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Crack Initiation and Crack Growth as the Problem of Localized Instability in Microcrack Ensemble

O. Naimark and M. Davydova

Institute of Continuous Media Mechanics, Ural Branch of the Russian Academy of Sciences, 1 Ak. Korolev Street, 614061 Perm, Russia

Abstract. Statistical theory of defect evolution allows us to obtain non-linear kinetic equations for tensor parameter of microcrack density. Investigation of non-linear properties of kinetic equation showed the existence of specific type of self-similar solution at the developed stage of damage, which is characterized by explosion-like kinetics of the microcrack growth on the spectrum of spatial scales. The system behaviour is controlled by the type of attractor determining non-linear dynamics of failure evolution, the scale transition due to the failure cluster formation and topological regularities of fracture. The scale distribution of damage localization corresponds to the laws of the free energy release in solids with microcracks. The laws of spatial damage localization on various structural levels are defined by the non-linearity of the microcrack accumulation in the condition of intensive interaction of the defects. This leads to the multiscale generation of failure centers. The relation between typical non-linearity of damage kinetics and spatial failure localization is the theoretical background for the explanation of experimental results and numerical simulation of fracture in heterogeneous materials. Topological features of fracture development were investigated numerically using percolation model of failure cluster growth.

1. STATISTICAL MODEL

It has been established that failure and deformation of solids are accompanied by multiple nucleation and growth of microshears and microcracks. Damage as result of evolution of these defects usually takes place due to heterogeneity or imperfection of solids. There are two typical ways of microcrack initiation: either from preexisting structural defects, or due to creation of new structural defects. In metals microcracks are caused by plastic deformation and the arise of the latter preceded by a critical structure formation [1, 2]. In polymers, ceramics, high strength composites microcracks are initiated as a result of the high initial structural heterogeneity [3, 4, 5]. It is reasonable concerning critical structure formation to introduce the conception of critical microcrack nuclei in the initial pile-ups of defects, grain boundaries, structural imperfections, which will be develop into a microcrack at specified conditions [6]. A detailed description of microcracks and microshears ensembles behaviour requires estimation of structural parameters which play role of independent thermodynamical variables. These variables can be determined in terms of dislocations structure characteristics of solids, taking into account that the microcracking process and plastic deformation are associated with evolution of dislocation ensembles [1,7]. There are two reasons for incorporating dislocation representations in the theory of continuum damage. One of their natural significance for physics of fracture and plastic flow and other is the possibility of using them as the base elements for the considered defects simulation. This can be explained by

the fact that microcracks as a kind of incompatibility in continuous medium are equivalent to some continuous distributions of dislocations [8]. The existence of different types of microcracks and diversity of mechanisms of their generation and development require the adequate choice of parameters characterizing the microcracks. It should be noted that microcracks, both in ductile and brittle materials, are oriented by the stress field and are characterized by the form anisotropy, which is higher for brittle solids ($\sim 1:10$) and lower for ductile ones ($\sim 1:2$) [1,9]. The volume concentration of these defects reaches the values of about $10^{12}-10^{14} \text{ cm}^{-3}$ and the evolution of mesoscopic defects is close to the evolution of thermodynamic systems but with very important difference: single mesoscopic defect represents the dislocation ensemble and possesses this ensemble properties. Each mesoscopic defect is the dislocation ensemble with the properties determined by the dislocation pile-up. Typical mesoscopic defects are the microcracks. These defects can be represented by symmetrical tensor [10,11,12].

$$s_{ik} = s n_i n_k, \quad (1)$$

Tensor s_{ik} corresponds to disk-shape microcracks with the volume $s = S_0 B$ where $S_0 = \pi R^2$ is the microcrack base and $\vec{B} = B\vec{n}$ is the total Burgers vector of the dislocation pile-up modelling mesoscopic defects. It is well known that collective properties of the dislocation pile-up are appeared in the creation of the long-range stress field, the collective mobility and the orientational instability [13]. Evolution of mesoscopic defects is caused by the statistical distribution of defect nuclei, interaction between defects and the latter with external fields. The distribution function $W(s_{ik})$ is given by the Fokker-Plank equation [14]

$$\frac{\partial}{\partial t} W = -\frac{\partial}{\partial s_{ik}} (K_{ik}(s_{lm})W) + \frac{1}{2} Q \frac{\partial}{\partial s_{ik}} \left(\frac{\partial}{\partial s_{ik}} W \right), \quad (2)$$

