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Mathematical modeling for the processes of strain hardening in heterophase materials with nanoparticles

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Abstract—An investigation of the process of deformation hardening and evolution of deformation defect medium in dispersion-hardened materials with face centered cubic matrices and nanoparticles was done. Mathematical model including balance equation for the deformation defects was used.

Keywords—deformation defects, dispersion-hardened materials, mathematical modeling, plastic deformation.

I. Introduction

PLASTIC deformation of face centered cubic (FCC) metals has been investigated for many years. Detailed descriptions have been developed to explain the basic process of plastic deformation which realise in single crystals of metallic materials [1]–[4]. The description of the macroscopic stress-strain behavior and deep understanding of the role of the different microscopic mechanisms are important from the viewpoint of both materials science and engineering applications.

An important role in wide range of deformation conditions in metals plays plastic deformation by crystallographic slip.

Although the basic mechanisms of plastic deformation have been known for a long time, the attempts of modeling the process of strain hardening and evolution of the defect medium taking into account the different mechanisms of generation and annihilation of deformation defects have only begun recently [5]–[10].

The primary goal of developing any mathematical models is to have a tool that can describe the behavior of material. One of the most important relationships that describe the material performance under loading is the stress-strain curve. Temperature and strain rate dependencies of the flow stress and densities of dislocations and concentrations of point defects also have great interest to researchers.

The mathematical models developed into different groups:

(a) Empirical models [11]–[14].

(b) Microstructurally-based models are based on the micromechanics of plastic deformation and are rooted in the thermally-activated motion of dislocations [15]–[19].

(c) Models based on the theory of thermal activation mechanism of dislocation motion, where the physical meaning of each model parameter will be shown by their relationships with microstructural characteristics [20].

The achievements in mathematical modeling and computational experiment have increasingly become in recent years. These achievements as information technology for obtaining new knowledge about the world around us are important for various fields of science. The apparatus of differential equations is used for the mathematical description of various natural phenomena and many fundamental laws [21]–[23]. Research evolution of a deformation subsystem, the roles of different mechanisms of generation and annihilation of various defects in the work hardening in FCC metals and alloys under loading are some examples of the problem where mathematical modeling can be effectively used. In this case differential equations of balance type widely use.

However exact solutions of differential equations are possible only for a limited class of problems. It is necessary a development of different methods for numerical solution of the system of ordinary differential equations (ODEs). The mathematical models of physical processes are often stiff. In this case it is important to made optimal choice of method for solution of ODEs and create new algorithms for analysis of physical process. The important role among the different numerical methods for solution of ODEs have difference methods. Their essential advantage is the simple algorithmization and the computer simulation [22].

Due to the unique properties nanostructure materials occupy a key position in modern materials science. Investigation of a role of the deformation defects in the regularities of plastic behavior is an essential component for the analysis of the physical properties of the materials. In this work we used a mathematical model, including the differential equations of balance of deformation defects [8], [24]–[28] to investigate temperature and strain rate dependencies of the flow stress and the role of different deformation defects in regularities of plastic behavior of materials with FCC matrix and nanodispersion hardening phase.

The dispersion hardening phase into the material leads to the considerable complication of a modeling object. Interaction of dislocations with the particles in the process of plastic deformation results not only in hardening effect, but also to appearance of new elements of dislocation structure. The scale characteristics of the hardening particles (size, shape and distance between them) can change the character and the result of this interactions.

The numerical experiments are simulated by the mathemat-

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ical model of the process of deformation hardening and evolution of defect medium in dispersion-hardened materials are done. The outline of this study is organized as follows: Section II gives a brief description of mathematical model; Section III presents the software for the numerical experiments; Section IV shows the results of experiments; and Section V presents the discussions and also conclusion.

