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CONDENSED-STATE PHYSICS

GENERATION OF INTERSTITIAL ATOMS IN FCC SINGLE CRYSTALS

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A mathematical model of generation and accumulation of interstitial atoms in plastically deformable pure FCC metals is suggested based on the concept of hardening and recovery that links the phenomena proceeding in the deformable crystal material with the behavior of crystal structure defects. The model comprises kinetics equations for point defects – mono- and bivacancies and interstitial atoms – written with allowance for mechanisms of their generation and precipitation on sinks. Special attention is given to investigation of the influence of the velocity and character of motion of helical segments of expanding dislocation loops on generation of interstitial atoms. Concentrations of interstitial atoms generated in the process of plastic deformation are calculated.

Keywords: concept of hardening and recovery, plastic deformation modeling, FCC metals, dislocation source, shear zone, dislocation density, interstitial atoms, vacancies, bivacancies, lattice defects, point defects.

INTRODUCTION

Plastic deformation of face-centered cubic (FCC) metals is accompanied by a number of substructural transformations [1]. Deformation in single crystals of these alloys causes substructural transformations which lead sooner or later to the loss of monocrystallinity of the material. In this case, the processes of return to intermediate and high temperatures are important. These processes can be realized in the process of interaction of point defects with a dislocation ensemble. This interaction provides arbitrary rearrangement of the dislocation structure that finally leads to substructure formation and, upon deeper deformation, to polycrystallinity. The rearrangement of the dislocation ensemble requires sufficiently high concentrations of point defects with high mobility. In many materials at room and low temperatures, the mobility of vacancies is insufficient to ensure these processes. The evolution of the dislocation ensemble can be provided by other defects having higher mobility [2].

Experimental observation of interstitial atoms is difficult and has not yet been performed *in situ*. In this regard, the theoretical consideration of the mechanisms causing generation of interstitial atoms becomes urgent. *In situ* accumulation of vacancies in the process of plastic deformation was studied experimentally in [3]. Therefore, a possible approach to a solution of this problem is to construct a model describing generation of not only vacancies, but also of interstitial atoms. If the model is in agreement with the available experimental data on the concentration of vacancies, it can be used for theoretical estimates of generation and accumulation of interstitial atoms.

The main physical prerequisite for a description of generation of point defects (vacancies and interstitial atoms) is the dislocation motion in an imperfect crystal comprising forest dislocations that lead to the formation of dislocation jogs and their motion. The motion of jogs in edge dislocations is of no interest in this sense, since it is exclusively conservative. In the case of helical and similar orientations, the newly formed jogs can move not only conservatively

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(along the dislocation line), but also non-conservatively (in the direction of dislocation motion). The non-conservative motion is accompanied by the formation of not only vacancies, but also interstitial atoms depending on the jog type. The main point in the description of this motion is a search for the conditions under which the conservative motion of jogs along the dislocation line becomes less favorable than their drawing with generation of point defects [4].

For pure metals, the condition of jog drawing is dynamical dislocation motion with high velocities, when the kinetic energy of a free dislocation segment is higher than the energy required for generation of point defects of one type or another. This process was discussed in detail in [4–6], where it was demonstrated that in this case, the rate of generation of point defects can be described with good accuracy by the expression $K_G\rho^{1/2}$, where the coefficient K_G is determined by the velocity of dislocation segments with helical orientation, the velocity of jog motion along the dislocation, and the distribution of jog-forming forest dislocations. Another factor stabilizing the position of jogs on moving dislocations of $L1_2$ alloys is the necessity of generation of anti-phase boundaries (APB) by moving jogs that leads to a more intensive generation of point defects. In this case, in [7] it was demonstrated that the generation rate is described by the expression $K_G(\zeta)\rho^{1/2}$, where ζ is the energy of the antiphase boundary.

These ideas provided the basis for the model of generation of point defects constructed in [8]. The present work is devoted to estimation of generation and accumulation of interstitial atoms in FCC single crystals taking into account interactions between ensembles of point defects and the dislocation ensemble and verification of the model by means of calculations of the vacancy concentration and its subsequent comparison with the available experimental data. For this purpose, based on the concept of hardening and recovery [9], calculations were performed of the following quantities: 1) rate of generation of interstitial atoms, 2) concentration of generated interstitial atoms, 3) concentration of interstitial atoms annihilated on dislocations, and 4) residual concentration of interstitial atoms.