where K_{ik} is the deterministic part of interaction forces, Q is the correlator which characterizes the potential relief of the initial structural heterogeneity (nonequilibrium potential). In [15] the statistical self-similarity of the defect distribution in solid was established for various conditions of the loading. Statistically self-similar solutions correspond to the stationary solution of the Fokker-Plank equation. The form of the solution follows from (2) for boundary conditions $W(s_{ik}) \rightarrow 0$ at $s_{ik} \rightarrow \pm\infty$

$$W = Z^{-1} \exp \left(\int_0^s 2K_{ik}(s'_{lm}) ds'_{ik} / Q \right), \quad (3)$$

where Z is the normalizing parameter. The hypothesis of the statistical self-similarity introduces into consideration the defect distribution for which the ratio of the energy $E = \int_0^s 2K(s'_{ik}) ds'_{ik}$ to

Figure 1: Nonlinear solid responses on microcrack growth.

the correlator Q is constant. The energy of the microcracks as a dislocation pile-up was estimated in [1] and can be represented in a form

$$E = \left(\frac{\mu}{\pi^3 R^3} \ln \frac{R}{r_0} \right) s^2, \quad (4)$$

where r_0 is the radius of the nuclei of the dislocation pile-up, μ is the shear modulus. The constraint parameter $\alpha = \mu / (4\pi^3 R^3) \ln(R/r_0)$ depends on the volume ($\sim R^3$) of structural elements (blocks or grains in solid). Taking into account (4) and the important role of long-range stresses produced by the defect ensemble the energy of the mesodefects was introduced

$$E = -H_{ik}s_{ik} + \alpha s_{ik}^2. \quad (5)$$

The effective stress field $H_{ik} = \gamma s_{ik} + \lambda n \langle s_{ik} \rangle$ determines the intensity of stress acting on the single mesodefect from the external stress field σ_{ik} and the "mean" stress field $\lambda n \langle s_{ik} \rangle$. Averaging s_{ik} with the distribution function W we obtain the self-consistency equation for microcrack density tensor $p_{ik} = n \langle s_{ik} \rangle$ (n is the microcrack concentration)

$$p_{ik} = n \int s_{ik} Z^{-1} \exp\left(\frac{E}{Q}\right) ds d^3 \vec{v} \quad (6)$$

Equation (6) was solved in [10] for the case of uniaxial and shear loading for various values of the dimensionless parameter $\delta = 2\alpha/(\lambda n)$ (Fig.1). The value $\lambda n \langle s_{ik} \rangle$ determines the intensity of long-range interactions in ensemble of mesodefects. There are three responses of material to the defect growth : monotonous ($\delta > \delta_*$), metastable ($\delta_c < \delta < \delta_*$) and unstable ($\delta < \delta_c$); δ_* and δ_c being the bifurcation points correspond to the change of the asymptotes. The monotonous response ($\delta > \delta_*$) is characteristic for a weak interaction between defects. In metastable area the jump-like change of p_{ik} corresponds to the orientation ordering of the mesodefect ensemble. The pass over the δ_c -asymptotics leads to the infinite jump of p_{ik} . The passes over the asymptotics can be recognized as topological transitions that lead to symmetry changes due to the new organization in the system. Mathematically speaking these transitions occur under the change of differential equation types and their group properties.

2. FRACTALITY AND DAMAGE LOCALIZATION

Kinetics of the damage accumulation was studied in [12] and based on the assumption that free energy Ψ of materials with considered type of defects is determined by the statistical model and depends on the parameter p_{ik} . When analyzing nonlinear regularities of the microcrack accumulation, especially, damage localization it is very important to take into consideration the spatial non-homogeneity of the defect distribution. The non-locality effect appears due to the high gradient of internal stresses caused by the non-homogeneous defect distribution at the mesoscopic level [16]. These gradients are determined by the scales from $1\mu m$ to $1cm$ and more.

Non-local potentials is written in the form $\Psi^* = \Psi + (1/2)\chi(\partial p_{ik} / \partial x_l)^2$, where the quadratic gradient term describes the non-local effect in the so-called long wave approximation, χ is the nonlocality parameter. To follow the Ginsburg Landau approach [17] we obtain as the consequence of the evolution inequality $\delta\Psi / \delta t = (\delta\Psi / \delta p_{ik})(\partial p_{ik} / \partial t) \leq 0$ ($\delta\Psi / \delta p_{ik}$ is the variational derivative) the kinetic equation for the p_{ik} tensor

$$\frac{\partial p_{ik}}{\partial t} = -\frac{1}{\tau_p} \frac{\partial \Psi}{\partial p_{ik}} + \frac{\partial}{\partial x_l} \left(\chi \frac{\partial p_{ik}}{\partial x_l} \right) \quad (7)$$

where τ_p is the relaxation time for p_{ik} . This equation coupled with the constitutive equation of elastic medium with microcracks [10]

$$u_{ik} = C_{iklm} \sigma_{ik} + \mathcal{P}_{ik} \quad (8)$$

where u_{ik} and C_{iklm} are the strain and elastic compliance tensors.

