Multiscale Damage Evolution as Structural-Scaling Transitions in Mesodefects Ensembles

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Keywords: Collective modes of mesodefect, structural-scaling transitions, crack dynamics, failure waves, seismic events.

Abstract. Statistical theory of mesoscopic defects (microcracks, microshears) allowed us to establish new type of critical phenomena– structural-scaling transitions, to develop thermodynamics of solid with mesodefects and to propose the phenomenology based on generalization of the Ginzburg-Landau theory. The key result of statistically based phenomenology is the interpretation of multiscale damage evolution in terms of characteristic collective modes of defects responsible for damage localization and transition to failure. Original experiments supported the linkage of these modes with material responses in large range of load intensity and allowed the interpretation of nonlinear crack dynamics, mechanisms of failure wave, scaling laws in seismic events.

Introduction

The problem of failure is one of the key problems of fundamental and applied physics and mechanics. Despite the large amount of experimental data and the efforts in materials science, there is no answer on some of the important questions conditioning progress in the estimation of reliability, prediction of fatigue and dynamic failure, as well as strength under intensive (shock wave) loading. To follow [1] the most basic questions still unanswered are: "What are the fundamental distinctions between brittle and ductile behaviors? Remarkably, we do not have a fundamental understanding of distinctions between these two behaviors. Moreover, the brittleness or ductility of some materials depends upon the speed of loading, which implies that a proper description of deformation and fracture must be dynamic, that is, it must be expressed in the form of equations of motion rather than the conventional phenomenological rules and yielding criteria." Our approach, which derives from the collective behavior of defects, is based on the statistical physics of mesoscopic systems with defects, which has already allowed the establishment of qualitative new features of failure as critical phenomena or structural-scaling transitions. The main ideas are based on the recognition that solids under loading demonstrate changes on all structural levels. These changes are associated with plastic deformation and damage processes, and result from the nucleation and growth of defects. Experimental studies of material responses in a large range of loading rates show that the behavior of solids is intimately linked with the evolution of typical mesoscopic defects (dislocation substructures, microcracks, microshears). This characterizes generically solids under dynamic and shock wave loading, when the internal times of the evolution of ensemble of defects for different structural levels are approaching the characteristic loading times. As a consequence, the widely used assumption in the phenomenology of plasticity and failure that structural (defect) variables can effectively be subordinated to the stress-strain variables (adiabatic limit) is not generally valid. In order to understand the nature of plastic deformation and failure, the key problem is to characterize the evolution of the statistics and the thermodynamics of typical mesodefects. This problem is intrinsically associated with an adequate description of the out-of-equilibrium system of evolving defects interacting over long ranges leading to the appearance of collective defect modes.

Statistical Mechanics of Solid with Mesodefects

Microcrack (microshear) ensemble may be considered as the representative for developed stage of failure. The rest of defects (point defects, dislocations, dislocation pile-ups) have smaller values of elastic fields and energies in the comparison with microcracks and microshears. Moreover, the nucleation and growth of these defects (that are closest to the macroscopic level) are some final acts of the previous rearrangement of the dislocation substructures, when all defects take part in the structural relaxation of elastic field. The density of microcracks (or microshears) reaches $10^{12} - 10^{14} cm^{-3}$, but each this mesoscopic defect, for instance, for crystalline materials, represents the dislocation pile-up and exhibits the properties of this ensemble. Structural parameters associated with microcracks and microshears were introduced [2] as the derivative of the dislocation density tensor. These defects are described by symmetric tensors of the form $s_{ik} = s\nu_i \nu_k$ or $s_{ik} = 1/2s(\nu_i l_k + l_i \nu_k)$ for microcracks and microshear correspondingly. Here $\vec{\nu}$ is unit vector normal to the base of a microcrack or slip plane of a microscopic shear; $\vec{l}$ is a unit vector in the direction of shear; s is the volume of a microcrack or the shear intensity for a microshear. The average of the "microscopic" tensor s_{ik} gives the macroscopic tensor of the microcrack or microshear density $p_{ik} = n\langle s_{ik} \rangle$, that coincides with the defect induced deformation, n is the defect concentration.

