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Crack patterns and strain energy distributions in model brittle systems in a random environment

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Monte Carlo simulations of crack growth are performed using simple two-dimensional model systems for brittle materials. Crack growth is modelled as a series of processes of release and transfer of strain energies on the system of square grains. The simulations are concerned with crack growth in a random environment. Considerable attention is paid to the correlation between crack patterns and strain energy distributions. It is shown that the model system settles into a stationary state. In this state, the features of crack pattern have a close relation to the characteristics of strain energy distribution. Some implications of the results are discussed in regard to crack patterns caused by heating, radiation, or random mechanical loading on the surface of real brittle materials.

1. Introduction

Various aspects of crack patterns on solid materials can be observed almost everywhere. These crack patterns may have been caused by particular loads, by random environments, or by unknown complicated influences. If the mechanical characteristics of a material and of a particular load are known, the mechanism of crack growth can be understood on the basis of fracture mechanics. There have been a number of investigations on the initiation and propagation of a single or a few cracks under particular loads. However, there is very little information on the global features of a spatial pattern of many cracks. Because real materials include various types of disorder, the behaviour of crack growth and the resultant crack patterns show intrinsically stochastic and intricate features. Different approaches to crack growth from conventional fracture mechanics would be required for an understanding of such crack patterns.

In recent years, there has been growing interest in crack patterns since the concept of fractals was proposed by Mandelbrot and co-workers to describe various intricate patterns in nature [1, 2]. Some models for crack growth have been explored in order to investigate the mechanism of fracture [3–8] and crack patterns [9, 10]. Meakin *et. al.* [9,10] performed computer simulations using a two-dimensional model in which a network of bonds of linear strings is broken with a bond-breaking probability. Skjeltorp and Meakin [11, 12] explored experimentally the development of crack patterns in monolayers of microspheres. These studies showed that crack patterns in the model and in the experiment are described in terms of fractal dimensionality.

Although the consideration of crack patterns in terms of fractality threw a new light on the understanding of the fracture mechanism, many questions about crack patterns still remain unsolved from the practical point of view. For example, how can we understand characteristics of materials from crack patterns? What can we say about a difference in environmental conditions from different crack patterns on materials with the same quality? If we can answer these questions to some extent, we would have a useful grasp of crack patterns in view of practical applications. The main purpose of the present work was to investigate global features of crack patterns in simple model systems and to give some responses to the above questions.

We modelled crack growth in brittle materials by a series of processes for strain energies in a system of grains. By performing Monte Carlo simulations of crack growth in the system subjected to random influences, we investigated especially the correlation between crack patterns and strain energy distributions. The results are discussed in connection with real materials, including some characteristic of our model.

2. Model and simulation

In general, the initiation and propagation of cracks are described in terms of stress–strain analysis based on fracture mechanics. In terms of energetics, crack growth may be regarded as processes of storage, release and transfer of strain energy in a material. Under an external influence, a material stores the strain energy. On the initiation of a crack, part of the strain energy is released as other energy forms, such as the surface energy of the crack and acoustic emission. The rest of the strain energy is spatially transferred. It is concentrated near the crack tips, as described by the stress intensity factor in terms of fracture mechanics. Therefore, these processes of strain energy will be incorporated in a simple model for crack growth.

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Consider a two-dimensional system of squares, as shown in Fig. 1. We call a square the grain, and a side of a square, the grain boundary. With this system, we conceive a model for crack growth [13]. We confine ourselves to crack growth on brittle materials, such as ceramics in which plastic deformation, associated with dislocations in metallic materials, can be disregarded. We also keep in mind the crack growth caused by random influences. Thus the grains in a system are supplied with strain energy at random from outside the system.

Our model is composed of the following processes. We select a grain at random and give a "strain energy", ΔE, to the grain. This process is repeated and each grain stores its strain energy. When the strain energies of the ith and the adjacent jth grains, E_i and E_j, satisfy the condition, $E_i E_j \geq E_t^2$, we generate a crack on the grain boundary of the two grains, as shown by a thick solid line in Fig. 1. E_t is a threshold energy for cracking, regarded as a measure of the strength of grain boundaries. On cracking, an energy, E_r, is released from the ith and jth grains. The strain energies of the ith and jth grains both reduce from E_i and E_j to E_s. The rest of the strain energies, $E_i + E_j - E_r - 2E_s$, is transferred equally to four grains contacted with the crack tips, i.e. to the grains shown by the shaded squares in Fig. 1. Then the criterion for cracking is examined for all grain boundaries belonging to the grains whose strain energies have been varied. If the condition is satisfied, further cracking follows. If it is not satisfied for any boundary, the process of strain energy input is repeated until the next crack occurs. In the case where two or more boundaries satisfy the condition, we preferentially chose a boundary having the largest value of $\{E_i E_j\}$. Also, in the case where two or more boundaries have the same largest value, we select one of them at random. Thus we proceed with the processes of energy input and cracking followed by energy release and transfer.

