Numerical simulation of evolution-induced catastrophe*

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Abstract A numerical simulation of damage evolution in a two-dimensional system of microcracks is presented. It reveals that the failure is induced by a cascade of coalescences of microcracks, and the fracture surface appears fractal. A model of evolution-induced catastrophe is introduced. The fractal dimension is found to be a function of evolution rule only. This result could qualitatively explain the correlation of fractal dimension and fracture toughness discovered in experiments.

Keywords: microcracks, numerical simulation, fractal dimension, evolution-induced catastrophe.

Essentially speaking, a fracture or a failure is caused by nucleation, growth, and coalescence of numerous microdamages in intact materials. This is a very complex nonlinear evolution process[1]. Statistical microscopic observations showed that the number of microdamages is very large. Under plate impact loading, the number density of microcracks on the cross-section of damaged material is about $10^2 - 10^3$ mm^2, i. e. $10^5 - 10^6$ mm^3, and the length of these microcracks ranges from one-tenth to a few micrometers. At incipient damage stage, the coupling effects of microcracks may be neglected, since randomly nucleated microcracks are quite sparse. As a simple approximation, Ke *et al.* recently proposed a statistical evolution model of ideal microcrack system, and studied the general features of the system under deterministic and stochastic growth[2, 3]. However, at the final stage, interaction and coupling effects become very strong, and damage localization occurs. Hence, the interactions between microcracks as well as the influence of various disordered effects must be considered.

As a typical nonlinear dynamic system, the study on disorder and fracture has been a hot topic in recent years[4, 5]. By considering crack as a growth process, great advances have been made in simulation of fracture patterns[6]. Some universal properties, such as fractal fracture surfaces[7] and scaling laws[8], indicate that fracture may result from simple mechanism.

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This paper presents a numerical simulation of damage evolution in a two-dimensional system of microcracks, in accordance with our experimental study of spallation in an aluminium alloy. The critical failure induced by evolution of microcracks is examined, a new model, evolution-induced catastrophe, is introduced, and comparison between simulated and experimental results is made.

1 Numerical simulation of evolution of microcracks

Spallation, resulting from tensile stress impulse, formed by reflection of compressive wave in explosion and plate impact tests at interfaces adjacent to low impedance media or free surfaces, is a typical dynamic failure. The tests reported in this paper were perfomed with a 101 mm bore single-stage light gas gun. The specimens (target plates), 70 mm in diameter and 2 — 10 mm in thickness, were taken from a piece of rolled aluminium alloy plate. Using the techniques to accurately control the stress amplitudes and pulse durations individually[9], we can freeze microscopic damage at different evolution stages, as shown in fig. 1, and proceed metallographic observation and statistical measurement. Investigation revealed that the spallation of the aluminium alloy is formed by microcrack nucleation in the second-phase particles, growth and coalescence in matrix. At the early stage, nucleation plays an important role and the nucleated microcracks are randomly distributed (see fig. 1(a)), whereas, at the final stage, the microcrack coalescence is limited to a narrow zone (see fig. 1 (b)), playing the key role. The nucleation and coalescence of microcracks are two main dynamic processes. In the following simulation, we chose the element size of the lattice as the smallest nucleated microcrack length, 2 μm[10], using a 500×500 square lattice to simulate the microcrack evolution in 1 mm^2 element on the cross-section.