Statistical mechanics of mesodefects was developed in [3] assuming the statistical self-similarity of defect distribution. Similar statistical approach was proposed in [4] for the formulation of the so-called "slip blocks" or "shear lattice" models in the application to the earthquake mechanics, where the role of fluctuations is also important. The Boltzmann type distribution of defects is discussed in "shears lattice" models $p(E_q) \propto \exp[-E_q/T_{sb}]$, where T_{sb} is the average energy (effective temperature) related to characteristic degrees of freedom in the system of shears. Definition of the effective temperature T_{sb} is linked with the energy functional $U(s)$ of blocks interacting in the course of sliding: $T_{sb} = \frac{1}{2}\{\langle U(s) \rangle\}$, where $\langle U(s) \rangle$ is the average energy in the block lattice and corresponding to the single block. This approach follows to the assumption that the system has the sensitivity to noise (similar to the Boltzmann fluctuations) that provides realization of all states in the phase space of mentioned variables. Such assumptions were analyzed using the cellular automata models to take into account long-range interactions in the sliding block system for the application of the "mean field" approach for the development of continuum models of the system of interacting sliding blocks ("coarse-grain models") [5]. This analysis established the existence of two critical points, where the cluster scaling was associated with the fluctuation induced criticality. Critical states correspond to the transition from disordered states at low stress to the metastability leading to the ordering states for high stress. Microscopic kinetics of s_{ik} corresponds to the Ito-Langevin equation

$$\dot{s}_{ik} = K_{ik}(s_{lm}) - F_{ik}\,, \tag{1}$$

where $K_{ik} = \partial E / \partial s_{ik}$ is the deterministic part of force field, influencing on the localized distortion. The energy of mesodefect can be represented as $E - E_0 = -H_{ik}s_{ik} + \alpha s_{ik}^2$, where the quadratic term reflects the energy fluctuation arising in the immediate vicinity of microcrack, the term $H_{ik}s_{ik}$ describes" the energy release due to the microcrack growth in the field of the "effective field" $H_{ik} = \sigma_{ik} + \lambda p_{ik}$, where σ_{ik} is the external stress; α, λ are the parameters related to the effective constrained constants; F_{ik} is the random δ-correlated part of the force field satisfying the relations: $\langle F_{ik}(t)\rangle = 0$ and $\langle F_{ik}(t')F_{ik}(t)\rangle = Q\,\delta(t-t')$. Here Q is the correlator of fluctuating forces induced by mesodefects. Macroscopic value of defect induced strain – the microcrack density tensor $p_{ik} = n\langle s_{ik}\rangle$ follows from the average $p_{ik} = n\int s_{ik}W(s,\vec{v},\vec{l})ds_{ik}$, where the distribution function has the form $W = Z^{-1}\exp(-E/Q); Z = \int\exp(-E/Q)ds_{ik}$ is the normalization factor. The definition of dimensionless variables $\hat{p}_{ik} = (1/n)\sqrt{\alpha/Q}\ p_{ik}$, $\hat{s}_{ik} = \sqrt{\alpha/Q}\ s_{ik}$, $\hat{\sigma}_{ik} = \sigma_{ik}/\sqrt{Q\alpha}$ allows the representation as the self-consistence equation

$$\hat{p}_{ik} = \int \hat{s}_{ik} Z^{-1}\exp\left((\hat{\sigma}_{ik} + \frac{1}{\delta}\hat{p}_{ik})\hat{s}_{ik} - \hat{s}_{ik}^2\right)d\hat{s}_{ik}, \tag{2}$$