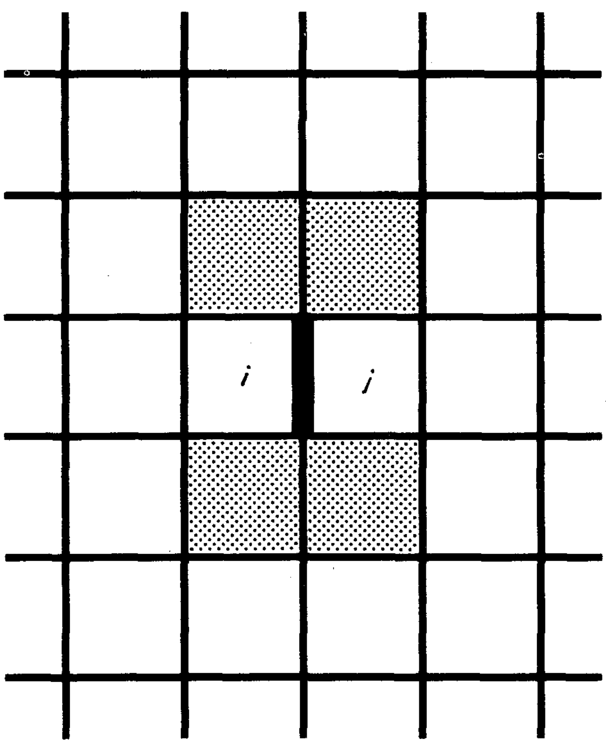

Figure 1 Part of a model system for crack growth. After a crack has been generated on the boundary between the ith and jth grains, as shown by a thick solid line, part of the strain energies of those grains is transferred equally to four grains shown by shaded squares.

The criterion, $E_i E_j \geq E_t^2$, has been introduced to take account of a co-operative effect of adjacent grains on cracking, that is, cracking is facilitated co-operatively by the product of strain energies of adjacent grains. For the boundary of the system, we have used periodic boundary conditions. The effect of system boundary conditions was examined by adopting other boundary conditions in which strain energies are absorbed at the system boundary. The characteristic features of crack patterns in the present model were not influenced by the choice of boundary conditions.

Simulations have been performed for systems of $120 \times 120 = 14\,400$ grains; the number of grain boundaries is 28 800. At the start of a simulation, the strain energy of any grain is zero. There are four parameters in our model: the input energy, ΔE, the grain boundary strength, E_t, the release energy, E_r, and the residual energy, E_s. We perform simulations for different sets of parameters to compare the results. We will investigate the evolution of the number of cracks, crack patterns, strain energy distributions, and the relationship between them.

3. Results

3.1. Stationary state

As a primary property of our model systems, we first show the evolution of the number of cracks, N_c, and the average strain energy per grain, $\langle E \rangle = \sum_i E_i/N_G$, where N_G is the number of grains in a system. Figs 2 and 3 show the dependences of N_c and $\langle E \rangle$ on the number of energy inputs, N, in the systems with $E_t = 5$ and 15, respectively; other parameters, $\Delta E = 1$, $E_r = 1$ and $E_s = 0$, are common to the two systems. At early stages, the strain energy stored by energy inputs is much larger than the energy released by crackings. Thus N_c increases slowly and $\langle E \rangle$ increases almost proportionally to N. The variations of N_c and $\langle E \rangle$ for $E_t = 5$ are relatively smooth, while those for $E_t = 15$ are rough; N_c increases in a step-like manner and $\langle E \rangle$ in a saw-toothed manner for $E_t = 15$. Because successive crackings decrease $\langle E \rangle$, the behaviour of N_c and $\langle E \rangle$ reflects a difference in crack growth between the two systems. The system with $E_t = 5$ alternates short crack propagations with energy inputs for a short time. The system with $E_t = 15$, on the other hand, alternates long crack propagations with energy inputs for a long time. This behaviour of crack growth will be seen clearly in the resulting crack patterns, as will be shown below. The present Monte Carlo simulations do not demonstrate the evolution of crack growth in real time. If we suppose that the crack propagation time is much shorter than the time interval between succeeding energy inputs, however, the N-dependences of N_c and $\langle E \rangle$ may be regarded as the real time evolution.

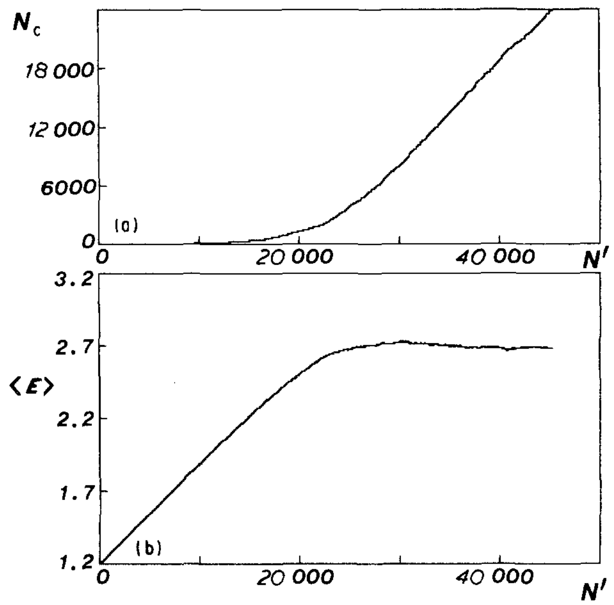

Figure 2 The dependences of (a) the number of cracks, N_c, and (b) the average strain energy per grain, $\langle E \rangle$, on the number of energy inputs, N, in the system with $E_t = 5$ under $\Delta E = 1$, $E_r = 1$ and $E_s = 0$. Note that the figure shows the dependence after the first crack initiation; the abscissa represents the number of energy inputs, N', after the first crack initiation (the first cracking at $N' = 1$).