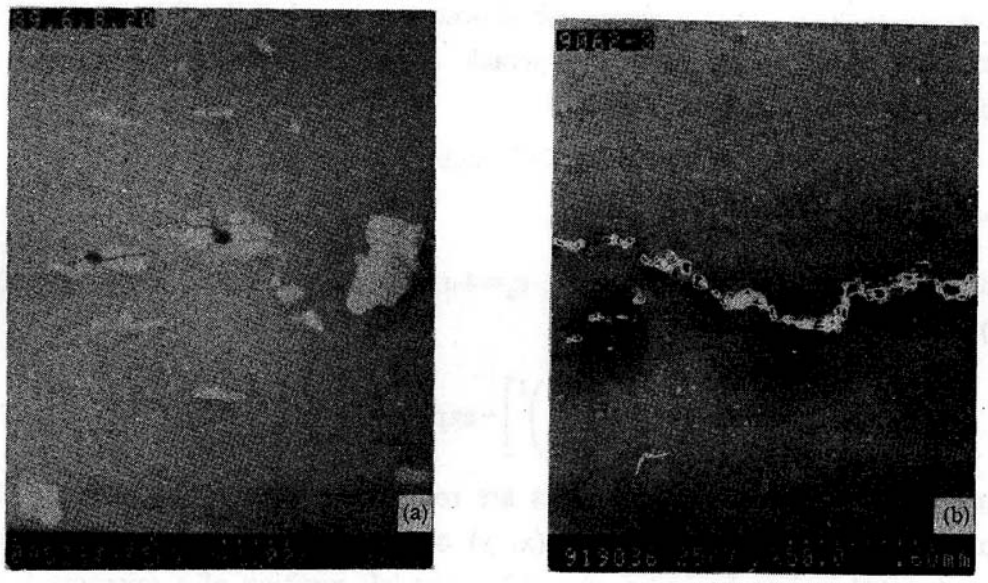

Fig. 1. Spall damage evolution process of an aluminium alloy.

1.1 Monte Carlo simulation of nucleated microcracks

In accordance with the experimental study of initial nucleation by Bai *et al.*[10], the distribution of nucleated microcracks is similar to that of the second-phase particles, and is random within the material. The randomly nucleated microcracks in physical space can be simulated by Monte Carlo method[11]. At first, a random series $\{r_i\}$ uniformly distributed in region (0, 1) is produced. Then, the random numbers are chosen as x and y coordinates evenly. Thus, the position of a microcrack in two-dimensional plane is

$$\begin{cases} x_i=[r_iL]+1, \\ y_i=[r_{i+1}L]+1, \end{cases} \quad (i=1,\ 3,\ 5,\cdots) \tag{1}$$

where [ ] stands for integering; L is the lattice length. Here $L=500$.

The corresponding microcrack length is determined by nucleation law. According to the statistical measurement of initial nucleation, the number density of nucleated microcracks may be approximately expressed by Rayleigh function[10]

$$\rho(c)=A\left(\frac{c}{c_0}\right)\exp\left[-\left(\frac{c}{c_0}\right)^2\right], \tag{2}$$

where c is the length of a nucleated microcrack, and c_0 is a characteristic length. Here, $c_0=3.4-4\ \mu m$, and $A=2/c_0$ is a normalized constant.

If the number of nucleated microcracks at time interval Δt is N, the microcrack number nucleated in $(c,\ c+\Delta c)$ is

$$N_N=\int_c^{c+\Delta c} N\rho(c)\mathrm{d}c=N\left\{\exp\left[-\left(\frac{c}{c_0}\right)^2\right]-\exp\left[-\left(\frac{c}{c_0}+\frac{\Delta c}{c_0}\right)^2\right]\right\}. \tag{3}$$

In order to remove the size effect, we choose the true length of lattice element Δx or Δy as reference. The normalized microcrack length is $\tilde{c}=c/\Delta x$, $\Delta\tilde{c}=\Delta c/\Delta x$. So the dimensionless form of expression (3) is

$$N_N=N\{\exp[-(r_0\tilde{c})^2]-\exp[-(r_0\tilde{c}+r_0\Delta\tilde{c})^2]\}, \tag{4}$$

where $r_0=\Delta x/c_0$.

In our simulation, choosing $\Delta x=2\ \mu m$, $c_0=4\ \mu m$, we have $r_0=0.5$, $\Delta\tilde{c}=1$. By making use of eq. (4), we get

$$N_N=N\left\{\exp\left[-\left(\frac{\tilde{c}}{2}\right)^2\right]-\exp\left[-\left(\frac{1}{2}+\frac{\tilde{c}}{2}\right)^2\right]\right\}. \tag{5}$$

Considering that the nucleated microcracks are roughly parallel, as shown in fig. 1(a), as a simple approximation, after the left end $(x,\ y)$ of microcrack $\tilde{c}$ is determined by eq. (1), we assume its right end to be $(x+\tilde{c},\ y)$. When the left position of a microcrack is located in the vicinity of the right boundary, a new random number is needed to assign the

microcrack a new position.

