Theoretical and Experimental Study of Nonequilibrium Structural-Scaling Transitions in Metals

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Abstract. Transition from thermally activated to the dislocation drag sliding for different stages of plastic deformation is discussed using the interpretation of mesodefect induced structural relaxation and plastic flow as structural-scaling transition in the ensemble of mesodefects. Thermodynamic state of plastically deformed solid is characterised in the terms of effective temperature – spatial-temporal invariant related to long-ranged interaction of mesodefects collective modes providing slow-driven dynamics of plastic flow.

Introduction

Mechanisms of plastic flow reveal qualitative different case of momentum transfer in comparison with momentum transfer in liquid that has the nature of momentum diffusion. This difference follows from the nature of plastic flow carriers – dislocations, dislocation substructures providing the flow under the dislocation motion in the field of structural elastic stresses and pronounced long-ranged interaction between the carriers. The configuration effects are important under realization of plastic flow that is realized in strained solid in the out-of-equilibrium states as the multiscale sliding of dislocation substructures. The motion of dislocation substructures with the energy exceeding kT essentially occurs in the conditions of finite-amplitude fluctuations related to structural stresses, dislocation ordering and the formation of characteristic collective modes playing the role of new independent variables for the out-of-equilibrium system. Generation of these modes characterizing by new spatial-temporal scales provides the so-called "slow dynamics" of out-of-equilibrium system related to the dynamics of collective modes. Statistical theory of mesoscopic defects allowed us to establish new type of critical phenomena – the structural-scaling transitions, that provides the explanation of multiscale nature of plastic flow and the formulation of statistically based thermodynamics and phenomenology as the generalization of the Ginzburg-Landau approach for the out-of-equilibrium states [1]. The principal question for this generalization is the definition of the activation law and "thermalization" conditions of out-of-equilibrium states of plastically strained materials with the freedom degrees related to the multiscale collective modes of mesodefects. The definition of the "effective temperature" was proposed for plastically deformed solid using generalization of the Fluctuation-Dissipation Theorem (FDT) that allowed us to realize the experimental program to identify the effective temperature in polycrystalline and mono-crystalline materials (aluminium) for different states on the stress-strain deformation diagram. Mesodefect induced fluctuations were identified by the surface roughness measurement due to the multiscale shear banding [2]. High resolution interferometer-profiler New View data and the following correlation analysis of 3D-image of relief roughness was used for the estimation of scale invariants and the effective temperatures for different plastically strained states of specimens. Interpretation of dislocation induced structure in terms of effective temperatures allowed us to estimate different activation scenario along the deformation diagram: the transition from thermally activated plastic flow to the dislocation drag controlled plasticity. Mentioned results were used to explain the structure induced relaxation mechanisms responsible for the structural relaxation and plastic flow mechanisms in the large range of strain rates.

Non-Equilibrium Free Energy. Collective Modes of Mesodefects

Statistical theory of collective behavior of mesodefects ensemble established new type of critical phenomena – structural-scaling transitions that is characteristic for out-of-equilibrium systems with mesodefects [1]. The phenomenology as the generalization of the Ginzburg-Landau approach was developed in the terms of two order parameters (mesodefect density tensor p_{ik} and structural-scaling parameter δ) that allowed one to propose the out-of-equilibrium potential (free energy). For the case of simple shear ($p = p_{xz}, \sigma = \sigma_{xz},$) the "minimal extention" for F is given by the 6th power polynomial presentation

$$F = \tfrac{1}{2} A(\delta, \delta_*) p^2 - \tfrac{1}{4} B p^4 + \tfrac{1}{6} C(\delta, \delta_C) p^6 - D\sigma\, p + \chi(\nabla_l p)^2 . \tag{1}$$

The gradient term describes the non-locality effect under the microshear interaction; A, B, C, D and χ are the parameters characterizing nonlinear properties of solid with mesodefects 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)

$$\frac{dp}{dt} = -\Gamma_p\left(A(\delta, \delta_*)p - Bp^3 + C(\delta, \delta_C)p^5 - D\sigma - \nabla_l(\chi \nabla_l p)\right), \tag{2}$$

$$\frac{d\delta}{dt} = -\Gamma_\delta\left(\frac{1}{2}\frac{\partial A}{\partial \delta}p^2 - \frac{1}{6}\frac{\partial C}{\partial \delta}p^6\right), \tag{3}$$

where Γ_p и Γ_δ are the kinetic coefficients. As it follows from the solution of equations (2), (3) 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 mesodefects. The type of transitions over the critical points is given by the bifurcation type – the group properties of equations (2), (3) for different ranges of the structural-scaling parameter δ ($\delta > \delta_*, \delta_c < \delta < \delta_*, \delta < \delta_c$). This equation has in the area $\delta > \delta_*$ the elliptic type with the eigen forms as spatial-periodic modes on the scales Λ with week anisotropy (orientation) determined mainly by the force field σ. For $\delta \to \delta_*$ the eigen forms of equation (2) 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. 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