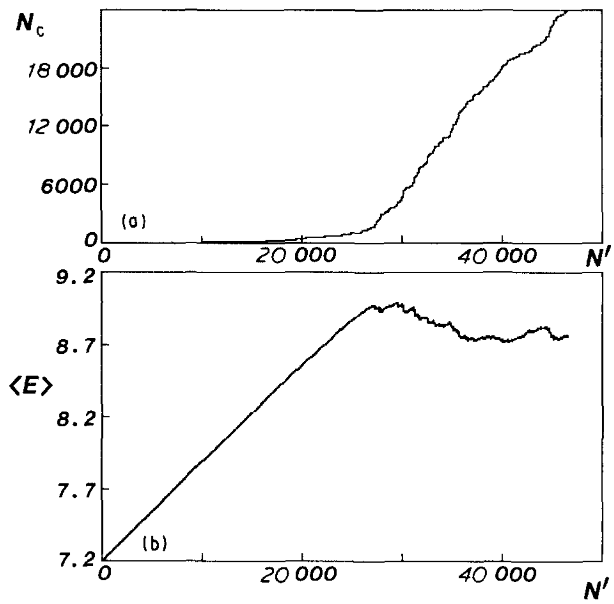

Figure 3 The dependence of (a) the number of cracks, N_c, and (b) the average strain energy per grain, $\langle E \rangle$, on the number of energy inputs, N, in the system with $E_t = 15$ under $\Delta E = 1$, $E_r = 1$ and $E_s = 0$. See also the caption of Fig. 2.

Our system settles into a stationary state at $N_c \sim 6000$. In this state, $\langle E \rangle$ is almost constant and correspondingly N_c increases proportionally to N, as shown in Figs 2 and 3. In other words, the strain energy stored by energy inputs is released by cracking, on average. In the system with $E_t = 15$, there are relatively large fluctuations of $\langle E \rangle$ in the stationary state, which reflect the behaviour of crack growth in this system, as described before. The average strain energies in the stationary state, $\langle E \rangle_s$, are listed in Table I for the systems with different values for E_t

TABLE I Average strain energies per grain in the stationary state, $\langle E \rangle_s$, in the systems with $E_t = 5$, 10, 15 and 20 under $\Delta E = 1$, $E_r = 1$ and $E_s = 0$. The values of $\langle E \rangle_s$ are the mean values obtained from five simulations for each value of E_t

	E_t			
	5	10	15	20
$\langle E \rangle_s$	2.7	5.7	8.8	11.9
$\langle E \rangle_s/E_t$	0.54	0.57	0.59	0.60

under $\Delta E = 1$, $E_r = 1$ and $E_s = 0$. The values of $\langle E \rangle_s/E_t$ are 0.54 to 0.60, being almost independent of E_t. The values of $\langle E \rangle_s/E_t$ do not depend appreciably on E_r, except $E_r \sim 0$ which is not practical. In the systems with $E_s \neq 0$, the values of $\langle E \rangle_s$ shift upwards by 0.4 E_s to 0.6 E_s.

3.2. Crack patterns and strain energy distributions

In the stationary state, the distribution of strain energies of grains in a system is stable; the distribution remains unchanged as the number of energy inputs increases. We will then see the correlation between crack patterns and strain energy distributions in the stationary states.

First we show the influence of the grain boundary strength, E_t. Figs 4 and 5 show the crack patterns at $N_c = 6000$, the magnitude distributions of strain energies, and the spatial distributions of strain energies in the stationary states of the systems with $E_t = 5$ and 15, respectively; other parameters, $\Delta E = 1$, $E_r = 1$ and $E_s = 0$, are common to the two systems. There is a clear difference in crack pattern between the two systems. The pattern for $E_t = 5$ has many short cracks, while that for $E_t = 15$ has relatively long cracks. They correspond to the behaviour of N_c and $\langle E \rangle$ shown in Figs 2 and 3. This difference in crack pattern is attributed to the magnitude of transfer energy on cracking and the strain energy distribution. To see that, we show in Fig. 6 the magnitude distributions of strain energies at $N_c = 1$ for both the systems; in the figures the mean magnitudes of the energy which is transferred to a grain at a crack tip, are shown by arrows. The probability of extending a crack is much higher in the system with $E_t = 15$ than in the system with $E_t = 5$, because the grains to which the strain energy is transferred are more probable to satisfy the cracking condition in the system with $E_t = 15$. Thus a system with a larger grain-boundary strength tends to reveal a spatially rough crack pattern.

