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A simple two-dimensional model for crack propagation

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Abstract. Simple models for crack growth which are closely related to the diffusion-limited aggregation (DLA) model have been explored using computer simulations. In these models the bond-breaking probabilities for bonds at the surface of a growing crack in a two-dimensional (triangular) network of bonds and nodes are proportional to $(\delta_i)^\eta$ and δ_i is the bond strain. Our results indicate that the cracks generated by these models have a fractal structure and that their effective dimensionalities depend on both the bond-breaking probability exponent (η) and the boundary conditions (which bonds are considered to be surface bonds that can be broken) at the crack surface. Very similar results were obtained using shear and dilational strain.

1. Introduction

The failure of materials under stress is a complex process involving a broad range of physical, chemical (Latanison and Jones 1987) and sometimes biological processes. Most failure processes of practical importance exhibit a rich phenomenology (Latanison and Pickens 1983, Ghandi and Ashby 1979, Ashby *et al* 1979) extending over a wide range of length scales from the atomic level to the overall size of the system. Because most failure processes involve complex interactions between a quite large number of processes, it has in most cases been difficult to develop understanding on a fundamental level. Nevertheless, considerable advances have been made towards developing a satisfactory understanding of mechanical failure processes on a phenomenological and/or statistical basis. Even in ideal homogeneous materials a complex non-local stress-strain field develops as the material begins to fail and an understanding of the evolution of the stress-strain field is an important ingredient in developing a better understanding of material failure. In this regard mechanical failure is similar to a variety of other processes which lead to the formation of complex patterns such as fluid-fluid displacement in a porous medium or Hele-Shaw cell and dielectric breakdown in which the complex structure is generated by amplification of growth instabilities. Under some conditions these processes can be understood in terms of the diffusion-limited aggregation (DLA) model of Witten and Sander (1981) in which the growth probabilities in a random growth process are controlled by a scalar field, ϕ, which obeys the Laplace equation ($\nabla^2\phi = 0$). In the case of fluid-fluid displacement in a porous medium (Paterson 1984, Maloy *et al* 1985) or Hele-Shaw cell (Nittmann

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et al 1985, Ben-Jacob *et al* 1985) the field obeying the Laplace equation is the pressure field in the viscous fluid which is being displaced by a non-viscous fluid. In the case of dielectric breakdown (Niemeyer *et al* 1984) the field obeying the Laplace equation is the potential field in the non-conducting dielectric medium. The DLA model has also been shown to provide a basis for understanding a variety of other random pattern formation processes in which the growth process is controlled by a field obeying the Laplace equation (see Ball (1986), Meakin (1988), Matsushita (1988) and Sander (1986) for reviews). In all of these processes the magnitude of the potential field ϕ at each point in the space surrounding the growing structure depends on the surface of the entire structure.

The success of the DLA model in describing random growth processes controlled by a Laplacian field suggests that a similar approach might be of value in developing a better understanding of mechanical failure processes controlled by the vector stress and strain fields in a linear elastic medium. In this case the stress and strain fields are related by the Navier equation (England 1971):

$$(\lambda+\mu)\partial_i\left[\sum_j \partial_j U_j\right]+\mu\left[\sum_j \partial_j^2\right]U_i=0 \tag{1}$$

where λ and μ are the Lame coefficients and U_i is the ith component of the displacement field (Landau and Lifshitz 1975). One of the most important characteristics of structures generated by DLA models is their fractal geometry (Mandelbrot 1982). In the absence of long-range anisotropy, the DLA model leads to the formation of patterns which have a fractal dimensionality (D) of about 1.71 for $d=2$ and about 2.50 for $d=3$ (Witten and Sander 1981, Meakin 1983a, b). These values are in quite good agreement with those measured in experimental realisations of the DLA process. The formation of fractal surfaces in mechanical failure processes is suggested by everyday experience and has been investigated more carefully for a variety of systems including steel (Mandelbrot *et al* 1984, Underwood and Banerji 1986), titanium (Pande *et al* 1987), and a two-dimensional array of polystyrene microspheres (Skjeltorp and Meakin 1988). Computer simulations have been used extensively to explore various aspects of mechanical failure. Most of these simulations have been carried out using a molecular dynamics approach (Alder and Wainwright 1957, Rahman 1964, Wood and Erpenbeck 1976, Jones and Gerberich 1985). This method has been used to explore hydrogen embrittlement (Grehlen *et al* 1976, other Rehbinder effect phenomena (Shchukin and Yushchenko 1981) and crack propagation in a two-dimensional Lennard-Jones solid (Puskin *et al* 1980, Chakrabarti *et al* 1986).