II. Description of the Mathematical Model

The mathematical model of plastic deformation in dispersion hardened materials with nanoparticles describe in this section. The research is based on the assumption that the particles are incoherent, non-deformed and spherical. It takes into account the main processes of generation and annihilation of dislocations and point defects of different type [29]. The differential equations of the balance of deformation defects are used in the following form [29]:

$$\begin{aligned}\frac{d\rho_m}{da} &= \frac{F}{Db}(1-\omega_s P_{as}) - \\ &- \frac{2\rho_m^2}{\dot{a}}(1-\omega_s)\,\min(r_a, 1/\sqrt{\rho_m}) \times \\ &\times (c_{2v}Q_{2v} + \tilde{c}_{1v}Q_{1v} + \tilde{c}_i Q_i) + \\ &+ \frac{2b}{\dot{a}}[\alpha\sqrt{\rho}\rho_p^v(c_{2v}Q_{2v} + \tilde{c}_{1v}Q_{1v}) + \rho_p^i\tilde{c}_iQ_i] + \\ &+ \frac{1}{r_a}[\rho_d^i\tilde{c}_iQ_i + \rho_d^v(c_{2v}Q_{2v} + \tilde{c}_{1v}Q_{1v})],\end{aligned} \quad (1)$$

$$\frac{d\rho_p^v}{da} = \frac{\langle\chi\rangle\delta}{2\Lambda_p^2 b} - \frac{2\alpha b}{\dot{a}}\sqrt{\rho}\rho_p^v(2\tilde{c}_iQ_i - 2c_{2v}Q_{2v} - \tilde{c}_{1v}Q_{1v}), \quad (2)$$

$$\frac{d\rho_p^i}{da} = \frac{\langle\chi\rangle\delta}{2\Lambda_p^2 b} - \frac{2\alpha b}{\dot{a}}\sqrt{\rho}\rho_p^i(2c_{2v}Q_{2v} + 2\tilde{c}_{1v}Q_{1v} - \tilde{c}_iQ_i), \quad (3)$$

$$\frac{d\rho_d^v}{da} = \frac{1}{\Lambda_p b} - \frac{2b}{\dot{a}r_a}\rho_d^v(\tilde{c}_iQ_i + c_{2v}Q_{2v} + \tilde{c}_{1v}Q_{1v}), \quad (4)$$

$$\frac{d\rho_d^i}{da} = \frac{1}{\Lambda_p b} - \frac{2b}{\dot{a}r_a}\rho_d^i(c_{2v}Q_{2v} + \tilde{c}_{1v}Q_{1v} - \tilde{c}_iQ_i), \quad (5)$$

$$\begin{aligned}\frac{dc_{1v}}{da} &= q\frac{\tau_{dyn}}{6G} - \\ &- \frac{1}{\dot{a}}[(((1-\omega_s)\rho_m + \rho_d + \rho_p)b^2 + \tilde{c}_{1v} + \tilde{c}_i) \times \\ &\times Q_{1v}\tilde{c}_{1v} + Q_i\tilde{c}_i\tilde{c}_{1v} + (Q_i + Q_{2v})\tilde{c}_ic_{2v}],\end{aligned} \quad (6)$$

$$\begin{aligned}\frac{dc_{2v}}{da} &= \frac{5q\tau_{dyn}}{6G} - \\ &- \frac{2}{\dot{a}}[(((1-\omega_s)\rho_m + \rho_d + \rho_p)b^2 + \tilde{c}_i \times \\ &\times Q_{2v}c_{2v} + Q_i\tilde{c}_ic_{2v}) + \tilde{c}_{1v}^2Q_{1v}],\end{aligned} \quad (7)$$

$$\begin{aligned}\frac{dc_i}{da} &= q\frac{\tau_{dyn}}{G} - \\ &- \frac{c_i}{\dot{a}}[((1-\omega_s)\rho_m + \rho_d + \rho_p)b^2Q_i + \\ &+ \tilde{c}_{1v}Q_{1v} + c_{2v}Q_{2v} + (\tilde{c}_{1v} + c_{2v})Q_i].\end{aligned} \quad (8)$$

The mathematical model also includes an equation that connects strain rate with the stress and the density of deformation

