Geometric and healing laws in simple stochastic models of fracture in a sputtering process

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We investigated two simple models of two-dimensional square lattice fracture under sputtering process conditions extending a previously studied model by Ausloos and Kowalski [Phys. Rev. B **45**, 12 830 (1992)]. The models differ by the particle displacement rules during the fracture. Healing of the medium is observed in both models. This effect implies the formation of several thresholds during sputtering process fracture. They are distributed as a size-dependent power law. An avalanchelike exponent is also obtained. We study this phenomenology within scaling arguments of classical percolation theory and mean-field arguments. [S1063-651X(97)04501-7]

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I. INTRODUCTION

Brittle fracture arises in materials incapable of much resistance to an external solicitation. On the contrary, a ductile sample means that the particles inside the medium can rearrange themselves in a way that the inner cracks tend to be repaired and that the inner empty sites are repelled towards the borders of the sample.

The distinction between ductile and brittle fracture is relevant from a practical and theoretical point of view [1]. There are several ways of approaching the problems of fracture. One of them is through algorithmic modelization [2], as followed here below. Therefore, neither an elasticity nor a continuum solid statelike approach are to be found here. Instead we follow the lines drawn in Ref. [3] in which a stochastic process, i.e., the most extreme situation, is considered in order to find whether general behaviors can be quantified and if so through which ingredients of the fracture phenomena. This extremal dynamics kind of studies is rather common nowadays [4] in order to find basic laws. One underlying concept is that of self-organization [5], well known in algorithmic models. This is known to be useful in related problems like sand pile, vortex pinning, and biological evolution, army combats, earthquakes, chemical reactions, economic features, etc. [4–10] and should be of interest in fracture problems. In such systems one avoids detailed microscopic approximations but rather concentrates on the basic geometric points, as found in fractal geometry [11]. Coarse grain investigations also allow for easy access to asymptotic time regimes due to intrinsic computational efficiency.

A very simple development of the percolation problem was found in Ref. [3]. A two-dimensional plane was supposed to be ''hit'' by ''particles'' of the same size as those filling the sites of the investigated lattice. The ejected particle from the ''target'' or ''substrate'' is allowed to jump towards the initial boundary of the finite size $L \times L$ (square) lattice and to find the closest empty site outside that initial boundary, the site on which the particle was then glued. The inner sites of the lattice were therefore slowly emptied and a ''percolationlike'' path, which was the signature of a crack throughout the sample, was found as a function of size. The process was continued in order to find whether a ''perpendicular crack'' could also occur and would have some general features. The concentration of both crack thresholds, the concentration of the remaining filled sites, the distribution of clusters, and the fractal dimension of the cracks were obtained. Power-law features were indicative of essential processes. The choice of processes was, however, very limited.

In the present work, we consider a softer set of rules about the site emptying process, allowing for the possibility of the hit particles still to remain in the target after a hit. Two probabilistic cases will be of interest. It will be found that the new rules give a new feature in this kind of research, i.e., a healing process.

II. THE MODEL FRACTURE RULES IN A SPUTTERING PROCESS

Following the model of Ref. [3], we consider a two-dimensional array of $N = L \times L$ particles on the sites of a square lattice. An external beam is supposed to hit the lattice sites at random. Once a target particle is hit, it is removed as described in the following paragraphs. A ballisticlike displacement of the hit particles is assumed. Each shot is taken into account and counted as a unit of time, even though the hit might have been without any effect on the lattice, e.g., if the hit is on an already emptied site.

In model I, if the randomly selected site is empty, nothing occurs. If the site is occupied by a particle, one of the four directions of the lattice is chosen at random and the particle is assumed to move in this direction. The particle is then assumed to stick on the first empty site that is encountered. This first empty site can be inside or outside the target. If the particle is ejected outside the target, the particle will never be selected again by the process.

