MATHEMATICAL MODELING OF TEMPERATURE AND RATE DEPENDENCIES OF STRAIN HARDENING IN FCC METALS

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ABSTRACT

The mathematical model for plastic deformation by slip is developed. The model is based on the balance equations for deformation defects. The deformation defects structure is characterised by slip-producing dislocations, dipole dislocations both of vacancy and interstitial type, interstitials, vacancies and bevacancies.
A package of applied programs for the description of plastic deformation by slip in f.c.c.-materials is developed. A package of applied programs is used for analysis of role of mechanisms of generation and annihilation of deformation defect in strain hardening and in evolution of defects structure. The calculations for single crystal of aluminum, copper and nickel, which are deformed with constant strain rate, were made.
The calculated temperature and rate dependencies of deforming stress are correspond to experimental data. The value of applied stress decreases when temperature increases. There are intervals of strong and weak temperature dependence. They correspond to the intensity of annihilation processes by means of deformation defects of various types. The dependencies of dislocation density and concentrations of point defects on strain for wide interval of temperature and strain rate are defined. The intervals of strong and weak temperature and rate dependence can be selected for all type of defects. These intervals correspond to the intervals of strong and weak temperature and rate dependence for applied stress.

1 INTRODUCTION

The crystallographic slip zone has been chosen as basic structural element for description of slip plasticity. The mechanisms and regularities of crystallographic slip are described on the base of [illegible]

fundamental physical and topological properties of crystal lattice defects realising the plastic mass [illegible]

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

$$\frac{dc_i}{da} = q\frac{\tau_{dyn}}{G} - \frac{1}{\dot{a}}c_i[([(1-\omega_s)\rho_m + \rho_d]b^2 + \tilde{c}_{1v} + c_{2v})Q_i + \tilde{c}_{1v}Q_{1v} + c_{2v}Q_{2v}]. \quad (3)$$

Here $Q_j = \nu_d Z\exp(-U_j^{(m)}/kT)$, k is the Boltzmann constant, T is temperature, $Z = 12$, ν_D is the Debye frequency, $U_k^{(m)}$ is the migration energy of the k-type point defect, $\dot{a}$ is the strain rate, $q = 8$ [3], $\beta = 1/6$, ω_s is the fraction of screw dislocations, τ_{dyn} is dynamical stress, b is the modulus of Burgers vector, G is the shear modulus.

2.2 The balance equation for dislocation dipoles

The dislocation loop emitted by a dislocation source expands in its slip plane with an acceleration. The segments of dislocation, whose orientation is close to screw one, draggs after some run owing to the point defects generation. When the non screw segments of dislocation loop bow out the stopping screw segments dislocation dipoles produce [2, 3].

It was taken into account the next mechanisms of dipole dislocations annihilation: the absorption of interstitials by vacancy dislocation dipoles leads to decreasing of the distance between dislocation in dipole and their annihilation; the absorption of interstitials on interstitials dipoles leads to increasing of distance between them and its transformation to slip-produsing dislocations; the absorption of vacancies and bevacancies by interstitials dipoles leads to decreasing of the distance between dislocation in dipole and there annihilation; absorption of vacancies and bevacancies on vacancies dipoles leads to increasing of distance between them and its transformation to slip-produsing dislocations.

The balance equations for dislocation dipoles are

$$\frac{d\rho_d^v}{da} = \frac{1}{6\gamma_d \ell_d(\rho)b} - \frac{8\pi\tau_f}{\dot{a}Gb^2}\frac{(1-\nu)}{(2-\nu)}[c_i\rho_d^v b^2 Q_i + \omega_{dv}^i c_i(\tilde{c}_{1v}Q_{1v} + c_{2v}Q_{2v}) + $$
$$+\omega_{dv}^{1v}c_{1v}((\rho_{ns}b^2 + 2\tilde{c}_{1v} + \tilde{c}_i)Q_{1v} + \tilde{c}_i Q_i) + 2c_{2v}(\rho_d^v b^2 + \tilde{c}_i)Q_{2v} + 2\omega_{dv}^{2v}c_{2v}\tilde{c}_i Q_i\,] , \quad (4)$$