that contains unit dimensionless parameter $\delta = \alpha/(\lambda n)$. Dimension analysis shows $\alpha \sim G/V_0, \lambda \sim G, n \sim R^{-3}$, where G is the effective constrained modulus solid with microcrack; $V_0 \sim r_0^3$ is the "nuclei volume" of microcrack; R is the correlation radius (mean distance) between microcracks. Finally the presentation for δ reads $\delta \sim (R/r_0)^3$, that reflects mentioned statistical self-similarity in the multiscale distribution of microcracks [3]. The solution of equation (2) for the case of uni-axial tension ($\mathrm{p} = \mathrm{p}_{zz}$, $\sigma = \sigma_{zz}$) is shown in Fig.1. The existence of three characteristic nonlinear responses were found corresponding to different values of structural scaling parameter δ ($\delta > \delta_* \approx 1.3$, $\delta_c < \delta < \delta_*$, $\delta < \delta_c \approx 1$), where δ_c and δ_* are the bifurcation points. Bifurcation points δ_*, δ_c play the role similar to critical temperatures in the Landau theory of phase transformations. Different non-linearity corresponding to the pass of critical points describe different scenario of defect ordering depending on material sensitivity to the defect growth in term of initial value of structural-scaling parameter. The structural scaling parameter δ has the meaning of the second order parameter and the value of δ determines the "thermalization" conditions (similar to the effective temperature) of mesoscopic out-of-equilibrium system. Taking into account the physical meaning of structural-scaling parameter the natural generalization for the distribution function can be introduced to assume the independent statistics for δ as the variation of structural scales R and r_0 in the initial state of system $\mathrm{N}(\hat{\mathrm{E}}) = \int \mathrm{d}\delta\, \mathrm{f}(\delta)\mathrm{Z}^{-1}(\delta)\exp(-\hat{\mathrm{E}}/\delta)$, where $f(\delta)$ is the distribution function for the initial "sensitivity" of the system to the defect growth in the term of δ; $\hat{E} = \delta(\hat{\sigma}_{ik}\hat{s}_{ik} - \hat{s}_{ik}^2) + \hat{p}_{ik}\hat{s}_{ik}$. The average assumes in this case the integrating over all order parameters of mesoscopic system

$$\hat{p}_{ik} = \int f(\delta)\int \hat{s}_{ik} Z^{-1}\exp\left((\hat{\sigma}_{ik} + \frac{1}{\delta}\hat{p}_{ik})\hat{s}_{ik} - \hat{s}_{ik}^2\right)d\hat{s}_{ik}\,d\delta. \tag{3}$$

The dependence of statistical integral on the unit structural parameter δ and corresponding non-linearity types reflect, probably, the universal properties of media with local change of symmetry under the generation of localized interacting distortions.

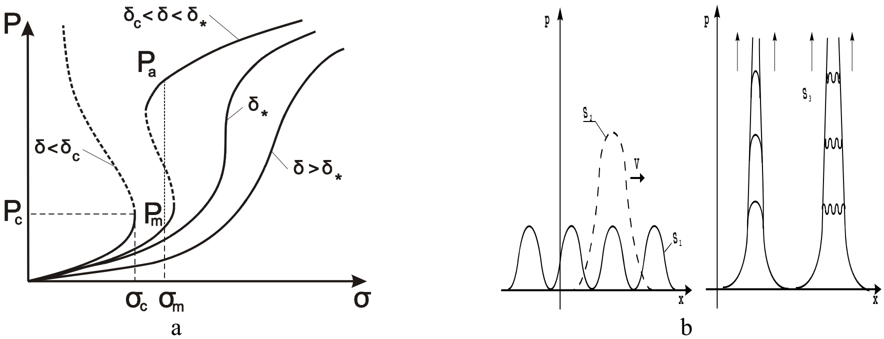

Fig.1. Nonlinear responses of system on the microcrack growth (a) and characteristic collective modes for different values of structural scaling parameter δ (b).

Mentioned non-linearity and related group properties of dynamic equations for p_{ik} define the types of collective modes that can subject the dynamics of entire system. With the evolution of these modes can be linked characteristic solid states in the presence of defects (quasi-brittle, ductile).