TABLE I
Description of Mathematical Model Parameters

Parameter	Description
ρ	total dislocation density
ρ_d^i	density of dislocation in the dipole configurations of the interstitial type
ρ_d^v	density of dislocation in the dipole configurations of the vacancy type
ρ_d	$= \rho_d^v + \rho_d^i$, density of dislocations in dipole configurations
ρ_m	density of shear-forming dislocations
ρ_p^i	density of prismatic dislocation loops of the interstitial type
ρ_p^v	density of prismatic dislocation loops of the vacancy type
ρ_p	$= \rho_p^v + \rho_p^i$, density of prismatic dislocation loops
c_{1v}	concentrations of monovacancies
c_{2v}	concentrations of bivacancies
c_i	concentrations of interstitial atoms
c_j^0	concentration of thermodynamically equilibrium point defects of the jth type $(j = i, v)$
$\tilde{c}_j$	$= c_j + c_j^0$ total concentration of point defects of the jth type $(j = i, v)$
a	shear strain
a_t	strain rate
t	time
B	parameter, which is determined by the probability of dislocation barriers limiting the shear zone [8]
F	parameter, which is determined by the shape of dislocation loops and their distribution in the slip zone [8]
q	parameter that determines the intensity of point defects generation
T	temperature
Λ	average length of free dislocation segment [8]
Λ_p	distance between the centers of the particles
δ	diameter of particle of hardened phase
α	parameter of dislocations interaction
α_a	parameter of athermal interaction of dislocations
b	Burgers vector
β_r	fraction of reacting forest dislocations
D	diameter of the slip zone
G	shear modulus
$\langle\chi\rangle$	parameter of geometrical characteristics of dislocations on the particles
k	Boltzmann constant
ξ	fraction of forest dislocations
ν	Poisson coefficient
ν_D	Debye frequency
ω_s	fraction of screw dislocations
P_{as}	probability of annihilation of screw dislocations
Q_j	$=Z_j\nu_D exp(-U_j^m/kT)$, $j = i, v$
r_a	critical capture radius
τ	flow stress
τ_{dyn}	stress excess over the static resistance to dislocation motion
τ_f	friction stress
τ_a	athermic component of the resistance to the dislocation gliding
U_j^m	activation energy of migration of point defects of the jth type $(j = i, v)$
Z_j	number of sites possible for the jump of the defect of the jth type $(j = i, v)$

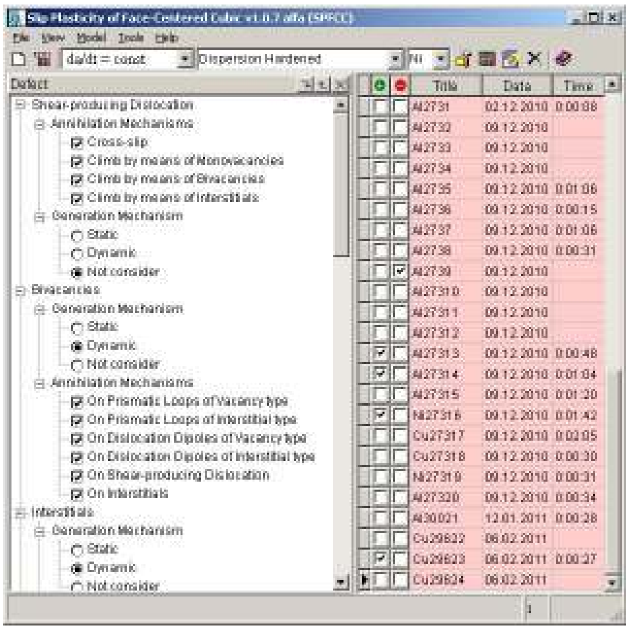

Fig. 1. Main Window of Software "Slip Plasticity of Face-Centered Cubic"