1. DISLOCATION MOTION IN A SHEAR ZONE

The loss of the shear stability of the crystal lattice under the influence of a deforming stress is accompanied by relay-race motion of localized shear deformation in the volume of the deformable material. The elementary shear instability – the spontaneous expansion of the dislocation loop from the Frank–Reed source up to obstacles that cannot be overcome (shear zone boundaries) – leads to the formation of a shear zone. Moreover, deformation defects such as dislocations with dynamical dipole configurations, dislocation fragments, and point defects (interstitial atoms, vacancies, and bivacancies) are generated in the shear zones. Superposition of mechanisms of generation, transformation, and annihilation of deformation defects leads to the formation of deformation substructures [1].

It is assumed that N dislocation sources emit during time Δt in unit volume Δn dislocation loops which form a cluster on the boundary of the shear zone. Climbing of edge dislocations in dislocation clusters leads to their rearrangement into dislocation walls at the boundaries of the shear zones. The formation of the dislocation walls leads to the removal of reverse stress fields and emission of the next portion of dislocation loops by the source.

During expansion of the dislocation loop, the work A of the external stress τ is spent on the creation of the kinetic energy E_k of the dislocation loop, overcoming various resistance forces, and increase of the intrinsic loop energy. Hence, we can write $\mathrm{d}E_k = \mathrm{d}A - \mathrm{d}A_R - \mathrm{d}A_\upsilon - \mathrm{d}A_j - \mathrm{d}A_\mu$ [10], where $\mathrm{d}A = \tau b\,\mathrm{d}S_D$, $\mathrm{d}A_R = \tau_R b\,\mathrm{d}S_D$, τ_R is the friction stress independent of the velocity of dislocation motion, $\mathrm{d}A_\upsilon = B_\upsilon \upsilon\,\mathrm{d}S_D$, B_υ is the viscous friction coefficient, and $\upsilon = \dot{R}$ is the velocity of motion. The kinetic energy E_k of the moving curved (with curvature radius R) segment of the dislocation loop can be represented as the product $E_k = R\theta_D e_k$ of the segment length $R\theta_D$ on the kinetic energy e_k of the unit dislocation length [10].

Let us write the system of differential equations describing the motion of the helical segments of the dislocation loop in the following form:

$$\dot{e}_k^s = \upsilon_s\left(\tau_{\text{eff}}\, b - 0.25Gb^2 c_j - B_\upsilon \upsilon_s - \left(\mu + e_k^s\right)R^{-1}\right),\ \dot{R} = c_t\sqrt{1-\left(1+e_k^s e_{\text{elast}}^{-1}\right)^{-2}}\,, \tag{1}$$

$$\dot{c}_j = \beta_j \xi \rho \upsilon_s - \left(w_j c_j\right)^2 \upsilon_j, \tag{2}$$

where $\tau_{\text{eff}} = \tau - \tau_R \approx 0.4Gb\rho^{1/2}$, $e_{\text{elast}} \approx 0.5Gb^2$, ξ is the relative fraction of forest dislocations, $\beta_j = 0.5\left(1-\beta_r\right)$ is the relative fraction of jog-forming forest dislocations, β_r is the relative fraction of reactive dislocations [12], and υ_j is the annihilation rate of jogs moving along the dislocation. For edge dislocation segments, the system of differential equations has the following form:

$$\dot{e}_k^e = \upsilon_e\left(\tau_{\text{eff}} b - B_\upsilon \upsilon_e - \left(\mu + e_k^e\right)R^{-1}\right), \ \dot{R} = \upsilon_e, \tag{3}$$

where $e_k^e = e_{\text{elast}}\left(1-\nu\right)^{-1}\left(c_t^2\upsilon_e^{-2}\left(8\gamma_\ell + 4\gamma_\ell^{-1} - 7\gamma_t - 6\gamma_t^{-1} + \gamma_t^{-3}\right) - 1\right)$, $\gamma_\ell = \left(1-\upsilon_e^2 c_\ell^{-2}\right)^{1/2}$, and $\gamma_t = \left(1-\upsilon_e^2 c_t^{-2}\right)^{1/2}$.