Non-equilibrium free energy. Phenomenology of solids with microcracks

Statistical approach allowed one to propose the mesoscopic out-of-equilibrium potential, which describes different scenario of microcrack ensemble evolution related to nonlinearity types. The curves, presented in Fig.1, corresponds to the solution of equation $\partial F/\partial p = 0$, where F is mesoscopic potential (nonequilibrium free energy). For the case of simple shear ($p = p_{xz}, \sigma = \sigma_{xz}$,) the "minimal extention" for F is given by the 6[th] power polynomial presentation and has the form similar to the Ginzburg-Landau expansion $F = \frac{1}{2}A(\delta,\delta_*)p^2 - \frac{1}{4}Bp^4 + \frac{1}{6}C(\delta,\delta_C)p^6 - D\sigma\ p\ + \chi(\nabla_l p)^2$ [3]. The gradient term describes the non-locality effect under the microcrack interaction; A, B, C, D and χ are the parameters characterizing nonlinear properties of solid with microcracks predicted in the frame work of the statistical description. Kinetics of mentioned order parameters p_{ik} and δ follows from the evolution inequality $\Delta F/\Delta t = \partial F/\partial p\, \dot{p} + \partial F/\partial \delta\, \dot{\delta} < 0$ and is given by the motion equations (the Ginzburg-Landau approximation)

$$\frac{dp}{dt} = -\Gamma_p\left(A(\delta,\delta_*)p\ - Bp^3 + C(\delta,\delta_C)p^5 - D\sigma\ - \nabla_l(\chi\nabla_l p)\right), \tag{4}$$

$$\frac{d\delta}{dt} = -\Gamma_\delta\left(\frac{1}{2}\frac{\partial A}{\partial\delta}p^2 - \frac{1}{6}\frac{\partial C}{\partial\delta}p^6\right), \tag{5}$$

where Γ_p и Γ_δ are the kinetic coefficients. As it follows from the solution of equations (4), (5) the transitions over the bifurcation points δ_c and δ_* result in sharp changes of the distribution function and the formation of collective modes of microcracks. The type of transitions over the critical points is given by the bifurcation type – the group properties of equations (4), (5) for different ranges of the structural-scaling parameter $\delta\,(\delta>\delta_*, \delta_c<\delta<\delta_*, \delta<\delta_c)$. This equation has in the area $\delta>\delta_*$ the elliptic type with the eigen forms as spatial-periodic modes S_1 (Fig.1b) on the scales Λ with week anisotropy (orientation) determined mainly by the force field σ. For $\delta\to\delta_*$ the eigen forms of equation (4) undergo qualitative changes in condition of the divergence of inner scale Λ: $\Lambda \approx -\ln(\delta - \delta_*)$. The periodic solution transforms into the "breathers" for $\delta \to \delta_*$ (in the area $\delta > \delta_*$) and the auto-solitary waves $p(\zeta) = p(x - Vt)$ in the orientation metastability area $\delta_C < \delta < \delta_*$, where the collective modes appear at the front of solitary wave (S_2, Fig.1b). The wave amplitude p, wave front velocity V and the width of wave front L_S are determined by the parameters of non-equilibrium transition

$$p = 1/2\left(p_a - p_m\right)\left[1 - tahn(\zeta L_S^{-1})\right], \qquad L_S = 4/\left(p_a - p_m\right)\left(2\chi/A\right)^{1/2}. \tag{6}$$

The velocity of wave fronts is $V = \chi A(p_a - p_m)/\Gamma_p^{\ 2}$, where $(p_a - p_m)$ is the jump in the value of p in the metastability area. A transition through the bifurcation point δ_c is accompanied by the appearance of spatio-temporal structures of a qualitatively new type characterized by explosive accumulation of defects as $t \to t_f$ in the spectrum of spatial scales ("blow-up" dissipative structures S_3, Fig.1b) [3]. It is shown in [6] that for equations (7) for $\delta < \delta_C$, $p > p_C$ the developed stage of kinetics of p in the limit of characteristic times $t \to t_f$ can be described by a self-similar solution of the form

