ФИЗИЧЕСКАЯ ХИМИЯ И ТЕХНОЛОГИЯ НЕОРГАНИЧЕСКИХ МАТЕРИАЛОВ

УДК 541.2: 548.4

THE SELF–ORGANIZATION AND EVOLUTION OF DISLOCATION STRUCTURES UNDER TREATMENT AND STRENGTH EFFECT ON METALS

A.K. EMALETDINOV
e–mail: emaletd@mail.ru

Technological Institute, Ufa, Russia

Article was presented in September 12, 2000

1. Introduction

The treatment and strength effect are used for the receipt of special physical and chemical properties of metals [1—3]. These properties are determined by the dislocation structures of materials. Under the treatment and strength effect of mono– and polycrystals of f.c.c. and b.c.c. metals it generate the 10^{11}—10^{12} cm^{-2} interactive with each other dislocations and it experimentally observed. the development and reorganization of dislocations substructure for materials with different type of crystalline lattice. The experimentally observed dislocation substructures constitute the hierarchical sequence and include homogeneous, mesh, cell, subgrain and other substructures. The change of one dislocation structure to another take place when stress σ (deformation ε) and density of dislocations ρ exceed the critical values : $\sigma \geq \sigma_C^{(i)}$, $\varepsilon \geq \varepsilon_C^{(i)}$, $\rho \geq \rho_C^{(i)}$ where $i = 1, 2, ...$ the number of structures. The type of dislocation structures are determined by the sequence of critical values of parameters $\sigma_{,,1} < \sigma_{,,2} < \sigma_{,,3} < \sigma_{,,4} < \sigma_{,,5} < ...$ (or $\rho_{,,1} < \rho_{,,2} < \rho_{,,3} < \rho_{,,4} < \rho_{,,5} < ...$). The experimental diagram [2, 3] of formation of various types of dislocation structures depending from temperature and stress is

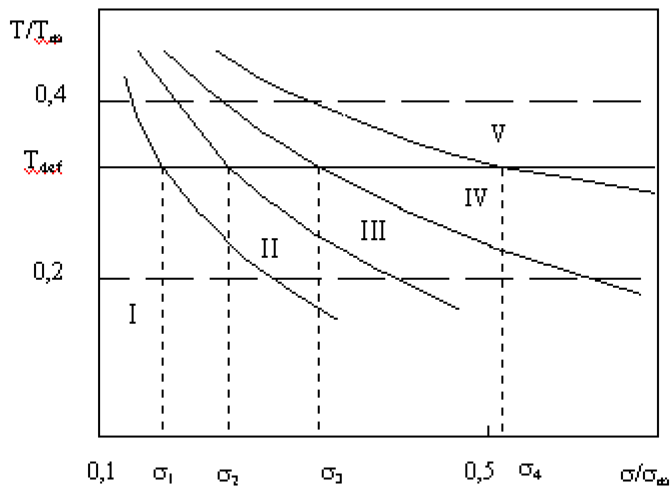

Fig. 1. Schematic representation of two variable (σ, T_0) diagram of dislocations structures

The self–organization of the spatial heterogeneous dissipative structures are observed at the deferent physical and chemical non–equilibrium systems, which include the huge amount of interactive elements [4]. Now the greater amount of work [2, 3, 5] have been appeared in which were proposed the equations of dislocation kinetics describing the main dislocation processes: multiplication, immobilization, diffusion, annihilation, etc. and were used the principles of synergetics and non–equilibrium thermodynamics for their analysis. On the basis of these equations were described the formation of some dislocation structures with the use of the harmonic appropriation for critical density of dislocation fluctuations at the fixed temperature T. At the same time it is necessary to know a two–parameter diagram of bifurcations of kinetic equation solutions depending from temperature and stress and to get the main types of solutions of the dislocation kinetic equations and to compare theirs with the structured dislocation conditions observed in the experiment.

2. Model of dislocation kinetic and basic equations

We shall consider kinetics of two slip systems of rectilinear infinite dislocation in two crossed planes and ensuring plastic deformation of a bidimensional polycrystal. One slip system with density of dislocations $\rho_1(x_1, x_2, t)$ is parallel to axis x_1. Second slip system with density of dislocations $\rho_2(x_1, x_2, t)$ is parallel to axis x_2. The immobile dislocations create the internal stresses which add to the effective stresses. This model is investigated in much tasks [2, 3, 5]. The exact description of elementary processes of multiplications, annihilations, mutual capture, movement and "diffusion" and others is very difficult problem and so in general case the system of kinetic equations is very complex. The equations of dislocations kinetics in a general kind have form [2, 3, 5]

$$\frac{\partial \rho_1}{\partial t} = A_1(\sigma - \sigma_{C1}) - M_1\rho_1^2 - K\rho_1\rho_2 + D_1\Delta\rho_1 + m_{11}\rho_1 - m_{12}\rho_1, \tag{1}$$

$$\frac{\partial \rho_2}{\partial t} = A_2(\sigma - \sigma_{C2}) - M_2\rho_2^2 - K\rho_1\rho_2 + D_2\Delta\rho_2 + m_{21}\rho_1 - m_{22}\rho_2. \tag{2}$$