1.2 Coalescence of microcracks

As the number of nucleated microcracks increases, a newly nucleated microcrack may coalesce with its neighboring microcracks. According to dimensional analysis and strength criterion, the coalescence condition of two microcracks shown in fig. 2 may be approximately expressed as[12]

$$\begin{cases} 0 \leqslant d/\bar{c} \leqslant L_c, \\ |\theta| \leqslant \pi/2, \end{cases} \tag{6}$$

where $\bar{c} = (c_1 + c_2)/2$ and d are the average length and the distance between the two microcracks, respectively, θ is the angle between the coalesced line of the two microcracks and extension line of a crack, and L_c is the critical coalescence conditon.

When two non-collinear microcracks get coalesced, the effective length of the formed irregular crack is approximately taken as the distance between its extreme left and right ends. When the number of microcracks is large enough, a newly nucleated microcrack may also satisfy the coalescence condition (6) like its several neighboring microcracks. In this case, we choose a pair of nearest microcracks. This is consistent with real processes. If the nearest microcracks are more than one, priority of coalescence is given to the microcracks that meet first. The further coalescence between a coalesced microcrack and other neighboring microcracks is similar to that described above.

In the numerical simulation, after one coalescence occurs, one needs to judge whether a main crack forms throughout the lattice. If there is such a main crack, the simulation stops, otherwise, nucleation or coalescence process continues (see fig. 3). Here, the main crack is the spalled profile.

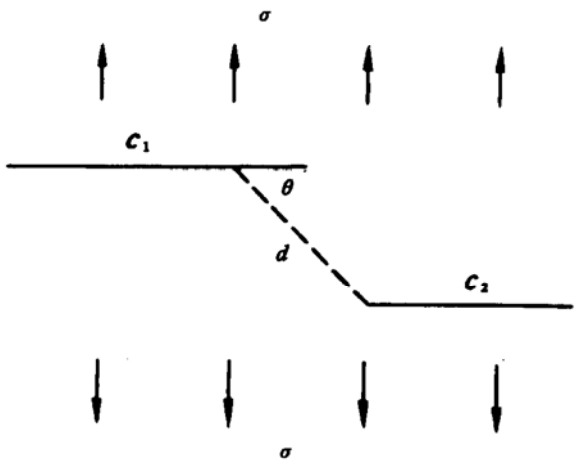

Fig. 2. Coalescence of two microcracks.

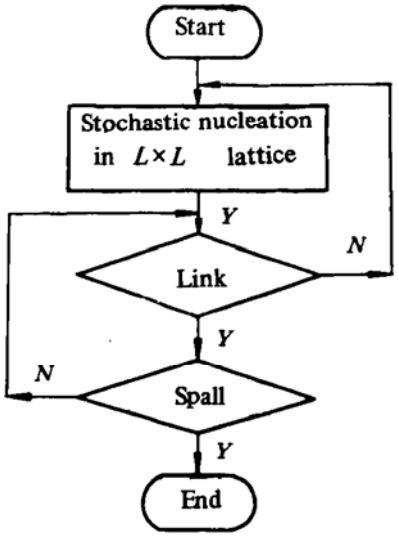

Fig. 3. Simple flow chart for computer simulation.

