Eq. (3), a new strain increase is generated.

We consider systems of elements whose breakdown thresholds are homogeneously distributed in the interval $[f_{\min},f_{\min}+W]$; for these the PD is

$$p(f^b)=\begin{cases}1/W & \text{for } f_{\min}<f^b<f_{\min}+W\\ 0 & \text{otherwise.}\end{cases} \qquad (4)$$

As we shall see in Sec. III, the strength of the disorder is characterized by the parameter $W/f_{\min}$. Systems with $f_{\min}=0$, i.e., with a rectangular distribution of the form

$$p(f^b)=\begin{cases}1/W & \text{for } 0<f^b<W\\ 0 & \text{otherwise,}\end{cases} \qquad (5)$$

contain elements with breakdown thresholds in the vicinity of zero and belong to the strong disorder case; see Ref. [10] and also Sec. III herein.

A measure for breakage is the mean size of the obtained fragments. In the case of complicated two-dimensional (2D) geometries, when the cracks are not continuous and do not lead to well-separated fragments, the determination of fragment sizes is ambiguous. Hence in two dimensions we focus on the distances of subsequent broken bonds measured along (arbitrarily drawn) straight lines and take as the characteristic length the average of such distances over the orientations of the lines and over the realizations of the system.

During our simulations we have found that although the visible crack pattern is rather insensitive to the quality of the relaxation [i.e., to the relative error ε in the numerical solution of Eq. (2)], the fragment size distribution depends strongly on ε. We determined the necessary accuracy ε through test runs in which we noted the sequence of breaking bonds for the same initial conditions under changes of ε. We found that taking ε as low as $\varepsilon=10^{-9}$ is sufficient in order to obtain unique sequences; higher ε values lead to ε-dependent sequences, evidently an artifact.

Before reporting the results of our simulations in two dimensions we focus in more detail on the parameters that govern the model's behavior. To do this we first turn to the consideration of a scalar 1D model. This will shed light on the interplay between the model's parameters and allow us to introduce as important notions the correlation length and the strength of the disorder.

III. ONE-DIMENSIONAL SYSTEMS

A 1D electrical analog for surface fragmentation was investigated by us both analytically and numerically in Refs. [11,12]. In one dimension the mechanical situation differs from an electrical scalar analog only in notation. Here we restrict ourselves to a summary of the findings, now adapted to the mechanical model, which is presented in Fig. 1(b). Moreover, we consider only the scaling aspects of the model, which can be generalized to two-dimensional coatings.

Starting from a single large fragment, one increases gradually the elongation ΔR of the substrate and reaches eventually a value at which the first spring fails. This spring is then removed from the system, by which (in general) two new fragments are created. A further increase in ΔR results in the splitting of these new segments, etc.

We focus on η_k, the elongation of the kth spring within an intact fragment of length N under the elongation of the substrate by ΔR. Now η_k depends on ξ, the correlation length in the problem,

$$\xi=\frac{2}{\operatorname{arccosh}\,[1+D/2\delta]}; \tag{6}$$

see Refs. [11,12]. For $\xi \ll N$ the elongation η attains the value ΔR almost everywhere inside the fragment, except near its ends. In the two end regions, of width around ξ, the stress follows an exponential law. In the opposite case $N \ll \xi$ (which always arises in the late stages of the fragmentation process), this distribution attains a universal parabolic form

$$\eta_k=\frac{N^2}{2\xi^2}\,(1-4\theta^2)\Delta R, \tag{7}$$

with $\theta=(k/N)-\frac{1}{2}$.

At the beginning of the process, as long as $\xi \ll N$, the stress is almost homogeneously distributed inside each segment and the weakest bond is the one that breaks, which gives rise to an approximately Poissonian distribution of fragment lengths. When the process goes on, the fragments' sizes get to be smaller than the correlation length ξ and the situation gets complex; it leads to nontrivial fragment size distributions and to power-law dependences of the mean fragment sizes.