Figure 2: Various complexity eigenfunctions of the microcrack evolution equation.

The characteristic features of microcrack ensemble evolution are associated with group properties of the non-linear operator (7), which in turn define the eigenfunction spectrum of a non-linear problem [18, 19]. These eigenfunctions correspond to the self-similar solutions of the equation (7) at the developed stage of the system behaviour ($\delta < \delta_c$, $p > p_f$) and define for a particular form of non-linearity the spectrum of spatial-time forms of solutions (dissipative structures of various complexity, Fig.2). The spatial-time invariants of these solutions at different scale-structure levels reflect the similarity that exists between mechanisms of defect accumulation, in particular between mechanisms of damage localization.

It was shown in [10] that there are several types of self-similar solutions, corresponding to a localized infinite growth of p_{ik} over a range of constant or "growing" space scales. This situation is typical for solid in case of initiation of stabilizing or extending fracture centers. The evolution of dissipative structures for equation (7) is described by the self-similar solution [19,20, 21]

$$p(x,t) = g(t)f(\zeta), \quad \zeta = x/\phi(t), \quad (9)$$

where $g(t)$ governs the growth law of parameter p and $\phi(t)$ defines variations over the half-width of the localization region. From equation (9) follows that the time dependence of p remain self-similar: this is simply an extension along the x and p -axes. The substitution (9) into the equation (7) allows to clarify the form of the function $g(t)$

$$g(t) = G \left(1 - \frac{t}{\tau_c} \right)^{-m}, \quad (10)$$

where τ_c is so called "peak time" ($p \rightarrow \infty$ at $t \rightarrow \tau_c$ [20]); $G > 0, m > 0$ are the parameters of nonlinearity, which characterize the rate of the free energy release $\partial \Psi / \partial p$ with the increase of the volume microcrack concentration in the region $p > p_f$, ($\delta < \delta_c$). Concurrently the eigenvalue problem is formulated for the eigenfunction $f(\zeta)$. Its solution gives the spectrum of eigenforms

$f_i(\zeta)$ "living" during τ_c^i time in the discrete ranges of eigenvalues ζ_i , specifying the damage localization scales. The solution (9) refers to the class of nonlinear singular solutions, describing an infinite growth of $p(t)$ over localization scale ζ_i (fundamentals lengths [20]) at $t \rightarrow \tau_c$.

The high-strength nonhomogeneous materials with multiple interacting microcracks are dissipative systems, the behaviour of which changes from a regular to a random one at small variations of certain parameters. This phenomenon is caused by local instabilities of p_{ik} beyond the thermodynamic branch of $p(\sigma)$ relation for $\delta < \delta_c$. Local instabilities in ensemble of defects are accompanied by alteration of the topological properties of the system. It is interesting that the same form of the relation (curve $\delta < \delta_c$, Fig.1.) between the scalar measure of damage P and stress was proposed by Bolotin [22]

$$P = F_r(g(\sigma, P)), \quad (11)$$

where

$$F_r[g(\sigma, P)] = 1 - \exp\left[-(g(\sigma, P)/r_c)^\alpha\right] \quad (12)$$

is the Weibull distribution function of the short-time strength, $g(\sigma, P)$ is the real stress in the structural elements, $r_c = r_s(V_s/V_c)^{1/\alpha}$ is a characteristic strength of the structural elements, r_s is the strength of the specimen, and α is the Weibull modulus. Assuming $g(\sigma, P) = \sigma \exp(\beta P)$, we obtain a concrete form of equation (11)

$$P = (\sigma/r_c \exp(\beta P))^\alpha, \quad (13)$$

where β is the parameter controlling the effective stress growth under damage accumulation. The relation such as equation (13) follows from (6) for the equilibrium condition of elastic medium with microcracks $\frac{d\Psi}{dp_{ik}} = 0$. Phenomenological analog of expression (7) appears from the above

$$\dot{P} = -\frac{1}{\tau_p} \left(P - \left(\frac{\sigma}{r_c} \exp(\beta P) \right)^\alpha \right) \quad (14)$$

