

Mathematical modeling of the deformation behavior of heterophase alloys at various characteristics of the strengthening phase

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Abstract. Further development of techniques and technologies urgently requires the creation of new materials with unique properties. One of the most popular and promising areas in materials science is the creation of composite materials with desired properties. Currently, in practice peening by dispersed particles is widely used to improve the properties of metal materials. It is necessary to investigate in detail the influence of various factors on the behavior of dispersion-hardened materials in a variety of conditions to control the properties of materials. Physical experiment, in addition to large investments, often takes a long time. This paper presents a mathematical model of plastic deformation of dispersion-hardened materials with a face-centered cubic (fcc) matrix and with incoherent and coherent nanoscale particles. Application of this model can significantly reduce the time of research and necessary amount of physical experiment. The results allow optimizing of experiment, identifying ways to improve the properties of the materials.

1. Introduction

Composite materials of various types are widely used in modern industry. The application of composites based on metal matrices strengthened by second phase remains of interest in materials science to improve the mechanical properties of materials for various applications. In this work, we present a model of plastic deformation in disperse-strengthened materials. Our investigation of the effect characteristics of the dispersed phase and conditions of deformation have on the plastic behavior of materials with FCC matrices is described. Mathematical modeling makes it possible to vary the characteristics of a material and the actions on it over quite wide ranges, anticipating and possibly even modifying the experiments. The mathematical model used here consists of a system of differential equations of balance of the elements of the deformational defect medium of the material.

2. The mathematical model

The mathematical model used here consists of a system of differential equations of balance of the elements of the deformational defect medium [1-3], allowing to conduct a study of the plastic behavior of a material with nanoscale particles of incoherent and coherent types [4, 5]. Dislocations bend around incoherent particles during plastic deformation, which, in addition to the hardening effect, causes the appearance of the new elements of the dislocation structure. Coherent zones and particles in the deformation process are cut by dislocations, and the work done during the passage through the



allocation of the first dislocation, further contributes to the flow stress [6-8]. Resistance to the motion of dislocations in the alloy with coherent and incoherent particles caused by stress of interaction with forest dislocations, by the friction stress τ_f , by the stress of cutting of particles, by the stress of bend around incoherent particles obtained in the form $\tau_a = \tau_f + \alpha Gb\sqrt{\rho} + (1-\mu)\Gamma_s\delta^2/2\sqrt{6}\Lambda_p^3 + \mu Gb/\Lambda_p - \delta$, where Γ_s is the surface energy of the matrix-segregation interface per unit area, Λ_p is the distance between particles of the second phase, δ is the diameter of the particles, α is the parameter of interdislocation interactions, G is the shear modulus, b is the magnitude of the Burgers vector, ρ is the density of dislocations, μ is fraction of incoherent particles in the material.

If the strengthening particles are coherent with the matrix, then in the course of the plastic deformation the emergence of the following types of defects is possible: shear-forming dislocations (we denote their density as ρ_m) and point defects: interstitial atoms (with concentration c_i), monovacancies (c_{1v}), and bivacancies (c_{2v}). If the material contains incoherent non-deformable hardening particles, the system of equations is supplemented by the balance equations of dislocation prismatic loops of interstitial (ρ_p^i) and vacancy (ρ_p^v) type, and by the dislocations in dipole configurations of vacancy (ρ_d^v) and interstitial (ρ_d^i) type. Moreover, in the equation for shear-forming dislocations the summands appear typical for materials with incoherent particles [1, 9-13]. The mathematical model in this case has the form:

$$\frac{d\rho_m}{da} = (1-\omega_s P_{as}) \frac{F}{Db} - \frac{2}{\dot{a}} (1-\omega_s) \rho_m^2 b \min(r_a, \rho_m^{-1/2}) (c_{2v} Q_{2v} + c_{1v} Q_{1v} + c_i Q_i) + \frac{2\alpha}{\dot{a}} b \sqrt{\rho} (\rho_p^v (c_{1v} Q_{1v} + c_{2v} Q_{2v}) + \rho_p^i c_i Q_i) + \frac{2b}{\dot{a} r_a} (\rho_d^i c_i Q_i + \rho_d^v (c_{1v} Q_{1v} + c_{2v} Q_{2v})), \quad (1)$$