The release energy, E_r, exerts an obvious influence on crack patterns and strain energy distributions. Fig. 7 shows the crack pattern and strain energy distributions in the system with $\Delta E = 1$, $E_t = 15$, $E_r = 15$ and $E_s = 0$. The figure should be compared with Fig. 5 in which $\Delta E = 1$, $E_t = 15$, $E_r = 1$ and $E_s = 0$; a difference in the values of parameters is only in E_r. The pattern for $E_r = 15$ is composed of many short cracks distributed uniformly. This is a consequence of the fact

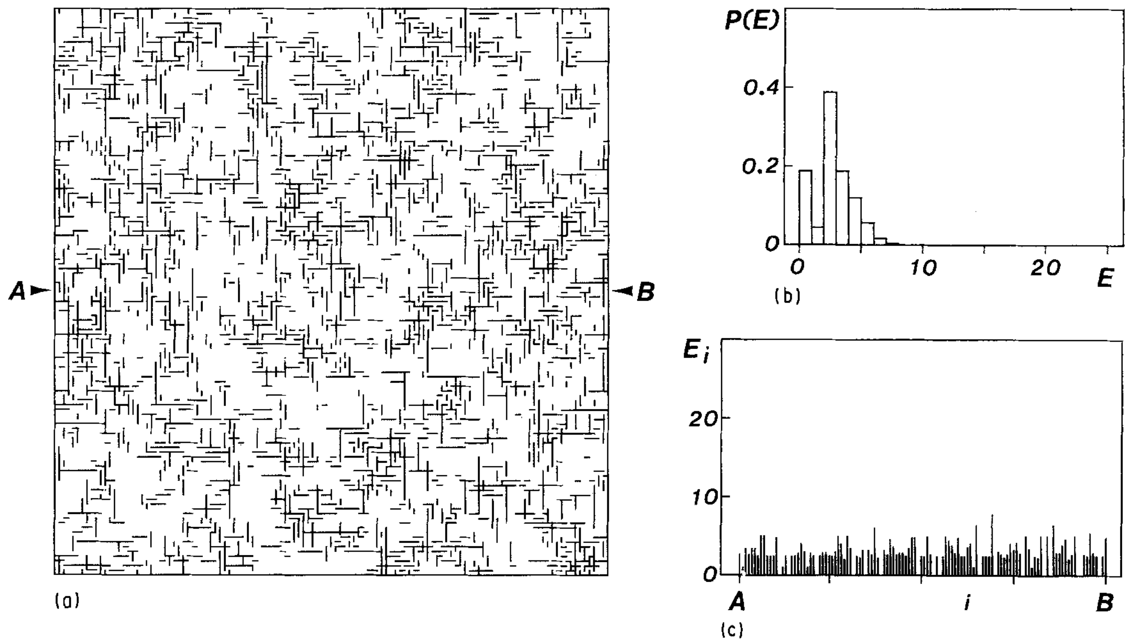

Figure 4 Crack pattern and strain energy distributions in a stationary state of the system with $E_t = 5$ under $\Delta E = 1$, $E_r = 1$ and $E_s = 0$; (a) crack pattern at $N_c = 6000$, (b) magnitude distribution of strain energies of grains, (c) spatial distribution of strain energies of grains along a line drawn between A and B in the pattern in (a).

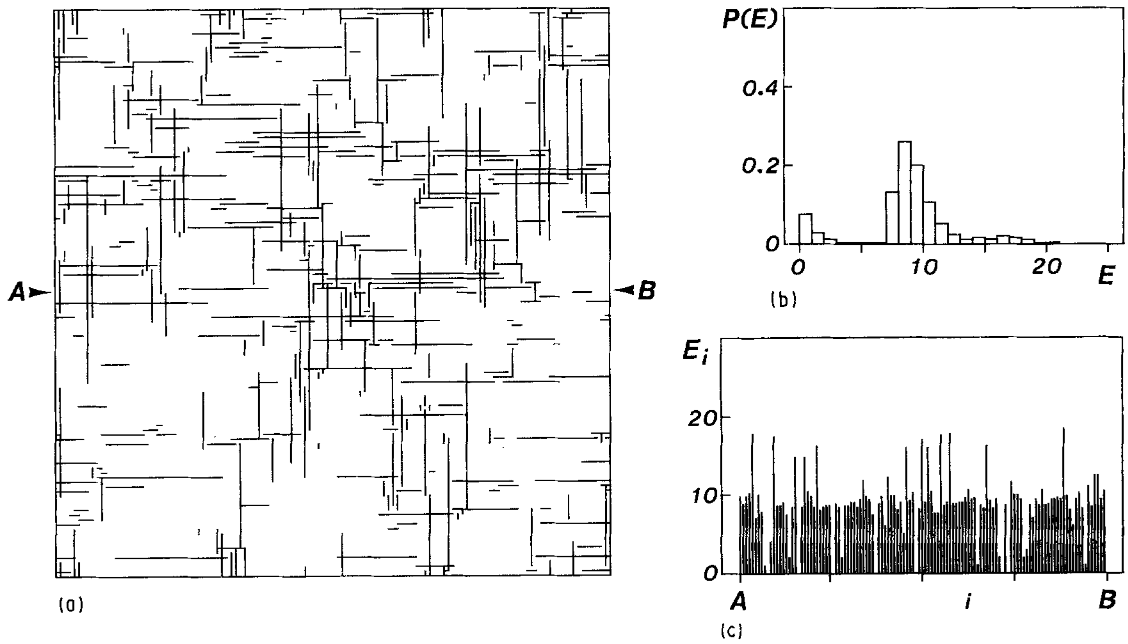

Figure 5 Crack pattern and strain energy distributions in a stationary state of the system with $E_t = 15$ under $\Delta E = 1$, $E_r = 1$ and $E_s = 0$. See also the caption of Fig. 4.

