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Description of Intermittent Plastic Flow

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Given the nanoscale point defects a transition from the solid state of the medium to state of ordinary and intermittent plastic flow was considered. Synergetic equations describing the self-organization of the particles and the vacancies of the system have been proposed. Phase diagram of the system and distribution function were constructed and analyzed.

Keywords: Nanoscale defects, Vacancy concentration, Langevin equation.

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1. INTRODUCTION

Deformation of solids has attracted attention of engineers, technologists and scientists for a long time [1]. The interest grows for a study of deformation of a continuous medium (granular materials, suspensions, etc), which are also characterized by elasticity and viscosity properties under certain conditions [2, 3]. But it is often necessary to know the subtle changes of the media (and increasingly at the nanoscale). Therefore, the task of studying the nano-level defects and their effect on deformation processes in solids and continuous media becomes actual.

In this the study of plastic flow – a change of solid state under external load, accompanied by significant residual deformations without destruction – particularly stands out. But the theoretical description of plastic flow is a difficult task despite the fact that there is a huge amount of numerical and theoretical methods [4-8]. In standard approaches for crystals plastic deformation is usually associated with the emergence and evolution of the dislocations within the grains. For amorphous materials and continuous media the plastic flow theoretical description remains a difficult challenge. Since plastic flow originates at the nanoscale, we decided to abandon the standard consideration of linear defects and study the effect of point defects (e.g. vacancies). Although for amorphous solids and granular medium the concept of vacancies is unacceptable, but the description of the local free volume is possible [9].

Usually to characterize the plastic deformation the dependence of the displacement (or strain rate) on the applied load is investigated. But since we want to investigate the effect of nanoscale defects, it is necessary to consider additional parameters and variables reflecting the presence of vacancies (in the case of crystalline solids).

2. THE LOCAL FREE VOLUME

The understanding of the basic laws of plastic flow can be achieved in the framework of the hydrodynamic theory [8,9], based on the parameter

$$m = \frac{n_0(r,t) - n(r,t)}{n_0(r,t)}, \qquad (2.1)$$

where $n_0(r,t)$ – is the density of lattice sites, which depends on both the temperature and the strain, and $n(r,t)$ is the number of particles per unit volume of material that depends from strain [8].

For crystalline solids Eq.(2.1) equation is associated with the concentration of vacancies. But for amorphous solids and continuous media the density of lattice sites makes no sense, so we can use another interpretation.

For crystals n_0 can still be interpreted as the density of particles, which will have a system with an infinite compression pressure at a constant value of the lattice constant. Accordingly, for amorphous solids n_0 can be defined as the particle density after compression with an infinite pressure at a constant distance to the nearest neighbor [9]. The last one, of course, is difficult to achieve experimentally, but nevertheless the accurate estimation of n_0 can be obtained under the condition that the compression is performed at a constant temperature and that the distance to the nearest neighbors correctly determined. As a result, to determine the n_0 at a given pressure P and temperature T with sufficient accuracy we can use the approximation [9]

$$n_0 = f(T,P) = \lim_{P'\to\infty}\left[\frac{r_s\ T,P'}{r_s\ T,P}\right]^3 n\ T,P' \ , \qquad (2.2)$$

where $r_s\ T,P$ is the distance between nearest neighbors. Then, in general, the parameter m may be defined as the free local volume.

Further, for simplicity, we will use the concept of vacancy concentration, but taking into account (2.2), all the results can be generalized to the case of a continuous medium or amorphous materials.

For the description of the plastic deformation the value of m will be critical. Indeed, in the absence of vacancies ($n = n_0$, $m = 0$) we have a solid state of the matter (the external stress gives rise to only elastic deformation); for the presence of vacancies ($n < n_0$, $m \le 1$) the external stress leads to plastic flow of the material.

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3. EVOLUTION EQUATIONS

The density and the momentum density is usually given by the dynamical equations [7, 10, 11]

$$\frac{\partial}{\partial t}\delta\rho = -\bar{\rho}\,\mathrm{div}\mathbf{v}, \tag{3.1}$$

$$\bar{\rho}\frac{\partial}{\partial t}\mathbf{v} = \nabla\sigma + \eta_0\nabla^2\mathbf{v}, \tag{3.2}$$

where $\bar{\rho}$ is an average density of the material, ($\delta\rho$ represents its changes), $\mathbf{v} = \frac{\partial \mathbf{u}}{\partial t}$ is the strain rate, σ is the elastic stress ($\nabla = \partial/\partial\mathbf{r}$), η_0 is the dynamic viscosity.