For a PD with a nonzero lower boundary $f_{\min}\neq 0$, Eq. (4), the distributions of the position of failure $Q_N(\theta)$ and of the breakdown threshold $R_N(s)$ are given by the expressions [11,12]

$$Q_N(\theta)=\tfrac{1}{2}\;\omega^{-1}\Gamma\left(\tfrac{2}{3},(|\theta|/\omega)^3\right) \tag{8}$$

and

$$R_N(s)=\frac{N}{W}\;\sqrt{\frac{s-f_{\min}}{f_{\min}}}\;\exp\left[-\frac{2N(s-f_{\min})^{2/3}}{3W\sqrt{f_{\min}}}\right], \tag{9}$$

where $s=D(N^2/2\xi^2)\Delta R$ corresponds to the local strain in the middle of a fragment. In Eq. (8) $\Gamma(x,y)$ is the incomplete gamma function and $\omega=[3W/(16f_{\min}N)]^{1/3}$ is the width of the distribution. Equation (8) leads to a bell-shaped function concentrated near the middle of the fragment. For $f_{\min}>0$ and N large the failures tend to occur near the middle of the fragment, which can be understood by realizing that a new failure occurs soon after the maximum of the strain distribution (basically a parabola) reaches the minimum of the PD of the breakdown thresholds.

Equations (8) and (9) are valid if the width of the distribution is smaller than the segments' length, i.e., if $\omega \ll 1$. This is the case when $W/f_{\min} \ll N$, where N is a typical size of a fragment. From Eq. (8) it follows then that failures occur near the middle of existing fragments, so that the overall fragmentation process follows a hierarchical pattern. The averaged pattern is then weakly disordered. In the limiting case in which $f_{\min}=0$ the distributions $Q_N(\theta)$ and $R_N(s)$ are given by [11,12]

$$Q_N(\theta)=\tfrac{3}{2}(1-4\theta^2) \tag{10}$$

and

$$R_N(s)=\frac{2N}{3W}\,\exp\left[-\frac{2N}{3W}\,s\right]. \tag{11}$$

In this case a fragment of length N breaks when $\Delta R_c=3D^{-1}W\xi^2/N^3$ and the point of failure can be situated anywhere inside the fragment. In general, for $W/f_{\min} \gg N$, failures are no longer concentrated near the fragments' centers. We denote this situation as leading to strong disorder in the distribution of patterns.

Inverting the relations between ΔR and the survival probability of a fragment of length N, one infers that for each value of ΔR_c there exists a characteristic fragment length N_c, such that fragments larger than N_c hardly survive and fragments smaller than N_c stay almost certainly intact; hence the mean fragment size is of the order of N_c. These considerations lead to the following dependences of $L=\langle N\rangle$ on ΔR:

$$L \cong \sqrt{2D^{-1}f_{\min}}\,\xi(\Delta R)^{-1/2} \tag{12}$$

for $W/f_{\min} \ll N$ and

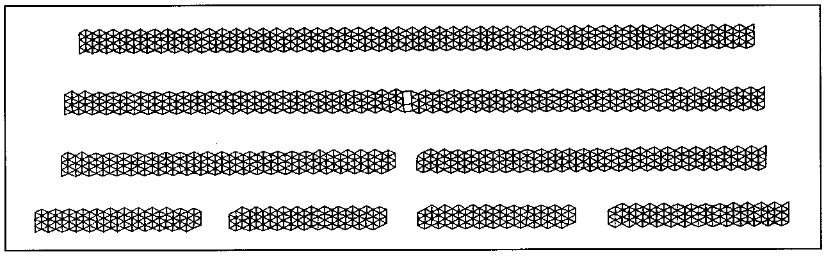

FIG. 2. Series of fragmentation stages of an elongated strip under uniaxial stress.

$$L \cong (3D^{-1}W\xi^2)^{1/3}(\Delta R)^{-1/3} \quad (13)$$

for $f_{\min}=0$.

Note that systems with $W<f_{\min}$ always belong to the class of weak disorder, while those with $f_{\min}=0$ are always strongly disordered. The dimensionless parameter $\zeta=W/f_{\min}L\propto\omega^3$, with L being the characteristic fragment size, typifies the situation. For $\zeta\ll1$ failures occur at the points of highest stress, while for $\zeta\gg1$ failures are associated with weakest bonds. The intermediate ζ domain leads to complex patterns of behavior, which depend on the correlation length, on N, and on $W/f_{\min}$. As we will show in Sec. IV, in two dimensions weak disorder leads to a brittle growth of straight cracks while stronger disorder lets the cracks get wavy. Summarizing, in one dimension we have found that L goes as $L\sim(\Delta R)^{-1/2}$ for weak and $L\sim(\Delta R)^{-1/3}$ for strong disorder.

