# The fractal nature of a fracture surface



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# The fractal nature of a fracture surface

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**Abstract.** A kinetic model is presented which simulates the propagation of cracks in solids composed of discrete atoms. The resulting fracture surface is found to be a fractal, the dimension of which depends on the elastic constants of the material.

It has been claimed recently [1-3] that frature surfaces in materials are fractal in nature, i.e. 'self-similar', over a wide range of scale. Differing from diffusion-limited aggregation (DLA) [4], dielectric breakdown [5] and viscous fingering [6], fracture surfaces are found to be another kind of fractal.

Fracture phenomena are some of the most intriguing processes in materials science. Many factors affect these processes, such as grain boundaries, environment, temperature and anisotropies [7]. A macroscopic treatment of the fractal nature of fracture has been carried out recently [8]. The present approach, which is based on a kinetic model, is entirely microscopic. Consider a two-dimensional ($xy$) square lattice of nodes. These nodes are linked in the $x$ and $y$ directions by harmonic springs with force constants $K_x$ and $K_y$. Suppose a bond in the centre of the network has been broken. We want to simulate the way in which the crack propagates, when a load is applied along the $y$ direction, until the network breaks into two parts.

We restrict ourselves to this case: only the bonds neighbouring the broken bonds are the candidates for subsequent breakage, so the crack propagates through the 'tips'. The bond breakage is controlled by thermal activation, and this process is examined with the help of the following kinetic model. The unbroken candidate is broken in the next step with a probability:

$$P_i \propto \exp[(-U_i + E_i)/KT] \tag{1}$$

where $U_i$ is an activation energy, $E_i$ is the elastic energy stored in the bond, $K$ is Boltzmann's constant and $T$ is the absolute temperature. $E_i$ is expressed as:

$$E_i = \tfrac{1}{2} K_i (\Delta l_i)^2. \tag{2}$$

Here $K_i$ is the force constant for bond $i$ and $\Delta l_i$ is the elongation. The total probability for all the candidates in one step is set to 1, i.e. one and only one bond is broken in one step. The nearest-neighbouring bonds of a chosen bond are illustrated in figure 1.

Our model thus resembles that of Termonia and Meakin (TM) [9]. But our work differs from theirs in at least three respects. First, in our model the crack propagates only through the crack tips, i.e. only the bonds neighbouring the broken bonds possess overwhelming probabilities of breakage, while the TM model assumed all the unbroken

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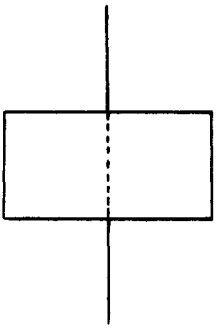