Using the definition (2.1), the relationship of the strain rate $\mathbf{v}$ and stress σ with the free energy, we can obtain [12] the equation

$$\dot{m} = \lambda_0\nabla^2\sigma + \lambda_0\nabla^2\left(\frac{\delta F}{\delta m}\right)_{\mathbf{u}} \tag{3.3}$$

Here λ_0 is a kinetic coefficient, the free energy of the system

$$F(m) = \frac{A}{2}m^2 + \frac{B}{4}m^4, \tag{3.4}$$

has the Landau expansion form for the second order phase transition ($A > 0$).

As a result, we can describe the transition from a solid state to a plastic flow as self-organization of particles in a medium with a particular set of vacancies. Parameter m can be chosen as an order parameter, which distinguishes the mentioned states.

It is known that the Lorenz system is a simple scheme, describing the self-organizing system [13]. On an example of the self-organization processes in particle ensemble [14] and solids [15, 16] the system of synergistic equations for our case becomes

$$\begin{aligned}
\dot{m} &= -\frac{m}{t_m} + \lambda_0\nabla^2\sigma + \lambda_0 A\nabla^2 m + g_m\nu\nabla^2\mathbf{v},\\
\dot{\mathbf{v}} &= \frac{1}{\bar{\rho}}\nabla\sigma + \frac{\eta_0}{\bar{\rho}}\nabla^2\mathbf{v} - g_{\mathbf{v}}m\sigma,\\
\dot{\sigma} &= \frac{\sigma_e - \sigma}{t_\sigma} - g_\sigma\nu m\nabla^2\mathbf{v} + \sqrt{I}\eta(t).
\end{aligned} \tag{3.5}$$

In contrast to equation (3.3) for the rate of change of the parameter m we took into account additionally the microscopic dissipation channel (t_m is a characteristic relaxation time) and the hydrodynamic contribution $\nu\nabla^2\mathbf{v}$ ($g_m > 0$ is the coupling coefficient, $\nu = \frac{\eta_0}{\bar{\rho}}$ is a kinematic viscosity). The strain rate $\mathbf{v}$ plays the role of a conjugated field, and the stress σ is a control parameter. The last one relaxes during time t_σ to the value σ_e, given by the external influences, ($g_\sigma, g_{\mathbf{v}}$ is a positive coupling constant).

At the distances of particle size the fluctuations occur, so to account them we add in the last equation of the system (3.5) the stochastic source $(\sqrt{I}/t_\sigma)\eta(t)$, which is characterized by intensity I and white noise $\eta(t)$:

$$<\eta(t)>=0,\ <\eta(t)\eta(t')>=\delta(t-t'). \tag{3.6}$$

Accounting that the relaxation time of the vacancy concentration is sufficiently larger than other time scales we can use an adiabatic approximation

$$\frac{\tau}{t_m} \ll 1;\ \frac{t_\sigma}{t_m} \ll 1. \tag{3.7}$$

As a result we can obtain the dependence of the conjugated field and control parameter:

$$\begin{aligned}
\sigma(t) &= \frac{\sigma_e}{1 + m^2/\gamma^2} + \frac{\sqrt{I}\eta(t)}{1 + m^2/\gamma^2},\\
v''(t) &= \frac{m\sigma_e}{\gamma^2 + m^2} + \frac{m\sqrt{I}\eta(t)}{\gamma^2 + m^2}.
\end{aligned} \tag{3.8}$$

Here we use dimensionless variables and the parameter γ is given by

$$\gamma^2 \equiv \frac{\eta_0\tau}{\bar{\rho}t_m\lambda_0 A}. \tag{3.9}$$

Further we use the notation

$$\begin{aligned}
f(m) &= -m + \frac{m\sigma_e}{\gamma^2 + m^2},\\
I(m) &= I\left(\frac{m}{\gamma^2 + m^2}\right)^2.
\end{aligned} \tag{3.10}$$

Substituting Eqs.(3.8) into the first equation of system (3.5) we obtain the Langevin equation

$$\dot{m} = m'' + f(m) + \sqrt{I(m)}\eta(t), \tag{3.11}$$

which has a set of random solutions with distribution given by Fokker-Planck equation:

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial m} - f(m)P + \frac{\partial}{\partial m}[I(m)P]. \tag{3.12}$$