$$p(x,t) = \phi(t) f(\zeta), \quad \zeta = x/\varphi(t), \quad \phi(t) \sim \left(t - t_f\right)^{-m}, \ \varphi(t) \sim \left(t - t_f\right)^{d}, \tag{7}$$

where m, d are the parameters related to the nonlinearity type of equation (4) for $\delta < \delta_C$, $p > p_C$; t_f is the characteristic temporal scale of self-similar solution (7). There are three types of self-similar solution (7) depending on the value of mentioned parameters m, d. The solution for represents the particular interest, when the self-similar solution has the form

$$p(x,t) = \left[C(\delta,\delta_C)(t - t_f)\right]^{-m} \left(\frac{2m(1+m)}{(1+2m)} \sin^2\left(\frac{\pi x}{L_f} + \pi\theta\right)\right)^m, \tag{8}$$

where θ is a random number in the interval (0,1). Specific form of the function $f(\zeta)$ can be determined by solving the corresponding eigen value problem. The scale L_f, so-called fundamental length [3], has the meaning of a spatial period of the solution (8): $L_f = 2\pi m\left((1/m + 1)\chi C^{-1}(\delta,\delta_C)\right)^{\frac{1}{2}}$. The self-similar solution (8) describes the kinetics of the microcrack ensemble in the "blow-up" regime $p(x,t) \to \infty$ for $t \to t_f$ on the spectrum of spatial scales $\mathrm{L_H = kL_f}$ $(\mathrm{k} = 1,2,\ldots\mathrm{K})$ and can be linked with multiscale damage evolution. In this case the complex "blow-up" structures appear on the scales $L_H = kL_f$ (Fig.1b), when the distance between simple structures L_C will be close to L_f. The set of eigenforms related to the spectrum of auto-solitary waves and blow-up dissipative structures represent the collective variables of nonlinear dynamic system "solid with mesodefects". Experimental program was realized to support theoretical prediction of the role of mentioned collective modes in relaxation ability of materials, nonlinear aspects of damage-failure transition, fragmentation statistics [3].

Fig.4 shows an example illustrating how the theory outlined in the previous sections provides an explanation for the transition from the steady-state to the branching regime, to fragmentation statistics and the failure wave phenomenon. High speed framing of crack dynamics was realized to analyze different crack dynamics in the preloaded PMMA plate [3]. Three characteristic regimes were observed in the different ranges of crack velocity: steady-state $V < V_C$, branching $V > V_C$ and fragmenting $V > V_B$, when the multiple branches of the main crack take an autonomous behavior.