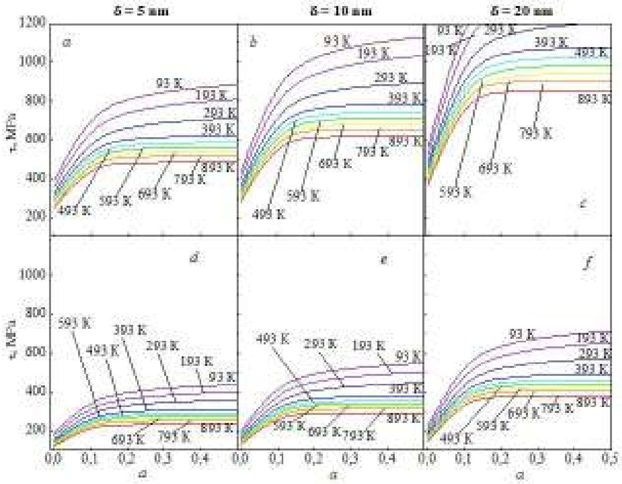

Fig. 2. Stress-strain curves of copper-based alloy. The distance between particles, nm: a, b, c – 50; d, e, f – 100. Strain rate is $10^{-3}s^{-1}$. The temperature and size of particles are shown in the figure

defects [29], [30]:

$$\dot{a} = \frac{8\nu B\beta_r^{1/2}\tau^3(((1-\beta_r)\rho_m + \rho_p + \rho_d)(\tau-\tau_a))^{1/3}}{\pi\xi^{1/6}F(1-\beta_r)G^{4/3}b^{1/3}(\tau^2 - G^2b^2\xi\beta_r\rho_m)\rho_m^{1/2}} \times \\ \times \exp\left(-\frac{0.2Gb^3-(\tau-\tau_a)\Lambda b^2}{kT}\right) \quad (9)$$

where $\tau_a = \tau_f + Gb/(\Lambda_p - \delta) + \alpha_a Gb\sqrt{\rho}$. The descriptions of mathematical model parameters are represented in Table I.

III. Software

The software "Slip Plasticity of Face-Centered Cubic" (SPFCC) for computer simulations of plastic deformation processes of strain hardening in heterophase materials with nanoparticles used in this study described in this section.

The software SPFCC are oriented for the users who has different qualification in programming and who has not an experience in solution of ODEs. In this software the mathematical models for various materials and loading similar to model (see the equations (1)–(9)) are realised in Delphi 2010 as integrated application package for Windows XP/Vista/7 [26], [27].

The package consists of four class hierarchies: first class for the representation of ODEs, a second class for the parameters of an ODEs problem, a third class hierarchy for solving initial value problems, and, at last, class for storing of result of experiments in data base. The software realization by class organization allows making the program more flexible for the further updating. The researcher must to choose the equations for numerical experiments. For viewing or change of variable, value of parameter, entry condition of model it is necessary to click mouse only (Fig. 1).

The equations of the model are stiff because the processes of generation and annihilation of deformation defects have essentially different rates. Use of implicit Gear's method of the variable order is more effective for solution of the model equations. The explicit Adams method with the step-by-step control of accuracy for the beginning of work is applied. The results of the carried out calculations together with the short description of the constructed model can be stored in data base or .txt files. The results of simulations can be represented as graphs of different type and save as .jpg file.

IV. Results and Discussion

Using the model (see the equations (1)–(9)), we studied the temperature and strain rate dependences on the curves of the flow stress and on the curves of densities of dislocation and on the curves of concentrations of point defect in dispersion-hardened materials with copper matrices and incoherent undeformable particles in condition of constant srain rate. The main computations were performed with software SPFCC using the following model parameters [3], [7], [31]: $b = 2.5\times10^{-10}m$, $F = 5$, $\alpha = 0.5$, $\nu_D = 10^{13}s^{-1}$, $\alpha_r = 0.3$, $\beta_r = 0.14$, $\xi = 0.5$, $\tau_f = 1\ MPa$, $\alpha_{dyn} = 0.33$, and $\omega_s = 0.3$. The initial conditions are as follows: $\rho_m = 10^{12}m^{-2}$, $\rho_d^v = \rho_d^i = \rho_p^v = \rho_p^i = 0$, $c_v = c_i = c_{2v} = 0$.