$$\frac{d\rho_p^i}{da} = \frac{\mu <\chi> \delta}{2\Lambda_p^2 b} - \frac{2\alpha}{\dot{a}} \sqrt{\rho} \rho_p^i b (2c_{2v} Q_{2v} + c_i Q_i + 2c_{1v} Q_{1v}), \quad (2)$$

$$\frac{d\rho_p^v}{da} = \frac{\mu <\chi> \delta}{2\Lambda_p^2 b} - \frac{2\alpha}{\dot{a}} \sqrt{\rho} \rho_p^v b (c_{2v} Q_{2v} + 2c_i Q_i + c_{1v} Q_{1v}), \quad (3)$$

$$\frac{d\rho_d^v}{da} = \frac{\mu}{\Lambda_p b} - \frac{2b}{\dot{a} r_a} \rho_d^v (c_{2v} Q_{2v} + c_i Q_i + c_{1v} Q_{1v}), \quad (4)$$

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

$$\frac{dc_i}{da} = q \frac{\tau_{dyn}}{G} - \frac{c_i}{\dot{a}} [((1-\omega_s)\rho_m + \rho_p + \rho_d)b^2 Q_i + Q_{1v} c_{1v} + Q_{2v} c_{2v} + Q_i (c_{1v} + c_{2v})], \quad (6)$$

$$\frac{dc_{1v}}{da} = \frac{q\tau_{dyn}}{6G} - \frac{1}{\dot{a}} [(((1-\omega_s)\rho_m + \rho_p + \rho_d)b^2 + c_i + c_{1v}) Q_{1v} c_{1v} + Q_i c_i c_{1v} - (Q_{2v} + Q_i) c_i c_{2v}], \quad (7)$$

$$\frac{dc_{2v}}{da} = \frac{5q\tau_{dyn}}{6G} - \frac{2}{\dot{a}} [(((1-\omega_s)\rho_m + \rho_p + \rho_d)b^2 + c_i) Q_{2v} c_{2v} + Q_i c_i c_{2v} - Q_{1v} c_{1v}^2]. \quad (8)$$

Here a is the shear strain, D is the diameter of the shear zone, τ_{dyn} is the excess tension over the static resistance to motion of dislocations, F is a parameter defined by the shape of the dislocation loops and their distribution over the shear zone, ω_s is the fraction of screw dislocations, q is a parameter defining the intensity of generation of point defects; $<\chi>$ is the mean value of a parameter characterizing the *geometry* of the dislocations on the particles, $Q_j = Z_j v_D \exp(-U_j^{(m)}/kT)$ is kinetic coefficient, $U_j^{(m)}$ is the activation energy of migration of point defects of j^{th} type, Z_j is the number of sites accessible for a jump of a defect of j^{th} type ($j = i, v$), v_D is the Debye frequency, k is the

Boltzmann constant, T is the deformation temperature, $\rho_p = \rho_p^i + \rho_p^v$ is the density of prismatic dislocation loops, $\rho_d = \rho_d^i + \rho_d^v$ is the density of dislocations in dipole configurations.

The model takes account of the main processes of generation, annihilation, and relaxational transformation of dislocations of various types and also of point defects. Mutual conversions are possible between the structural elements in the course of deformation and subsequent relaxation processes. Here the nature and result of interactions of elements of the dislocation structure with the particles can vary with variation of the relationships between the scale characteristics of the strengthening phase (size and shape of particles and distance between them) and the distance between dislocations [3]. The balance equations of the dislocations take into account annihilation of screw dislocations by cross-slip and of non-screw dislocations by climb on account of precipitation on them of point defects. The balance equations of the shear-forming dislocations take into account the fact that with growth of the prismatic dislocation loops and increase in size of the shoulder of the dislocation dipoles, they lose stability and in their subsequent behavior become similar to shear-forming dislocations [1, 2]. The balance equations of the point defects take into account the full set of pairwise interactions between point defects.

The model takes into account that when the critical density of dislocations ρ_c (whose magnitude is determined by the scale characteristics of the strengthening phase) is reached in the material [1], dislocation dipole structures begin to form as a result of incomplete annihilation of the dislocation branches bending the non-deformable particles as they overcome them.