The average free path lengths for helical and edge segments of dislocation loops are determined by sizes of the shear zone estimated for the model of interdislocation interaction, according to which $D = 2\left(\beta_D\beta_r\xi\rho\right)^{-1/2} \approx 80\rho^{-1/2}$ [13]. Calculations by formulas (1)–(3) demonstrated [14] that the edge segments move with higher velocities and reach the shear zone boundaries before the helical segments; therefore, the area enclosing edge segments can be neglected in the first approximation.

2. RATE OF INTERSTITIAL ATOM ACCUMULATION

For stationary segment motion, it is assumed that the stable jog density $c_j = \left(p_j\xi\rho\right)^{1/2}$ is established on the segments and that the jog drawing causes generation of vacancy chains with the intensity $\Delta c_i/\Delta a \approx 0.25b\left(p_j\xi\rho\right)^{1/2}$, where b is the Burgers vector modulus, $p_j \approx 0.5$ is the relative fraction of jog-forming forest dislocations, c_i is the concentration of interstitial atoms forming chains, and a is the shear deformation. The factor 0.25 takes into account that half the jogs generate vacancy chains and that the average chain length is half the free path length of the helical segments.

The helical segments of the dislocation loop emitted by the Frank–Reed source move with high average velocity υ_s reached during time which is by an order of magnitude smaller than the total time of dislocation motion to the shear zone boundary [14]. In this case, the stationary jog density $c_j = \left(\beta_j\xi\rho\upsilon_s/\upsilon_j\right)^{1/2}$ determined from Eq. (2) is formed on the helical segments. The ratio of the increment of the interstitial atom concentration $\Delta c_i \approx 0.5b^2 c_j S_D^s \Delta nN$ in chains formed during jog drawing to the increment of the shear deformation $\Delta a \approx bS_D\Delta nN$ gives the expression for the rate of interstitial atom generation in the following form:

$$G_i = 0.5bc_j S_D^s S_D^{-1} \approx 0.5bc_j = 0.5b\left(\beta_j\xi\rho\upsilon_s/\upsilon_j\right)^{1/2}. \tag{4}$$

Limiting cases were considered in [5, 6] for the ratio υ_s/υ_j when $\upsilon_s = \upsilon_j$ and $\upsilon_s = c_t$, and the phenomenological dependence was suggested in [8, 11], according to which the rate first increases exponentially, then the rate of increase slows down, and in the limit the rate of increase for helical segments of the dislocation loop tends to a certain constant value $\upsilon_m\left(T\right) = w_j^2\beta_j^{-1}\xi^{-1}\upsilon_j K_\upsilon^2$ for a given deformation temperature. The relative fraction of jogs that can annihilate was $w_j \approx 0.25$. It was determined by their distribution over the helical dislocation line [11]. The rate $\upsilon_m\left(T\right) \approx 3.56\upsilon_j$ which can be determined experimentally or by modeling of dislocation motion [11, 15, 16] depends

on the jog distribution, annihilation rate υ_j of jogs during their motion along the dislocation line, and on the deformation temperature.

If we assume that the average velocity of dislocation motion is defined as a harmonic average of the average velocity of *quasi-viscous* dislocation motion through a random field of strong point barriers $\upsilon_T(\tau,T)=\upsilon_0\exp\left(-k_{\mathrm{B}}^{-1}T^{-1}\left(U_0-\gamma\tau\right)\right)$ at a certain value τ of the deforming stress [17] and the average velocity $\upsilon_m(T)$ of viscous dislocation motion between the barriers, we obtain the following expression for the helical dislocation velocity [8]:

$$\upsilon_s(\tau,T)=\left(\upsilon_m^{-1}(T)+\upsilon_T^{-1}(\tau,T)\right)^{-1}=\left(\upsilon_m^{-1}(T)+\upsilon_0^{-1}\exp\left(k_{\mathrm{B}}^{-1}T^{-1}\left(U_0-\gamma\tau\right)\right)\right)^{-1}$$
$$=w_j^2\beta_j^{-1}\xi^{-1}\upsilon_j V_a\left(V_aK_\upsilon^{-2}+\exp\left(V_a\left(\tau_n-\tau\right)\right)\right)^{-1}. \quad (5)$$

Here U_0 is the activation energy of thermally activated dislocation motion, γ is the activation volume, T is the temperature, and k_{B} is the Boltzmann constant.