In model II, a site of the target is randomly chosen at each time step. If this site is empty, nothing occurs. If this site is occupied, one of the four directions [3] of the square lattice

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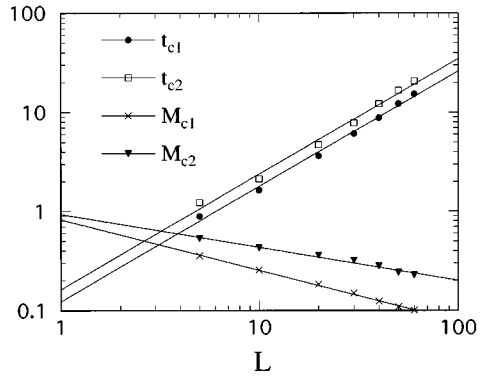

FIG. 1. Lattice size dependence of the parameters t_{c1}, t_{c2}, M_{c1}, and M_{c2} for model I.

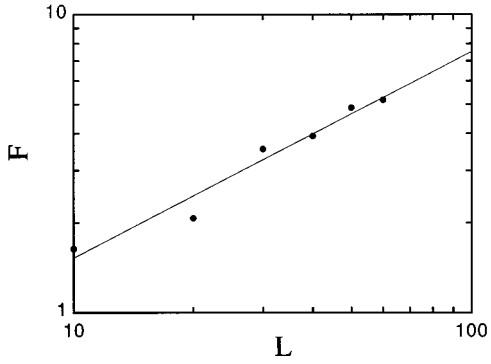

FIG. 2. Log-log plot of the lattice size dependence of the number F of first-cracklike thresholds for model I. The continuous line is a guide for the eye.

is randomly chosen and the particle is assumed to move along this direction (as for model I). The particle is assumed to stick on the first encountered empty site with a probability $\frac{1}{2}$ or is ejected outside the target with a probability $\frac{1}{2}$. Model II represents thus an intermediate situation between model I and the model of Ausloos and Kowalski (AK) [3].

III. NUMERICAL RESULTS

We numerically investigated several targets of sizes ranging from 10×10 to 120×120. For both models, 100 or so simulations were made for each investigated lattice size. It will be seen that such a range of sizes is already sufficient for observing interesting features and laws.

A. Model I

The first hit particle is obviously ejected outside the target. After a few hits, a few holes appear in the target. After a number t_{c1} of hits, a cluster of empty sites is seen to extend from one border to the opposite one of the target. The target is said to be fractured and t_{c1} is called the ''first crack threshold.'' Figure 1 presents this first crack threshold normalized by the size L^2 of the target as a function of L. One observes that t_{c1}/L^2 increases with L and behaves as a power law

$$\frac{t_{cl}}{L^2}\sim L^{\alpha_1}, \tag{1}$$

where the exponent α_1 is estimated to be $\alpha_1=1.16\pm0.04$.

By analogy with percolation phenomena [12], we characterized this first crack threshold by measuring the ''mass'' M_{c1} of the empty cluster that crosses the lattice, renormalized by the total ''mass'' L^2, and by measuring the size (s) distribution $N_1(s)$ of the remaining clusters of particles on the target. One should remark that M_{c1}/L^2 is a constant for percolation and is equal to 0.593 [12]. Figure 1 presents the mass M_{c1} of the ''percolating'' cluster of empty sites as a function of L. This concentration M_{c1} behaves as a power law

$$M_{c1}\sim L^{\beta_1}, \tag{2}$$

where we found numerically that $\beta_1=-0.51\pm0.05$. The distribution of leftover particle clusters strictly in the target at t_{c1} is also found to be a power law

$$N_1(s)\sim s^{-\tau_1} \tag{3}$$

with an exponent $\tau_1=1.27\pm0.07$.

After the first crack is reached, the simulation is nevertheless pursued until another cluster of empty sites connects the four borders of the target. This is called ''the second crack threshold'' occurring at time t_{c2}. Figure 1 presents also t_{c2}/L^2 as a function of L. One observes a power law

$$\frac{t_{c2}}{L^2}\sim L^{\alpha_2}, \tag{4}$$

with an exponent α_2 that was estimated numerically to be $\alpha_2=1.16\pm0.04$, i.e., comparable to α_1.