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

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) [1]. It is shown that for equations (2), (3) 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

$$p(x,t) = \phi(t) f(\zeta), \quad \zeta = x/\varphi(t), \quad \phi(t) \sim (t - t_f)^{-m}, \ \varphi(t) \sim (t - t_f)^{d}, \tag{5}$$

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 (5) depending on the value of mentioned parameters m, d. There is the case of the particular interest, when the self-similar solution has the form

$$p(x,t) = \left[C(\delta,\delta_C)(t - t_f)\right]^{-m} \left(\frac{2m(1+m)}{(1+2m)} \sin^2\left(\frac{\pi x}{L_f} + \pi\theta \right) \right)^m, \tag{6}$$

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 (6): $L_f = 2\pi m\left((1/m+1)\chi C^{-1}(\delta,\delta_C)\right)^{\frac{1}{2}}$. The self-similar solution (6) 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 $\mathrm{L_H} = \mathrm{kL_f}$ $(\mathrm{k} = 1,2,...\mathrm{K})$ and can be linked with multiscale damage evolution. In this case the complex "blow-up" structures appear on the scales $L_H = kL_f$, 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".

Effective Temperature of Slow Driven Systems

Intensively studied question during last decades is the definition of thermalization conditions for the out-of-equilibrium systems revealing the so-called slow dynamics. The behavior of these systems allows the definition of the effective temperatures as spatial-temporal invariants related to the current thermodynamic state using the analysis of fluctuations revealing the long-ranged correlations in the slow driven states. Definition of the effective temperature was proposed first by Leontovich [1] under the formulation of non-equilibrium thermodynamic potentials using the idea of the effective field and generalization of the Fluctuation-Dissipation Theorem. Similar approach is based on the generalization of the Boltzmann-Gibbs statistics for the out-of-equilibrium states revealing the slow driven dynamics [3]. This approach is well-known as the non-extensive statistics (the Tsallis statistics) and superstatistics). The objective of the Fluctuation-Dissipation Theorem is the link of mean square fluctuations of any internal parameter s of the near equilibrium thermodynamic system with temperature and the current susceptibility of system.

$$\overline{(S-s)}^2 = \frac{T}{\left(\partial^2 F \middle/ \partial s^2\right)}, \tag{7}$$

where F is the thermodynamic potential (free energy in our case).

The definition of non-equilibrium free energy using the effective field conception allows the application of generalized version of the Boltzmann-Gibbs statistics for the estimation of the effective temperatures of the current states of slow driven systems related to the long range correlations and corresponding spatial invariants of mesodefects collective modes.

Effective Temperature of Material in Plastically Strained States

Metals in the conditions of plastic deformation represent the typical case of out-of-equilibrium system with slow dynamics. Deformation diagrams of typical ductile materials demonstrate the weak sensitivity in the large range of strain rates. This feature of plastic flow is in the correspondence with the "slow driven system" conception and result from the slow dynamics of collective modes of mesodefects that subject the macroscopic behavior of entire system. Spatial-scale invariants related to the mesodefect collective modes were calculated using the New View profilometry data of surface roughness for strained specimens.

The aluminium monocrystal (Fig.1) was used for the study of mesodefect induced thermodynamic state.

Fig.1 Monocrystalline aluminium specimen (180x10x4 mm) prepared by Zhochralsky method

The plastic straining and the following study of surface roughness were realized for the specimens (Fig.2) that were machined from the monocrystal and the following surface polishing including electro-polishing.

Fig.2. Monocrystalline aluminum specimen (41x3.8x1.8 mm)

Stress-strain diagram for the clumps velocity V= 0.22mm/min is presented in Fig.3 for 6 load-unload tests.