3. KINETIC EQUATIONS FOR DEFORMATION DEFECTS

The elementary act of work of dislocation sources increased the deformation products by $\Delta a=S_Db\Delta n\,N$ (shear plastic deformation), $\Delta\rho_m=P_D\Delta n\,N$ (density of the shear-forming dislocations), $\Delta\rho_d=\Delta\rho_d^{\upsilon}+\Delta\rho_d^{i}=n_d\ell_d\Delta n\,N$ (density of dislocations in the vacancy and interstitial dipole configurations), $\Delta N_W=d_WF_eD_s\Delta n\,N$ (density of misorientation boundaries), $\Delta c_k=w_kc_jS_D^sb^2\,\Delta n\,N$ (concentrations of point defects, including interstitial atoms c_i for $k=i$, monovacancies $c_{1\upsilon}$ for $k=1\upsilon$, and bivacancies $c_{2\upsilon}$ for $k=2\upsilon$).

The ratios of $\Delta\rho_m$, $\Delta\rho_d$, ΔN_W, and Δc_k to Δa give expressions for deformation defect generation rates (G) [8 9, 14]: $G_m=\left(F_sD_s^{-1}+F_eD_e^{-1}\right)b^{-1}$ for shear-forming dislocations, $G_d^i=G_d^{\upsilon}=F_dS_D^sS_D^{-1}\ell_d^{-1}b^{-1}\approx 2F_db^{-1}\rho^{1/2}$ for dislocations in dynamical dipole configurations, $G_W=2d_WF_eD_e^{-1}b^{-1}$ for low-angle tilt walls, and w_ic_jb, $w_{1\upsilon}c_jb$, and $w_{2\upsilon}c_jb$ for point defects. Considering that the numbers of vacancy and interstitial jogs are the same, we take $w_i=1/2$. Due to higher mobility of bivacancies, vacancy chains break so that most of them escape from the chains in the form of bivacancies ($w_{2\upsilon}=5/12$), and the rest vacancies escape as single vacancies ($w_{1\upsilon}=1/12$) [8].

The deformation-induced point defects are precipitated on sinks representing edge dislocation segments and point defects of alternative type. We define the power of sinks of a certain type as the squared precipitation surface of the point defect per unit volume. Let us use the following designations for the power: ($\beta_m=2\pi bw_e\rho_m$, $\beta_{id}=2\pi b\rho_d^i$, and $\beta_{\upsilon d}=2\pi b\rho_d^{\upsilon}$) for dislocation sinks of different types and ($\beta_i=4\pi r_{\mathrm{R}}^2b^{-1}c_i$, $\beta_{1\upsilon}=4\pi r_{\mathrm{R}}^2b^{-1}c_{1\upsilon}$, and $\beta_{2\upsilon}=4\pi r_{\mathrm{R}}^2b^{-1}c_{2\upsilon}$) for point defects of different alternative types. The sums of sink powers for point defects are $\beta_i^{\mathrm{sum}}=\beta_m+\beta_{\upsilon d}+\beta_{2\upsilon}+\beta_{1\upsilon}$, $\beta_{1\upsilon}^{\mathrm{sum}}=\beta_m+\beta_{id}+\beta_i+\beta_{1\upsilon}$, and $\beta_{2\upsilon}^{\mathrm{sum}}=\beta_m+\beta_{id}+\beta_i$. We denote by $w_{\bar{k}}^{k}=\beta_{\bar{k}}\big/\beta_k^{\mathrm{sum}}$ the ratio of the sum of the surface areas of sinks of the *k*th type to the sum of the surface area of all sinks for point defects of the *k*th type.