where A_i $(i = 1, 2)$ is speed of dislocation generation by sources, $M_i \approx M_{0i}T$ is are constant of mutual annihilation of dislocations determined by temperature T, physical characteristics of dislocations and elastic properties of metal and investigated in [2, 3, 5], K is constants describing the mutual reactions of dislocations of different slip system; $m_{ii} \approx m_{0ii}T$ $(i = 1, 2)$ is constants describing the multiplication of dislocation due the double cross sliding [5], $\Delta = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2$ is Laplas operator, x_1, x_2 are rectangular Cartesian coordinates, $D_i \approx D_{0i}T$ is coefficient of "difussion" of fluctuation of dislocation density [2, 5]. The constants D_i, M_i, K, m_{ij}, D_i were investigated in much works above and have the complex form.

The first member of the right part of the equations of system (1), (2) describes generation of dislocations, second and third — annihilation and both mutual capture, fourth — diffuse, the member fifth — multiplication of dislocations due to double cross sliding, sixth — absorption in grain boundaries. At the analysis of the solution types of system of stationary equations (1), (2) were used: numerical modeling, construction of phase trajectories and diagrams, Lypunov factors, reflections of Puankare [2, 4]. The solutions were searched of two kind:

a) similar,

б) of periodic nonlinear waves on the time and space.

At numerical modeling the system was resulted to undimension form with parameters: $\dot{\varepsilon}t$, ρ_i/ρ_c, $\sigma/\sigma_p = 0{,}1$ to $0{,}6$ and $T/T_m = 0{,}2$ to $0{,}4$, where σ_p is stress of destruction, T_m is temperature of melt, $\dot{\varepsilon} = 0{,}001$ s^{-1}, $\rho_c = 10^{12}$ m^{-2} are the typical magnitude. The estimations of coefficients of equation system (1) are obtained for the typical metals Al, Cu, Fe. The coefficient A is equal to the generation dislocation speed on the initial stage of deformation at $\varepsilon \approx 0{,}02$ to $0{,}05$, $\sigma/\sigma_p \approx 0{,}1$ and has estimation $A \approx 10^4$ to 10^5 s^{-1}Pa^{-1}. The coefficients M are equal to $M_i \approx 10^{-12}$ to 10^{-13} m^{2}s^{-1}K [2]. The coefficient

K is equal to $K \approx 10^{-14}$ to 10^{-15} m^{2}s^{-1}. The coefficients D_i are equal to $D_i \approx 10^{-14}$ to 10^{-15} m^{2}s^{-1}K. The coefficient m_{11}, m_{12}, m_{21}, m_{22} are equal to [4, 10] m_{11}, $m_{22} \approx 10$ to 100 m^{2}s^{-1} and m_{12}, $m_{21} \approx 0{,}1$ to to 1 m^{2}s^{-1}.

3. Results of numerical modeling of equation system

It installed the stationary conditions. The method of [5] was used for a finding the positions of stationary points. For the determination of area of stability of stationary points for parameters (σ, T) we research a dependency of own values of Jakoby matrixe from these parameters using the linear equation system obtained from system (1) near the stationary point. The changing of nature of stability of stationary point occurs in consequence of direct or inverse Turing bifurcations when $\mathrm{Re}\lambda_i = 0$, λ_i is own values of matrixes. In initial area on the parameter σ system (1), (2) has a single unstable stationary point O_1 of type a unit — saddle. The unstable stationary point O_2 of type a saddle — focus depending from the values of parameter T arise in the system. The two–parameters diagram of system state are shown on the Fig. 2

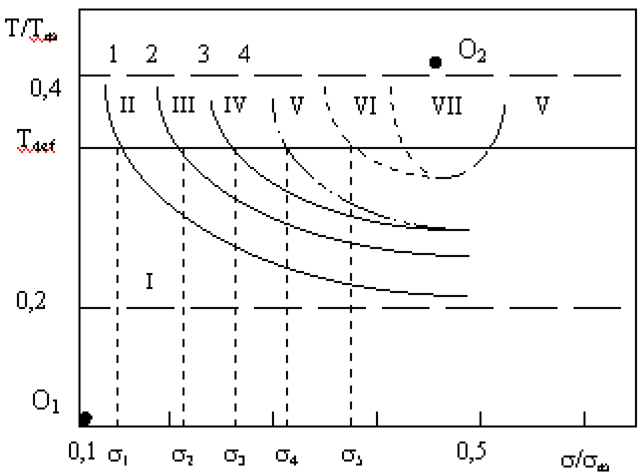

Fig. 2. Schematic representation of two variable (σ, T_0) diagram of basic type of solutions of system

Paint O_1 is of type unit — saddle, O_2 is saddle — unstable focus. Magnitudes σ_{C1}, σ_{C2}, σ_{C3}, σ_{C4} are critical stress and curve 1, 2, 3, … are the line of transition from one type solutions to another