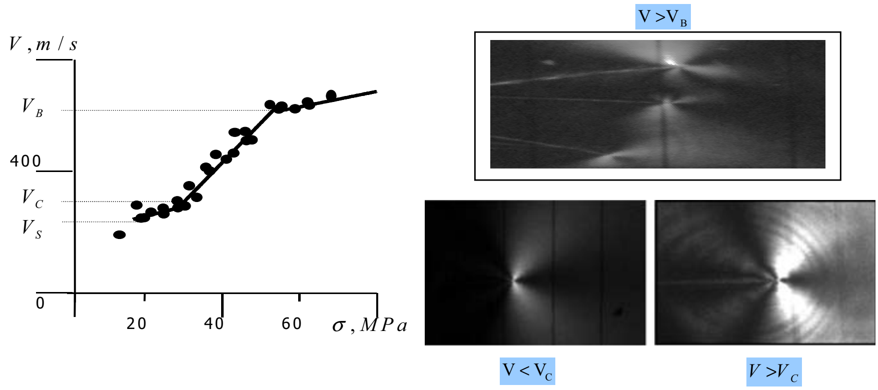

Fig. 2. Characteristic regimes of crack dynamics

High speed framing experiment (resolution 10^7 frames per second, coupled with polarization scheme) for crack dynamics in the preloaded PMMA plate allowed to confirm the transition from the steady-state to the branching dynamics for characteristic crack velocities $V_C \sim 0.4 V_R$ and to discover according to the theoretical prediction the second critical velocity V_B as the onset of fracture controlled by the "blow-up" dynamics of daughter cracks originated in the process zone. Three mentioned regimes of crack dynamics is the consequence of existence of two self-similar solutions (two attractors) for dynamic variables: long range self-similar stress distribution at the process zone (as the basis for stress intensity factor conception, $V < V_C$) and self-similar solutions corresponding to the set of "blow-up" collective modes of defect density tensor ($V > V_B$). The link of self-similar solutions (attractor types) and statistics of failure depending on the energy density imposed into material was established: energy dependent statistics ($V < V_C$), the Poisson statistics ($V > V_B$) and the intermediate (Weibull) statistics in the range of the co-existence of two mentioned attractors. The degeneration of the Poisson statistics into the uniform distribution of fragments with the scales corresponding to simplest "blow-up" eigenforms allowed the explanation of the "failure wave" as the phenomenon of "delayed failure" under the resonance excitation of "blow-up" collective modes of damage localization with delay time given by solution (7). Experimental validation of this theoretical prediction was realized as the high-speed framing of failure wave generation and propagation in fused-quartz rods loaded in the condition of the symmetric Taylor test. Processing of high-speed photography of the flyer rod traveling at 534 m/s at impact shows (Fig.3) three dark zones corresponding to the image of the impact surface (green triangles), the failure wave (red squares) and the shock wave (blue diamonds). The initial slope for the failure wave gives the front velocity $V_{fw} \approx 1.57\, km/s$, which is close to traditional measures in the plate impact test. However, the analysis reveals the increase of failure front velocity up to the value $V_{fw} \approx 4\, km/s$. This convergence of the velocity of the failure wave front towards the shock front velocity supports the theoretical description of the failure wave as a "delayed failure" with the limit "delay time" τ_D corresponding to the "peak time" in the blow-up self-similar solution shown. τ_D represents generally the sum of the induction time τ_I - the time of the formation of the spatial distribution of damage close to the self-similar profile, and the "peak time" τ_C - the time of the "blow-up" damage kinetics. A steady-state regime for the propagation of failure wave fronts can be linked with the successive activation of "blow-up" dissipative structures with the condition $\tau_D \approx \tau_C$.

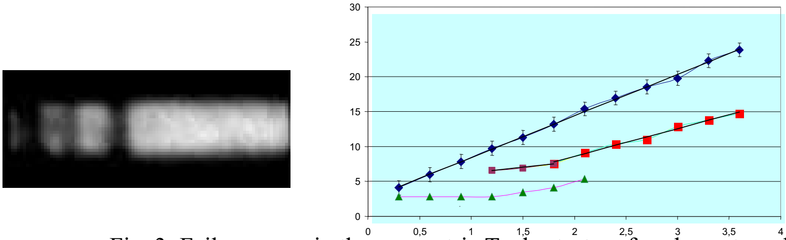

Fig. 3: Failure wave in the symmetric Taylor test on fused-quartz rods

This experiment provides one step towards validating the failure wave phenomenon as the consequence of the generation of collective burst modes of mesodefects. In this theory, the failure waves represent the specific dissipative structures (the "blow-up" dissipative structures) with "slow dynamics" in the microshear ensemble that can be excited due to the passing of the shock wave.

