EFFECTS OF STOCHASTIC EXTENSION IN IDEAL MICROCRACK SYSTEM*

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Received April 4, 1990.

ABSTRACT

The effects of stochastic extension on the statistical evolution of the ideal microcrack system are discussed. First, a general theoretical formulation and an expression for the transition probability of extension process are presented, then the features of evolution in stochastic model are demonstrated by several numerical results and compared with that in deterministic model.

Keywords: ideal microcrack system, stochastic extension, transition probability, evolution equation of number density.

I. INTRODUCTION

One of important damage mechanisms in materials subjected to external loading claims that numerous microcracks, owing to nucleation, extension and coalescence, can eventually lead to fracture of materials. So far the understanding of the evolution of microdamages and their effects on macroscopic mechanical properties remains still quite superficial. Nevertheless, the interest in this subject is increasing.

The evolution of the ideal microcrack system was discussed in [1] by the statistical description based on the deterministic extension model. The deterministic extension model means that the extension rate of a microcrack with length scale c may be expressed as

$$\frac{dc}{dt} = A, \tag{1}$$

where A is a deterministic function depending on material properties, loading stress, and length scale of microcrack c.

In this paper we intend to explore the effects of possible stochastic fluctuations in extension rate of microcracks on the evolution of the ideal microcrack system. For this purpose, a generalized model, the stochastic extension model, is proposed.

* Project partly supported by the National Natural Science Foundation of China.

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Instead of Eq. (1), the meso-dynamic equation should be

$$\frac{dc}{dt} = a \tag{2}$$

where a is a stochastic variable. As in Ref. [1], a cutoff length scale c_1 is assumed, i. e. $a = 0$ for $c \leqslant c_1$.

Obviously, the stochastic fluctuation of extension rate is closely related to the stochastic deviations of local conditions from the macroscopic average ones. The stochastic fluctuations of local conditions may result from the following factors: (i) the small-scale inhomogeneities in material and stress, (ii) the interaction, or coupling, between microcracks distributed stochastically, and (iii) the stochastic orientations of microcracks. The stochastic fluctuations can appear not only because of the microcracks on the same scale in the microcracks system, but also in the extension process of a special microcrack due to the stochastic fluctuation of local conditions at the tip of microcracks. In this sense, the deterministic extension model in [1] is a simplified one in the limit without fluctuations. The aim of this paper is to demonstrate the effects of the local stochastic fluctuations on the evolution of the microcrack system.

In the deterministic extension model[1], an individual microcrack was depicted by its length scale c, and the statistical description was made in 1-dimensional phase space $\{c\}$ using the number density $n(c,t)$. In the stochastic extension model, however, an individual microcrack should be specified by two independent variables, the length scale c and the extension rate a. Hence the phase space must be generalized to 2-dimensional (c, a), and the statistical description should be given by distribution function $f(c, a, t)$.

The evolution equation of the microcrack system in deterministic extension model was a partial differential equation[1]

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial c}[An] = s, \tag{3}$$

where s is the rate of nucleation density in phase space $\{c\}$, depending on material properties, loading stress, and length scale of microcrack c. In this paper, nucleation rate s is still adopted to describe the nucleation process. But the governing equation of n will not maintain the previous form of Eq. (3) due to the stochastic extension rate. Therefore, we have to deduce another evolution equation, with which we could further discuss the feature of evolution analytically and numerically, and compare it with that of the deterministic extension model.

II. Effects of Stochastic Extension of Microcracks

Now we start from the distribution function $f(c, a, t)$ in phase space (c, a), which can be limited to the region $c_1 \leqslant c$ and $0 \leqslant a$ because of the cutoff length scale c_1 and the negligible probability of the contraction process (i.e $a < 0$).

The lowest order moment of $f(c, a, t)$ is the average number density in sub-phase space $\{c\}$, relevant to $n(c, t)$ in the deterministic model, i. e.

$$n(c, t) = \int_0^\infty f(c, a, t)da. \tag{4}$$

n is closely related to the macroscopic properties of materials, we have to deduce the evolution equation of n.