**Figure 1.** Eight nearest-neighbouring bonds (solid line segments) of a chosen bond (broken line segment).

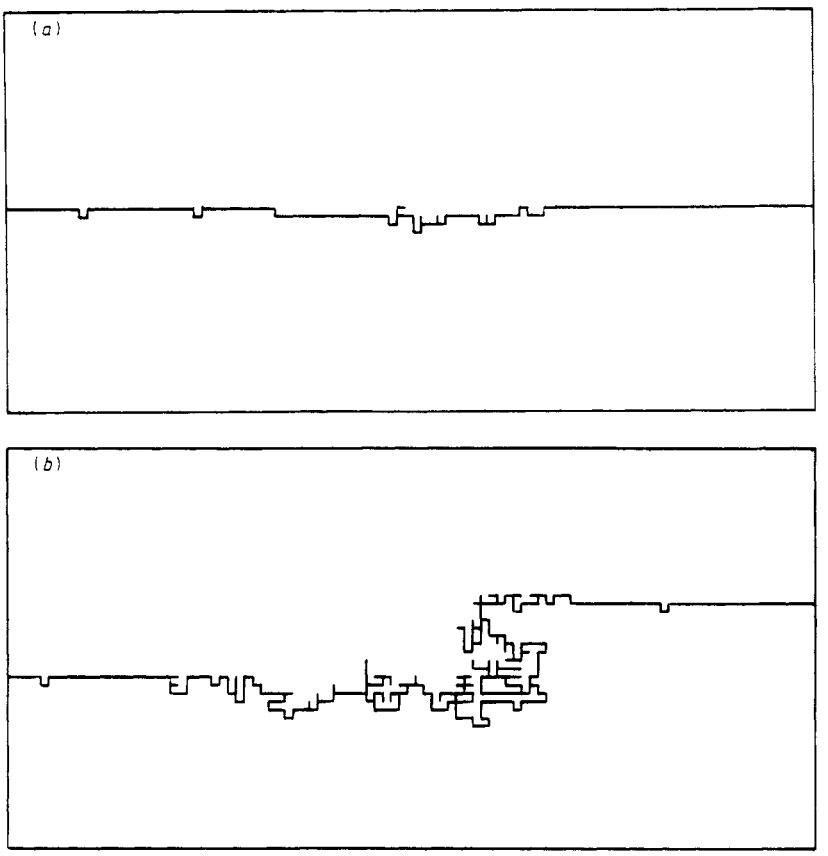


**Figure 2.** (*a*) The fracture surface for case a: $K_x = K_y = 20$. (*b*) The fracture surface for case b: $K_x = 200$, $K_y = 20$.

bonds to have some breakage probabilities similar to (1). In reality, the existing defects (or cracks) can assist the breakage of the material near the defects [10]. Second, the normalisations of the probabilities are different. In the TM model, the most stressed bond breaks with probability of 1. Third, in the work of TM, the node had non-zero size, in contrast to our 'point' node.

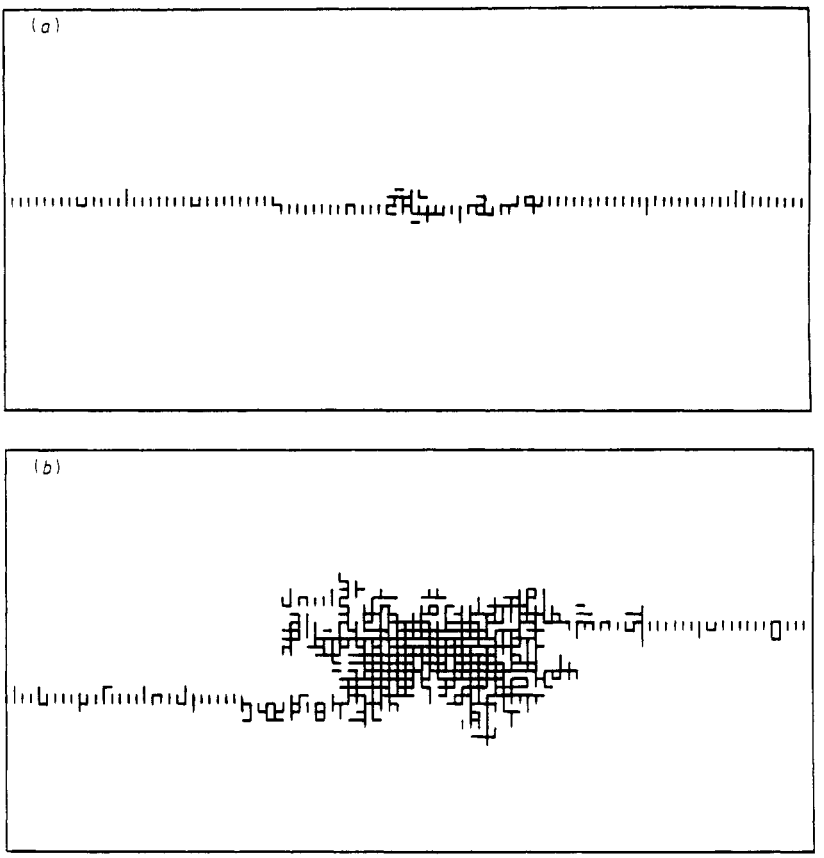


**Figure 3.** (*a*) The graph of broken bonds for case a: $K_x = K_y = 20$. (*b*) The graph of broken bonds for case b: $K_y = 200$, $K_x = 20$.