The recombination (R) and annihilation rates (A) can be written in the form [8, 9]

$$R_{i1\upsilon}=K_Rw_{1\upsilon}^ic_ic_{1\upsilon}D_i\ ,\ R_{i2\upsilon}=K_Rw_{2\upsilon}^ic_ic_{2\upsilon}D_i\ ,\ R_{1\upsilon i}=K_Rw_i^{1\upsilon}c_ic_{1\upsilon}D_i\ ,\ R_{\upsilon\upsilon}=K_Rw_{1\upsilon}^{1\upsilon}\left(c_{1\upsilon}\right)^2D_{1\upsilon},$$

$$R_{2\upsilon i} = K_R w_i^{2\upsilon} c_i c_{2\upsilon} D_{2\upsilon},\ A_{i\rho} = \left(w_e \rho_m + \rho_d^{\upsilon}\right) c_i D_i,\ A_{1\upsilon\rho} = \left(w_e \rho_m + \rho_d^{i}\right) c_{1\upsilon} D_{1\upsilon},\ A_{2\upsilon\rho} = \left(w_e \rho_m + \rho_d^{i}\right) c_{2\upsilon} D_{2\upsilon},$$

where $K_R = 28\pi r_R b^{-3}$, $r_R \approx 8.38b/\sqrt[3]{T}$, $D_k = D_0 \exp\left(-U_k^m k_{\rm B}^{-1} T^{-1}\right) m\tau b^3 k_{\rm B}^{-1} T^{-1}$ is the diffusion coefficient of the point defects of the *k*th type ($k = i, 1\upsilon, 2\upsilon$) drifting to sinks under the action of internal stresses $m\tau$, and $D_0 = 12b^2\nu_D$ is the pre-exponential factor.

If we denote generation rates of point defects as follows: $G_i = K_{Gi}(\rho_m)\sqrt{\rho_m}$, $G_{1\upsilon} = K_{G1\upsilon}(\rho_m)\sqrt{\rho_m} + \dot{a}^{-1} w_i^{2\upsilon} R_{i2\upsilon}$, and $G_{2\upsilon} = K_{G2\upsilon}(\rho_m)\sqrt{\rho_m} + \dot{a}^{-1} w_{1\upsilon}^{1\upsilon} R_{\upsilon\upsilon}$, where $K_{Gk} = w_k b c_j S_D^s S_D^{-1}$, then we obtain ***the balance equations for point defects*** in the form

$$\dot{c}_i = \dot{a} G_i - A_{i\rho} - R_{i1\upsilon} - R_{i2\upsilon},\ \dot{c}_{1\upsilon} = \dot{a} G_{1\upsilon} - A_{1\upsilon\rho} - R_{1\upsilon i} - R_{\upsilon\upsilon} + w_i^{2\upsilon} R_{i2\upsilon},$$

$$\dot{c}_{2\upsilon} = \dot{a} G_{2\upsilon} - A_{2\upsilon\rho} - R_{2\upsilon i} + w_{1\upsilon}^{1\upsilon} R_{\upsilon\upsilon}.$$

Let us write down the balance equation for the shear-forming dislocations in the form

$$\dot{\rho}_m = \dot{a}\left(G_m^e + G_{mW}\right) - \sum_k \sqrt{8 w_e \rho_m}\, w_e w_m^k \rho_m c_k D_k / b.$$

Here we have taken into account that $G_m^e = w_e \left(1 - w_W^m\right) F D^{-1} b^{-1}$ is the rate of generation of edge dislocations whose relative fraction $w_W^m = \Delta n / n$ forms nuclei of fragment boundaries, $\Delta n \approx D\pi(1-\nu)\alpha_{\rm dyn} \times \sqrt{\rho_m}\left(\ln 8 - \ln\left(3\beta_j \xi b \rho_m D\right)\right)^{-1}$ is the number of dislocations emitted during one act of source operation, $n \approx 1000$ is the number of dislocations emitted by the source, $G_{mW} = \dot{a}^{-1} K_\tau N_W / d_W$ is the rate of wall decay, K_τ is a constant, $d_W = 0.125 K_{aW} \beta_j \xi \rho_m D^2 b (\Delta n + 1)^{-1}$ is the distance between dislocations in the wall, $\xi\beta_j \approx 0.22$ is the relative fraction of jog-forming forest dislocations, and the factor K_{aW} takes into account the effect of annihilation on the wall formation.

The balance equation for the density of misorientation boundaries can be written in the form

$$\dot{N}_W = \dot{a}\left(G_{Wm}^{\rm dyn} + G_{Wm}\right) - A_{W\tau}.$$

Here $A_{W\tau} = K_\tau N_W$ is the decay rate of misorientation boundaries, $G_{Wm} = \dot{a}^{-1} b^{-1} w_{Wm} D_W \times \sum_k D_k w_m^k c_k d_W w_e \rho_m N_W$ is the rate of their expansion, and $G_{Wm}^{\rm dyn} = d_W w_e w_W^m F D^{-1} b^{-1}$ is the rate of their dynamical nucleation.