The system of equations of the mathematical model also includes an equation linking the strain rate with the applied action and characteristics of the defect medium [2]:

$$\dot{\alpha} = \frac{8}{\pi} \frac{\nu_D B \beta_r^{1/2}}{\xi^{1/6} F(1 - \beta_r)} \frac{\tau^3 ((1 - \beta_r) \rho_m + \rho_p + \rho_d)(\tau - \tau_a))^{1/3}}{G^{4/3} b^{1/3} (\tau^2 - G^2 b^2 \xi \beta_r \rho_m) \rho_m^{1/2}} \exp\left[-\frac{0,2Gb^3 - (\tau - \tau_a)\Lambda b^2}{kT}\right].$$

Here B is a parameter defined by the probability of formation of the dislocation barriers bounding the shear zone, β_r is the fraction of reacting forest dislocations, ξ is the fraction of forest dislocations, Λ is the average length of a free dislocation segment and τ is the applied tension.

3. The results of research

The calculations assumed that deformation of the crystal occurs to a constant strain rate $\dot{\alpha}$. The initial concentration of point defects is determined by the thermodynamic equilibrium concentration of point defects of the corresponding type at a given temperature, the initial density of shear-forming dislocations taken equal to 10^{12} m^{-2} . The size of hardening particles varied from 10 to 50 nm, the distance between the particles varied from 200 to 1000 nm.

Consider a material with hardened coherent and incoherent particles (Figure 1), deforming stress in the material increases during the whole process of plastic deformation. However, at temperatures above room temperature rate of increase the deforming stress is reduced. Decrease in the flow stress caused by more intense annihilation processes in dispersion-hardened material at temperatures above 293 K, compared with low temperatures (Figure 1).

Form of the curves of the flow stress depends strongly on the ratio of scale characteristics of the hardening phase (Figure 1). If the material in the deformation process has not achieved the critical density of dislocations, the stress-strain curves are smooth and monotonically increasing (Figure 1 *a, b, c, e*). If the material reaches a critical density of dislocations, the stress-strain curves have a kink due to appearance of new types of defects, it is the dislocation dipoles. With increasing temperature the length of the subcritical region increases. When the distance between the particles (Figure 1 *c, f, i*), as well as particle size increases, the critical density of dislocations is attained with a smaller amount of deformation (Figure 1 *g, h, i*), i.e. begin to form dipoles. Thus the rate of generation of dislocation dipoles is significantly higher in materials with a smaller distance between the particles. Consequently, when dipoles are begun to be formed, their density increases rapidly and becomes higher than the density of dislocation dipoles in the material with a large distance between the particles. This causes the greater

strain hardening in the transcritical region in materials with a smaller distance between the strengthening particles (Figure 1 *c, f, i*).