Like for the first crack threshold, we determined the size distribution of the particles clusters $N_2(s)$ and the relative ''mass'' M_{c2} of the empty cluster that extends throughout the target. Figure 2 presents M_{c2} as a function of L. One observes a power law

$$M_{c2}\sim L^{\beta_2}, \tag{5}$$

with an exponent $\beta_2=-0.33\pm0.06$, a value which is quite different from β_1. The size distribution $N_2(s)$ of particle clusters at the second crack threshold is found to behave as a power law

$$N_2(s)\sim s^{-\tau_2}, \tag{6}$$

with an exponent $\tau_2=1.37\pm0.09$, i.e., different from τ_1, and greater.

The exponents seem to be different from a crack threshold to another one. Moreover, the values of these exponents are different from two-dimensional percolation exponents [12].

However, it was found that the above laws do not completely describe model I. An interesting new phenomenology takes place between t_{c1} and t_{c2}. Indeed, several secondary cracks of the ''first type,'' i.e., connecting one border of the target to the opposite one, are observed before the second crack threshold connecting the target four borders is reached. Some particle displacements after the first crack threshold can fill the holes of the first spanning (percolation) cluster

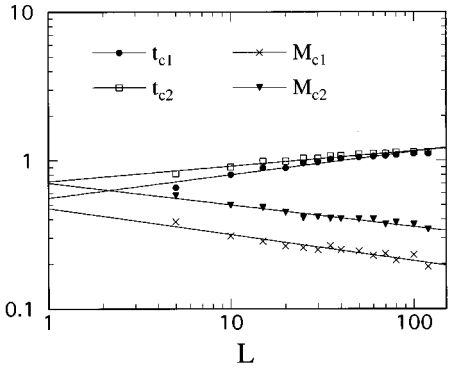

FIG. 3. Lattice size dependence of the parameters t_{c1}, t_{c2}, M_{c1}, and M_{c2} for model II reported on a log-log graph.

indeed and thus repair the fracture. In this way, many first cracklike thresholds can exist before reaching the second crack threshold, depending on the lattice size. Notice that the crack of the first type can rotate with time after healing and can thus be found to be connecting different opposite borders of the target.

Figure 3 presents the number F of fractures before t_{c2} is reached as a function of L. A power law is observed, i.e.,

$$F \sim L^{\varepsilon}, \tag{7}$$

with an exponent $\varepsilon = 0.69 \pm 0.07$.

The mean-time interval Δt between two following crack thresholds is

$$\Delta t = \frac{t_{c2} - t_{c1}}{F}. \tag{8}$$

Again, a power law is found

$$\Delta t \sim L^{\delta}, \tag{9}$$

with an exponent δ numerically estimated to be $\delta = 2.59 \pm 0.09$.

Thus,

$$F \sim \Delta t^{\varepsilon/\delta} = \Delta t^{\mu}, \tag{10}$$

with $\mu = 0.69/2.59 = 0.27$ which can be called the number of avalanche time distribution exponent in the self-organized criticality (SOC) language [5].

B. Model II

In model II, in the same way as for model I, we determined numerically t_{c1}, M_{c1}, and $N_1(s)$ at the first crack threshold. Lattice size dependences are found, characterized by power laws with respective exponents $\alpha_1 = 0.16 \pm 0.04$ (for t_{c1}), $\beta_1 = -0.18 \pm 0.05$ (for M_{c1}), and $\tau_1 = 1.69 \pm 0.09$ [for $N_1(s)$]. These values of α_1 and β_1 are intermediate between those of the AK model (where all the above exponents are trivially zero, showing the independence of these parameters as a function of the lattice size L) and those estimated for model I. This is consistent with the conception of model II as an intermediate case between the two others.

Similarly, at the second crack thresholds, power laws for the lattice size dependence are obtained for t_{c2}, M_{c2}, and $N_2(s)$. The exponents are numerically found to be $\alpha_2 = 0.10 \pm 0.05$ for t_{c2}, $\beta_2 = -0.15 \pm 0.07$ for M_c, and $\tau_2 = 1.68 \pm 0.08$ for $N_2(s)$, i.e., again intermediate values for α_2 and β_2.

Unlike for model I, only a few intermediate thresholds occurred for very long time Monte Carlo simulations. Thus, no characteristic behavior can be proposed for F in model II within a reasonable time investigation.