Balance equations for the densities ρ_d^i and ρ_d^{υ} of the interstitial and vacancy dislocation dipoles have the form

$$\dot{\rho}_d^i = \dot{a} K_{Gd} \rho_m^{1/2} - w_d^{\upsilon} < h >^{-1} b^{-1} \rho_d^i \left(D_{1\upsilon} c_{1\upsilon} + D_{2\upsilon} c_{2\upsilon}\right),\ \dot{\rho}_d^{\upsilon} = \dot{a} K_{Gd} \rho_m^{1/2} - w_d^i < h >^{-1} b^{-1} \rho_d^{\upsilon} c_i D_i.$$

4. RESULTS OF MODELING

The above-discussed balance equations for deformation defects and the expression for the deforming stress

$$\tau = \tau_f + \alpha G b \sqrt{\rho_m} + \alpha_1 G b \sqrt{\rho_\pm} - 0.25\pi^{-1} G b N_W \ln\left(N_W b\right),$$

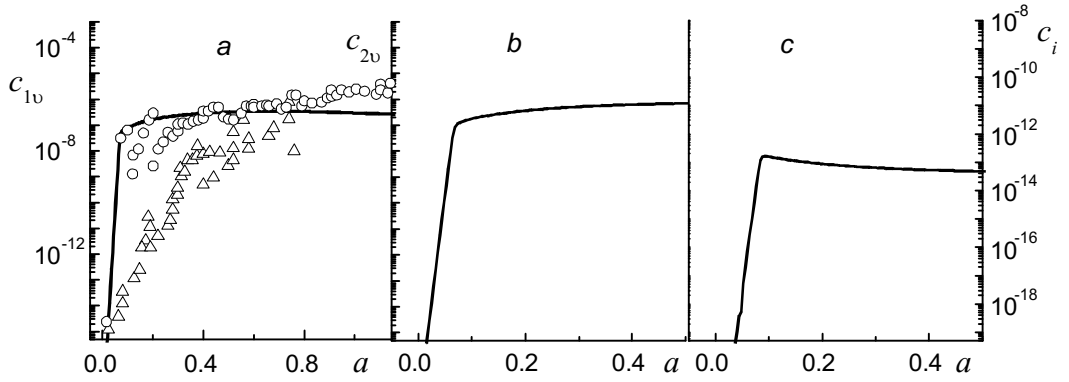

Fig. 1. Dependences of the concentrations of accumulated monovacancies (*a*), bivacancies (*b*), and interstitial atoms (*c*) on the deformation degree. Solid curves are for calculated results, and symbols are for the experimental data [3].

where $\rho_{\pm} = w_W^m \rho_m + N_W / d_W$ is the excess dislocation density, form the closed system of equations whose solution allows theoretical dependences of the densities of deformation defects on the deformation degree and deforming stress to be obtained. Calculations were performed for uniaxial deformation of a copper single crystal at the constant temperature $T = 300$ K and $\dot{a} = 10^{-4}\ \mathrm{s}^{-1}$ with the deformation axis oriented along the [001] direction with the following initial conditions: $\rho_m(0) = 10^6\ \mathrm{mm}^{-2}$, $\rho_d^{\upsilon}(0) = 0$, $\rho_d^{i}(0) = 0$, $c_k(0) = 0$, and $N_W(0) \approx 0\ \mathrm{mm}^{-1}$ and the following parameter values: $G \approx 55710$ MPa; the Burgers vector modulus $b \approx 2.56 \cdot 10^{-7}$ mm; the interdislocation interaction parameter $\alpha = \alpha_1 \approx 0.25$; $B_r \approx 200$, $F \approx 5$, $K_{Gm} = F/(\alpha\, b\, B_r) \approx 0.1/b$; the relative fraction of helical dislocation components $w_s = 1 - 2/\pi$; $\tau_n = 4$, $V_a = 16$, $\nu_D \approx 10^{13}\ \mathrm{s}^{-1}$; the energy of point defect migration $U_i^m \approx 1.87 \cdot 10^{-20}$ J, $U_{1\upsilon}^m \approx 14 \cdot 10^{-20}$ J, and $U_{2\upsilon}^m \approx 11 \cdot 10^{-20}$ J; and $\zeta \approx 29$, $K_{\tau} \approx 0.00029$, $K_W \approx 4$, $< h > \approx 6b$, and $K_D \approx 0.39$.