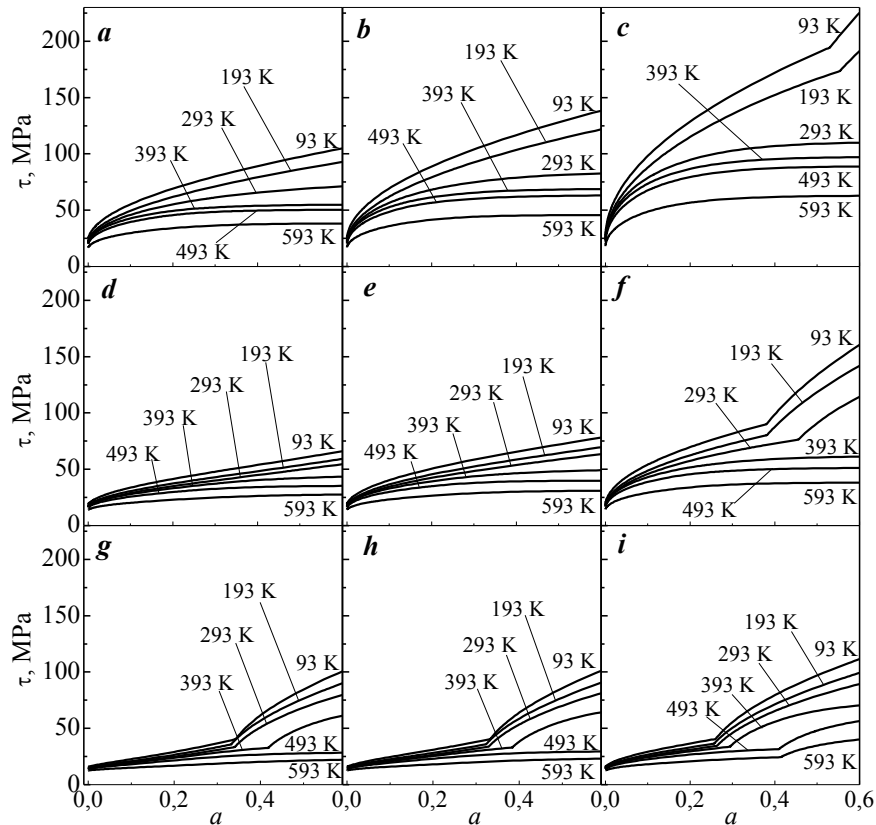


Figure 1. Stress-strain curves on the strain for an aluminum-based alloy at different temperatures. The fraction of incoherent particles is 25%. Distance between particles, nm: *a, b, c* – 200, *d, e, f* – 400, *g, h, i* – 1000; particle diameter, nm: *a, d, g* – 10, *b, e, h* – 20, *c, f, i* – 50. Strain rate 10^{-2} s^{-1} .

The greatest strain hardening at all temperatures is observed in the material having the greatest volume fraction of the strengthening phase (Figure 1 *c*). When increasing the size strengthening particles and reducing the distance between them the strain hardening increases in the subcritical region of dislocation densities. But when the critical density of dislocations is reached in the material, this dependence is not unequivocal (compare curves at temperatures of 93-393 K in figure 1 *b, e, h*).

The density of shear-forming dislocation (Figure 2 *a-c*) increases during deformation, where in the shape of the curves are different dependence on the temperature of deformation. The density of shear-forming dislocations as a function of the scale characteristics the strengthening phase is ambiguous: at low temperatures (93-193 K) the density decreases with increasing size of strengthening particles, whereas at higher temperatures (293 K or more) it increases.

The dependence of the density of shear-forming dislocations on the temperature is nonmonotonic. This is due to the fact that at moderate temperatures the contribution from the transition of the dislocations of prismatic loops and dipole configurations in the category of shear-forming dislocations is quite large, and at high temperatures it is reduced due to increased intensity of the annihilation process (Figure 2 *a, b, c*). At low temperatures the density of shear-forming dislocations is the lowest, since the contribution from the transition of prismatic loops and dipole configurations is negligible.

The dislocation density in the prismatic loops decreases with increasing strain temperature and decreasing the size of strengthening particles (Figure 2 *d-f, g-i*). At high temperatures the annihilation processes are more intensive. Dipole configurations begin to form in materials with larger reinforcing particles (Figure 2 *j-l*), at low temperatures it occurs earlier than at high. In the material with

strengthening particles of diameter 50 nm (Figure 2 *l*), the contribution of dislocation dipoles in the total dislocation density becomes dominant at low and medium temperatures, but at a lower particle size dipole configurations in the material is absent.