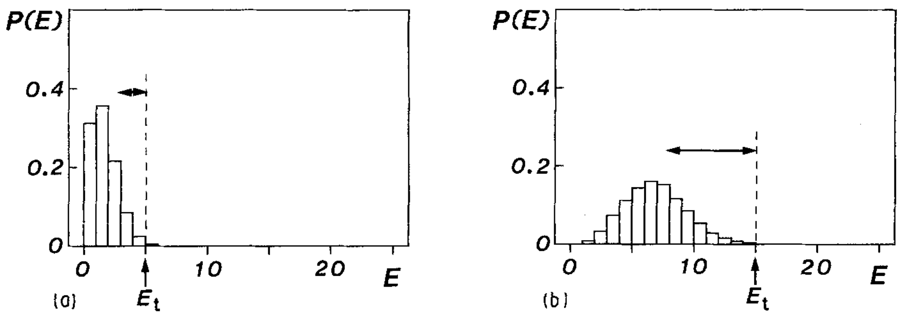

Figure 6 Magnitude distributions of strain energies of grains at $N_c = 1$ in the systems with (a) $E_t = 5$ and (b) $E_t = 15$ under $\Delta E = 1$ ($E_r = 1$ and $E_s = 0$). In each figure, the mean magnitude of the energy which is transferred to a grain at a crack tip is shown by an arrow drawn from the location of E_t.

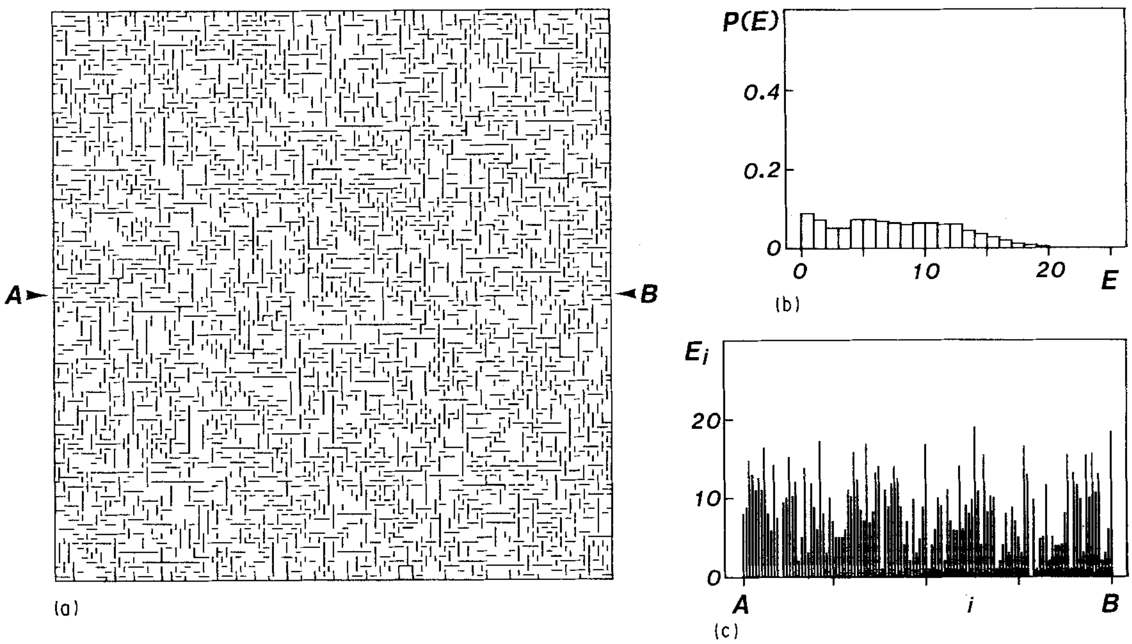

Figure 7 Crack pattern and strain energy distributions in a stationary state of the system with $\Delta E = 1$, $E_t = 15$, $E_r = 15$ and $E_s = 0$. For (a), (b) and (c), see Fig. 4.