Figure 1 shows the dependences of the concentrations of accumulated point defects on the deformation degree. The calculated results are in agreement with the experiment not only qualitatively, but also quantitatively. Results of theoretical calculation predicted the two-stage increase in the point defect concentration depending on the deformation degree, including the stage of fast increase in the point defect concentration for intermediate deformation degree followed by the stage of saturation during which the point defect concentration varies slightly. This is in agreement with observations. The good agreement between the calculated results and the experimentally observed dependence (Fig. 1*a*) [3] as well as the agreement with the experimental data on dislocation densities, parameters of substructure fragments, and macroscopic hardening curves [8, 9] allows the model to be considered as well verified that can be used to analyze the process of generation and accumulation of deformation interstitial atoms.

Figure 2 shows the dependences of the current concentrations of accumulated (curves *1*) and generated mono- and bivacancies (curves *3*) and of the concentration of mono- and bivacancies annihilated on dislocations (curves *2*) on the deformation degree. Analogous dependences for the residual concentration of interstitial atoms, concentration of generated interstitial atoms, and concentration of interstitial atoms annihilated on dislocations are shown in Fig. 3*a*. The concentrations of annihilated point defects were close in values to the concentration of generated ones, which led to a significant decrease of the current concentrations. The overwhelming majority of the generated point defects were spent on relaxation. The interstitial atoms take more active part in the annihilation and relaxation processes. The concentration of accumulated interstitial atoms is by many orders of magnitude lower than concentrations of mono- and bivacancies. It should be noted that the accumulated point defects were in a nonequilibrium state, and after the termination of deformation, the relaxation processes continued. Hence, experimental observations of point defects can provide reliable information only when measurements are performed in the process of deformation.

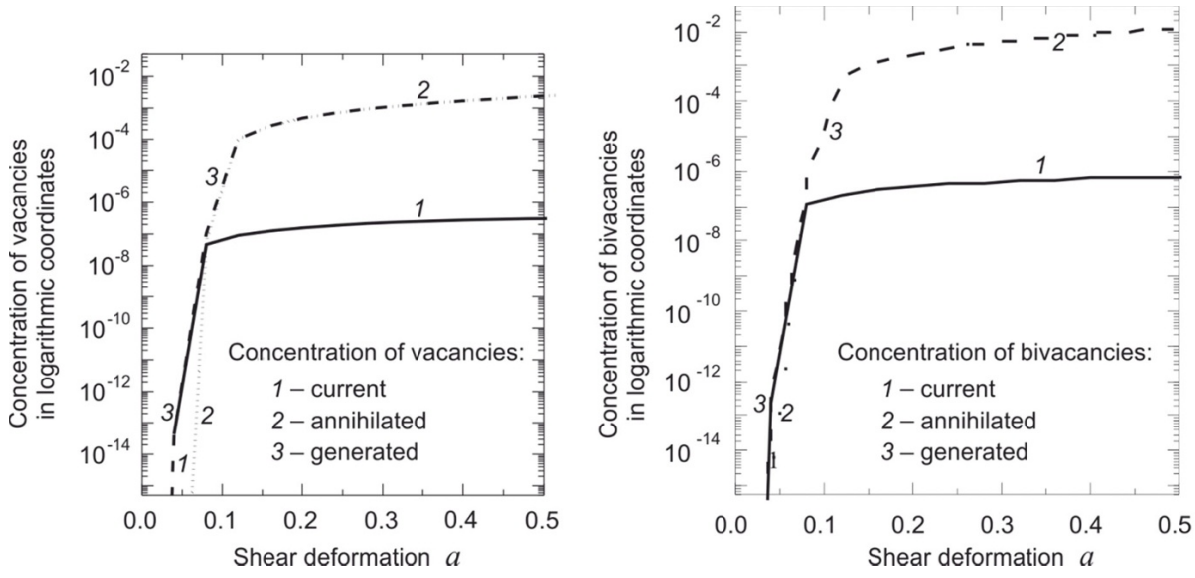

Fig. 2. Dependences of the concentration of generated (curve *3*) and annihilated (curve *2*) vacancies and bivacancies and of their current concentrations on the deformation degree (curve *2*).