A second approach is to represent the elastic medium by a network of nodes joined by Hookean springs (Kausch 1978, Mikitishin *et al* 1969, Dobrodumov and Elyashevich 1973, Louis *et al* 1986, Termonia and Meakin 1986, Louis and Guinea 1987, Meakin 1987). In particular, the model of Louis and Guinea is quite closely related to DLA (particularly the dielectric breakdown model implementation of DLA introduced by Niemeyer *et al* (1984)). The models used in the work described in this paper are very closely related to the crack propagation model of Louis and Guinea. In this model the probability that a bond at the surface of a propagating crack will break is proportional to the strain (δ) associated with that bond. Here we investigate models in which the bond-breaking probability is given by

$$P_i \sim \delta_i^{\eta} \tag{2}$$

where P_i is the bond-breaking probability for the ith surface bond.

For the closely related dielectric breakdown model (Niemeyer *et al* 1984) the fractal dimensionality of the breakdown pattern changes continuously as the exponent η in equation (2) is changed. Similar behaviour is expected for the crack growth models which are the subject of this work. In general, we might expect that the dependence of the bond-breaking probability P_i on the bond strain δ_i could be almost any monotonically increasing function of δ_i ($f(\delta_i)$). We restrict ourselves to the case $f(\delta_i) = (\delta_i)^\eta$ since only simple homogeneous functions of δ_i are expected to generate cracking patterns with simple geometric scaling properties. In addition, the effects of different local 'growth rules' at the propagating crack surface are explored. This work was stimulated when substantial discrepancies were found between two independently developed cracking models. These discrepancies were eventually traced to different local growth rules at the crack surface. Similar effects are found for the DLA and dielectric breakdown models, but the effects are quite small and both models appear to give the same asymptotic fractal dimensionality. The cracking models investigated in this work are considerably more sensitive to the local boundary conditions.

2. Computer models

In all of our simulations a two-dimensional elastic medium is represented by a triangular network of nodes connected by Hookean springs which have an equilibrium length of l_0. At the start of a simulation, each of the nodes (except for those at the edge of the system) is connected to six nearest neighbours. For the system the elastic energy E is given by

$$E = \tfrac{1}{2} \sum_{ij} k_{ij} (l_{ij} - l_0)^2 \tag{3}$$

where l_{ij} is the length of the bond joining the ith and jth nodes and k_{ij} is the force constant associated with the bond joining these nodes. Here $k_{ij} = k$ if the nodes are joined and $k_{ij} = 0$ otherwise. At the start of each simulation the array of bonds and nodes is either isotropically dilated (typically by 0.1%) or sheared in either the X or Y directions by the transformation $(X_i, Y_i) \rightarrow (X_i + \alpha Y_i, Y_i)$ or $(X_i, Y_i) \rightarrow (X_i, Y_i + \alpha X_i)$. In most of our simulations a value of 0.01 was chosen for α. For both dilation and shear, small strains were used to ensure that our simulation results were not influenced by non-linear effects. We also carried out simulations with larger strains to explore the effects of these non-linearities. The results from these simulations indicated that for the values of the dilation and shear strains indicated above, we are well within the linear regime. Under these conditions, the elastic energy can be written, within the harmonic approximation, as

$$E = \tfrac{1}{2} \sum_{ij} k_{ij} [(\boldsymbol{U}_i - \boldsymbol{U}_j) \cdot \boldsymbol{r}_{ij}]^2 \tag{4}$$

where $\boldsymbol{U}_i$ and $\boldsymbol{U}_j$ are the displacements of the ith and jth nodes and $\boldsymbol{r}_{ij}$ is a unit vector in the direction of the bond joining these nodes.