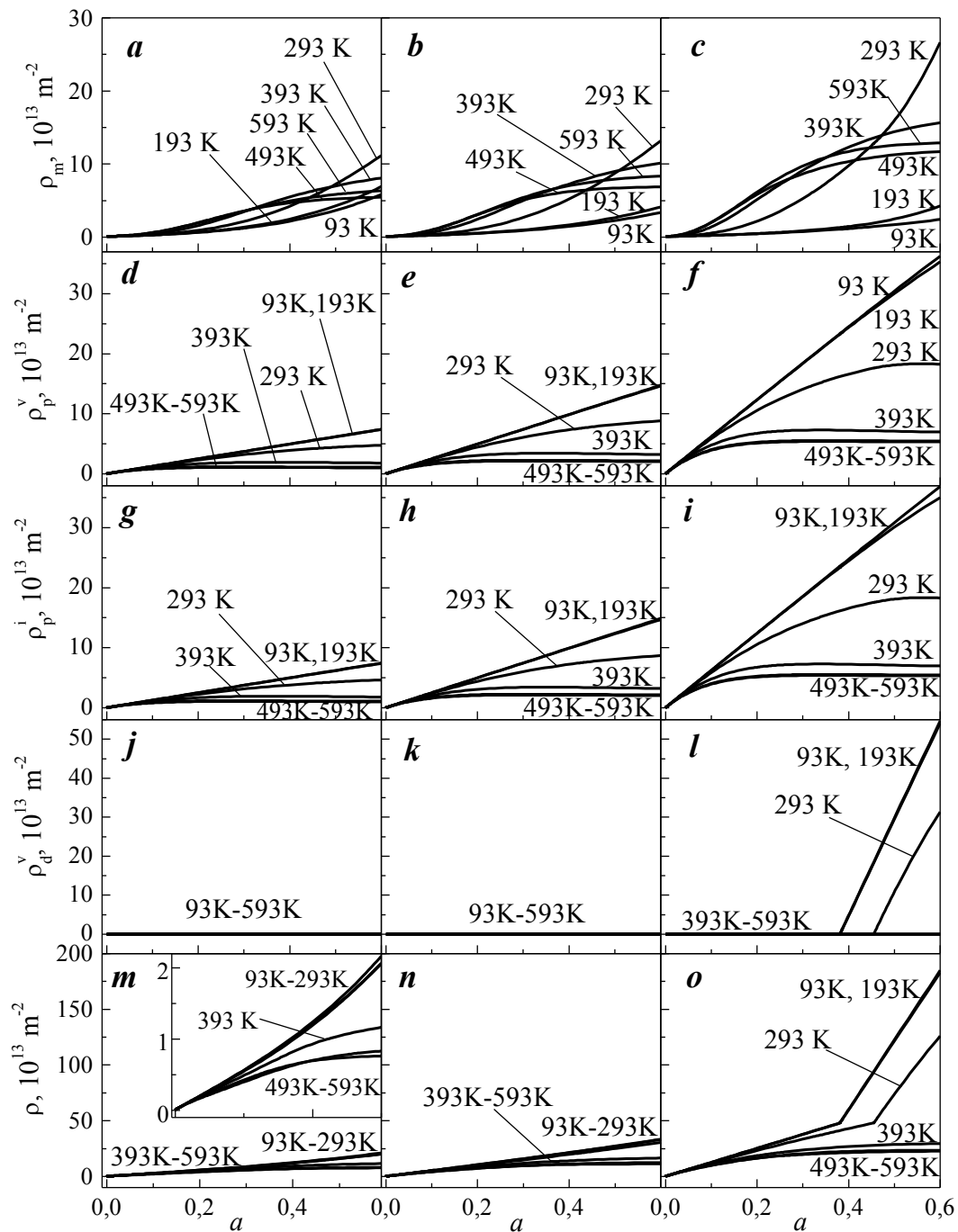


Figure 2. The dependence of the density of the shear-forming dislocations (*a, b, c*), dislocations in prismatic loops of vacancy (*d, e, f*) and interstitial (*g, h, i*) types, dislocations in dipoles (*j, k, l*), and total dislocation density (*m, n, o*) on the strain for an aluminum-based alloy at different temperatures. The fraction of incoherent particles is 25%. Particle diameter, nm: *a, d, g, j, m* – 10, *b, e, h, k, n* – 20, *c, f, i, o* – 50. Distance between particles is 400 nm. Strain rate 10^{-2} s^{-1} .

In a material with a particle size of 10 nm and 20 nm when the dislocation dipoles are not formed, the prismatic loops are dominant element of the dislocation structure (Figure 2). In view of the fact that the shear-forming dislocations behave in a complicated manner, at certain temperatures deformation they contribute more to the total dislocation density. Thus, at medium (293 K-393 K) and high (493 K-593 K) temperatures in the material with particle size of 10 nm and a distance between them of 400 nm contribution to the total dislocation density is greater of the shear-forming dislocation (Figure 2 *a*) than the contribution of prismatic dislocation loops (Figure 2 *d*). Such situation is observed for the material with strengthened particles of size of 20 nm at medium and high temperatures (Figure 2 *b*, *e*). In a material with a particles size of 50 nm is achieved critical dislocation density at temperatures of 93 K - 293 K, there are dislocations in dipole configurations, which become the dominant type of defects and make a decisive contribution to the total dislocation density. At higher temperatures the dislocation dipoles are not formed, and shear-forming dislocations become by dominant element of the dislocation structure.

4. Conclusions

Studies have shown that in materials with nanodispersed phase ($\delta = 10\text{-}50$ nm) at a fixed volume fraction of the strengthening phase a material with smaller particle sizes reaches the greatest strain hardening in the subcritical region of dislocation densities. On reaching a critical dislocation density the dislocation dipoles begin to form in the material with the larger strengthening particles. This is reason of the enough strong strain hardening, which is ahead of the strain hardening of material with smaller particles. Such a pattern is observed at all temperatures of deformation.

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