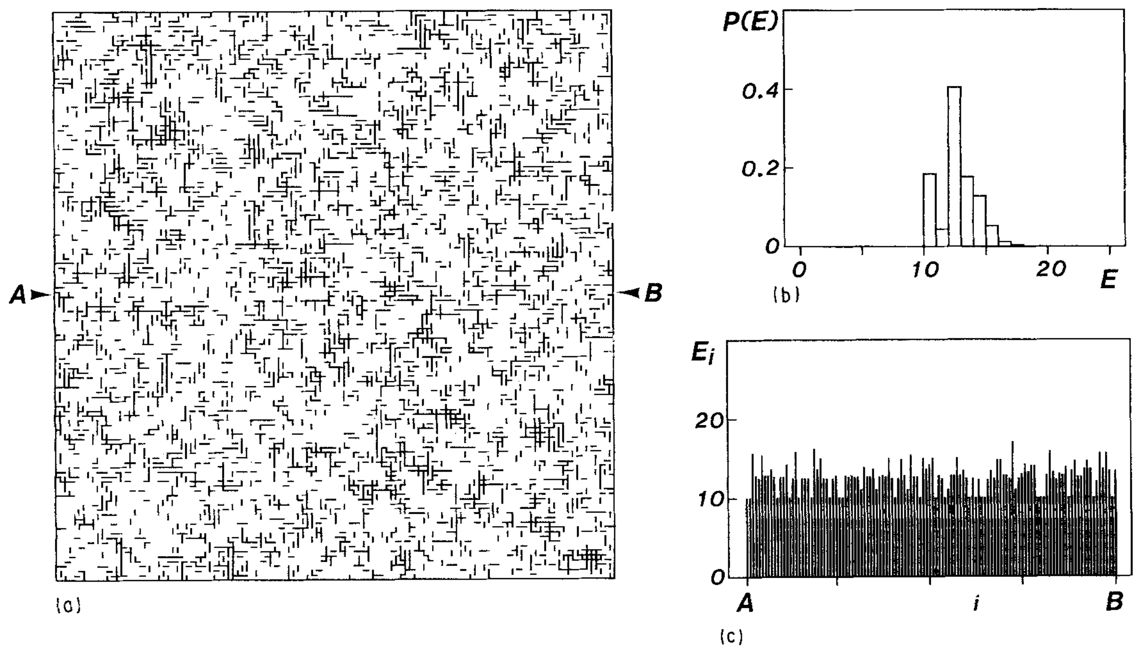

Figure 8 Crack pattern and strain energy distributions in a stationary state of the system with $\Delta E = 1$, $E_t = 15$, $E_r = 1$ and $E_s = 10$. For (a), (b) and (c), see Fig. 4.

that cracks are caused mostly by random energy inputs, because crack extension is restrained by a large release energy. The strain energy distributions for $E_r = 15$ characteristically have a uniformly wide magnitude distribution and a randomly fluctuating spatial distribution.

The residual energy, E_s, also has some effect on crack patterns and strain energy distributions. Fig. 8 shows the pattern and the distributions in the system with $\Delta E = 1$, $E_t = 15$, $E_r = 1$ and $E_s = 10$. The figure should be compared with Fig. 5 in which $E_r = 1$ and $E_s = 0$ and also with Fig. 7 in which $E_r = 15$ and $E_s = 0$. The crack pattern in Fig. 8 has many short cracks, but they are distributed nonuniformly in comparison with those in Fig. 7. Although the system with a large E_r or a large E_s shows crack patterns with many short cracks, the spatial arrangement of cracks is clearly different between the two systems. The strain energy distributions for $E_s = 10$ are characterized by a narrow magnitude distribution and a nearly uniform spatial distribution with small fluctuations. These are due to the fact that cracks are likely to grow within local regions as a result of a large residual energy and a small transfer energy.

The input energy, ΔE, has an influence on the crack pattern, but not on the strain energy distributions. Fig. 9 shows the pattern and the distributions in the system with $\Delta E = 3$, $E_t = 15$, $E_r = 1$ and $E_s = 0$; the

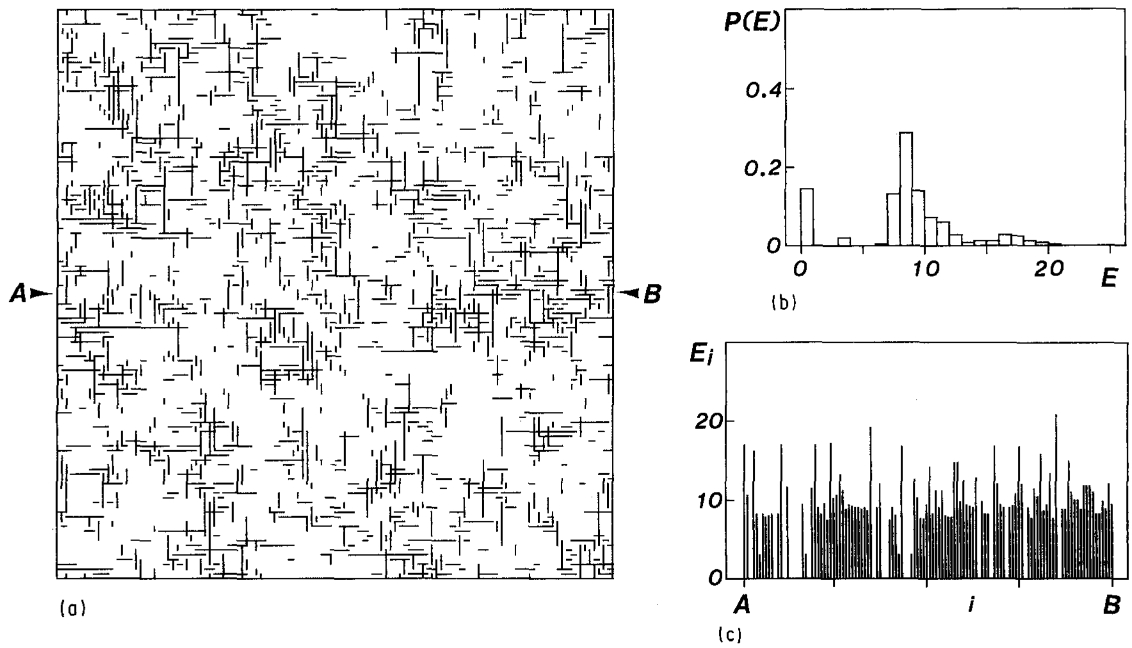

Figure 9 Crack pattern and strain energy distributions in a stationary state of the system with $\Delta E = 3$, $E_t = 15$, $E_r = 1$ and $E_s = 0$. For (a), (b) and (c), see Fig. 4.

figure should be compared with Fig. 5 in which $\Delta E = 1$ with other parameters being the same. A larger ΔE leads to larger spatial fluctuations of strain energies of grains at early stages of energy inputs. This results in a short crack pattern, because large spatial fluctuations of strain energies are likely to arrest crack extension. The strain energy distributions in the stationary state are, however, almost the same as those for $\Delta E = 1$ shown in Fig. 5b and c.

