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EQUATIONS OF STATE OF PLASTICALLY DEFORMED POLYCRYSTALLINE MEDIUM CONSIDERING PLASTIC DEFORMATION THERMAL EFFECT

Alexander I Khaimovich and Stanislav R Abulhanov
Samara State Aerospace University, Moskovskoye shosse, Samara, Russia
E-Mail: berill_samara@bk.ru

ABSTRACT

The article suggests a modeling method and shows relations of state of a polycrystalline body under severe plastic deformation in temperature range outside the sphere of phase transformations, where the body constitutes heterogeneous medium created by two interacting components - continual medium and grain boundaries structure imbedded into this medium. Evolution of grain boundaries, temperature and internal energy connected with changes of stress-strain state inside of and at grain boundaries are regarded from the point of view of regulations of thermodynamics of irreversible processes.

Keywords: polycrystalline body, grain boundaries, severe plastic deformation, equations of motion, Gibbs energy, stress-strain state.

INTRODUCTION

Mechanical properties of steel and alloys to a large extent depend on construction of their grain structure formed at a stage of workpieces plastic shaping in hammering and presswork and subsequent thermal treatment. In this regard, to optimize deformation technological parameters and to obtain required properties of workpieces, it is important to model their microstructure. Polycristalline material microstructure may be modelled directly, via dynamics of dislocation motion and crystals plasticity, and indirectly, via relations based on dislocation density. Models using dislocation density are developed in works of Bergström [1, 2, 3] and so on. Direct relations require extensive computing resources; therefore nowadays indirect models are the ones that are developed to the fullest extent. In the sphere of polycrystalline bodies evolution phenomenological modelling the most popular approach is the approach based on Avraami's works [4]. We know a dynamical recrystallization model based on a mesoscale mechanism (MesoScaleUnitsmodel), which gives more precise results, in particular for processes with repeated straining impact [5, 6]. The advantage of MSU-models and the same-name method is a combination of phenomenological approach to the dynamical recrystallization process, which is based on Avraami's models, and physical principles considering grain evolution process driving force connected with dislocation density, and that combined provides a method which is more universal than Avraami's formulas complex. But MSU-models, let alone Avraami's models consider grain boundaries evolution, temperature and internal energy connected with changes of stress strain state inside of and at graing boundaries from the viewpoint of regulations of thermodynamics of irreversible processes, which ties these processes into a unified system of equations. It is evident that this determines a disadvantage of the mentioned models. The approach given in this article is an attempt to obtain such equations system.

What concerns internal energy; crystalline ordered structure inside of grain and non-ordered structure at its boundaries are heterogeneous substances. Thermomechanical interaction of heterogeneous substances during deforming is studied in heterogeneous media mechanics. In particular, in the work [7] deformed medium is regarded as a 2-components model consisting of springing frame saturated with liquid. Medium's behaviour is defined by consolidation equations describing thermomechanical interaction of components which have permanent weight. In the same way, let's regard polycrystalline body as a medium with two components of variable mass – a continual isotropic constituent inside of grain and a constituent of grain boundaries. Particular equations describing medium's state were obtained in an early work [8]. Later we will give some relations from [8] which are necessary for presentation of further conclusions.

Theoretical part

Conditions of dynamic equilibrium of the system of continual medium and grain boundaries constituent will be written in formula (1).

$$\begin{cases} \sigma^{v}_{ij,j} + \sigma^{w}_{ij,j} - \rho[(1-f_\rho)v_i - (f_\rho + \delta\Omega_0)\Delta w_i]_{,t} = 0, \\ \sigma^{w}_{ij,j} - \rho[(f_\rho + \delta\Omega_0^{(m,n,p)})\Delta w_i]_{,t} - F_{\Omega_i} = 0. \end{cases} \quad (1)$$

where $\delta\Omega_0$ is change of local volume due to grain boundaries migration;

F_{Ω_i} is force of interaction between two components of the deformed medium;

ρ is deformed medium density (taken as an invariant one). From now on in subindex at a variable a we accept designator of the operator $a_{,j} = \dfrac{\partial a}{\partial x_j}$, so for components

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of tensor a_{ij} in space D_3 taking into account Einstein notation for repeated indices is denoted as: $a_{ij,j} = \sum_j^3 \left(\frac{\partial a_{ij}}{\partial x_j} \right)$.