Results obtained for dispersion-hardened materials with the nanosize hardening phase indicate that the influence of the temperature and scale characteristics of the hardening phase on the flow stress is single-valued, but multidirectional. The flow stress is reduced with reduction of the particle size or with increase of the distance between them, or with rise of the deformation temperature (Fig. 2).

The analysis of dependence of the dislocation of different type and the total dislocation density (Fig. 3, scale characteristics of the hardening phase corresponding to Fig. 2 (b)) shows that with the rise of the temperature the dislocation density in the prismatic loops of vacancy and interstitial types are reduction (Fig. 3 (c), (d)), the density of shear-forming dislocations changes complex (Fig. 3 (b)). This is due to the

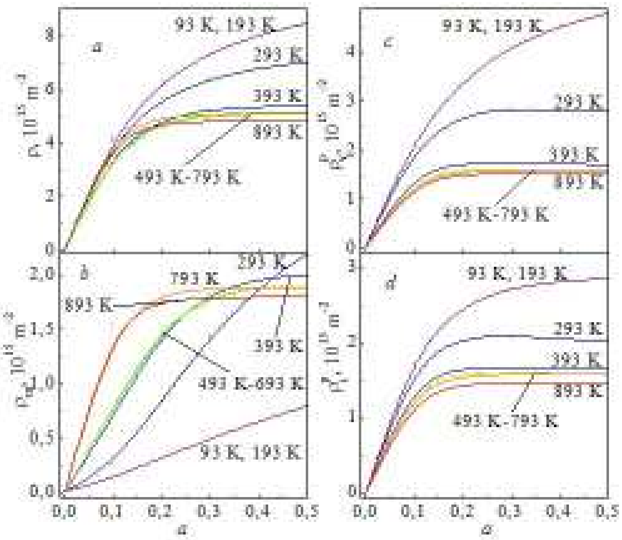

Fig. 3. The dependence of the total dislocation density (a), the density of shear-forming dislocations (b), the density of prismatic dislocation loops of vacancy (c) and interstitial (d) type on strain. The distance between the particles is 50 nm, the particle diameter is 10 nm. The temperature is shown in the figure

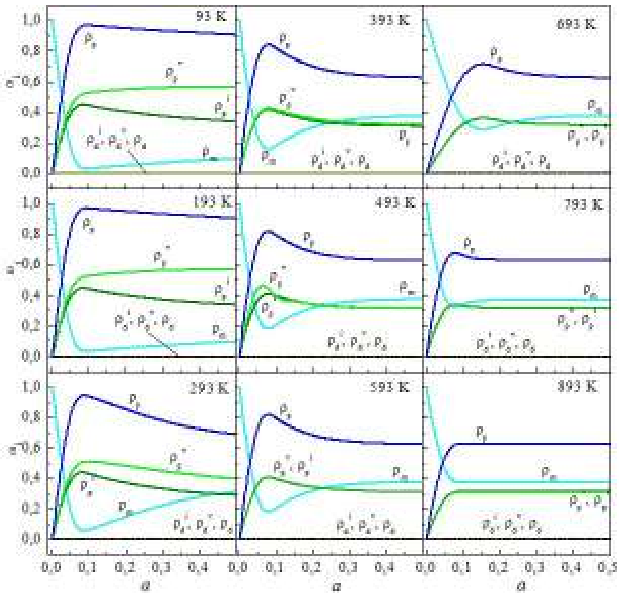

Fig. 4. Contribution from dislocations of different types to the total dislocation density in a dispersion-hardened material. The particle size is 10 nm, and the distance between the particles is 50 nm. The deformation temperature is shown in the figure