TABLE I. Averaged results for the first (1) and second (2) crack percolation thresholds. For models I and II, the characteristic features are found to follow power laws showing a lattice size dependence. The corresponding exponents are given in the table. The values reported for the AK model are the values of the parameters. The number in parentheses corresponds to the uncertainty in the last digit.

	AK model	Model I	Model II
t_{c1}	0.783	1.16(4)	0.16(4)
M_{c1}	0.310	−0.51(5)	−0.18(5)
D_{f1}	1.31	1.49(8)	1.72(7)
$N_1(s)$	1.17	1.27(7)	1.69(9)
t_{c2}	0.898	1.16(4)	0.10(5)
M_{c2}	0.66	−0.33(6)	−0.15(7)
D_{f2}	1.80	1.67(8)	1.85(11)
$N_2(s)$		1.37(9)	1.68(8)
F		0.69(7)	

IV. DISCUSSION

For both models, it was impossible to obtain an unambiguous estimation of the fractal dimension of the percolating cluster by the usual method of the embodied boxes. However, by a simple reasoning taking into account the behavior of $M_{ci}(i=1,2)$, it can be easily argued that

$$M_{ci} \sim \frac{L^{D_{fi}}}{L^2}, \tag{11}$$

thus $D_{fi} = 2 + \beta_i$ in order to evaluate a ''mean-fieldlike'' fractal dimension. It can be so called indeed because M_{ci} is measured without taking into account the geometric features of the empty site distribution at the considered threshold. The values evaluated in this way seem reasonable (Table I).

To examine the temporal dependence of the particle concentration, remembering that a shot is a unit of time, we investigated the relation $n = n(t)$, where n is the number of occupied sites renormalized by the total site number, i.e., the concentration at a definite time t. We use a mean-fieldlike approach.

To estimate a mean-field probability P_m for a chosen particle to be ejected from the target, we assume this particle to be on site (x,y) where both x and y can only take integer values from 1 to L, i.e., the maximum target size. The probability P_s for the hit particle to stay in the target is

$$P_s = \tfrac{1}{4} P_{\mathrm{rel}} \sum_{i=1}^{4} P_s^i, \tag{12}$$

where P_s^i is the probability that there is an empty site in one of the four equivalent directions of diffusion ($i = 1,4$ means

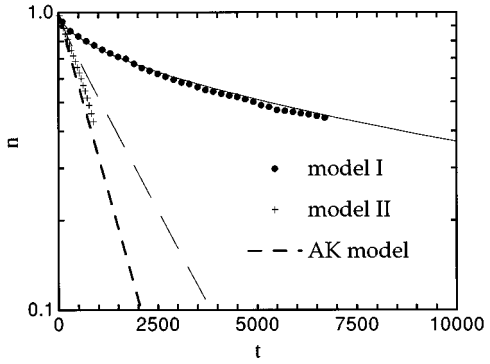

FIG. 4. Time decreasing law for the particle concentration $n(t)$ for a 30×30 target: analytical result for the AK model; analytical and numerical results for models I and II. The continuous line is the analytical mean-field results for model I; the long-dashed line is the one for model II; the short-dashed line is the one for the AK model. Numerical results end as the second crack threshold is reached.

up, right, down, and left, respectively) and $P_{\rm rel}$ the relative probability that the particle moves to the inside or outside of the target available site. $P_{\rm rel}$ takes the value 0 in the AK model, the value 1 in model I, and the value 0.5 in model II. Notice that the probability for a chosen particle to be ejected is $1-P_s$. If we denote by v the number of empty sites, we have

$$P_s=\frac{P_{\rm rel}v}{4N}\left(\sum_{k=0}^{L-y-1}+\sum_{k=0}^{y-2}+\sum_{k=0}^{L-x-1}+\sum_{k=0}^{x-2}\right)\left(1-\frac{v}{N}\right)^k. \tag{13}$$