The average extension rate of microcracks, relevant to A in the deterministic model, may be calculated from the first-order moment of $f(c, a, t)$

$$\langle a \rangle = A(c, t) = \frac{1}{n(c, t)} \int_0^\infty af(c, a, t)da. \tag{5}$$

Now we shall split the extension rate a into two parts

$$\frac{dc}{dt} = A + \tilde{a}, \tag{6}$$

where A is the average part, and the fluctuation part $\tilde{a}$ is a stochastic variable, $\langle \tilde{a} \rangle = 0$. Generally speaking, A is a slow variable, and $\tilde{a}$ is a fast variable, both belonging to different time scales. Let t_c be the characteristic time of $\tilde{a}$ and r be the scale of the fluctuations under local conditions, t_c may be estimated as

$$t_c \sim \int_c^{c+r} \frac{dc'}{A(c')} \equiv r/\bar{A}, \tag{7}$$

i. e. t_c is the average extension time of microcracks from c to $(c + r)$, and the barred quantity in Eq. (7) is a mean value in the region $(c, c + r)$.

Define autocorrelation function of $\tilde{a}$ as

$$G(t_1, t_2) = \langle \tilde{a}(t_1)\tilde{a}(t_2) \rangle, \tag{8}$$

In view of the characteristic time t_c of $\tilde{a}$, the approximate form of G may be written as

$$G(t_1, t_2) \cong \langle \tilde{a}^2 \rangle \theta\left(\frac{t_1 - t_2}{t_c}\right), \tag{9}$$

where $\theta(y)$ is a function with a half width 1/2 centered at $y = 0$, and $\int_{-\infty}^{\infty} \theta(y)dy = 1$.

On average, the stochastic behavior of $\tilde{a}$ appears only in the period $\Delta t > t_c$. The intensity of fluctuations can be described by $\langle \tilde{a}^2 \rangle$, which is a slow variable with a time scale longer than t_c. Then the relative intensity of the fluctuations is characterized by

$$\beta = \sqrt{\langle \tilde{a}^2 \rangle}/A. \tag{10}$$

In general, $\beta < 1$ or $\beta \ll 1$, determined by the real conditions of materials.

Usually $f(c, a, t)$ is a complex function of a, which is determined by a large amount of data. But roughly speaking, f is a function centered at $a = A$ with a relative deviation β. It might become a wide distribution if β is not small enough, which will not be discussed in this paper. Now a new stochastic variable with simpler probability distribution will be derived from the original stochastic variable a. The distribution function of the new stochastic variable could be determined by only a few parameters or functions.

Define the increment of the length scale in duration $(t, t+\Delta t)$:

$$\Delta c = \int_t^{t+\Delta t} a(t')dt', \tag{11}$$

where Δt satisfies the condition

$$\Delta t \gg t_c. \tag{12}$$

Δc is a stochastic variable related to the mean value of a in the duration Δt. The condition (12) means that Δc is the stochastic accumulation of a during Δt. We will determine the probability distribution $W(c, t; c+\Delta c, t+\Delta t)$.

The mean value of Δc is

$$\langle \Delta c\rangle = \int_t^{t+\Delta t} \langle a\rangle dt' \cong \int_t^{t+\Delta t} A dt'. \tag{13}$$

which may be calculated from equation

$$\Delta t = \int_c^{c+\langle\Delta c\rangle} \frac{dc'}{A(c')} \cong \frac{\langle \Delta c\rangle}{\bar{A}}, \tag{14}$$

if the function $A = A(c)$ is given. In Eq. (14), $\bar{A}$ is a mean value of A in region $(c, c+\langle\Delta c\rangle)$.

The variance of Δc is given by

$$\langle(\Delta c - \langle\Delta c\rangle)^2\rangle = \int_t^{t+\Delta t} dt_1 \int_t^{t+\Delta t} dt_2 G(t_1, t_2). \tag{15}$$

Substituting Eq. (9) into (15), we have

$$\langle(\Delta c - \langle\Delta c\rangle)^2\rangle = \bar{\beta}^2\bar{A}^2 t_c \Delta t, \tag{16}$$

again the barred quantities are the mean values in region $(c, c+\langle\Delta c\rangle)$. By using the variance of Δc, the diffusion coefficient can be defined as

$$D = \frac{1}{2\Delta t}\langle(\Delta c - \langle\Delta c\rangle)^2\rangle = \frac{1}{2}\bar{\beta}^2 t_c \bar{A}^2. \tag{17}$$

Introduce parameter

$$g = 2\bar{\beta}^2 \frac{t_c}{\Delta t}. \tag{18}$$

D may be rewritten as

$$D = g\frac{(\langle\Delta c\rangle)^2}{4\Delta t}. \tag{19}$$

From the condition (12), $g \ll 1$. As a matter of fact, we have neglected in Eq. (13) the contribution of diffusion to the mean increment $\langle\Delta c\rangle$, whch is related to $\partial D/\partial C$ and the relative magnitude is about $\frac{1}{8} g \frac{\langle\Delta c\rangle}{c} \ll 1$.