Structural-scaling transitions and scaling laws in seismicity

Scale analysis of the Earth core rupture gives the information concerning the large spectrum of scales: from few millimeters to some hundreds kilometers. It means that seismic events related to earthquakes are the consequence of blocks interaction in the large range of scales and the meaningful of laboratory tests to analyze the mechanisms related to the earthquakes. The understanding of role of collective modes in mechanisms of structural relaxation (plasticity and damage) can be considered as the basis for the interpretation of phenomenological scaling laws (Gutenberg-Richter, Omori, Bach), the prediction of criticality stages related to seismic events [7]. Frequency N-magnitude m scaling (Gutenberg-Richter law) for the after-shock sequence is observed in the large range of the earthquake power recorded on some temporal scale with magnitude m, $\mathrm{N}(\geq \mathrm{m})$: $\mathrm{N}(\geq \mathrm{m}) = 10^{\mathrm{a}-\mathrm{bm}}$. Parameter b corresponds to the range $0.8 < \mathrm{b} < 1.2$ and the constant a determines the logarithm of the earthquake number with magnitudes $\mathrm{m} > 0$. This relation has also equivalent representation as the fractal distribution $\mathrm{N} = \mathrm{CA}^{-D/2}$, where *A* is characteristic area of seismic ruptures due to the earthquakes, *D* is fractal dimension $\mathrm{D} = 2\mathrm{b}$ with variation of *D* in the range $1.3 < \mathrm{D} < 2.1$. Seismic events under the earthquakes are characterized by the decay of after-shocks according to the Omori law [7] $\mathrm{N} = \mathrm{K}/(\mathrm{c}-\tau)^{\mathrm{p}}$, where K, c and p are parameters ($\mathrm{p} = 1.0 \pm 0.1$). The existence of systematic delay times shows on the self-similar character of after-shock dynamics. The correlation relation for temporal sequences of after-shocks generation in the form of the Omori law includes two characteristic times τ and c, where c plays the role of characteristic temporal scale in the Gutenberg-Richter law. The Bath law for aftershocks establishes the universality of magnitude difference $\Delta\mathrm{m}$ between mainshocks with the magnitude m_{ms} and maximum value of aftershocks with magnitude $\mathrm{m}_{\mathrm{as}}^{\max}$: $\Delta\mathrm{m} = \mathrm{m}_{\mathrm{ms}} - \mathrm{m}_{\mathrm{as}}^{\max}$,which is practically independent on the mainshock magnitude, $\Delta\mathrm{m} \approx 1.2$. The features of ranged metastability, the power laws of main phenomenological laws, role of "noise" in the development of seismic events give the impact to consider the link of seismic events with critical phenomena in out-o-equilibrium systems that reveal the property of the so-called self-organized criticality SOC [7]). The initiation of blow-up structures under auto-solitary transforming can be considered as the scenario of pre-shock sequence. The shear transfer by auto-solitary waves can initiate the blow-up regime for the minimal time that is close to $\tau \sim \tau_c$. This regime corresponds to the limit case of spinodal decomposition under maximal depth of penetration into metastability area, when the resonance excitation of blow-up structure can be realized on corresponding "critical nuclei" on the core fault. The resonance excitation of blow-up dissipative structure for the minimal time $\tau \sim \tau_c$ can be identified with the main-shock. The number of seismic events corresponding to pre-shocks for the magnitudes exceeding some characteristic one is determined by the number of blow-up structures exciting on the set of scales $L_H = kL_f$ $(k = 1,2,...K)$ under the transforming of auto-solitary waves into blow-up structures in the δ_c- critical point. The constant difference of main-shock magnitude m_{ms} and maximum value of the after shock with magnitude m_{as}^{max} (the Bath law) is determined by the minimum stress increment providing the transition from the auto-solitary wave dynamics under realization of structural-scaling transition in the metastability range $\delta_c < \delta < \delta_*$ to the resonance excitation of blow-up dissipative structures corresponding to the main-shock. Qualitative transition between two these regimes, that is caused by different nonlinear asymptotic explains the universality of magnitude difference on the main-shock amplitude.

Summary

Statistical theory allowed definition of order parameters for mesodefects ensemble and formulation of nonequilibrium potential as generalized Ginzburg-Landau expansion. Kinetics of parameters determines relaxation property during plastic slip and damage-failure transition. Generation of mesodefects collective modes is the consequence of nonlinear properties of solid with defects, leads to steady-state (auto-solitary) wave of shear transformation, blow-up kinetics of damage-failure transition. The role of collective modes was studied experimentally for the explanation of nonlinear crack dynamics, failure wave generation, interpretation of the empirical scaling laws in seismicity.
The research was supported in part by grants of the Russian Foundation of Basic Research (07-01-96004-р_урал_а, 08-01-00699-а, 07-01-91100-АФГИР_а).

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