At the start of a simulation, a bond near to the centre of the network is broken and the system is relaxed to mechanical equilibrium (the elastic energy in equation (3) is minimised) using standard relaxation methods (de G Allen 1954) including block relaxation and overrelaxation. In addition, extra relaxation cycles were used for those

bonds in the vicinity of the (last) broken bond. The relaxation procedure was stopped when the largest displacement of any node from its local equilibrium position is smaller than 0.01 times the initial bond strain. This would not ordinarily be sufficient to guarantee an accurate convergence, but relaxation of the whole system continues as other bonds are broken and the additional relaxation near to the last broken bond ensures almost complete relaxation in this region. Tests with different values for the largest local displacement indicated that our criterion for stopping the relaxation was adequate. Similar results were obtained without overrelaxation using simulations in which Gauss-Seidel iteration was continued until the maximum force in any node was less than 0.001 times the initial force on the boundary nodes. After the network has been relaxed, the strains (δ_i) associated with each of the bonds at the surface of the 'crack' formed by the broken bond(s) are obtained and one of these bonds is randomly selected with probabilities given by $P_i/\Sigma_i P_i$. The process of crack propagation is then simulated by a sequence of random bond-breaking and relaxation events. Throughout the simulations, the positions of the nodes at the edges of the network are fixed.

Several versions of the model were investigated in which different definitions of the crack surface bonds (bonds which may be broken) were used, as shown in figure 1. In model I only those bonds which are at the edge of the crack may be broken. In model II those bonds associated with 'damaged' nodes (nodes for which one or more of the associated bonds is already broken) may be broken, and in model III all of the bonds associated with all of the nodes at the crack surface may be broken.

In most of the simulations, the triangular network of bonds and nodes consisted of 160 rows and 160 nodes (the equilibrium size of the system is $160l$ in the X direction

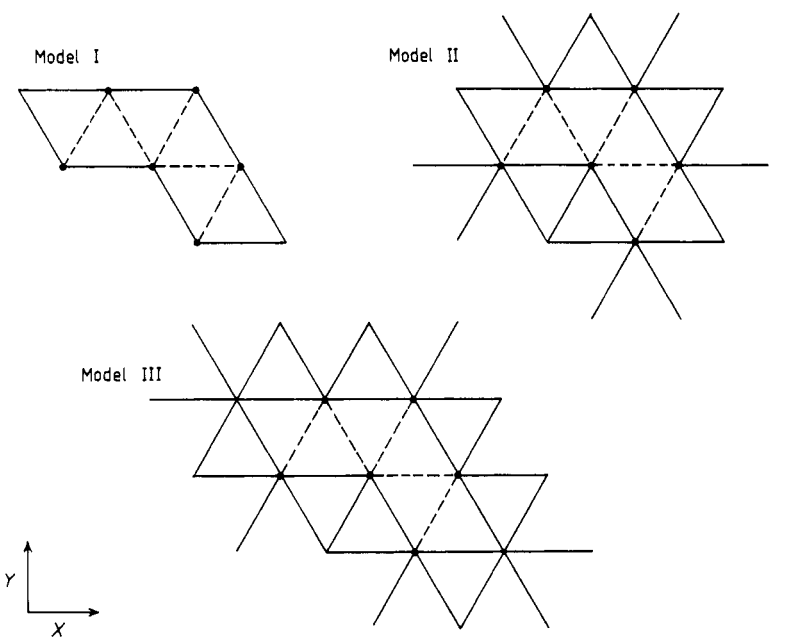


Figure 1. Definition of the surface bonds used in models I, II and III respectively. The broken bonds are indicated by broken lines and the damaged nodes by large dots. The full lines indicate those bonds (the crack surface bonds) in the triangular network which may be broken in the next stage of the crack growth simulations.

and $160(\sqrt{3/2})l$ in the Y direction). The crack propagation process was stopped before the crack tips approached closely to the edges of the network.