The probability distribution function W has a form centered at $\Delta c = \langle\Delta c\rangle$ with a relative deviation $\sqrt{g/2} = \bar{\beta}\sqrt{\dfrac{t}{\Delta t}}$, which is much narrower than that of $f(c, a, t)$. Essentially, this result comes from the central limit theorem.

Let us introduce the characteristic function[2] defined by

$$\Phi(k) = \langle e^{ik\Delta c}\rangle = \int d(\Delta c) W e^{-ik\Delta c}, \tag{20}$$

where W is the Fourier transform of Φ:

$$W(c, t; c + \Delta c, t + \Delta c) = \frac{1}{2\pi}\int dk e^{-ik\Delta c}\Phi(k). \tag{21}$$

Now, we write $\Phi(k)$ in term of a cumulant expansion

$$\Phi(k) = \exp\left[\sum_{m=1}^{\infty}\frac{(ik)^m}{m!}u_m(\Delta c)\right], \tag{22}$$

where $u_m(\Delta c)$ is the m-th cumulant. Comparing Eqs. (20) with (21), we obtain the expressions of the first three cumulants

$$u_1 = \langle \Delta c\rangle, \tag{23}$$

$$u_2 = 2D\Delta t = \int_t^{t+\Delta t} dt_1 \int_t^{t+\Delta t} dt_2 \langle \tilde{a}(t_1)\tilde{a}(t_2)\rangle, \tag{24}$$

$$u_3 = \int_t^{t+\Delta t} dt_1 \int_t^{t+\Delta t} dt_2 \int_t^{t+\Delta t} dt_3 \langle \tilde{a}(t_1)\tilde{a}(t_2)\tilde{a}(t_3)\rangle. \tag{25}$$

If the fluctuations are not very strong and the autocorrelation time is not very long, the higher-order cumulant may be neglected, and a good approximation to $\Phi(k)$ can be obtained by retaining only the first few cumulants. Notice that the first cumulant $u_1(\Delta c)$ is just the mean value of Δc and the second cumulant $u_2(\Delta c)$ is the variance.

Retaining the first two cumulants, we have the characteristic function

$$\Phi(k) = \exp(ik\langle \Delta c\rangle - k^2 D\Delta t). \tag{26}$$

From Eqs. (21), (26), and the assumption of the zero probability of the contraction process of microcracks (i. e. $\Delta c < 0$), an approximate expression of W is obtained

$$W(c, t; c + \Delta c, t + \Delta t) = \begin{cases} \dfrac{\eta}{\sqrt{4\pi D\Delta t}}\exp[-(\Delta c - \langle \Delta c\rangle)^2/4D\Delta t], & for\ \Delta c \geqslant 0, \\ 0, & for\ \Delta c < 0, \end{cases} \tag{27}$$

where η is the normalization factor that is close to 1 as $g \ll 1$. We can see that W given by Eq. (27) is a Gaussian function centered at $\Delta c = \langle \Delta c\rangle$ with a cutoff for $\Delta c < 0$, and its relative deviation can be estimated by $\sqrt{g/2}$. W is determined by the average extension rate $A(C)$ and the fluctuation parameter g, which are related to the real conditions of materials.

For the microcrack system, the length scale c is also a stochastic variable, and its probability distribution density is proportional to $n(c, t)$

$$\rho(c, t) = n(c, t) \Big/ \int_{c_1}^{\infty} n(c', t)dc'. \tag{28}$$

Whereas, $W(c, t; c + \Delta c, t+\Delta t)$ is the conditional probability, i. e. the probability density of length scale $c + \Delta c$ at time $t + \Delta t$ if the scale is c at time t. Because Δt is taken to be much longer than the autocorrelation time t_c, the conditional probability is only determined by the value of c at time t, and is independent of the earlier information. Therefore, the extension process, described in this way, appears to be Markovian. Therefore, given the number density of microcrack system $n(c, t)$ at time t, the extension-induced evolution can be calculated according to $W(c, t; c + \Delta c, t + \Delta t)$. So W is also called the transition probability.