IV. SCALING AND PATTERNS IN TWO-DIMENSIONAL SURFACE LAYERS

The findings for the scalar one-dimensional model are reproduced in simulations of a quasi-one-dimensional system (elongated strip); see Fig. 2. The dependence of L on the elongation is given in Fig. 3 in double-logarithmic scales and shows the cases of weak and strong disorder. We note that square plates under uniaxial stress behave similarly; in this case the majority of cracks are nearly perpendicular to the direction of the stress.

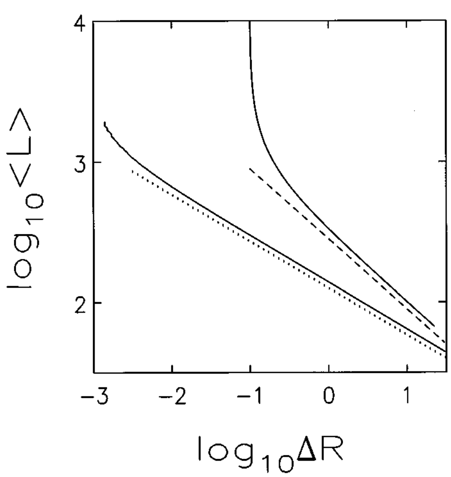

FIG. 3. Mean fragment size L as a function of ΔR (the elongation of the substrate) in a quasi-1D geometry (a 50×25000 strip) plotted in double-logarithmic scales. The upper curve corresponds to the PD Eq. (4), with $f_{\min}=100$ and $W=10$, the lower curve to the PD Eq. (5) with $W=100$. The numerical results were obtained using an average over ten realizations each. The slope of the dashed line is $-\frac{1}{2}$ and that of the dotted line is $-\frac{1}{3}$.

The situation for two-dimensional layers under isotropic stress is considerably more complex than in elongated strips or in layers under uniaxial stress. Here a different, very important feature appears, namely, the propagation of cracks. In Fig. 4 we display a mosaic of patterns that emerge when the breaking systems have different PDs, here obtained for several values of W in Eq. (4). For $W/f_{\min}\ll1$ [Fig. 4(a)] the cracks are mostly straight lines, which follow the lattice structure closely. For stronger disorder the cracks become wavy, but fragmentation still proceeds through crack growth. The overall picture [Fig. 4(b)] is very reminiscent of the desiccation in thick layers of coffee-water mixtures; see Ref. [14]. For $W/f_{\min}\gg1$ [Fig. 4(c)] the parquet pattern of Figs. 4(a) and 4(b) is no longer visible. Cracks develop now through the coalescence of pointlike defects, which at first arise independently of each other. We remark that such a scenario of crack growth through the coalescence of defects was observed in random networks of fibers [15]. Furthermore, the lack of a parquet pattern and a finding similar to Fig. 4(c) were observed in the desiccation of very thin (and probably more inhomogeneous) coffee layers; see Ref. [14]. In Fig. 5 we show the time evolution of crack patterns for weak ($W\ll f_{\min}$) disorder.

We analyze now the dependence of L, the average fragment cross section, on ΔR; see Fig. 6. For weak disorder we find, paralleling the 1D and quasi-1D results, that the power law $L\sim(\Delta R)^{-1/2}$ holds. The fact that the exponent retains its value is rather unexpected; it means that surface fragmentation is mainly due to the formation of new defects rather than to crack propagation.

For weak disorder fragmentation proceeds through defect formation (a seed "microcrack"); this is followed almost immediately by fast crack propagation and by the mechanical relaxation of the film near the "banks" of the newly formed crack. Seed formation is thus the rate limiting process for fragmentation. These facts may be inferred readily from Fig. 4(a): in the late fragmentation stages only very few cracks with free ends are present in the system.