3. Results

The results obtained from typical simulations carried out with isotropic dilation (0.1%) and a value of 1.0 for the exponent η are shown in figure 2 for models I, II and III. In this figure (and in other figures in this paper) the locations of the broken bonds in the original (undistorted) network are indicated. It is evident from this figure that these three models lead to similar randomly branched structures, but the different local rules for the bonds which may be broken at the crack surface have a substantial effect on the crack structure (at least on short length scales).

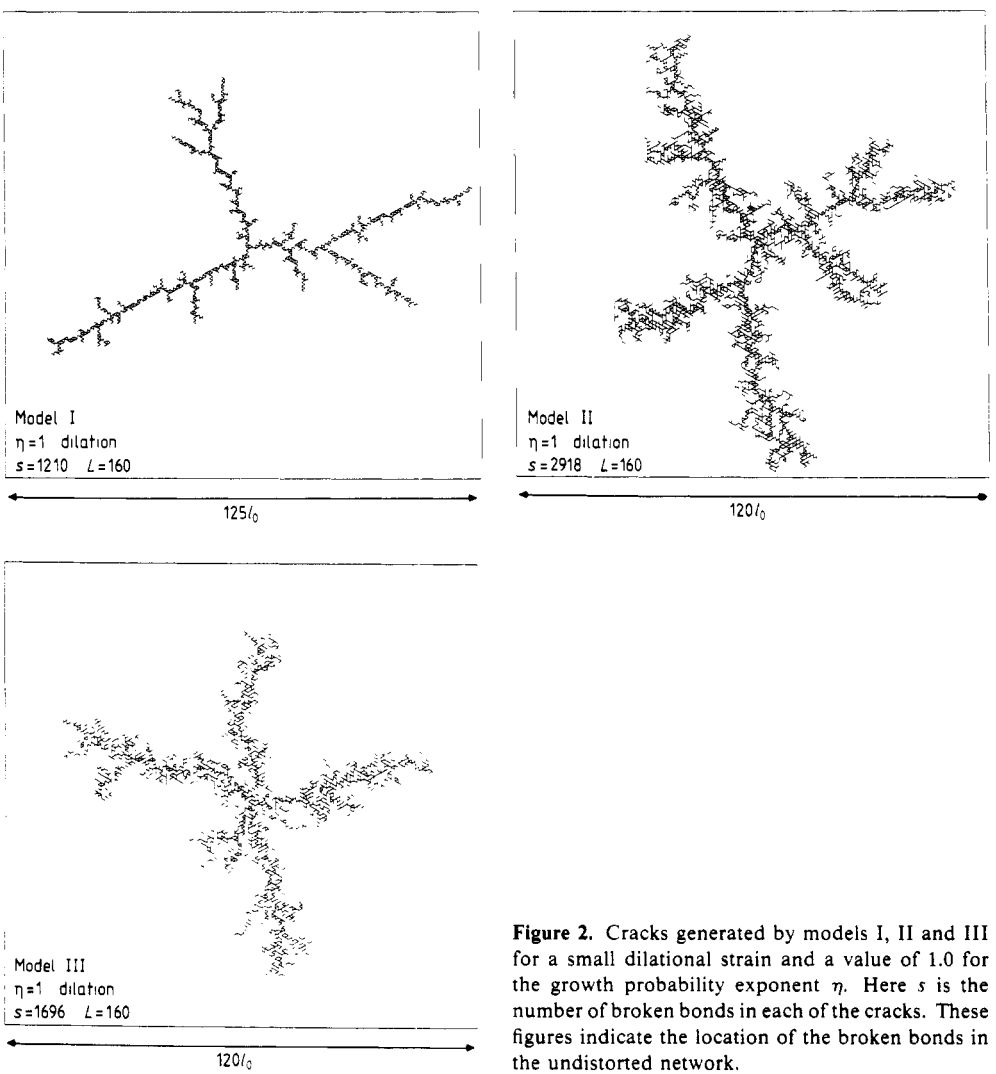
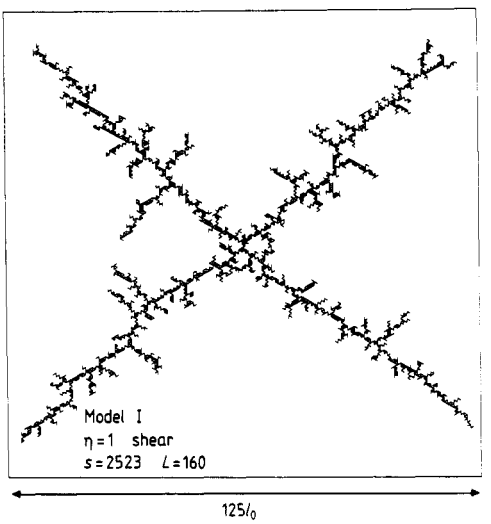
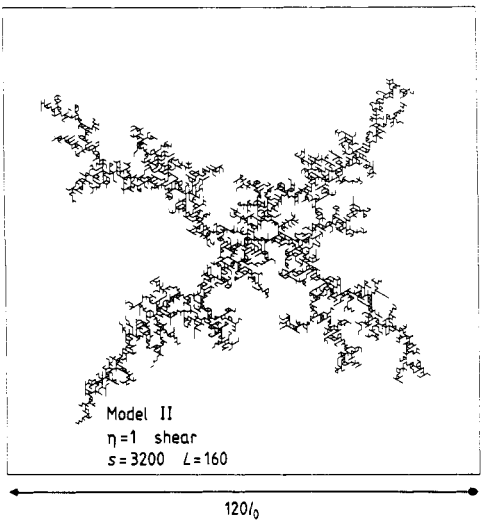