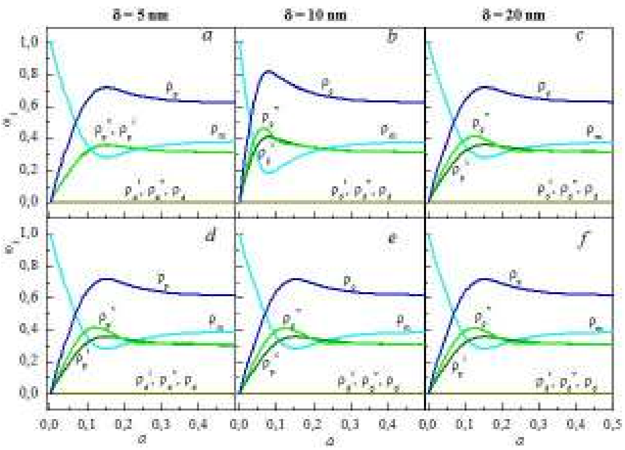

Fig. 5. Contribution from dislocations of different types to the total dislocation density during deformation at temperature 493 K. The distance between the particles, nm: a, b, c – 50; d, e, f – 100. The particle size is shown in the figure

fact that the density of shear-forming dislocations considerably depends on the intensity of generation and annihilation of defects of different types. On the one part, shear-forming dislocations annihilate as a result of climb of unscrew dislocations due to the accumulation of point defects on their extraplanes. On the other part, the density of shear-forming dislocations increases due to the fact that prismatic loops growing in the result of accumulation of point defects on them, lose stability and transform into shear-forming dislocations.

At low temperatures (93–293 K) prismatic dislocation loops of the vacancy type give the greatest contribution to the total dislocation density (Fig. 4). At meddle and high temperatures the dislocation densities in prismatic loops of the vacancy and interstitial types become approximately equal. Dislocation dipoles are not formed at wide range temperature and strain rate, and, as a result, do not contribute to the work hardening of material with nanoparticles.

For less deformation (0.05 and below) the dominating element of the dislocation subsystem is shear-forming dislocations for all studied temperatures and scale characteristics of the hardening phase. The contribution of shear-forming dislocations and dislocations in prismatic loops of the vacancy and interstitial types to the total dislocation density rise with increasing of deformation (Figs. 4 and 5). For larger particle and smaller distances between them, and different strain rates for different values of strain higher deformation hardening shows (Fig. 6). The most temperature dependence of flow stress in nanodispersed material for low temperatures (below 293 K) shows. This is due to the fact that at higher temperature more point defects participate in annihilation processes. It is one more range of the temperature dependence of flow stress for a low strain rate at high temperatures (Fig. 6 (g), (h), (i)). In this range of temperatures thermodynamically equilibrium point defects play a significant role in the annihilation of dislocations. For this reason at high temperatures the strain rate dependence of flow stress is obtained.

The form of the curves of temperature dependence for the density of shear-forming dislocation practically independs on the scale characteristics of the hardening phase. The dislocation density in the prismatic loops decreases with the rise of temperature in materials with different scale characteristics (Fig. 7 (d–f)).

For rise of temperature from 93 to 393 K the density of shear-forming dislocations increases and the density of dislocations in prismatic loops of the vacancy type decreases

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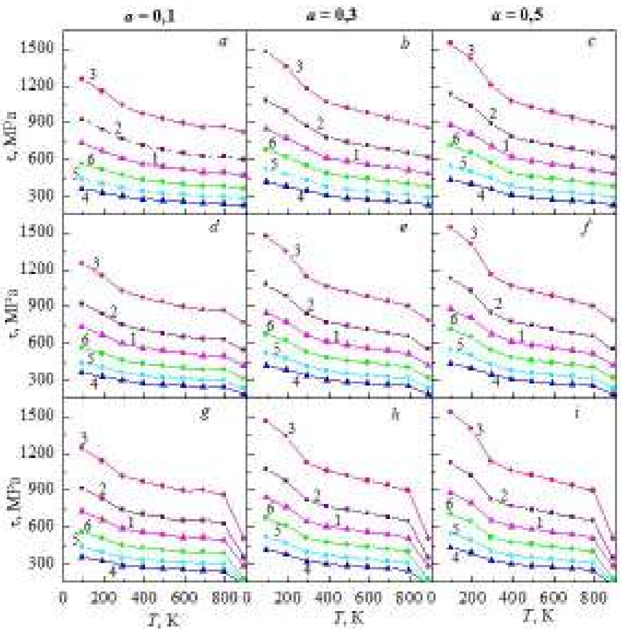