The parameter, ΔE, may be regarded as a unit of strain energy. Then the system with $\Delta E = 3$, $E_t = 15$, $E_r = 1$ and $E_s = 0$ is quite the same as that with $\Delta E = 1$, $E_t = 5$, $E_r = 1/3$ and $E_s = 0$. A larger ΔE therefore, corresponds to smaller E_t, E_r and E_s. However, one physical significance of ΔE is an external influence on a system, while other parameters may be concerned with the system itself. Therefore, we will regard ΔE as an independent parameter in connection with real materials and real environmental effects.

4. Discussion

4.1. Implications in real materials

The present simulations have revealed some correlations between crack patterns and strain energy distributions. The results are summarized as follows. The larger the grain-boundary strength, E_t, the rougher is the crack pattern, and the longer are the cracks. An increase in the release energy, E_r, causes many short cracks, resulting in a uniformly-distributed fine pattern. Then the strain energy distribution is uniformly wide in magnitude and randomly fluctuating in space. An increase in the residual energy, E_s, also causes many short cracks, but results in a nonuniformly distributed fine pattern. Then the strain energy distribution is narrow in magnitude and almost uniform in space. Increasing the input energy, ΔE, generates nonuniform crack patterns with short cracks, but does not influence the strain energy distributions.

In regard to real materials, the present results are implicated in various crack patterns on the surface of non-metallic materials in a random environment. For example, drying materials which include water causes spatially random stresses and strains in the materials. Gradual heating or thermal shock (rapid heating) has an effect which corresponds to random inputs of strain energy. Spatial randomness of stress and strain may be ascribed to various types of disorder in a material itself, instead of the environment. In any case, the present model simulates qualitatively crack growth on the surface of brittle materials subjected to spatially random influences. Thus soils or concretes in drying or heating environments are possible candidates for consideration. Paint surfaces and ceramic coating films may also be considered.

Now we suppose different materials to be subjected to random influences and to expose different crack patterns in them. If the mechanical properties of these materials are not known, we will speculate some distinguishable properties among them in view of our simulations. For example, the material which has a very rough crack pattern with long cracks is expected to have a large crack resistance of grain boundaries. If there is a material showing a fine crack pattern with spatially uniform distribution, we would identify the material as a medium which has a large release energy on cracking on average. Furthermore, we infer that the strain energies of grains (which are invisible) in the material are distributed over a wide range in magnitude and at random in space.

We may conjecture a difference in the environment from the exposed crack patterns. Suppose that two materials with the same quality exhibit different crack patterns in different random environments and that no difference in environment is known. Then we will infer that a material with a fine pattern and short cracks has been subjected to an influence with larger random fluctuations than the other material with a relatively rough pattern and long cracks. For example, soil surfaces appear to show many shorter cracks when they are dried at higher temperature. A higher drying temperature tends to cause larger local fluctuations in strain energies on the surface. This situation corresponds to the case of a larger value for the input energy, ΔE, in our model. Our simulations show that a larger ΔE results in many shorter cracks, therefore, being qualitatively consistent with observations.

The aspect of fragmentation under a strong impact on materials, i.e. impact fracture, is an important topic in fracture phenomena. In view of our results of strain energy distributions, although our simulations, as they stand, are not concerned with fracture itself, we make the following suggestion. We contrast two different features in spatial distribution of strain energies as shown in Figs 7c and 8c. The former distribution fluctuates considerably in space, while the latter is relatively even in space. If a strong impact is given to the two systems, in other words, an input of a large strain energy is given in a moment, then the system of Fig. 8c is ready to initiate a crack immediately. Therefore, we speculate that a material with a fine and nonuniform crack pattern is likely to be broken into finer fragments than a material with a fine and uniform pattern.

Fatigue crack growth is caused by weak regular or irregular loading over a long time. In our model, strain energies are stored in a system by random inputs, and cracks are generated by excess local strain energies over a threshold. This situation may be interpreted in the sense that strain energies are fixed evenly in space and grain boundary strengths are weakened randomly in space. The present simulations are, then, similar to a situation of fatigue crack growth. The results would, therefore, be useful in understanding fatigue crack patterns in brittle materials under random weak loads.

4.2. Some characteristics of the model

In the present model, we have not taken account of a stochastic variation of the grain-boundary strength, E_t. Real materials involve various types of disorders which result in spatial fluctuations of the strength. Because the present simulations are concerned with crack growth in a random environment, the stochastic effects were taken into account only through strain energy inputs into a system. Consideration of the stochastic effects of the grain-boundary strength in our model would result in quantitatively different strain energy distributions. We expect, however, that the correlation between crack patterns and strain energy distributions, as shown in the previous section, is not modified qualitatively. Investigation to confirm this is in progress.