Figure 2. Cracks generated by models I, II and III for a small dilational strain and a value of 1.0 for the growth probability exponent η. Here s is the number of broken bonds in each of the cracks. These figures indicate the location of the broken bonds in the undistorted network.

Figure 3 shows similar results obtained from models I, II and III for the case of shear strain. In all three cases the cracks have a characteristic branched X shape. These results were obtained using shear in the X direction, but very similar results were also obtained with shear in the Y direction (for a triangular lattice the X and Y directions are not equivalent—see figure 1).

Simulations have also been carried out using models I, II and III for both dilation and shear with values of 0.5 and 2.0 for the growth exponent η. Typical results are shown in figure 4 for model I and dilational strain. Figure 5 shows the results obtained from other simulations with both shear and dilational strain with different models and exponents η. A qualitative comparison of the cracks shown in figures 2-5 suggests that the exponent η has a large effect on the crack morphology and that the fractal dimension of the cracks can be decreased by increasing η. Similar results have been obtained previously for both the DLA (Matsushita *et al* 1986) and dielectric breakdown





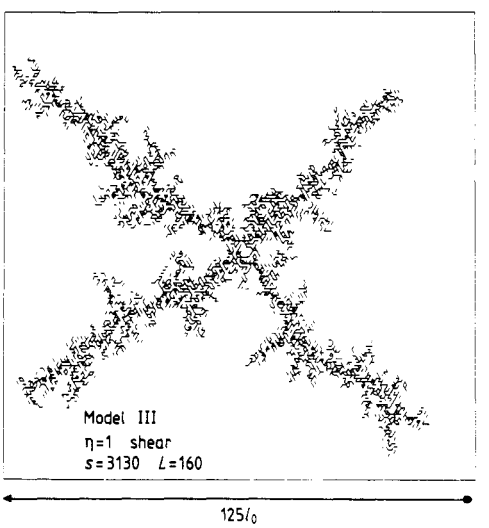


Figure 3. Cracks generated using models I, II and III with a small shear strain in the X direction and a value of 1.0 for the growth exponent η. Very similar results were obtained with shear in the Y direction.