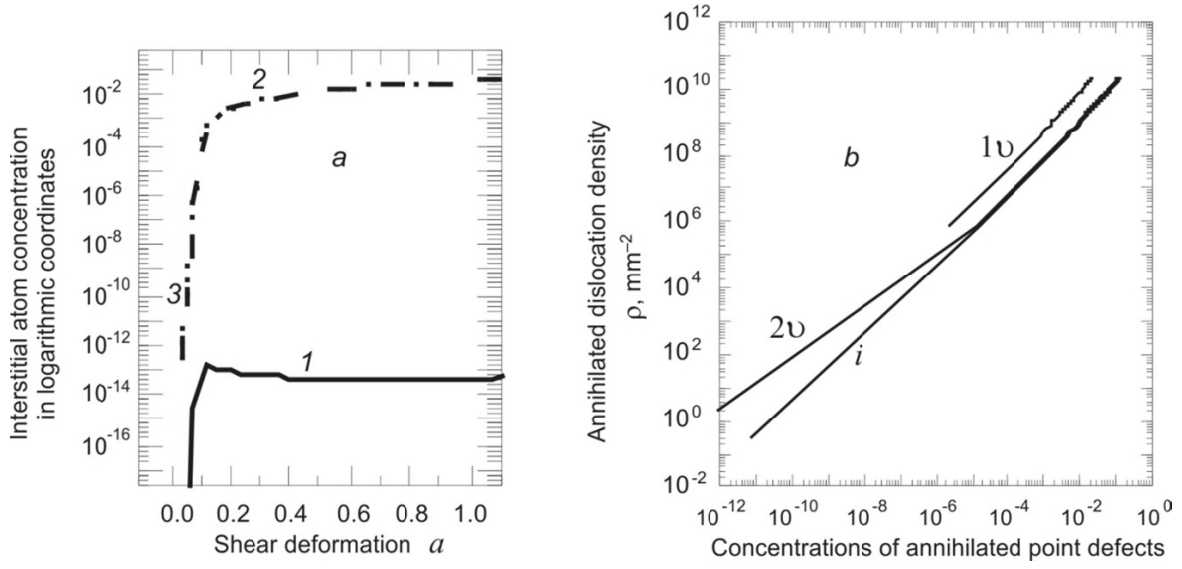

Fig. 3. Dependences of the concentrations of generated (curve *3*) and annihilated (curve *2*) interstitial atoms on the deformation degree together with their current concentration (curve *1*) (*a*); dependences of the annihilated dislocation density on the point defect concentrations (*b*).

Figure 3*b* shows the dependences of the annihilated dislocation density on the point defect concentrations. Interstitial atoms annihilate with a high rate, thereby leading to the decrease of their concentration by more than ten orders of magnitude. We can consider that all generated interstitial atoms annihilate on dislocations or vacancies. Interstitial atoms bring the main contribution to annihilation at the initial deformation stage, and then their contribution becomes comparable with that of bivacancies. The contribution of monovacancies to annihilation becomes noticeable only at high dislocation density, but still remains by an order of magnitude lower than the contribution of interstitial atoms.

Results of modeling demonstrated that by the end of the third deformation stage, the concentration of point defects in the absence of mechanisms of annihilation on dislocations can reach values of 10^{-3}–10^{-2} physically unrealistic for the crystalline state. However, the precipitation of point defects on dislocations does not allow this to be the case by reducing the density of point defects down to actually observed values. A significant part of interstitial atoms (6%) is involved in the dynamical formation of nuclei of the dislocation walls.

Interstitial atoms have a very strong effect on dislocations. This can be the determining factor in the evolution of dislocation substructures. Consideration of this circumstance is particularly important for an analysis of processes of nanostructure formation in materials subjected to intensive treatment with high degree of plastic deformation. The interaction of interstitial atoms with the dislocation ensemble remains intensive at low temperatures. This is due to retention of the mobility by interstitial atoms at low temperatures due to low activation energy of their drift. High concentration of interstitial atoms generated in the process of deformation can be the important factor causing the occurrence of dislocation substructures in materials deeply deformed at low temperatures.

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