$$\frac{d\rho_d^i}{da} = \frac{1}{6\gamma_d \ell_d(\rho)b} - \frac{8\pi\tau_f}{\dot{a}Gb^2}\frac{(1-\nu)}{(2-\nu)}[\omega_{dv}^i c_{1v}((\rho_{ns}b^2 + 2\tilde{c}_{1v} + \tilde{c}_i)Q_{1v} + \tilde{c}_i Q_i) + $$
$$+2c_{2v}\rho_d^v b^2 Q_{2v} + 2\omega_{dv}^i c_{2v}\tilde{c}_i Q_i + c_i\rho_d^i b^2 Q_i + \omega_{di}^i c_i(\tilde{c}_{1v}Q_{1v} + c_{2v}Q_{2v})] . \quad (5)$$

Here ω_j^m is the friction of the m-type point defect, which annihilate on the j-type sink.

2.3 The balance equation of slip-producing dislocations

The rate of slip-producing dislocations generation depends of the diameter of a slip zone. The diameter D of a slip zone is determined by formation of long dislocation barriers [1-2].

The basic mechanisms of annihilation of dislocations are cross slip of screw dislocations and climb of non-screw dislocations [1-3]. We assume, that screw dislocations do not annihilate up to the temperature T_{cs}; the cross slip at temperatures higher T_{cs} is athermal [1-3].

The intensity of transformation of dipole dislocations to slip-producing dislocations is taking into account. The balance equation of slip-producing dislocations is

$$
\begin{aligned}
\frac{d\rho_m}{da} = & (1-\omega_s P_{as})\frac{F}{Db} - \frac{2}{\dot{a}b}\rho_m \min(r_a, \rho_m^{-1/2})[(1-\omega_s)\rho_m b^2 (c_i Q_i + +2c_{2v}Q_{2v}) + \\
& + c_i \tilde{c}_{1v}\omega'^{i}_{m} Q_{1v} + c_{2v} c_i \omega'^{i}_{m} Q_{2v} + c_{1v}\omega_m^{1v}(\rho_{ns} b^2 + 2\tilde{c}_{1v} + \tilde{c}_i) Q_{1v} + \tilde{c}_i c_{1v}\omega_m^{1v} Q_i + \\
& + 2\tilde{c}_i c_{2v}\omega_m^{2v} Q_i] + \frac{8\pi\tau_f}{\dot{a}Gb^2}\frac{(1-\nu)}{(2-\nu)}[\omega_{dv}^{1v} c_{1v}(\rho_{ns} b^2 + 2\tilde{c}_{1v} + \tilde{c}_i) Q_{1v} + \omega_{dv}^{1v} c_{1v}\tilde{c}_i Q_i + \\
& + 2c_{2v}\rho_{dv} b^2 Q_{2v} + 2\omega_{dv}^{2v} c_{2v}\tilde{c}_i Q_i + c_i \rho_{di} b^2 Q_i + \omega'^{i}_{di} c_i \tilde{c}_{1v} Q_{1v} + \omega'^{i}_{di} c_i c_{2v} Q_{2v}\ ]
\end{aligned} \qquad (6)
$$

Here [1-3] the parameter F is defined by geometry of dislocation loops and their allocation in slip zone, D is the average diameter of a slip zone, ν is Poisson ratio, τ_f is the stress of friction, $P_{as} = \begin{cases} V_{as}, \text{ if } V_{as} < 1, \\ 1, \text{ if } V_{as} \le 1, \end{cases}$ $\quad V_{as} = \left(\frac{Gb}{\pi}\right)^2 \frac{\rho\omega_s}{12\tau_f(\tau-\tau_f)}$, P_{as} is the probability of annihilation of screw dislocations. The diameter can be estimated as $D = B_r\tau/(Gb\rho_m)$ where B_r is a parameter, which is defined by the probability of a long dislocation barrier formation, τ is the applied stress.