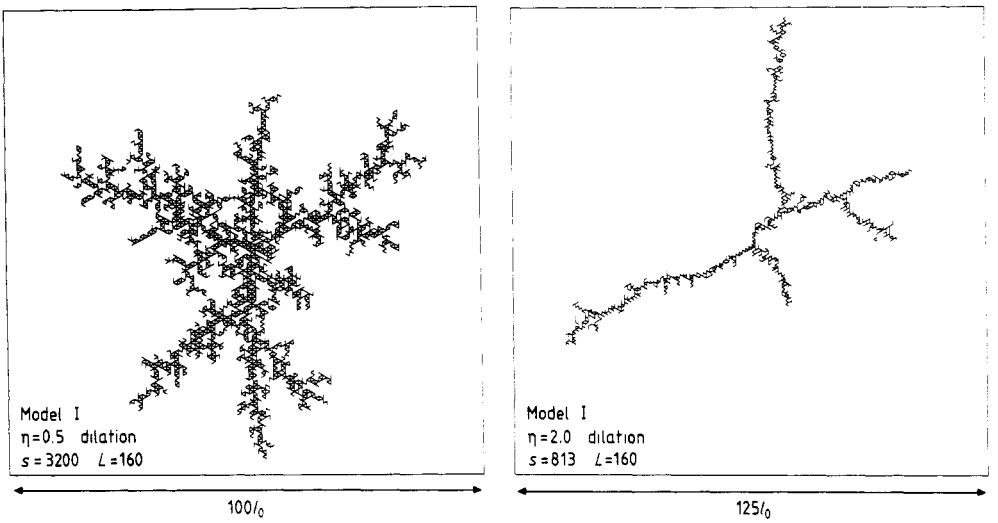


Figure 4. Cracks generated using model I and dilational strain for growth exponent $\eta = 0.5$ and 2.0.

models (Niemeyer *et al* 1984). A more quantiative assessment of the effects of model parameters on the cluster geometry can be obtained from the dependence of the radius of gyration of the crack (R_g) on the number of broken bonds. Figure 6 shows the results obtained from eight simulations carried out using model III with a value of 1.0 for the exponent η. The dashed line has a slope of 0.601 corresponding to an effective fractal dimensionality (D_β) of 1.66 which is quite close to the fractal dimensionality of 1.71 associated with the two-dimensional DLA model (Meakin and Sander 1985). The results obtained from this and the other models (for $\eta = 1$ and $\eta = 2$) are shown in table 1. For $\eta = 0.5$ all of the models generated cracks with effective fractal dimensionalities in the range 1.90–2.0. Each of the results shown in table 1 was obtained using between three and ten simulations. The statistical uncertainties are typically 0.05–0.10 (depending on the model and the number of clusers used). The results shown in table 1 indicate that D increases continuously as η is decreased. Similar behaviour is associated with the dielectric breakdown model (Niemeyer *et al* 1984). For both models $D = 2$ for $\eta = 0$ and $D = 1$ for $\eta \to \infty$. However, we do not know if a fractal dimensionality of 1 is reached only for $\eta = \infty$ or for $\eta > \eta_0$ where η_0 has a finite value. Similarly, for small values of η we expect that the limiting value $D = 2$ is reached only for $\eta = 0$, but the possibility that $D = 2$ for $\eta > 0$ cannot be eliminated using computer simulation results alone.

4. Discussion

Using a model closely related to model III, Louis and Guinea (1987) generated cracks with an effective fractal dimensionality of 1.55 ± 0.05 (for $\eta = 1$ with dilation). They found that essentially the same fractal dimensionality was obtained with shear strain ($D = 1.60 \pm 0.05$) and suggested that both models may generate cracks with the same asymptotic fractal dimensionality as DLA clusters (Witten and Sander 1981). The results obtained here are in quite good agreement with this earlier work. However, the results shown in table 1 suggest that the fractal dimensionality of cracks generated using