The line 1 is bifurcation line of transformation stationary point unit into saddle. Line 2 of Turing bifurcations separates stable and unstable area of system conditions. The line 3 is the line of change of type of stability of stationary point O_2 from the saddle to a focus and in system the different wave and dissipative modes exist. As is seen from Fig. 2. the theoretical lines of bifurcation of solutions describe the experimental diagram of dislocation substructures (Fig. 1) well enough. In central area on the parameter T the system has a single unstable stationary point and consequently different complex nonhomogeneous periodic spatial dislocation dissipative structures. By use of numerical modeling the basic kind of solutions of equation system (1) were obtained and which can describe dislocation substructures known at experiments and depending from parameters σ and T. There are next basic kind of solutions: (I) steady, stationary, homogeneous solutions; (II) quasi–harmonic wave, (III) bi–harmonic, (IV) alternate, (V) sub–harmonic, (VI) nonlinear waves, (VII) chaotic waves. It is obtained the following hierarchical sequence of critical stress at fixed temperature $T = 3{,}5T_m$:

$$\sigma_{,,1} < \sigma_{,,2} < \sigma_{,,3} < \sigma_{,,4} < \sigma_{,,5} < \ldots$$

of occurrence of new types of modes which reflected change of dislocations substructures:

$$\mathrm{I} \Rightarrow \mathrm{II} \Rightarrow \mathrm{III} \Rightarrow \mathrm{IV} \Rightarrow \mathrm{V} \Rightarrow \mathrm{VI} \Rightarrow \mathrm{VII} \Rightarrow \mathrm{IV} \Rightarrow \ldots$$

At $\sigma < \sigma_{C1}$ the density of dislocations is homogeneous ρ_1, $\rho_2 \cong \text{const}$ (solution of type I). At $\sigma < \sigma_{C2}$ the solution of type II has the quasi–harmonic form. At $\sigma < \sigma_{C3}$ the solution of type III has the biharmonic form. At $\sigma < \sigma_{C4}$ the alternate solution of type IV. At $\sigma < \sigma_{C5}$ the solution of type V has the sub–harmonic form. At $\sigma < \sigma_{C6}$ the nonlinear solution of type VI has the form of knoidal waves. At $\sigma < \sigma_{C6}$ the solution of type VII has the form of stochastic waves. It is possible to consider that quasi–harmonic distribution II describes the polarization on dislocations of a different sign [2, 3, 5]. The two–periodic waves III are represented high–frequency fluctuations modulated low–frequency making. It is possible to consider that solutions III describe the formation of dipol structures. The alternate structures IV has the form including the periodically located the areas of high–frequency and low–frequency modes. The solutions IV describe the undislocation channels or the cell structures. The sub–harmonic solutions V having the high–frequency and low–frequency modes can describe the intermediate structures. The nonlinear waves VI consist from periodic narrow region of high density of dislocations and fluent wide region of low density dislocations The solutions VI can be interpreted as subgrain dislocation structure.

It gets [4] that the dissipate structures are generated in that cases only when a system size L exceeds the certain critical value L_m. The minimum system size (sample) is defined the minimum of dislocation density in the system which it is possible the generation of the collective modes of motion and self–organisation. Used the system (1), (2) it get that in first approximation the critical size has of the form $L \geq L_m \approx \sqrt{(D_1 + D_2)\pi^2 m_2 / 2M_1 A\sigma_i^2 - m_1 m_2}$.

4. Conclusions

When a temperature is changed it observed the more complex sequences under high temperatures or simple sequences under more low temperatures. At temperatures $0{,}2 \leq T/T_0 \leq 0{,}35$ it were observed more simple types of development of solutions: $\mathrm{I} \Rightarrow \mathrm{II} \Rightarrow \mathrm{V}$ and the others. At temperatures $T/T_0 \leq 0{,}2$ it was observed only uniform solution. The calculation of first Lypunov coefficients have shown that they are accordingly: $\lambda_1 / b \cong 0{,}0823$, $\lambda_{21} / b \cong -0{,}16$ under $T/T_m = 0{,}3$. The calculation length of period (size) dislocation structure equal to $l_d \cong b/\lambda_1 \approx 6 \cdot 10^{-6}$ cm that good agree with experimental data.

References

1. Meyer T. *Physicist–chemical crystallography* // M.: Metallurgy, 1972. — P. 480.
2. *Deformation Strenthening and Fracture Polycrystal Materials* / Ed. by Trefilov V.I. // Kiev: Naukova Dumka (in Russian), 1987. — P. 326.
3. Lihkachev V.A. and et al. *Cooperative Deformation Process and Localization of Deformation* // Kiev: Naukova Dumka (in Russian), 1989. — P. 320.
4. Nicolis G, Prigogine I. *Self–Organization in Nonequilibrum Systems* // Moscow: Mir, 1979. — P. 512 (Rus).
5. Malygin G.A. *Self–Organization Dislocation and Slip Localization in Plastic Deformed Crystals* // Fiz. Tverd. Tela. — 1995. — Vol. 37, No 1. — P. 3—42. (Rus).