For simplicity, we assume that the motion of the nodes along the $x$ and $y$ axes are mutually independent [11], and we focus on their displacements along the $y$ axis where the network is strained. We start with a network with one broken bond (crack embryo) in the centre. The network is loaded along the $y$ axis so that the length of the network in this direction is stretched by 20%, and the uppermost and lowermost lattice points are then fixed throughout the process, the free boundary condition is assumed for the leftmost and rightmost lattice points. Then the network recovers its equilibrium state, i.e. the force acting on every node equals zero (equation (3)). The simulation is completed in a series of steps. At each step, one bond out of the candidates breaks according to (1), (2), and then the network proceeds to its new equilibrium state which is characterised by the following equation:

$$\sum_j K_{ji}(y_j - y_i) = 0 \tag{3}$$

where $y_i$ is the $y$ coordinate for node $i$, $K_{ji}$ is the force constant of the bond connecting nodes $i$ and $j$ ($K_{ji} = 0$, if the bond is a broken bond), the sum index $j$ runs over all the nearest nodes of node $i$. These steps are repeated until the network breaks. The network is considered to be broken into two parts when the elongation of all the bonds are zero to within an error of $10^{-3}$ unit length (we assume the lattice constant to be

unit). Under the assumption of nearest-neighbour interaction, (3) is a block-tridiagonal equation. It can be solved by the block-overrelaxation method [12], and the coordinates $y_i$ in (3) were calculated to within an error of $10^{-4}$. In this work, a network consisting of 50 nodes in the $y$ direction and 100 nodes in the $x$ direction was used. The CPU time taken was 4-11 hours on a FACOM M340. For simplicity, we chose equal activation energy for all the bonds (equation (1)) and took $KT = 1$. In order to compare our model with TM model effectively, the force constants were adopted from TM [9], i.e., $K_x = K_y = 20$ for case a, $K_x = 200$, $K_y = 20$ for case b. After fracture, the fracture surface is not strictly 'smooth'. Figure 2 shows two typical fracture surfaces. The corresponding graphs of broken bonds are shown in figure 3. The irregularity of the surface can be characterised by its fractal dimension [1-3]. The fractal dimension was obtained by measuring the length of the fracture 'surface' (which was a curve in our two-dimensional simulation) using yardsticks of different sizes. The fractal dimension of the 'surface' $D$ was obtained by the following equation:

$$n \sim r^{-D} \tag{4}$$

where $n$ is the number of the yardsticks of size $r$ needed to cover the fracture 'surface'. Figure 4 shows the log-log dependence of $n$ on $r$ for case a and case b. Fitting a straight line in the range $2 < r < 30$ gives $D = 1.011 \pm 0.003$ for case a and $D = 1.248 \pm 0.017$ for case b, in contrast to the result of TM [9]. From the log-log linearity, the fractal nature of the fracture surface is evident.

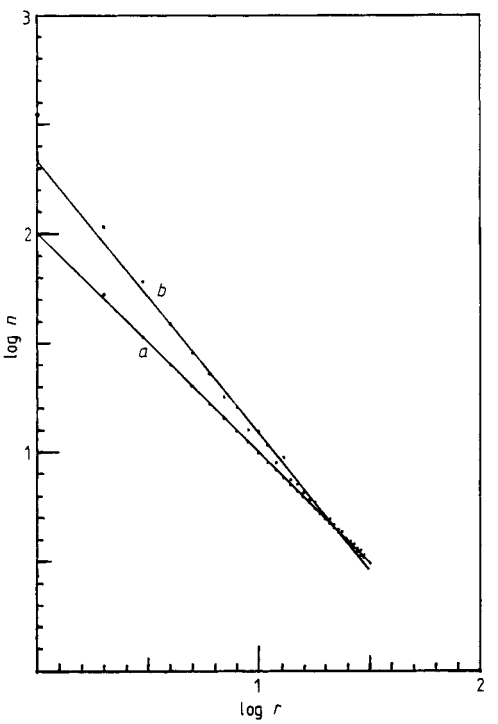


**Figure 4.** Log-log dependence of $n$ on $r$ (equation (4)): ($a$) $K_x = K_y = 20$, ($b$) $K_x = 200$, $K_y = 20$.

Admittedly our model may be only a crude representation of real experimental systems. Nevertheless, our results show the dependence of fractal dimension on the force constants of the materials, i.e. $D$ does not have a universal value for all materials. Thus one may understand why the experimental values of the fractal dimension are so scattered [1-3].

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