In our quasistatic model the only relevant parameter describing the relaxation of stress is the correlation length ξ, which determines the distance (measured from the free boundary) at which the local strain becomes almost constant. Note that ξ is also an estimate for the distance at which two separately growing cracks start to "feel" each other's presence. Within fragments whose sizes are larger than ξ the local strain attains a plateau, while for the fragments whose sizes are much smaller than ξ the strain shows a paraboloidal form. For two fragments similar in form, the maximal value

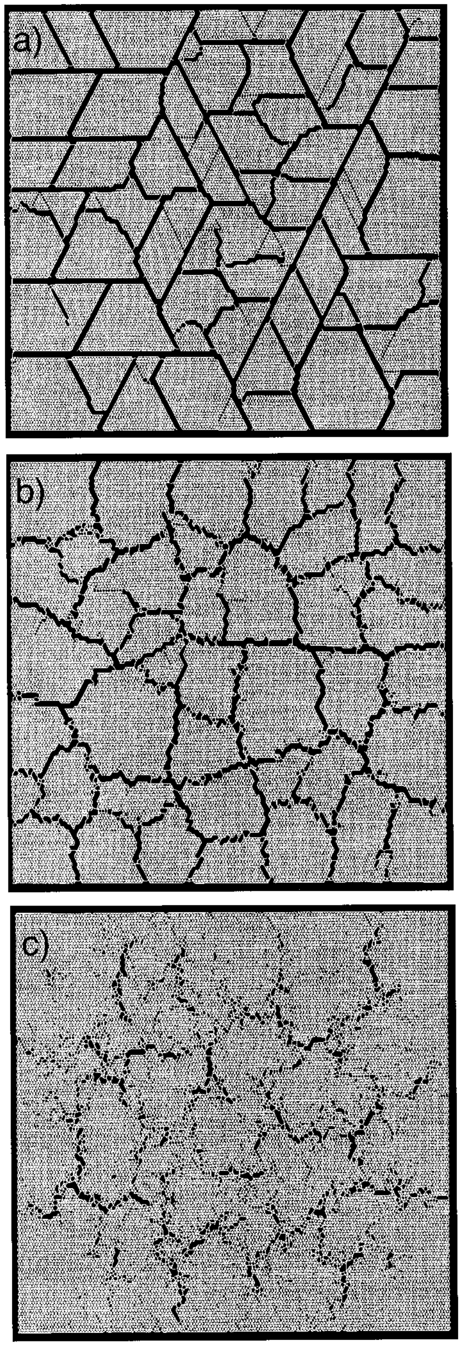

FIG. 4. Fragmentation patterns on a 150×150 lattice with $\xi=20$ after 4000 bonds have failed; the PD is Eq. (4), with $f_{\min}=100$. Furthermore, W is 15 in (a), 100 in (b), and 400 in (c).

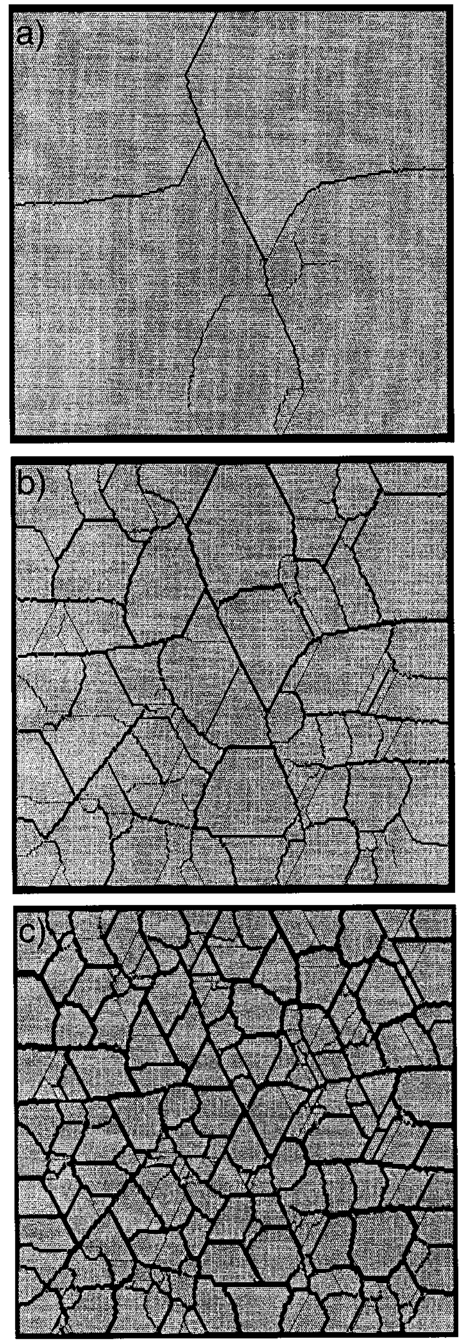

FIG. 5. Fragmentation patterns on a 200×200 lattice with $\xi=150$ after 1000, 5000, and 10 000 bonds have failed. The PD is Eq. (4) with $f_{\min}=200$ and $W=10$.

