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Stochastic models of two-dimensional fracture

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Two statistical models of (strictly two-dimensional) layer destruction are presented. The first is built as a strict percolation model with an added "conservation law" (conservation of mass) as physical constraint. The second allows for damped or limited fracture. Two successive fracture crack thresholds are considered. Percolation (i.e., fracture) probability and cluster distributions are studied by use of numerical simulations. Different fractal dimension, critical exponents for cluster distribution, and universality laws characterize both models.

I. INTRODUCTION

The fracture surface of a piece of metal is rough and irregular.[1] Fracture is dynamic in nature and results from cooperative effects in which material bonds are broken. Thus, the dynamical as well as the kinetic aspect of fracture have to be understood. The first aspect is essentially studied through solid-state physics ideas and techniques.[2] The second aspect has received much impetus due to simulation techniques on (fast) computers.[3,4] Analytical models are based on statistical-mechanics development, in particular, along the lines of those developed for first-order phase transitions.[5] Simulation models are, however, the best suited to economically give many interesting results.

Two models are presented here. Several extensions can be envisaged. The models differ from others by a realistic physical constraint: we have imposed "mass (or number) conservation."

To put this work into proper perspective, let us briefly recall previous work on fractal and other simulation models of fracture. A *modern* model is that of Takayasu[3] who has developed an elastic model from his previous work on electric breakdown.[6] He considered a random distribution of microcracks and solved elastic equations at each node—breaking bonds when the stress is greater than a given threshold. He obtained a percolation-like threshold.[7]

Lung[8] observed that the fracture surface (of planar grains) is composed of microscopic dimples resulting from holes forming ahead of the (main) crack. He characterized the fracture "surface" by a fractal dimension[9] ranging (for planar systems) from 1.26 to 2.23. The minimum value (1.26) characterizes pure intergranular brittle fracture—though different grain sizes are expected to lead to this same value.

Recently, Louis and Guinea[4] observed self-similar patterns with fractal dimensions *nearly independent* of the elastic constants, i.e., $D=1.55-1.60$ for a model of a perfectly elastic solid containing a single crack propagating in a defect-free medium according to (static) elasticity, i.e., equilibrium equations.

The above models consider the solid to be a lattice governed by specific constitutive equations, and thus pertain to a line of investigations admitting a *deterministic* ingredient, even though stochasticity enters through the inherent kinetic and irreversible crack pattern. It is therefore natural to obtain for these crack patterns a fractal dimension similar to that of the diffusion-limited aggregation (DLA) model of Witten and Sander,[10] for which $D=1.70$.

Although in such simulation experiments it is conceptually difficult to see what basic difference exists between diffusion-limited *aggregation* and diffusion-limited *decay* (DLD), Banavar, Muthukumar, and Willemsen[11] have examined the two-dimensional reverse process of DLA and of the Eden model.[12] In the DLD case, for a square lattice, the fractal dimension of the cluster is $D=2$. In another experiment called the random-walk decay (RWD), a diffusing particle is infinitely potent and allowed to annihilate as many particles of the original cluster as it is possible before this cluster falls apart. (Periodic boundary conditions are used.) The fractal dimension of the pervading cluster is found to be equal to 1.75.

Related to these models are the dielectric breakdown[13] and electrodeposition[14] phenomena.

The models we introduce here are of the purely stochastic class. They were specifically imagined to be of interest for fracture and decay processes.

In some sense, only geometrical aspects are considered. They can serve as paradigms for molecular beam destruction of thin films, but also for the reverse process, i.e., sputtering, as well as for the description of ion-ion explosive reactions. However, besides the purely kinetic growth (or fracture) models, there exists a class of energetic models.[15] Here we try to combine both aspects by "perturbing" the purely kinetic process in requiring an energetic constraint, i.e., mass (or number) conservation. This serves to investigate a constraint effect on the universality class of growth models through the calculation of the growth exponent. This mass conservation condition exists in order to describe processes which occur and remain on a given energy shell. We force the nucleon target to escape and to stick to the border, i.e., the external destroying beam is not energetically too strong. In so doing we are only "perturbing" the kinetic model.