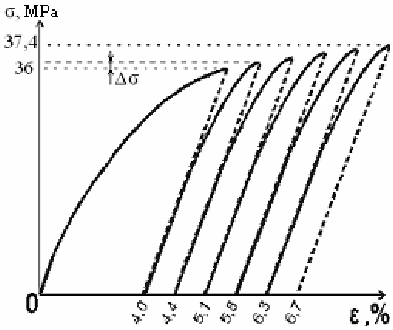


Fig.3. Load-unload tests for plastically strained specimens

3D roughness fluctuations along the strain axis were measured by the interferometer-profiler New View 5000 with vertical resolution ~ 1nm and horizontal resolution ~ 1 μm. Characteristic roughness profile is presented in Fig.4.

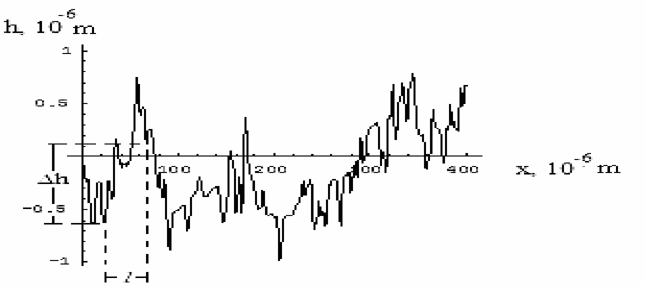


Fig.4. Characteristic roughness profile for aluminium moocrystal

Fluctuations of plastic strains were estimated according to the New View data using the formula

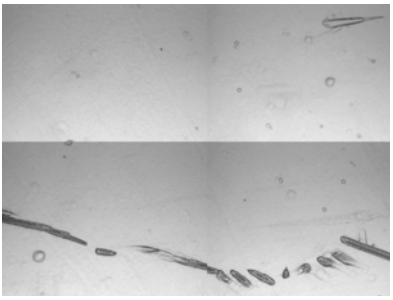
$$\Delta\varepsilon = \frac{\Delta h(l)}{l}, \tag{8}$$

where l is the selected spatial scale of the New New resolution; Δh is the roughness increment.

The mean-square strain fluctuations were determined according to formula

$$\overline{(S-s)}^2 = \left\langle \ \left\langle \Delta\varepsilon(l) \right\rangle_x^{\ 2} - \left\langle \Delta\varepsilon^2(l) \right\rangle_x \ \right\rangle_{l'}, \tag{9}$$

where $l^{'}$ is the number of traces cutting the 3D roughness profile along the strain axis. The average was realized in the initially marked area of the New View window for different strains (Fig.5).


a

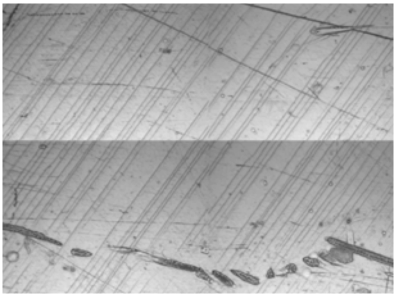

b

Fig.5. Surface pattern of aluminium specimen in initial (a) and strained state (b): ε= 0,044 (x400)

The structural susceptibility reads according to the definition

$$\chi = \left(\frac{\partial^2 F}{\partial^2 \varepsilon} \right)^{-1} = \frac{1}{V_a} \frac{\Delta\varepsilon}{\Delta\tau}, \tag{10}$$

where $\tau = \tau_{\max} = \sigma/2$ is the maximum value of the shear stress providing the orientation of slip bands, V_a is the effective activation volume. The increments of stress and strain were calculated according to the formulas for each state

$$\Delta\tau = \tau_{i+1} - \tau_i, \quad \Delta\varepsilon = \varepsilon_{i+1} - \varepsilon_i, \tag{11}$$

where the index corresponds to the points along the deformation diagram.

Activation volume V_a was estimated as $V_a = lb^2$, where b is the value of the Burgers vector given by the formula $b = a/2 < 110 >$ according to the slip orientation in the crystals strained in the direction <110>.

To follow the generalized version of the Fluctuation Dissipation Theorem the presentation of the effective temperature is given by the formula

$$T_{eff}(l) = \frac{V_a \ \Delta\tau \left\langle \left\langle \Delta\varepsilon(l) \right\rangle_x^2 - \left\langle \Delta\varepsilon^2(l) \right\rangle_x \right\rangle_{l'}}{\kappa_B \Delta\varepsilon}, \tag{12}$$

where κ_B is the Boltzmann constant. The plots of the effective temperature versus scale are presented in Fig.6 for different strains along the deformation diagram.