Our model allowed any grain boundary to be cracked two or more times. Two grains between which a crack was generated are allowed to store the strain energy due to energy inputs and energy transfer; the boundary between them can be cracked again when the cracking condition is satisfied. Thus crackings in the model do not mean the separation of adjacent grains. This corresponds to the situation of cracking on the surface of real materials. The present two-dimensional systems, therefore, may be considered as quasi-two-dimensional systems.

The crack patterns in the present model, as shown in Fig. 5 a, appear to be similar. We have examined the patterns in terms of fractality. The procedure is based on the dependence of the number of cracks, $N_c(R)$, inside a square of "radius" R, on R. Fig. 10a explains the procedure and Fig. 10b shows the relationship between $N_c(R)$ and R for the crack pattern shown in Fig. 5a. From the power-law relationship, $N_c(R) \propto R^D$, the pattern may be regarded as a fractal with the fractal dimension, $D = 1.6$. The present model seems to generate crack patterns characterized

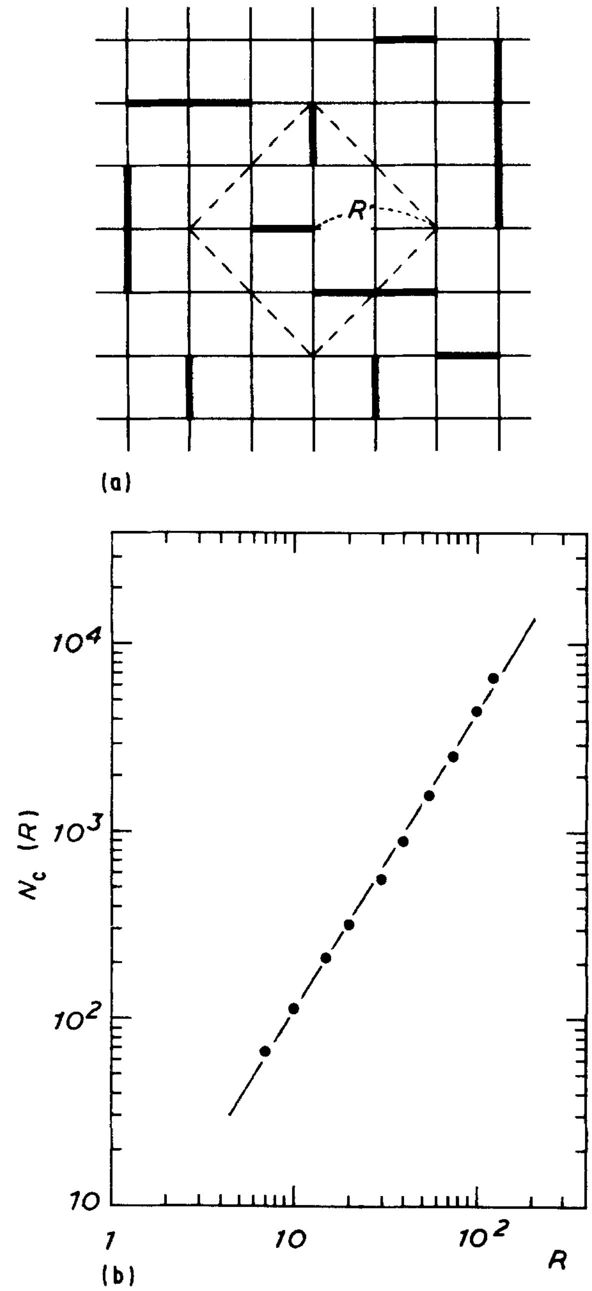

Figure 10 Explanatory figure for investigating fractality of crack patterns (a), and the result (b), for the pattern shown in Fig. 5a. The number of cracks, $N_c(R)$, inside the square (dashed lines) of "radius" R is counted as a function of R. The slope of $\ln[N_c(R)]$ versus $\ln(R)$ is 1.6.

by fractal geometry. However, the differences in features of the pattern, such as fineness and uniformity, have not been identified definitely by the present examinations. A more detailed consideration would need much larger-sized systems than the present one. This is an open subject for the future.

Our model for crack growth can be regarded as one of cellular automata in which the time evolution of a system of cells is determined by an algorithm defining a change in the state of a cell [14]. The characteristics of a stationary state, such as the stability of the strain energy distribution, could be described in terms of cellular automata. Although the consideration of our systems in terms of cellular automata is of theoretical interest, it would be beyond the scope of the present interest in the crack patterns as relating to real materials. This subject will also be left for future study.

5. Conclusion

We have shown the results of simulations in a simple model for crack growth in brittle materials in a random environment. In particular, the crack patterns have been related closely to the strain energy distributions. The crack pattern is a trace of the past influences on a material and is also an indication of the present mechanical properties of the material. In this sense, our results shed some light on an understanding of crack patterns observed in real materials. They are complementary with conventional approaches based on fracture mechanics.

The present model is, of course, too simple to simulate details of crack growth in real materials. Global features of crack patterns, however, should be appreciated in terms of qualitative characteristics of materials and environments. From this point of view, we expect systematic investigations of crack patterns from the experimental side, in which various kinds of materials are exposed to different environmental situations. Possible candidates for materials are ceramic coating films and the possible environmental set-up is a thermal or radiational one.

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