II. F_1 MODEL

Consider a finite two-dimensional array of particles on a (hereafter square) lattice of size L_0. This array is either seen as the "target" or the "film" or the "nucleus." Each element of the target can be called a nucleon. The target is supposed to be placed in front of a "gun" shooting at random on the target. When a site particle is hit, it supposedly escapes along a straight line toward one of the four borders of the target [Fig. 1(a)]. This direction is chosen randomly (out of four possibilities). The escaping nucleon is then *forced to stick* to the first available (i.e., empty) lattice site *outside* the "target." Another shot is then taken at the target, and is successful if there is a "hit" on an occupied site. The hit nucleon is then removed toward one of the borders, a.s.o. It can occur that the shot is unsuccessful because the nucleon has already been removed. *Both* types of events are counted for future statistical analysis.

After many hits, it occurs that the original "sheet" (or "nucleus") is made of clusters. After a (to be determined) number of hits p_{c1}, the target falls apart because an ("empty") "fracture crack" extends from one of the *original* borders toward the *opposite* one. This *first fracture crack* extends, i.e., from "north" to "south" or from "east" to "west," but there is no distinction to make between the "polar crack" or the "equatorial crack." (A diagonal-like crack is not considered: indeed, the smallest diagonal crack would occur when one of the corner nucleons would be hit. This is trivial and statistically irrelevant.) Statistics of the (empty) cluster crack, its "mass" M, its fractal dimension, and those of the remaining clusters is made then, together with the measurement of the radius of gyration R_G of the cluster assembly, with

$$R_G^2 = \frac{1}{N}\sum_i r_i^2 , \tag{1}$$

where r_i is the position of the elementary nuclei with respect to the center of gravity of the cluster, and N is the number of particles of the target ($N = L_0^2$). It is, of course, faster to calculate $\Delta(R^2)$ with respect to the initial gyration radius of the defect-free target.

The random walk dimension D_W of the fracture crack[11] has also been calculated. Such a dimension measures the relationship between the number of steps N_W of a random walker and its rms displacement R_W, i.e.,[7,15]

$$N_w = (R_w)^{D_w} . \tag{2}$$

However, fracture processes may continue *after* the first crack has reached opposite sides. The *second percolation threshold* p_{c2}, i.e., for the crack extending in the "*perpendicular* direction," has also been considered, and the "mass" of the new total crack and clusters has also been estimated. It is obvious that such cracks intersect each other in this geometry. Results averaged over several simulation runs are given in Table I. Five runs were made for each lattice size with, respectively, $L_0 = 10$, 20, 40, and 60. The same five initial seeds were used for the random number generator. The choice of the target nucleus coordinates and of the escape direction was always made in the same order.

The fractal dimension of the crack increases from 1.65 to 1.89 (after analysis from a $\log M$-$\log L_0$ plot). The "mass" of the crack (i.e., the number of empty sites belonging to the crack) grows from 33.7% of the original mass to 52.9% (see Table I). Notice that the relation[15] between the number of nearest neighbors z, the (Euclidean) dimension (d), and p_{c1}, i.e.,

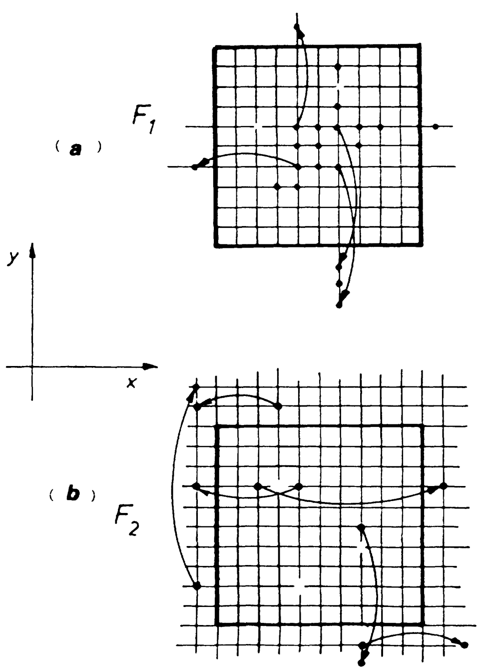

FIG. 1. A hit "nucleon" is removed toward the border in the $\pm x$ or $\pm y$ direction and is trapped at the closest vacant site to its original site but outside the target border: (a) F_1 model, i.e., for constant target size, (b) F_2 model, i.e., when a nucleon can be hit several times, i.e., the target size grows with the number and type of hits.