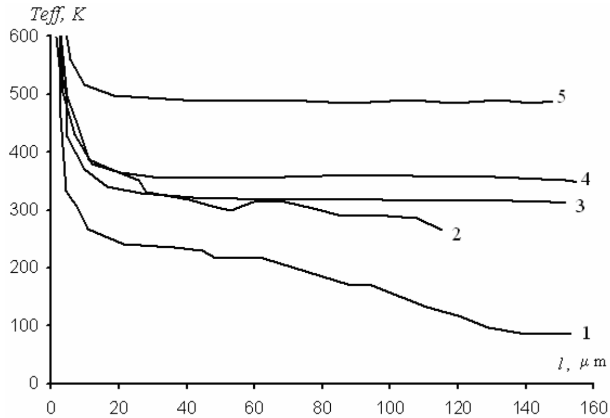


Fig.6. Effective temperature T_{eff} versus scale l for the strains: 1 - ε = 4.0%; 2 - ε = 4.4%; 3- ε = 5.1%; 4 - ε = 5.8%; 5 - ε = 6.3%.

The initial states of plastic flow (curves 1, 2) are characterized by the dependence of the effective temperature T_{eff} on the scale l that is in the contradiction with the definition of thermalization condition of strained specimen as thermodynamic system. The sensitivity of the effective temperature to the scale reflects the weak correlations between the dislocation carriers and realization of plastic flow as thermally activated discrete activation slips of dislocations. The roughening of dislocation substructures under the straining and the formation of collective modes of mesodefects lead to the increase of structural stresses and long-ranged correlation spreading on the entire specimen length. The effective temperature as the spatial-temporal invariants can be introduced in this case to characterize the thermodynamic state of plastically strained material. The independence of the effective temperature T_{eff} on the scale l for the strains that exceed ε = 5.1% supports this theoretical prediction.

Discussion

Variety of systems with slow dynamics, and plastically strained materials are the typical case, demonstrate asymptotically power statistical distribution of entirely measured variables. These distributions are characteristic for out-of-equilibrium systems revealing the violation of significant thermodynamic property – the entropy additivity that follows from the Boltzmann-Gibbs statistics. The entropy additivity for the equilibrium (or near-equilibrium) thermodynamic systems is the consequence of local interaction between the system elements. However, the large class of phenomena represents the interest when the elements reveal long-ranged interaction. This situation is typical for mesoscopic systems, for instance "solids with mesodefects", when the generation of collective modes of mesodefects and long-ranged interaction lead to the decrease of the system symmetry and slow driven dynamics related to the kinetics of collective modes. Generalization of the Boltzmann-Gibbs statistics for the out-of-equilibrium systems with slow dynamics is discussed in [3] and it is well-known as non-extensive statistics or superstatistics. The idea of superstatistics is the assumption concerning the possible generalization of the Boltzmann factor under the definition of distribution $B(E)=\int_0^\infty d\beta\, f(\beta)e^{-\beta E}$ related to the independent β statistics. The discussion of possible reasons of reformulation of the Boltzmann-Gibbs statistics [*] is related to the typical case of the behavior of out-of-equilibrium systems revealing stationary states or slow driven dynamics when the ergodicity assumption can be not generally used. As it was shown in [2] the generalization of the Boltzmann-Gibbs statistics (non-extensive statistics or superstastistics) corresponds to early developed extension of classical version of thermodynamics using the method of effective field for the definition of non-equilibrium free energy. The comparative analysis of two approaches was developed using the results of statistically based thermodynamics of mesoscopic defects that allowed one to establish new class of critical phenomena – structural-scaling transitions. These transitions allowed the explanation of the self-criticality scenario of plastic flow, generation of collective modes of mesodefects related to long-ranged interaction in the dislocation substructures that provides the introduction of spatial-temporal invariants in the term of effective temperature to characterize the thermalization conditions of plastically strained solid.

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References

[1] O.B.Naimark, in: Advances in Multifield Theories of Continua with Substructure, edited by G.Capriz and P.Mariano, Birkhauser, Boston (2004), p.75-114

[2] Yu.V.Bayandin, V.A.Leontiev, S.L.Permjakov and O.B.Naimark: Physical Mesomechanics Vol. 8, No. 5, (2005), p. 39

[3] C. Beck and E.C.D.Cohen: Physica A 322 (2003), p.267