2 Evolution-induced catastrophe

In this work, the numerical simulation was performed with Alliant FX/40, a mini-super computer. Fig. 4 shows a typical evolution process of microcrack system. In this simulation, (i) the number of nucleated microcracks per unit time interval is $N=100$; (ii) microcrack nucleation proceeds from small to large according to eq. (5); (iii) the critical coalescence condition is $L_c=1$[12]. When a new microcack nucleates, the following cases may happen:

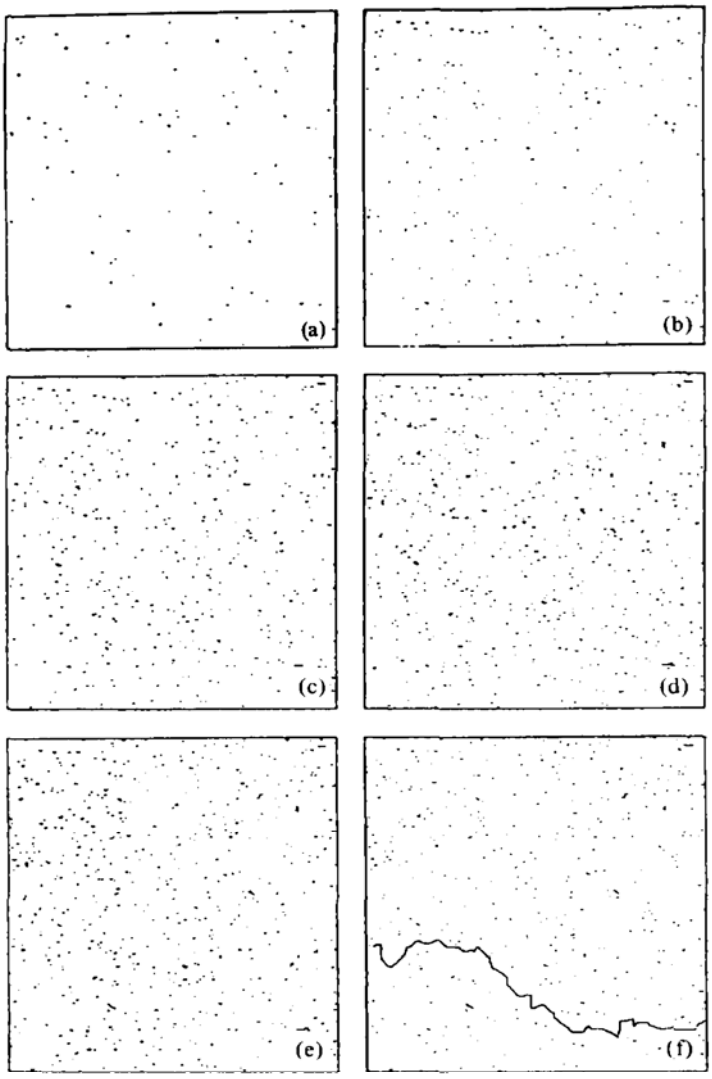

Fig. 4. Computer simulation of EIC. The numbers of nucleated micorcracks are (a) 100, (b) 300, (c) 500, (d) 700, (e) 831 and (f) 832.

Case A. Locally stable: a nucleated microcrack remains isolated and there is no coalescence.

Case B. Globally stable: there is local coalescence, but after several coalescences, the system remains stable, although larger crack forms. So both Cases A and B are globally stable.

Case C. Globally unstable: the cascade coalescence occurs and a throughout crack forms.

From the example in fig. 4, we can get more details of the evolution. At the initial stage, there were few coalescences (see fig. 4(a)). As the number of nucleated microcracks increased, coalescences of microcracks of different scales occurred in some local regions (see fig. 4 (b) — (d)). As the evolution process continued, though there were more local coalescences, the system still remained globally stable until the number of nucleated microcrack reached 831 (see fig. 4(e)). Noticeably, the state shown in fig. 4(e) was a critical state. Then, the randomly nucleated microcrack (No. 832) triggered a cascade of coalescences and formed a main crack, thus resulting in eventual failure (see fig. 4(f)). This phenomenon is consistent with that discovered in the experiment of

spallation[13].

It is found that the system of microcracks evolves irreversibly to a critical state as the damage accumulates. At the critical state, very small fluctuation can result in a catastrophic failure. Thus, we call this phenomenon evolution-induced catastrophe (EIC)[14, 15].