The regularities of transitions from damage to fracture were examined numerically for carbon-carbon composites. Tensile loading tests of carbon-carbon specimens demonstrate characteristic

Figure 3: Typical deformation curves of the carbon-carbon specimens.

features of deformation and fracture: the presence of microcracks in the bulk of the specimen; the influence of microcracking on the deformation behaviour of materials; fragmentation of the specimen across the regions subject to damage and highly statistical scattering of the specimen strength (Fig. 3). For the case of uni-axial tension only the component p_{yy} of the tensor p_{ik} is sufficient to characterize the microcrack accumulation process. The problem of quasi-brittle fracture of the carbon-carbon composite has been solved numerically [18,19] by the finite

Table 1: Statistics of tensile test measurements

N series	dispersion	characteristic strength r_s , MPa	Weibull modulus α
1	360	79	4
2	130	83	8
3	45	88	16
4	25	77	17
5	43	117	20
6	19	81	23
7	20	91	25

element method based on the equilibrium equation $\partial \sigma_{ik} / \partial x_{ik} = 0$ ($k=1,2$), the constitutive equation of elastic medium with microcracks (8), the kinetic equation of damage accumulation (14), and boundary condition and initial conditions. Phenomenological parameters (α, β, r_c) were determined from the results of statistical analysis (Table 1, Fig. 3, Fig. 4) of tensile test

Figure 4: Distribution function of the specimen strength for one series (a); distribution function of characteristic strength for all series (b).

measurements on carbon-carbon composite specimens (Fig. 3). Simulation of the deformation and fracture processes starts with random assignment of (according to Table 1 and Fig.4) the strength

r_s and Weibull modulus α to each element of the finite element approximation (number of the elements is 5000). At every step of the time we calculate a new value of the elastic modulus taking into account the influence of microcrack accumulation, and solve the elasticity problem and define the value of parameter p_{yy} . The element is broken, when p_{yy} reaches the critical value p_c .

($p_c = 3 \cdot 10^{-4}$ is an experimental estimate). The macroscopic fracture corresponds to the formation of a percolation cluster that consists of fractured elements. The final step of fracture simulation is the fractal analysis of the percolation cluster. The cluster appears to be fractal in nature and with an increase of linear dimension L of the damaged array [23] its mass M (the number of failed elements) increases on the average as:

$$M(L) = AL^D, \quad (15)$$

where D is the fractal dimension, A is the effective amplitude. The mean value of A is obtained by averaging over the manifold realization of the percolation cluster. This approach was used to simulate failure development in carbon-carbon specimens with an initial macroscopic defect located in the center (the macrocrack is normal to the tension direction) with characteristic size N_a (Fig. 5). The dependence $M(L)$ consists of two linear parts with the slopes determined by the fractal dimension D . Simulation of damage has demonstrated that under loading the initial stage is accompanied by preferential failure of elements located in the vicinity of the macroscopic defect ($D=1$). The percolation cluster across the specimen results from coalescence of the cluster originating from the initial macrodefect with clusters in its immediate

Figure 5: Topological characteristics (fractal dimensions) of the damage cluster growth.

neighbourhood ($D = 1.4 - 1.7$). This is indicative of the qualitative change in the topology of damage accumulation process and the fracture mechanism replacement. The fractal dimension $D = 1$ supports the validity of approaches of fracture mechanics only at the initial stage of crack evolution.

The results of statistical simulation for the time of complete formation of the main cluster are plotted in Fig. 6. This dependence involves two parts with two asymptotics x_c^n and x_c^d . The right part corresponds to the formation of branched cluster with the fractal dimension $D = 1.4 - 1.7$. The transient region between these parts defines the critical size N_a^c of the initial defect, which specifies two qualitatively different mechanisms of fracture according to the size of initial defects. It means that the highest reliability of materials is reached when the size of initial defect is not larger than N_a^c . In this case, the material exhibits the maximum of "dissipative capacity" and the damage accumulation in the specimen is more homogeneous.

Figure 6: Dependence of critical concentration of failed elements X_c on initial macrodefect size N_a .

A fracture zone formation is connected with the nucleation of localized damage zones in the form of dissipative structures which are developed in a peak regime. This is accompanied by the generation of simple and complex structures of the localized failure and it reflects the self-similarity of damage development at various scale levels.

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