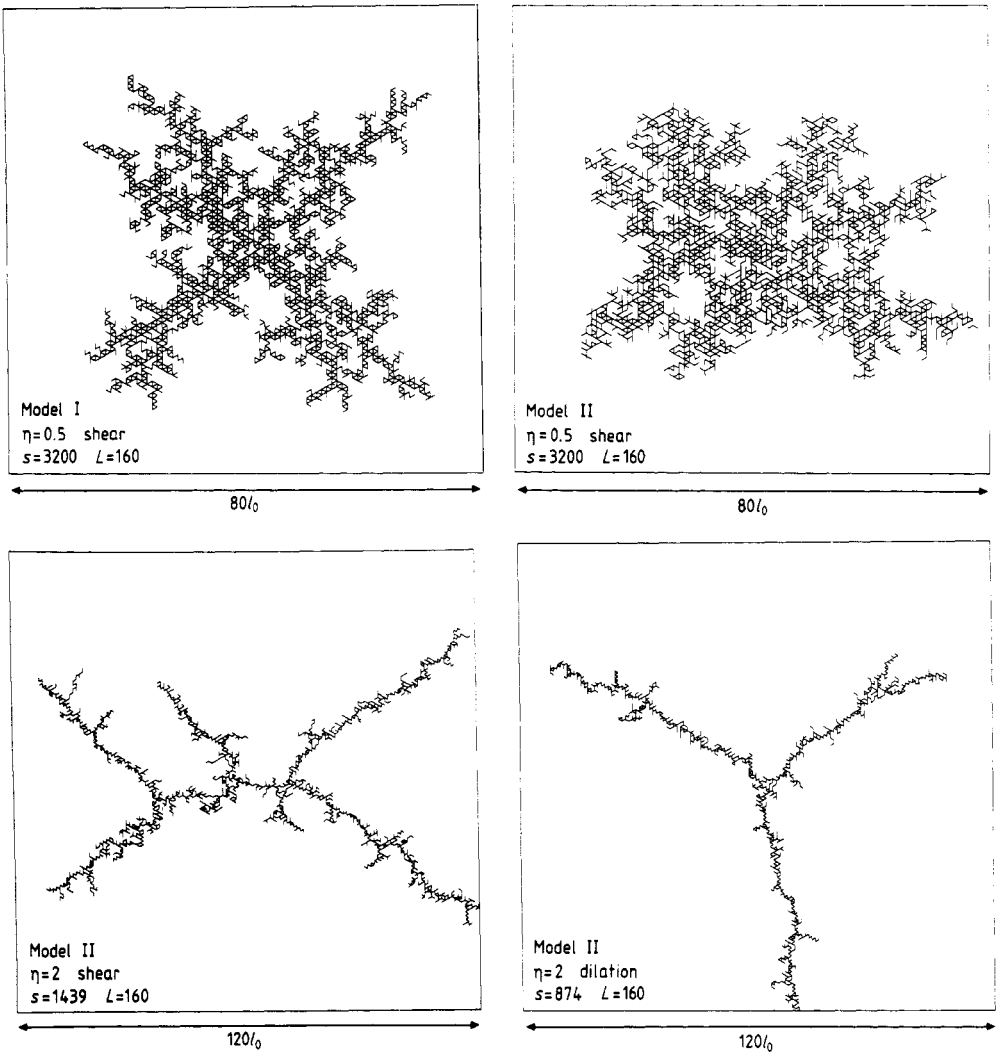


Figure 5. This figure shows the effects of the bond-breaking probability exponent η on simulations carried out with shear and dilational strain.

model I is smaller than that obtained using model II. There is also evidence that the fractal dimensionality associated with model III might be larger than that found for model II.

As we have noted above, the relationship of these models to DLA and other (scalar Laplacian) growth mechanisms is unclear at the moment. It is interesting to note, however, that many of the qualitative features of our simulations can be compared to corresponding features of the better-known DLA problem. For example, it is clear from our simulations that the effect of the underlying lattice is not negligible and, in fact, depends on the boundary conditions at the surface of the crack (i.e. whether we are using models I, II or III). Something of this sort is known in DLA-type simulations (Nittmann and Stanley 1986). In fact, the apparent difference in fractal dimension between the models may be a result of this sort of effect, i.e. model III may be the least sensitive to lattice perturbations. Similarly, the introduction of external shear