Fig. 6. The dependence of flow stress on deformation temperature. The size of strengthening particles, nm: 1, 4 – 5; 2, 5 – 10; 3, 6 – 20. The distance between the particles, nm: 1, 2, 3 – 50, 4, 5, 6 – 100, the strain rate, s^{-1}: a, b, c – 10^{-3}; d, e, f – 10^{-4}; g, h, i – 10^{-5}

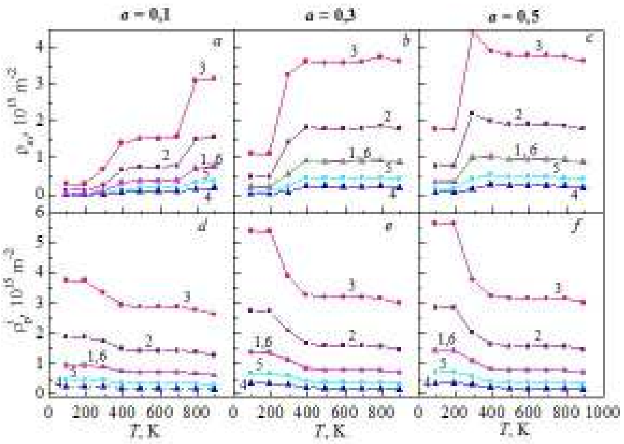

Fig. 7. The temperature dependence of the shear-forming dislocations density and density of the dislocations in prismatic dislocation loops of interstitial type. The distance between the particles, nm: 1, 2, 3 – 50; 4, 5, 6 – 100; particle diameter, nm: 1, 4 – 5; 2, 5 – 10; 3, 6 – 20. The strain rate is $10^{-3}s^{-1}$

at the different strain rates (Fig. 8). At meddle temperatures (393–793 K) the strain rate dependence and temperature dependence of the densities of both shear-forming dislocations and dislocations in prismatic loops of the vacancy type are not distinct (Figs. 7 and 8). At high temperatures (793–893 K) a decrease in densities of shear-forming dislocations and dislocations in prismatic loops occurs, which is caused by the involvement of thermodynamically equilibrium point defects in the annihilation processes. This is especially visible at high strain rate (Fig. 8 (a), (b), curve 3).

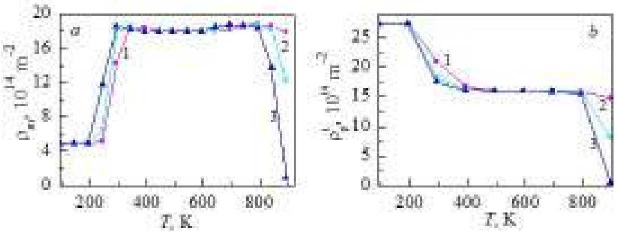

Fig. 8. The temperature dependence of: a – density of shear-forming dislocations, b – density of dislocation in prismatic loops of interstitial type. Particle size is 10 nm, the distance between particles is 50 nm, the strain is 0.3, the strain rate is: 1 – $10^{-3}s^{-1}$, 2 – $10^{-4}s^{-1}$, 3 – $10^{-5}s^{-1}$

V. Conclusion

The software Slip Plasticity of Face-Centered Cubic (SPFCC) for computer simulations of plastic deformation processes for research of strain hardening in heterophase materials with nanoparticles is used.

In dispersion-hardened materials with the nanodispersion hardening phase the flow stress and density of the components of the deformation defect subsystem are significantly higher than ones in materials with larger particles for the same volume fraction of the hardening phase.

For nanoscale characteristics of the hardening phase the generation of dislocations in dipole configurations is absent during deformation.

The various mechanisms of generation and annihilation of dislocations of various types dominate at different temperatures; it is results to the complex temperature dependence of the density of shear-forming dislocations.

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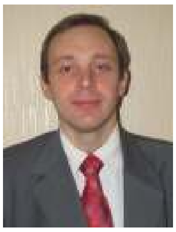

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