The average of P_s over the whole target is found to be

$$P_m=1-P_{\rm rel}+P_{\rm rel}\frac{N^L-(N-v)^L}{vLN^{L-1}}. \tag{14}$$

To deduce the temporal dependence of the particle concentration $n(t)$, we suppose that the number of empty site dependence is given by the discrete time master equation

$$v(t+dt)=v(t)+\left(1-\frac{v(t)}{N}\right)P_m dt \tag{15}$$

keeping in mind that

$$n(t)=1-\frac{v(t)}{N}. \tag{16}$$

The solution $n(t)$ for the three investigated values of $P_{\rm rel}$ (i.e., for $P_{\rm rel}$ equal 0, 0.5, and 1) is shown in Fig. 4 where arbitrarily chosen simulation examples for models I and II are also shown. The theoretical laws from Eqs. (15) and (16) are given for both models. The theoretical law for the AK model is also shown for comparison. The fit is excellent for model I. In the AK model, the theoretical law fits the data since the solution is then found exactly and analytically. In the case of model II, the theoretical law departs from the data at finite time, and surprisingly the data are closer to the AK law. This indicates that the neglect of correlations in Eq. (15) is a severe approximation. In principle, one should take v as a function of the coordinates, hence the environment of the hit site should be included in more elaborate work.

For $P_{\rm rel}=1$, from Eq. (15), we obtain $t=t(v,L)$ and taking for v the values $M_{c1}L^2$ and $M_{c2}L^2$, respectively, t_{c1} and t_{c2} are found. The lattice size dependences are indeed extremely good approximations with power laws like Eqs. (1) and (4) but the values of the exponents (i.e., $\alpha_1=1.81$ for t_{c1} and $\alpha_2=2.2$ for t_{c2}) obtained in the above mean-fieldlike framework differ from the numerical data (Table I) for the same reasons as described in the preceding paragraph.

For model I, a finite lower size effect was observed. The first intermediate threshold appears for lattices about 7×7 (i.e., $F=1$ for $L=6.8$). Hence the maximum probability that a hit site particle reorganizes the target and heals the fracture can be estimated to be the critical probability P_m(crit). This probability should be the one permitting healing in the case of 7×7 lattices for model I; thus from Eq. (14), taking $v=M_{c1}L^2\approx15$, we obtain $P_m(\text{crit})\approx0.43$. This predicts (in the limit of a mean-field reasoning) that for all models with $P_{\rm rel}<0.57$, no reorganization is to be expected. This is found for model II, indeed. The critical value of $P_{\rm rel}$ in Eq. (12) is thus conjectured to be $P_{\rm rel}(\text{crit})=0.57$. In other words, for $P_{\rm rel}$(crit) target reorganization is only possible for infinite lattices. This is similar to a usual phase transition between two different symmetry behaviors.

By analogy between geometrical percolation theory and critical thermodynamic phenomena [13], we can identify the intratarget motion as a sort of thermal activation process characteristic of ductile fracture. The energy given by the external ''field'' is dissipated by the particles inside the target, due to ''thermal motion.'' At high temperatures, a situation equivalent to the case of large $P_{\rm rel}$, the target (always) behaves like a ductile material. On the other hand, for small $P_{\rm rel}$, the target falls apart irremediably and behaves like a brittle material. The ''temperature'' is thus the analog to $P_{\rm rel}$ and the transition temperature corresponds to $P_{\rm rel}$(crit).

V. CONCLUSION

Numerical analysis of two generalized stochastic fracture models under particle hits as in a sputtering process shows that a new type of behavior is obtained. It is connected to the notion of ductibility. Introducing a kind of mean-field analysis, we predicted the critical value for the relevant parameter of a transition between material features when a certain parameter $P_{\rm rel}$ reaches a definite value $P_{\rm rel}(\text{crit})=0.68$.

To decide whether a material is brittle or ductile, and whether a ''material transition'' occurs requires a test of physical (mechanical here) properties and then energy and volume time dependence under a permanent external stress. More elaborate elastic models should require interacting particles. Possible ways to explore the models are easily thought of. This philosophy has already been tested in other growth models, like the magnetic Eden or the magnetic diffusion-limited aggregation models [14].

For the size distribution of the remaining particle clusters inside the target, the results for the three models are quite different: this is a clue to the varied behavior of the particles inside the target.

ACKNOWLEDGMENTS

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