2.4. The equation for strain rate

The equation which connects the strain rate, applied stress and the defect state of crystal for quasistatic deformation was considered by many writers [1-5]. In the paper the equation for strain rate is obtained under assumption of thermally activated movement of a dislocation source up to critical configuration, which is a semicircle. Past critical configuration dislocation source move dynamically [5]. The time of slip zone formation is defined by the time of the movement of the dislocation source up to critical configuration [5]. In this case the equation for strain rate has the next form [5]:

$$
\dot{a} = A_0 \exp\left[-\frac{U-(\tau-\tau_a)\lambda(\tau,\rho)\rho^{-1/2}b^2}{kT}\right], \qquad (7)
$$

where $A_0 = \frac{8\beta_r^{1/2}(\tau-\tau_a)^{1/3}\nu_D b^{2/3}\rho^{1/3}}{\pi(1-\beta_r)^{2/3}\xi^{1/6}G^{4/3}\lambda(\tau,\rho)}\frac{B_r\tau}{F}$; $\lambda(\tau,\rho) = \left\{(\alpha_r\beta_r\xi)^{1/3} + \left[\frac{(\tau-\tau_a)(1-\beta_r)}{\xi^{1/2}Gb\rho^{1/2}}\right]^{1/3}\xi^{1/2}\right\}^{-1}$,

β_r is the fraction of reacting forest dislocations, α_r is the parameter, characterizing of intensity of dislocation interaction with reacting forest dislocations, τ_a is athermic component of dislocation slip resistance.

3 THE PACKAGE OF APPLIED PROGRAMS FOR THE DESCRIPTION OF PLASTIC DEFORMATION BY SLIP IN FCC MATERIALS

The set of ordinary differential equations (1-7) is stiff and their decision is a rather nontrivial problem. Now the specialized mathematical software which allows to decide stiff equations are existed (for example, Maple, Mathematica, MathCad, MATLAB etc). As a rule, applied programs use classical methods from Runge-Kutta's method family. These methods allow decision of a rather wide class of tasks. Also specialised methods for the decision stiff systems of ODE may be used. But to use this applied software a user must has some experience in work with ODE and applied programs. The created package of applied programs for the description of plastic deformation by slip in f.c.c. materials is not required an experience in work with ODE deciding [6].

In this package the set of mathematical models for various materials and influences as (1-7) is realised in language Object Pascal in Delphi 5 as integrated application package under Windows.

The package consists of 4 class hierarchies: one for the representation of ODE systems, a second for the parameters of an ODE problem, a third class hierarchy for solving initial value problems, and, at last, class for storing result of experiments in data base. The applied program realisation by class organisation allows to make the program more flexible for the further updating.
The researcher must to generate the ODE system for compute of laws of plastic deformation in f.c.c.-materials under deformation. For viewing or change of a set variable, meanings of parameters, entry conditions of model it is necessary to click mouse only. At formation of the right part of the ODE system of deformation defects balance the cross effects are taken into account (see fig 1).