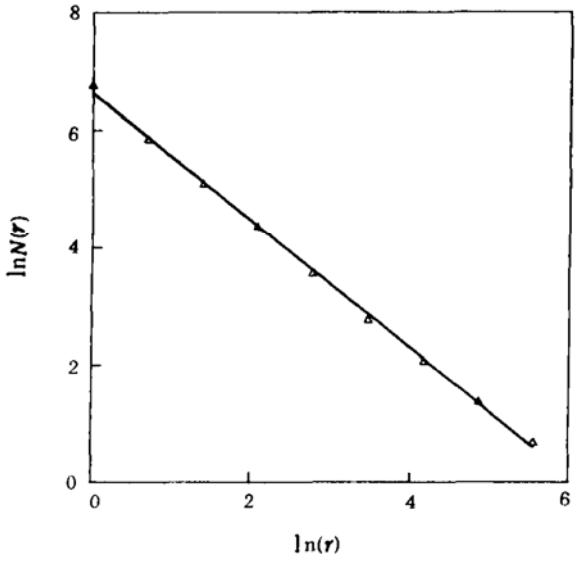

Fig. 5. Fractal plot of a main crack. Here, $N \approx r^{-D}$, where r is yardstick, N is the measured number and D is fractal dimension.

The experimental measurements of spalled profiles of the aluminium alloy have shown that the spalled surfaces have fractal character. In the $10 - 1000\,\mu m$ length scale regime, spalled profiles may be well quantitatively described by fractal dimension $D = 1.09 \pm 0.01$[12]. Intuitively, the pattern obtained in the simulation (fig. 4(f)) is very similar to the observed spalled profile (fig. 1(b)). Further quantitative calculation of the fractal dimension $D = 1.09 \pm 0.01$ of the main crack, as shown in fig. 5, is in good agreement with the experimental result. Therefore, although it is very simple, the numerical model simulates the microcrack evolution process in spallation quite well.

In the simulation, the random number series must satisfy some good statistical properties. We examined the influence of different random number series on the simulation. For instance, we randomly chose 10 random number series to carry out the above-mentioned simulation. The results showed that the fractal dimensions of the main crack were approximately constant for different random number series. But we could not determine, *a priori*, the position where a main crack appeared (see fig. 6).

In addition to fractal dimension, another key characteristic parameter is the accumulative damage value at the critical failure. Here, we define this value as the fraction occupied by the effective length of microcracks in the lattice. The calculated results show that the critical value is not a constant, but there is a critical region $(0.20 - 0.28)$. This fact is very different from the phenomenon of percolation.

Besides, the simulations show that both rate and order of nucleation, as well as different microcrack distributions with the same characteristic length do not obviously affect the results[1]; that is to say, the fractal dimension of a main crack is not sensitive to the form of microstructural distributions; but decisively determined by parameter L_c.

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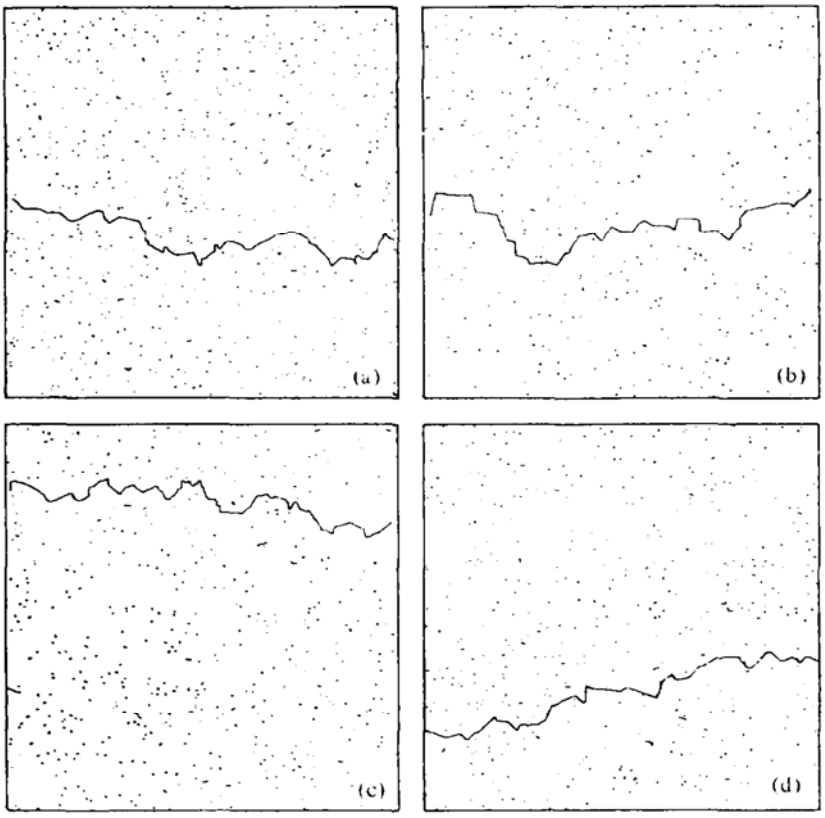