4. PHASE DIAGRAM AND PROBABILITY DISTRIBUTION

Let us investigate the stationary distribution case ($\partial P/\partial t \equiv 0$). Then the distribution of homogeneous solutions of the Langevin equation (3.11) has a form

$$P(m) = \frac{1}{I(m)}\exp(-U(m)), \tag{4.1}$$

where $U(m)$ is an effective energy of vacancies and is defined by the equation

$$U(m) = \frac{1}{2}\frac{\gamma^4}{I}\left[\frac{1}{2}\frac{m^4}{\gamma^4} + \left(2 - \frac{\sigma_e}{\gamma^2}\right)\frac{m^2}{\gamma^2} + \ln\left(\frac{m^2}{\gamma^2}\right)\left(1 - \frac{\sigma_e}{\gamma^2}\right)\right] \tag{4.2}$$

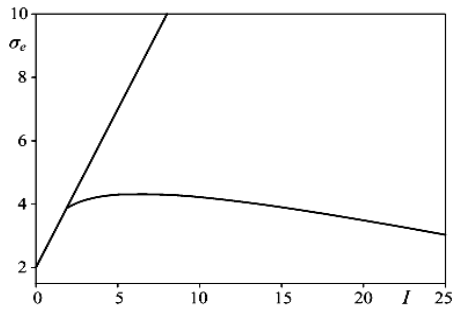

Fig. 1 – Phase diagram of the system at γ^2=2.

Maximum of the distribution (4.1) is given by the system parameters and demonstrates the phase diagram of the system (see Fig.1).

$$\left(\frac{I}{\gamma^2}\right)^2 - I\left[\frac{27}{2} - \frac{1}{8}\frac{\sigma_e^2}{\gamma^4} + \frac{9}{2}\frac{\sigma_e}{\gamma^2}\right] + \frac{\sigma_e^3}{2\gamma^4} = 0 \qquad (4.3)$$

The corresponding dependencies of the distribution function of the vacancy concentration and the energy of vacancy formation are shown in Fig. 2.

As seen from phase diagram three domains is realized: the lower domain of the phase diagram characterizes solid state, as evidenced by the distribution function (curve 1 in Fig.2a has a maximum value for zero concentration of vacancies); at the top domain the plastic flow is realized (curve 3 in Fig.2a has a maximum for sufficiently large values of the concentration of vacancies); and finally the largest domain of the phase diagram corresponds to intermittent motion, when the distribution of vacancies has two maxima (curve 2 in Fig.2a).

Thus knowing the external load and parameters of the medium and manipulating them we can achieve the transition from the solid state to the plastic flow or intermittent flow regime (the so-called stick-slip regime).

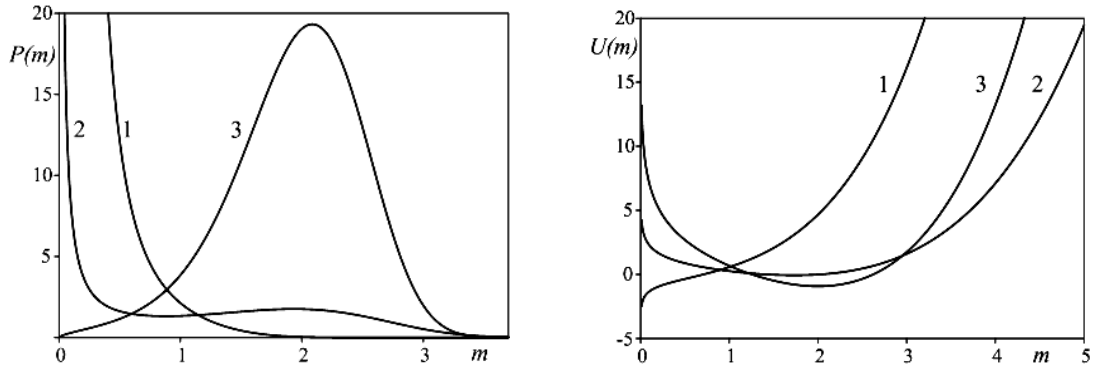

Fig. 2 – a) The dependence of the probability of vacancies concentration at γ^2=2, b) the dependence of the effective energy. Curve 1 corresponds to the values $\sigma_e = 5, I = 7$; curve 2 – $\sigma_e = 2, I = 1.5$; curve 3 – $\sigma_e = 6, I = 3$.

5. CONCLUSION

A result of the study it was shown that the description the intermittent plastic flow of the media is possible within synergetic representation. At the same time, not to limit the consideration by linear defects, the nanoscale defects were taken into account, resulting in the concentration of point defects, which was taken as a basis of our analysis.

The results obtained can be used for modeling the processes occurring during machining, surface treatment selection modes in micromechanical technologies (grinding, rolling out the ball, and ultrasonic vibrotreatment effects, etc.), in order to reduce errors in the experiments on friction coefficient, microhardness, adhesion and others, as well as to predict the behavior of micromechanical systems.

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