III. Evolutionary Features of Microcrack System in Stochastic Extension Model

In the ideal microcrack system, the evolution of number density $n(c, t)$ is mainly controlled by the nucleation and extension process of microcracks, which are independent of each other statistically. The evolution equation may be expressed as

$$n(c, t + \Delta t) = \Delta n_s(c, t) + \int_{c_1}^{c} dc' n(c', t) W(c', t; c, t + \Delta t), \tag{29}$$

where the first term on the right-hand side indicates the contribution of nucleation in the duration from t to $t + \Delta t$, and the second comes from the extension process.

The nucleation term can be calculated from the rate of nucleation density S.

$$\Delta n_s(c, t) = S(c, t)\Delta t, \tag{30}$$

where the extension effect in the duration from t to $t + \Delta t$ for the cracks created just during this period is neglected. In order to include this effect, we utilize the solution of Eq. (3) given in Ref. [1] to obtain a modified expression of nucleation term as

$$\Delta n_s = \frac{1}{A(c)} \int_{c_0}^{c} S(c')dc', \tag{31}$$

where, $c_0 = c_1$ for $\int_{c_1}^{c} \frac{dc'}{A(c')} \leqslant \Delta t$, otherwise c_0 is defined by $\int_{c_0}^{c} \frac{dc'}{A(c')} = \Delta t$. Expression (31) includes the average effect of extension, and the higher-order modifications induced by fluctuations are neglected.

In the limit case without fluctuations (i. e. $D \to 0$), the transition probability W becomes the δ-function, and the evolution equation (29) reduces to Eq. (3), i. e. the evolution equation in the deterministic model. Because the evolution of n is related to an integral of W, the behavior of n is not very sensitive to the details of W. Hence, the features of the behavior of $n(c, t)$ in deterministic and stochastic model might be more or less alike. Some important differences, however, do exist between these two models.

A remarkable feature of the deterministic model is the saturation in the behavior of $n(c, t)$[1]. The saturation time for length scale c is given by

$$t_{st}(c) = \int_{c_1}^{c} \frac{dc'}{A(c')}, \tag{32}$$

which is just the extension time from cutoff scale c_1 to c. The appearance of saturation means that the effect of the initial state vanishes, and the effects of nucleation and extension balance each other.

In stochastic extension model, the extension time from c_1 to c

$$T(c) = \int_{c_1}^{c} \frac{dc'}{a} = \int_{c_1}^{c} \frac{dc'}{A(c') + \tilde{a}} \tag{33}$$

is a stochastic variable, and its probability distribution is a function centered at $T = \langle T \rangle \sim t_{st}(c)$ with characteristic width $t_{st}(c)\ \bar{\beta}\sqrt{t_c/t_{st}} = t_{st}\sqrt{g\Delta t/2t_{st}}$. The effect of the initial state vanishes only when $t \to \infty$ due to finite probability for any value of T. Then the saturation becomes an asymptotic process in the stochastic model. The effective saturation time may be estimated by

$$t_{st}^*(c) \sim t_{st}(c)[1 + \gamma\sqrt{g\Delta t/2t_{st}(c)}\,], \tag{34}$$

where γ is a numerical factor, typically $\gamma \sim 3$—4. (The probability for $T > t_{st}^*$ is estimated by $e^{-\gamma^2/2}$, and for $\gamma = 3.7$ we have $e^{-\gamma^2/2} \sim 10^{-3}$, which measures the difference from the saturation value of n).

In the stochastic model, the boundary between saturation and non-saturation region becomes a transitional layer, and the effective boundary may be estimated by

$$c_{st}^*(t) \sim c_{st}(t)[1 - \gamma\sqrt{g\Delta t/2t_{st}(c)}], \tag{35}$$

where $c_s(t)$ is the boundary of saturation region in the deterministic model.