of the local forces f is proportional to the elongation ΔR and to the squared cross section l, i.e., $f \propto l^2 \Delta R$. A new defect forms inside an initially intact fragment as soon as f gets to be larger than $f_{\min}$. This gives an estimate for L_c, the characteristic size of fragments that break under the elongation ΔR: $L_c \cong \sqrt{f_{\min} \Delta R}$. Supposing that (apart from their characteristic length) the geometrical properties of the crack patterns do not change, one obtains $L \sim (\Delta R)^{-1/2}$, in full agreement with the findings of Fig. 6.

Even more astonishing is the fact that for very strong disorder ($f_{\min}=0$), in two dimensions the mean distance between defects also follows the trend found in one dimension. From Fig. 6 we infer readily that in this case $L \sim (\Delta R)^{-1/3}$ holds. As in one dimension, for $f_{\min}=0$ the probability of forming a new defect follows the stress pattern in the system, so that this probability is proportional to the maximal stress inside the fragment and obeys essentially the same laws as in one dimension. The defect coalescence, which leads to the mesoscopic pattern, is a spectacular but rather subordinated process: most of the defects belong to small clusters, not forming any medium-scaled connected structure, but being sufficient for the local relaxation of the stress.

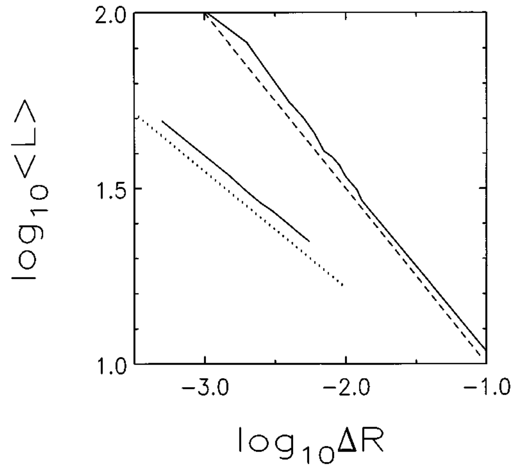

FIG. 6. Same as in Fig. 3, but now for a square 200×200 plate with the PD Eq. (4) with $f_{\rm min}=100$ and $W=10$ (upper curve) and with the PD Eq. (5) with $W=100$ (lower curve). Note the double-logarithmic scales. Again, the dashed line has a slope $-\frac{1}{2}$, the dotted line a slope $-\frac{1}{3}$.

Our simulations show both for $W \ll f_{\rm min}$ (weak disorder) and for $f_{\rm min}=0$ (very strong disorder) that surface fragmentation in two dimensions is controlled by the formation of local defects. For $f_{\rm min} \cong W$ (due to the complex interplay between defect formation and crack propagation) this is no longer the case.

V. CONCLUSION

In this work we studied a model for the fragmentation of surface layers under quasistatical, slowly increasing strains. We analyzed the pattern of cracks and the dependence of the fragment sizes on the strain. We find that the mean fragment size obeys power laws whose exponents are related to the strength of the disorder, i.e., to the relative width of the assumed PD for the breakdown thresholds. Both in quasi-one-dimensional (narrow strips) and in two-dimensional (square plates) geometries the mean fragment's cross section L (the distance between two successive defects along a straight line) follows $L \sim (\Delta R)^{-1/2}$ for weak and $L \sim (\Delta R)^{-1/3}$ for strong disorder. Moreover, the mode of fragmentation depends on the disorder's strengths: for weak disorder the system breaks through crack propagation, whereas for strong disorder the cracks form through the coalescence of initially independent point defects.

ACKNOWLEDGMENTS

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