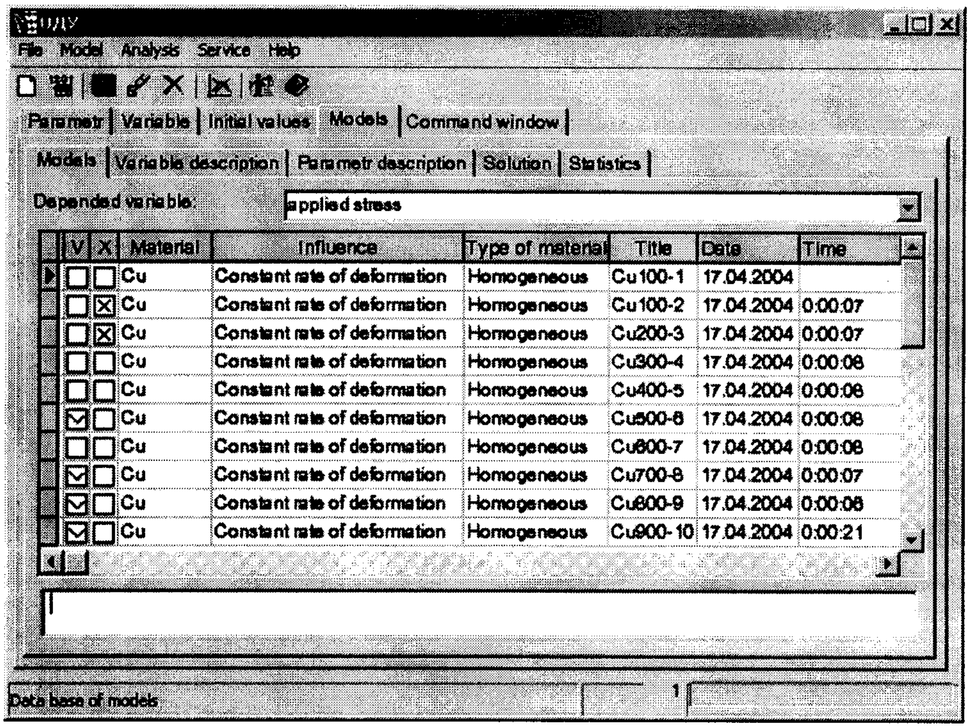

Figure 1: The widow of package interface

The ODE system is 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 for decision the system of ODE is more effective in this case [7], for the beginning of work the explicit Adams method with the step-by-step control of accuracy is applied.
The results of the carried out calculations, together with the short description of the constructed model, can be stored in txt-format or with full description in xml files. Besides, the opportunity of preservation of results as graphic files of a format *.wmf with the graphic information is stipulated.

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The results of calculation for deformation with constant strain rate are shown in the fig. 2-4. The set of equations for calculations include the equations (1-7) and the condition $\dot{a} = const$. In this case the equation (7) for the strain rate is the transcendental equation allowing finding the value of the deforming stress.

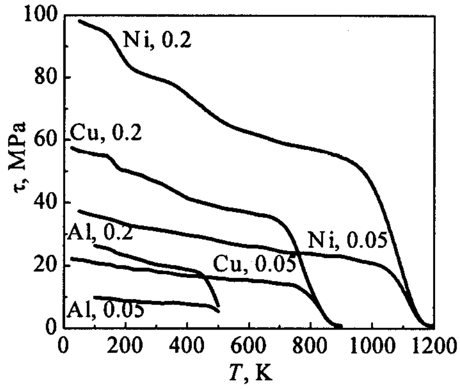

Figure 2: The dependence of applied stress on temperature for different metals and for two strain values.

The calculations are carried out for values of model and material parameters, which are characteristic of copper, nickel and aluminum single crystals [1-3]: $b = 2{,}5\cdot10^{-10}$ m^{-2}, $F = 4$, $\nu_D = 10^{13}$ s^{-1}, $\alpha_a = 0{,}45$, $\alpha_r = 0{,}3$, $\beta_r = 0{,}14$, $\xi = 0{,}5$, $\tau_f = 1$ MPa, $\nu = 1/3$, $\alpha_{dyn} \approx 0{,}33$, $k = 1{,}38\cdot10^{-23}$ J/K, $p_j = 0{,}5$, $\gamma_d = 2{,}5$, $\omega_s = 0{,}3$, $\tau_{dyn} = \alpha_{dyn} G b \rho^{1/2}$, $\alpha_{dyn} \approx 0{,}3$. The initial density of slip-producing dislocations is equal to 10^{12} m^{-2}, the initial densities of dislocation dipoles of interstitial and vacancy type and the initial concentrations of deformation point defects both type are equal to zero.