Now we show some numerical results about the evolution of number density

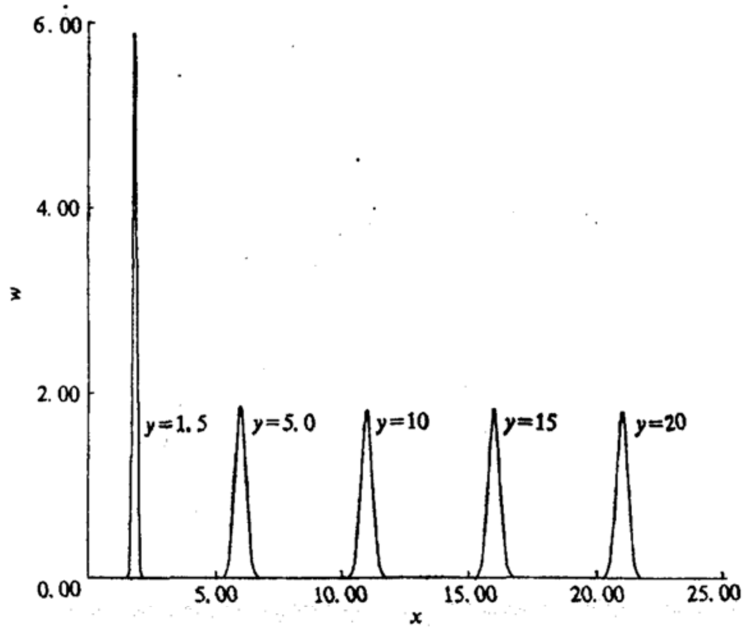


Fig. 1. Transition probability $W(y,\tau;\ x,\ \tau+1)$, $b = 1.5$ and $g = 0.1$.

$n(c, t)$. The trial models

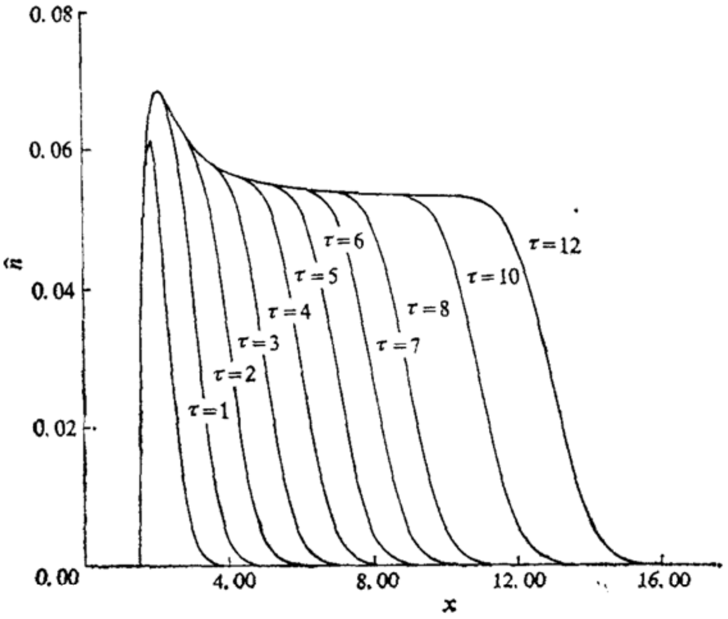
$$A = \alpha\sqrt{1 - c_1^2/c^2}, \tag{36}$$

$$S(c) = S_0 \frac{c}{c_2} \exp(-c^2/c_2^2) \tag{37}$$

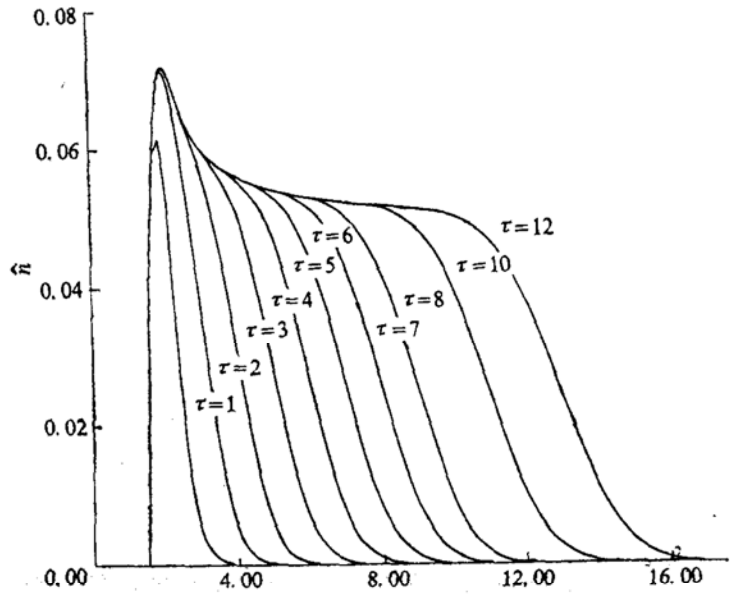
are adopted, where Eq. (36) is from Ref. [3]. Several trial values of fluctuation parameter g are used.

