Fractal Shapes of Deterministic Cracks.

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Abstract. – By solving the full elastic equations on a two-dimensional lattice we grow cracks under various breaking conditions for a system that is submitted to external shear. We find that deterministic fracture patterns are in general branched and can be fractal. This effect is due to the competition between the direction of global stress and the local growth direction imposed by the lattice anisotropy. In scalar models this novel type of patterns cannot be observed.

Fracture, i.e. the formation of cracks in an elastic medium and its subsequent failure, is a question of widespread interest. The mechanisms leading to fracture are highly material dependent and have been studied quite extensively [1]. Despite the diversity of experimental situations one can hope to find generic features due to the underlying instabilities and their interplay with noise, anisotropy or memory effects. Recently two new approaches in this direction have been proposed [2], one inspired from random resistor networks [3, 4] and another using DLA [5] as a guideline [6, 7].

In this letter we will focus on the growth of one single crack in the spirit of the second approach. There have been numerical indications that cracks grown in central-force media with a probability proportional to the elongation of the springs are fractal [6, 7]. There is some evidence from small-scale simulations [7] that the fractal dimension of these cracks depends considerably on the type of external force that is applied (uniaxial tension, shear, uniform dilatation) but since only very small cracks can be grown, precise statements are difficult to make. We will investigate some of the origins of this fractal behaviour and obtain much better accuracy by considering deterministic models. In addition, in our studies we solve the full elastic equations which contain automatically angular forces and two elastic moduli, as compared to the central force model that has been studied before and which shows pathologies on some lattices.

The elastic medium is usually described by the field of displacement vectors \( \mathbf{u} \) which obeys an equation of motion which in the case of symmetric elasticity is the Lamé
equation [8]

\[(\lambda + \mu) \nabla(\nabla u) + \mu \nabla^2 u = 0,\]  \hspace{1cm} (1)

where \(\lambda\) and \(\mu\) are the Lamé coefficients. On the external boundary an imposed displacement is fixed. Suppose that in this medium one has already a crack and one wants to study how this crack grows. Then one will have on the surface of the crack the boundary condition that the stress normal to the surface of the crack is zero and the crack will grow in the direction perpendicular to the surface at the point where the strain parallel to the surface is largest. The detailed growth law depends on the microscopic mechanism like how the elastic energy is transported away from the growing tip. One can use a normal growth velocity \(v_n\) of the form

\[v_n \propto ((\partial_i u_i)^2 + q \cdot \mathbf{\sigma}^0 \cdot \mathbf{u})^\gamma,\]  \hspace{1cm} (2)

where \(q\) and \(\gamma\) are material-dependent parameters. For \(\gamma = 1\) this growth law is inspired by the von Mises yielding criterion [1], but we cannot derive it from first principles. \(\gamma\) is just an additional free parameter of the model that makes the growth law more general. Physically \(q\) is the affinity of the breaking process to the bending mode (second term on the r.h.s. of eq. (2)) as compared to cleavage (first term on the r.h.s. of eq. (2)). In the above approach we have assumed that the relaxation of the local strain due to the growth of the crack is much faster than the velocity of the crack so that in eq. (1) we do not need to consider a time derivative. We also do not consider plasticity or nonlinear elasticity.

We discretized these elastic equations on a square lattice by using the beam model [9] which is in fact a little richer than eq. (1) because it also allows for local rotations in the material. This discretization introduces anisotropy and a cut-off at small length scales, two physical effects that are very often present in real materials.

A detailed description of the implementation of the beam model is given in ref. [2]. For each beam that is eligible for being broken one calculates the quantity \(p\) defined by

\[p = (f^2 + q \cdot \max(|m_1|, |m_2|))^\gamma,\]  \hspace{1cm} (3)

where \(f\) is the traction (and/or compression) force applied on the beam and \(m_1\) and \(m_2\) are the moments that are acting at the two ends of the beam. Equation (3) again follows from the von Mises yielding criterion for beams [2] and represents a heuristic way of implementing eq. (2) on a lattice. The \(p\) of eq. (3) determines if the beam will be broken. Each time a beam is broken the shape of the crack and consequently the boundary condition of the equation of motion has changed and one has to solve the discretized equation again if one wants to know which beam to break next.

We consider a finite square lattice of linear size \(L\), with periodic boundary conditions in the horizontal direction. On top and on bottom we impose an external displacement, usually a shear. We remove one beam in the centre of the lattice which is the original microcrack. Next we consider the six nearest-neighbour beams of this broken beam. These include the two beams that are parallel to the broken beam and the four perpendicular beams that touch a common site with the broken beam. This choice of nearest-neighbours is due to the fact that the actual crack consists of the bonds that are dual to the set of broken beams [2]. Other connectivity conditions have also been used [7]. The equation of motion is solved by a conjugate gradient method [10] to very high precision \((10^{-20})\) and the \(p's\) of eq. (3) are calculated for each of the nearest-neighbour beams. We set \(p = 0\) for a beam that is not a nearest-neighbour to the crack. Now various criteria for breaking are possible: 1) one breaks
the beam with the largest value of \( p \); II) one breaks the beam for which \( q_0 = p + f_0 \cdot p_{-1} \) is largest, where \( p_{-1} \) is the value of \( p \) that this beam had before the previous beam was broken; \( f_0 \) is, a memory factor; III) on each beam of the lattice we put a counter \( c \) which is set to zero in the very beginning. Each time one has obtained the \( p \)'s one calculates \( \alpha = (1 - c)/p \) and breaks the beam which has the smallest \( \alpha \), namely \( \alpha_{\text{min}} \). After the beam has been broken each counter \( c \) is set to \( c = \alpha_{\text{min}} \cdot p + f \cdot c_{-1} \), where \( c_{-1} \) is the value the counter had before the breaking and \( f \) is another memory factor.