Fig. 6. Various cracking patterns.

3 Fractal dimension spectrum

We have seen that the fractal dimension of main cracks appears to be a function of coalescence condition $L_c=d/\bar{c}$. In order to study it in more detail, the following coalescence conditions ($L_c=0.5$, 1.0, 1.5, 2, 3, 4) are simulated. Here, the form of microcrack distribution, nucleation order as well as the rate of nucleation, etc. remain unchanged. A fractal dimension spectrum, i.e. fractal dimensions of main cracks versus coalescence parameter L_c, is shown in fig. 7(a). The tendency of the variation is qualitatively consistent with that obtained by a statistical fractal model given by the present authors[12].

Recently, Williford summarized some experimental results of fractal fracture, and discovered that the data of fractal dimension versus fracture toughness lies in a unimodal curve (see fig. 7(b))[16]. It is very interesting that for ductile materials such as metals, fracture toughness decreases as fractal dimension increases, but for brittle materials like ceramics, rock, etc., fracture toughness increases as fractal dimension increases. At present, there is no reasonable explanation for this phenomenon.

Although there are some differences in the definitions and measurements of fractal

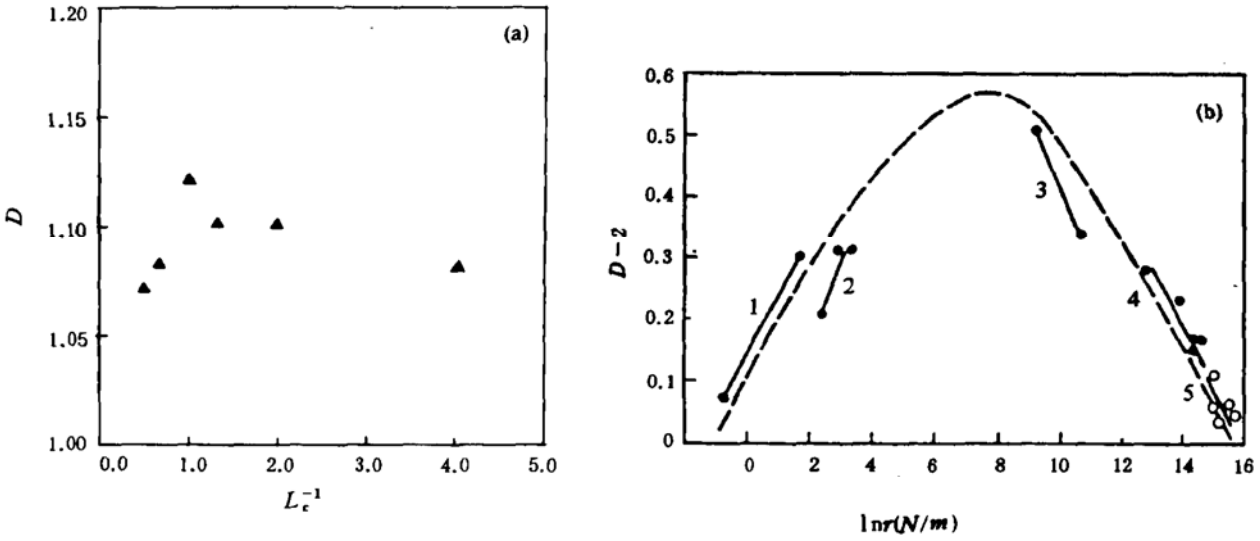

Fig. 7. (a) Relation of fractal dimension to critical coalescence condition. (b) Experimental results of fractal dimension varying with fracture toughness[17]. 1, ZnSe; 2, alumina; 3, 4 340 steel; 4, 300 grade maraging steel; 5, titanium alloys.

dimension and toughness, our simulations seem capable of qualitatively explaining the above experimental results. According to fig. 7[16], it is easy to see that the fractal dimension versus critical coalescence condition L_c is also a unimodal curve. Clearly, the larger the critical L_c, the wider the influence zone of a microcrack, implying that the more brittle the material, and *vice versa*[12].

4 Discussion and conclusion

In this paper, based on the statistical measurement of damage evolution of spallation in an aluminium alloy and the mechanical analysis of two main dynamic processes (nucleation and coalescence), we have constructed a numerical model for the evolution of a two-dimensional microcrack system. The calculated results agree well with the fractography and fractal character of spalled profiles and are confirmation for critical failures discovered in the experiment.