TABLE I. Averaged results for the first (1) and second (2) crack percolation threshold: p_{c1} and p_{c2}, percolation threshold; M_{c1} and M_{c2}, the relative number of sites belonging to be crack; D_{f1} and D_{f2}, fractal dimension; D_{w1} and D_{w2}, random walk dimension.

	F_1	F_2
p_{c1}	0.584	0.783
p_{c2}	0.652	0.898
M_{c1}	0.337	0.310
M_{c2}	0.529	0.66
D_{f1}	1.65	1.31
D_{f2}	1.89	1.80
D_{w1}	2.20	
D_{w2}	2.52	

$$zp_{c1}=d/(d-1)\ , \tag{3}$$

is not well verified ($p_{c1}=0.584$). This measures either the "accuracy" of our results with respect to the exact result of classical percolation without constraint which gives $p_c=0.60$, or shows that the constraint has moved the model to another (though related) universality class.

III. F_2 MODEL

In the second model (F_2), an (at first) apparently mild restriction on F_1 is removed. In contrast to the F_1 model, where the target is always of the same (initial) size, the target *size* is allowed to vary with "time" and grows with the number of hits. In F_2, a hit nucleon when placed just outside the border *remains* part of the target [Fig. 1(b)]. The target is thus supposed to become a rectangle of variable size for which the long and short widths depend on the number of particles which have been removed in the "east-west" or "north-south" direction. It may happen that the rectangle widths do not change during several hits because the escaping nucleon is removed in the opposite direction along which it has escaped. Similarly, the rectangle longest width can turn with time. In so doing, the size of the target might also grow anisotropically, and the fracture might be quite different.

This model has been imagined in order to maintain mass conversation *and* to simulate cooperative slowing down in fracture crack propagation. In particular, F_2 can simulate the case of heavy-ion reactions in which "energy waves" may propagate in the composite nucleus. In this work, nucleons are, of course, indistinguishable.

In the F_2 model, the crack (percolation) threshold is thus much more difficult to reach. This is due to the "bouncing effect," but also to the existence of many (small) clusters which may appear *outside* the *initial* target region and which push further and further away the borders of the target. Nevertheless, a percolation crack threshold [Fig. 2(a)] has been found in each case (five runs were made for the same lattice sizes as F_1). It is found that $p_{c1}=0.783$. The "empty mass" of the crack is *smaller* in such a case ($M_{c1}=31\%$ of the initial mass $M_0=N$) than in the F_1 case. The fractal dimension obtained from a $\log M$-$\log L_0$ plot is $D=1.31$, which is much smaller than in the F_1 case (Table I).

A "perpendicular" crack is also expected to develop, as in the F_1 case. However, the border of the target (or of the original "nucleus") becomes very diffuse when the number of hits grows. Aggregation effects between "escaped clusters" can sometimes be observed. They may become reconnected to the initial target. Hence, it has been necessary to define the 'first-second percolation crack threshold extending between the *original* borders" [Fig. 2(b)]. The largest size of investigated lattices does not permit one to conclude whether an unambiguous second percolation crack threshold exists. It may also happen that the above value of p_{c1} is, in fact, only a lower bound. The "empty" mass of such a second crack is $0.66M_0$.

Important observations which do not seem to be infirmed by further investigations are the inequalities

$$M_{c1}^{(F_1)}>M_{c1}^{(F_2)}$$

and

$$M_{c2}^{(F_1)}<M_{c2}^{(F_2)}\ .$$

The fractal dimension of the second crack (as defined above) is 1.80. Notice that the fractal dimensions are systematically smaller for the F_2 model than for the F_1 model (Table I).