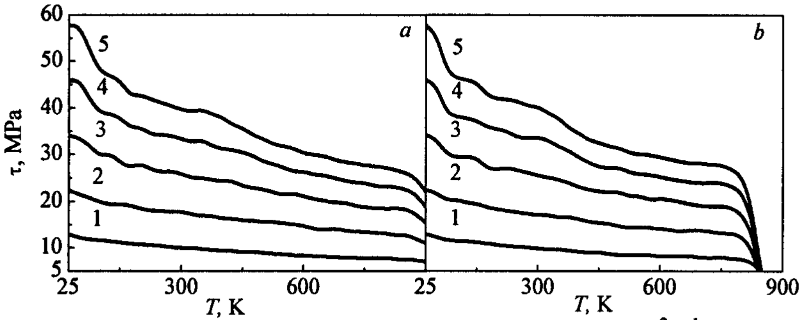

Figure 3: The dependence of stress on temperature for strain rate 10^{-2} s^{-1} (*a*) and 10^{-4} s^{-1}, (*b*) for Cu and for strain values: 1 – 0,01; 2 – 0,05; 3 – 0,1; 4 – 0,15; 5 – 0,2.

The dependencies of applied stress on temperature and strain rate are shown in the fig. 3. The calculated temperature and rate dependencies of deforming stress are correspond to experimental data. The value of applied stress decreases when temperature increases. There are intervals of strong and weak temperature dependence (fig. 3, 4). They correspond to the intensity of annihilation processes by means of deformation defects of different types. The dependencies of dislocation density and concentrations of point defects on strain for wide interval of temperature and strain rate are defined. The intervals of strong and weak temperature and rate dependence can be selected for all type of defects (fig. 4). These intervals correspond to the intervals of strong and weak temperature and rate dependence for applied stress.

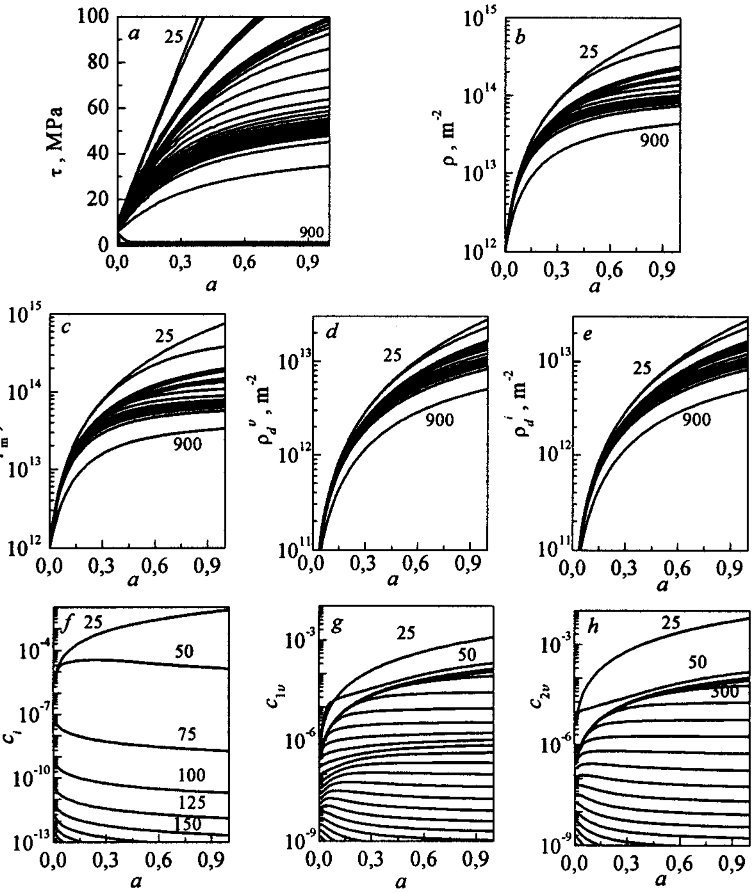

Figure 4: The dependence of density of different type defects on strain. The strain rate is 10^{-4} s^{-1} for Cu and temperatures from 25 to 900 K by step 25.

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