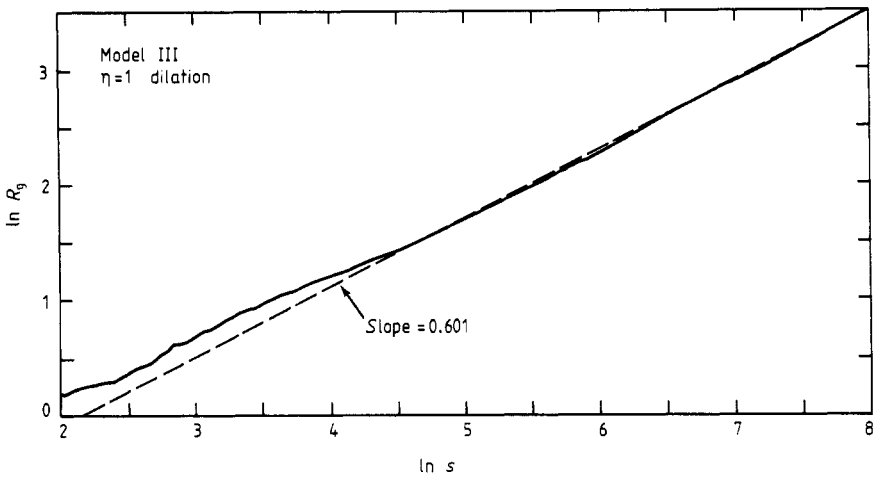


Figure 6. Dependence of the radius of the crack gyration (R_g) on the number of broken bonds (s) obtained from eight simulations carried out using model III with dilational strain and a bond-breaking exponent $\eta = 1$.

Table 1. Effective fractal dimensionalities obtained from the crack growth models.

Growth exponent	Stress field	Model	D_{eff}
1	Dilation	I	1.35
1	Dilation	II	1.51
1	Dilation	III	1.66
1	Shear	I	1.42
1	Shear	II	1.62
1	Shear	III	1.65
2	Dilation	I	1.12
2	Dilation	II	1.16
2	Dilation	III	1.45
2	Shear	I	1.17
2	Shear	II	1.49
2	Shear	III	1.40

corresponds to the introduction of a preferred direction in the material. In the case of DLA, when there is a preferred direction in the sticking probability, the structure crosses over into a non-fractal pattern which reflects the anisotropy of the sticking (Ball *et al* 1985). This may be a clue that the apparent change in fractal dimension in this case may be a crossover to a lattice-dominated pattern.

Our results also indicate that the fractal dimensionality is sensitive to the value of the growth probability exponent η. This is not surprising in view of the well established fact that D depends on η in the dielectric breakdown (Niemeyer *et al* 1984) and DLA (Matsushita *et al* 1986). All of our estimates for the fractal dimensionality are based on the observation of a power-law relationship between the radius of gyration R_g of the crack (broken bonds) measured on the unstrained network (R_g) and the number of broken bonds s:

$$R_g \sim s^{\beta}. \tag{5}$$

In all cases the dependence of ln R_g on ln s was quite linear for the larger values of s (see figure 6 for a typical example).

Hinrichsen *et al* (1988) have carried out similar simulations using model I and model II boundary conditions with uniaxial compression and shear strains. Using model I boundary conditions with shear strain, they find an effective fractal dimensionality $D_\beta = 1.35 \pm 0.05$ from the dependence of R_g on s. This result is in reasonably good agreement with the value of 1.42 (with similar statistical uncertainties) found in this work. However, Hinrichsen *et al* also measured the dependence of the principal values of the inertial tensor on s and obtained a fractal dimensionality of 1.28 ± 0.06 from the scaling of the largest value with s. They argue that the cross-shaped cracking patterns generated by shear strain consist of two cracking patterns having the structure of uniaxial compression cracks for which they measured a fractal dimensionality of 1.22 ± 0.05. Based on these results Hinrichsen *et al* suggest that the fractal dimensionalities of the cracks produced by these models may have a universal value independent of the strain boundary conditions. A more detailed theoretical analysis and/or much larger-scale simulations will be needed to determine if these ideas are correct.

In order to draw more definitive conclusions, much more extensive, larger-scale simulations would be needed. This is not possible with our present algorithms and computer resources. It is clear from this work that much more efficient algorithms will be needed to make further progress. We are now working in this direction.

Acknowledgments

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