Cluster statistics has also been examined at the first crack percolation threshold (Table II). As in DLA,[16] clusters containing a percentage s of nucleons (with respect to the initial value N) obey a different law depend-

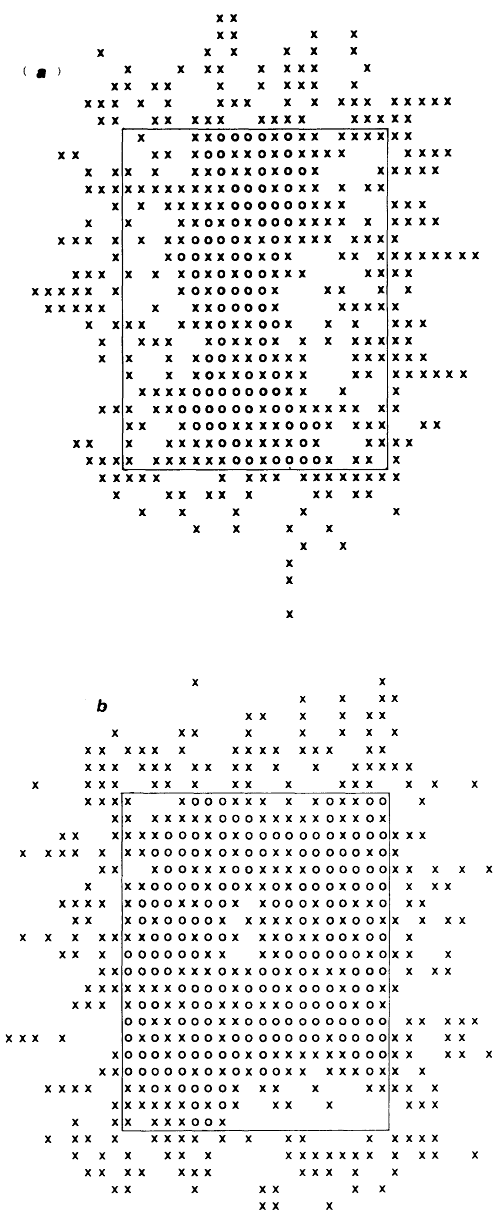

FIG. 2. Typical configuration at the (a) first and (b) second crack threshold for the F_2 model showing ($\times$) cluster fragmentation and the crack ($\circ$).

TABLE II. Parameter value of the data cluster size distribution [Eq. (5)] in the F_1 and F_2 model.

	F_1	F_2
τ	1.17	1.25
σ	(1.0)	(1.0)
s_c	0.03	0.01

ing on their size distribution. Many *small* clusters are formed, and below a critical size s_c obey the relation

$$n_s(p_{c1}) \approx s^{-\tau} \quad (s < s_c) , \tag{4a}$$

while very few *large* and sparsely distributed clusters exist but obey the law

$$n_s(p_{c1}) \approx \exp(s/s_c)^{\sigma} \quad (s > s_c) . \tag{4b}$$

Such a three-parameter (σ, τ, s_c) distribution cannot be obtained unambiguously from the data. It is thus usual to assume $\sigma = 1$. In so doing, the τ ($\cong 1.2$) and s_c ($\cong 0.02$) values are of the correct order of magnitude (Table II) to describe the distribution of (mass) events found in (Au-Au or Mn-Mn) heavy-nuclei collisions,[17,18] but not for sol-gel polydispersity examples ($\tau \cong 2.5$ in mean-field theory[19,20] and 2.2 for classical percolation.[7]

Notice also that it is easy to obtain the critical exponent δ defined by Hermann[15] for the gyration radius

$$R_g = N^{\delta} A(p) , \tag{5}$$

where $A(p) = (p - p_c)^y$. One finds $\delta = 0.5$. This is a consequence of the mass conservation condition.

IV. CONCLUSION

Two simple models which can be the source of many further investigations have been investigated to describe decay or fracture models. A specific mass "conservation law" has been imposed. The notion of the "second perpendicular crack threshold" has been introduced. Data on cluster fragmentation are consistent with observed phenomena (e.g., heavy-ion reaction). It appears that geometrical (or probabilistic) considerations are basically more important than dynamic ones, and that cluster statistics is not controlled by dynamics. Fractal dimension and cluster statistics results seem to indicate the existence of various universality classes different from percolation and/or invasion and usual kinetic growth models.

Investigations of percolation models under conservation-law constraints thus seem of interest for understanding other peculiar physical phenomena. Other applications beside layer fracture might be related to growth such as nucleation "mechanisms" at first-order transitions.[21]

Extensions of these models can be imagined, e.g., (i) the escaping nucleon would not escape to the outside border but could be trapped at the first available site, or (ii) the hit nucleon would randomly push one of its neighbors (and the others in some way of another up to the border) in order to escape. Moreover, the gun might be placed in the target plane, while three-dimensional cases, shells, other lattices, and so on, can be considered.

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