In calculation, the following reduced quantities are used:

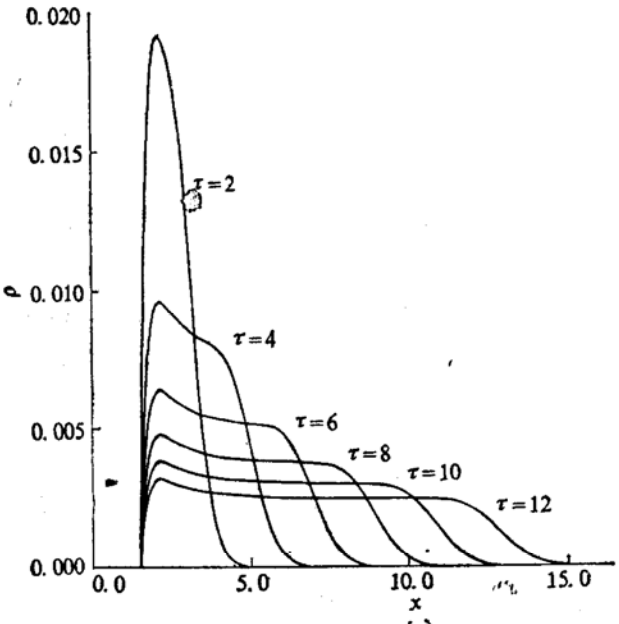
$$x = c/c_2,\quad \tau = \alpha t/c_2,\quad \hat{n} = \alpha n/S_0 c_2,\quad b = c_1/c_2.$$



(a)



(b)



(c)

Fig. 2. (a) Number density for the stochastic model, $b = 1.5$ and $g = 0.1$;

(b) Number density for the stochastic model, $b = 1.5$ and $g = 0.3$;

(c) Probability distribution ρ, $b = 1.5$ and $g = 0.1$.

We take $b = 1.5$, $g = 0.1$ or 0.3, the initial condition is $\hat{n}(x, 0) = 0$, and the time step $\Delta\tau = 1$. From Eq. (18), if $t_c/\Delta t = 0.1$, $g = 0.1$ means a relative fluctuation of about 0.7, which is not too weak.

Fig. 1 shows the transition probability $W(y, \tau; x, \tau + 1)$ with $b = 1.5$ and $g = 0.1$, where the curves for $y = 1.5, 5, 10, 15$, or 20, respectively, are given.

The evolution of number density for the stochastic extension model with $g = 0.1$

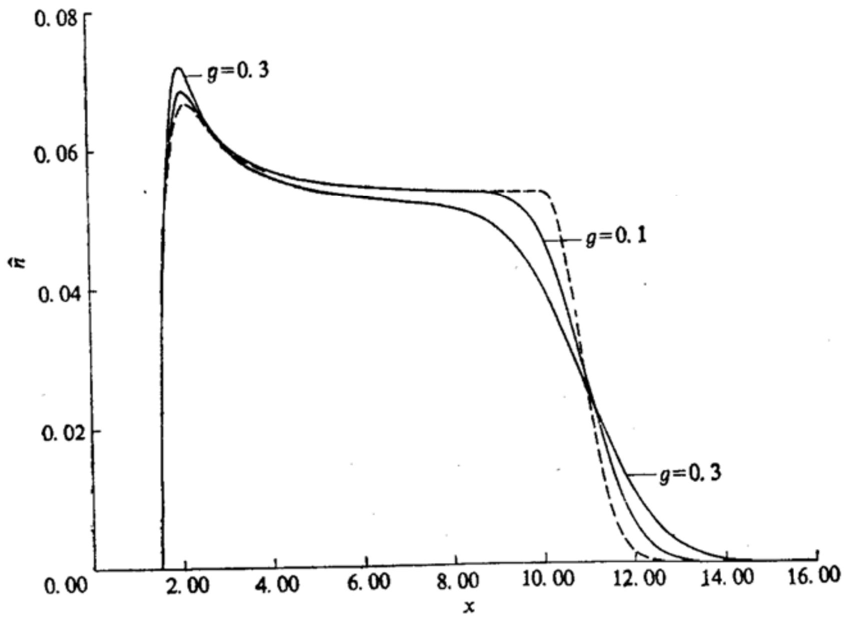


Fig. 3. Curves of $\hat{n}$-x at $\tau = 10$.