The fractal character of main cracks indicates that damage evolution is scaling-invariant. It is obvious that the coalescence condition given by eq. (6) is of geometrical similarity; that is to say, the longer the crack, the longer the coalescence length or the larger the influence zone will be. This is equivalent to a positive feedback mechanism. As the coalescence of microcracks occurs, the real area supporting the load decreases, as a result the stress acting on the residual material increases. At the final damage stage, the positive feedback becomes more obvious. The self-similarity in damage evolution provides us a simple way to deal with the relationship between microstructures and macroscopic mechanics.

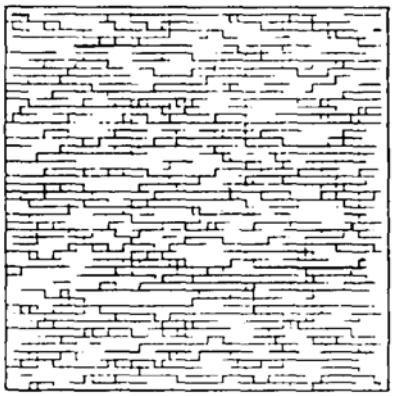

Fig. 8. Evolution pattern under a local coalescence condition.

The EIC model given in this paper is different from self-organized criticality (SOC) presented by Bak *et al.*[17] to describe the evolution of a dynamic system. In our model the coalescence condition is nonlocal. In order to have a more intuitive understanding, fig. 8 illustrates an evolution pattern under local coalescence condition

$$0 \leqslant d \leqslant d_c. \tag{7}$$

Here $d_c = 1$. The lattice size is 50×50 and other conditions are the same. Obviously, fig. 8 is rather close to percolation than to the pattern of spallation.

In summary, EIC as a model describing a nonequilibrium and nonlinear evolution process of damage-fracture has the following features: (i) Before final catastrophic failure, the system remains in a globally stable state although local unstability occurs. (ii) At critical point, a newly nucleated microcrack can trigger a cascade of coalescence and form a main crack catastrophically. (iii) Coalescence remains scaling-invariant and fracture surfaces are fractal. The fractal dimension of fracture surfaces is an intrinsic parameter, which seems to be independent of nucleation distribution functions, etc. The fractal dimension depends on coalescence parameter only and is a unimodal function of coalescence parameter. (iv) For a specific sample, the critical damage is a deterministic value, but for different samples (the dynamic parameters keep constant), critical fractions of damage are not a constant and there is a transition region.

The EIC model given in this paper may help us understand the inherent mechanism of damage evolution in materials, and give us a useful tool to deal with the failure of disordered media as well as some natural evolution and catastrophe, such as earthquakes and landslides.

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