All three breaking criteria described above are deterministic. Criterion III) corresponds for \( f = 1 \) to the limit of infinite noise reduction [11, 12]. Noise reduction has been invented to reduce statistical noise in DLA simulations and has also been applied recently to central-force breaking [13]. What noise reduction certainly does is to introduce a memory effect with long-range time correlations. Physically the three breaking criteria defined above correspond to three different situations. Criterion I) describes ideally brittle and fast rupture. Criterion II) contains a short-time memory one would expect in cracks that propagate slower and produce strong local deformations at the tip of the crack as happens in many realistic situations. One could imagine applying this criterion to situations with very fast stress corrosion effects. Criterion III) could be applied to situations of relatively slow stress corrosion, crazing of polymers or static fatigue. The memory factors \( f_0 \) and \( f \) measure the strength of these time correlations. In criterion III) the limit \( f \to 0 \) gives criterion II) with \( f_0 = 1 \), and in criterion II) the limit \( f_0 \to 0 \) gives criterion I).

Fig. 1 - Crack grown in a 50 x 50 system if an external shear is applied. Beams break under traction or with an affinity of \( q = 0.28 \) in the bending mode. Only the bond with the largest value of \( q \) breaks (criterion I). The first broken beam was vertical.

In fig. 1 we see a crack broken according to criterion I) under external shear for \( L = 50 \) and \( q = 0.28 \). Cleavage tends to have the crack grow in the diagonal direction, while the bending mode favours a horizontal rupture. The competition between these two effects can lead as seen in the figure to complex branched structures. The exact shape of these cracks depends strongly on \( q \) and the system size. For any finite \( q \) the horizontal rupture will eventually win if the system is large enough, while for \( q = 0 \) one obtains diagonal cracks with eventual kinks. For this reason the cracks will not be fractal. However, we point out that in the analogous scalar model (i.e. DLA) only straight lines will be formed in criterion I); the different behaviour here is due to the fact that competing directions are possible in a vectorial model.

In fig. 2 we see a crack grown using criterion II) with \( q = 0 \), \( \gamma = 0.7 \) and a size \( L = 118 \). Over four hours on one CrayXMP processor were needed to generate this structure. We count the number of broken beams inside a box of length \( l \) around the first broken beam and
plot it as a function of \( l \) in a log-log plot ("sand box method"). The result is shown in fig. 3 which gives a good evidence that this structure is fractal with a fractal dimension \( d_f \) of \( d_f = 1.25 \pm 0.05 \). It is self-similar around the origin and probably a directed fractal [14]. Within the numerical accuracy the envelope of the cluster has the form of a wedge with a width roughly proportional to the distance from the origin. The structure shown in fig. 2 is the upper half of the crack. The lower part is totally inversion symmetric because the pattern is grown deterministically, i.e. no random numbers are used and the results are independent of the roundoff errors of the computer. The very slight curvature of the crack is a finite-size effect of the lattice but the fractality is not altered if the system size is changed. Changing the elastic constants (i.e. the Lamé coefficients) just changes the opening angle of the crack, while changing \( \eta \) also changes the fractal dimension (we find \( d_f = 1.15 \) for \( \eta = 0.5 \)). If in eq. (3) one uses an exponential instead of a power law, the structures seem to be dense [15].

The effect that using criterion II) gives fractal structures is novel and very distinct from what is seen in the scalar case of DLA. It shows that neither noise nor long-range time correlations are necessary to obtain fractal breakdown. The origin of fractality is the competition between a global stress perpendicular to the diagonal and a local stress that tends to continue a given straight crack due to tip instability. Again we see the important role of the interplay of different directions which is only possible in a truly vectorial model. The relevance of a short memory in criterion II) indicates that there might be a relation between this case and the models that have been put forward for snow flakes [16].

In fig. 4a) we show a crack grown using criterion III) for \( q = 0, f = 1, \eta = 1 \) and \( L = 60 \). The physical situation is similar to that seen in criterion II), only the fractal dimensions are
higher. This case can be directly compared to results obtained for DLA in the limit of infinite noise reduction [18, 17] where needles, not fractals are predicted.

In fig. 4 we also show our deterministic cracks next to an experimental example of stress corrosion cracking in an alloy [18]. Due to the heuristic nature and simplicity of our model it makes no sense to compare numerical values of fractal dimensions. It seems also clear that the inhomogeneities of the medium in the experimental crack are important. The vague similarity that one can see between the patterns in fig. 4 seems to indicate that the effects found in our model may explain to a certain degree the branching behaviour of experimental cracks.

In conclusion, we have treated the problem of deterministic single crack propagation for finite square, lattice samples. The patterns of cracks can become very complex and in particular they can be fractal with a fractal dimension that depends on the breaking criterion, i.e. the effect of memory. This phenomenon is due to the competition between the direction of global stress and the direction of local growth imposed by the lattice anisotropy. Therefore the vectorial nature of the elastic medium leads to crucially different results from what is known to occur in the analogous model of scalar DLA. These differences must be taken into account also when randomness is introduced either quenched in the form of random elastic constants [19] or annealed in the form of breaking probabilities [6, 7]. The dependence of shapes and fractal dimensions on the various parameters as well as the influence of noise, i.e. of a probabilistic growth rule, will be described elsewhere [15].
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