Solid lines for stochastic model with $b = 1.5$, $g = 0.1$ or 0.3, respectively, and dashed line for the deterministic model with $b = 1.5$.

and $g=0.3$ is shown in Fig. 2(a) and 2(b), respectively. We can see that the curve is composed of an approximate saturation part in the small-scale region, a non-saturation part in the large-scale region, and between them exists a transitional region, which moves forward to a large length scale. Fig. 2(c) shows the probability distribution ρ defined by Eq. (28) with $b=1.5$ and $g=0.1$.

In Fig. 3 we compare the curves $\hat{n}$-x of stochastic model ($g=0.1$ and $g=0.3$, respectively) with those of deterministic model at $\tau=10$. The result shows that three curves are more or less alike, however, remarkable differences exist in the vicinity of the boundary between the saturation and non-saturation regions. Comparing the calculated data with Eqs. (34) and (35), we find that $\gamma \sim 3.7$ is reasonable.

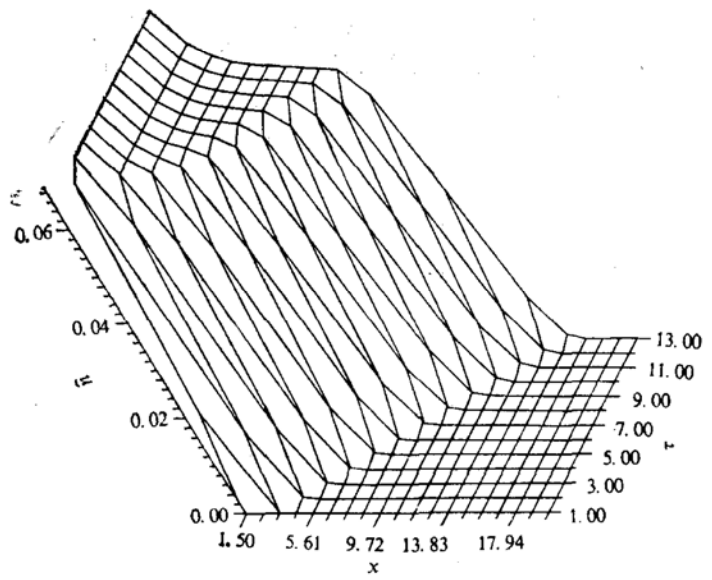


Fig. 4. 3-D graphics of $\hat{n}$-x-τ in the stochastic model with $b=1.5$ and $g=0.1$.

Fig. 4 shows a 3-dimensional graphics for the stochastic extension model with $b=1.5$ and $g=0.1$, in order to demonstrate the global characteristics of the evolution of microcrack distribution.

IV. Conclusion

This paper presents a statistical description of an ideal microcrack system. The theory is based on the probability description of nucleation and the stochastic extension model. The main points of stochastic extension model are as follows: (i) the extension rate of microcracks is a stochastic variable; (ii) the phase space $\{c, a\}$ and the distribution function $f(c, a, t)$ are introduced; (iii) the transition probability $W(c, t; c+\Delta c, t+\Delta t)$ and the evolution equation of number density $n(c, t)$ are derived.

The deterministic extension model[1] is merely the limit case without fluctuations.

The evolutionary features of $n(c, t)$ are discussed in this paper. In numerical calculations, we adopted trial models of nucleation rate S and average extension rate A, and trial values of fluctuation parameter g. The results show that the behaviors of $n(c, t)$ calculated from the stochastic and deterministic models are more or less alike, even for the case with strong fluctuations in the stochastic model. The differences for these two models, however, do exist, especially in the vicinity of the boundary between saturation and non-saturation regions. It is believed that the gained information about evolutionary features of the microcrack system would help us further investigate the microdamage in materials. S, A and g in our theory should be determined according to practical conditions of materials. Such a problem is beyond the scope of this paper, the discussion will be given elsewhere.

In this paper we have discussed the ideal microcrack system, which is suitable to the early stage of damage, when the microcracks are sparse. With the development of the damage, however, the density of cracks increases, and the interaction and coalescence between cracks, will become dominant, especially at the stage close to fracture. These effects will be discussed elsewhere.

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