Unknown variable of interaction F_{Ω_i} in (1) will be defined using methods of thermodynamics of irreversible processes. Total entropy S in medium's volume Ω limited by size of a grain (or several grains), with surface A, segregates into entropy $\dot{S}_l$, changed by the environment via this surface, and irretrievably increasing entropy S_i. According to Clausius–Duhem inequality:

$$\dot{S}_i = \dot{S} - \dot{S}_l \geq 0 \ . \tag{2}$$

Inequality (2) transformed into a local shape at grain boundaries leads to the following ineqaulity:

$$\dot{S}_i^{loc} = \dot{S}^{loc} + \left[\frac{q_l - \rho c \Delta w_l \Delta T}{T} \right]_{,l} \geq 0 \, , \tag{3}$$

Omitting derivation of the energy balance equation, let's put the first law of thermodynamics for local volume, solving it regarding internal energy U :

$$\begin{cases} \dot{U} = (\sigma_{ij}^v \dot{\varepsilon}_{ij}^v (1 - f_\rho) + \sigma_{ij}^w \dot{\varepsilon}_{ij}^w f_\rho) + F_{\Omega_i} [f_\rho \Delta w_i - (1 - f_\rho) v_i] - (q_{i,i} + \rho c \Delta T_{,i} \Delta w_i) \\ \delta \dot{U} = \rho \delta \Omega_{0,t} [\Delta w_i \delta_{ij} + c \Delta T \ ] \end{cases} \tag{4}$$

where $\{\delta_{ij} \mid \delta_{ij} = 0 \text{ when } i \neq j, \quad \delta_{ij} = 1 \text{ when } i = j\}$ is a Kronecker symbol.

From (4) it follows that change of internal energy is caused by the work of external forces (summand in first brackets), internal friction caused by grain boundaries moving (second summand), and also conducted and delivered heat (last summand). Second equation in (4) is connected with change of internal energy δU , caused by heat transport during grain boundaries migrations and change of mass $\delta \Omega_{0,t}$, located at grain boundaries.

Let's define $\frac{\dot{U}^{loc}}{T}$ in (4) via Helmholtz free energy: $F = U^{loc} - S^{loc} T$, which will be represented in the form of a functional $F = (\varepsilon_{ij}^v, \varepsilon_{ij}^w, T, f_\rho)$, such one that there is a linear combination $F = (1 - f_\rho) F^v (\varepsilon_{ij}^v, T) + f_\rho F^w (\varepsilon_{ij}^w, T)$. In this case change of free energy F will be equal to:

$$\dot{F} = (1 - f_\rho) \left[\frac{\partial F^v}{\partial (\varepsilon_{ij}^v - \delta_{ij} \dot{\varepsilon}^v)} (\dot{\varepsilon}_{ij}^v - \delta_{ij} \dot{\varepsilon}^v) + \frac{\partial F^v}{\partial \varepsilon^v} \delta_{ij} \dot{\varepsilon}^v \right] + f_\rho \left[\frac{\partial F^w}{\partial (\varepsilon_{ij}^w - \delta_{ij} \dot{\varepsilon}^w)} (\dot{\varepsilon}_{ij}^w - \delta_{ij} \dot{\varepsilon}^w) + \frac{\partial F^w}{\partial \varepsilon^w} \delta_{ij} \dot{\varepsilon}^w \right] + S^{loc} \, , \tag{5}$$

where $\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij} - \delta_{ij} \dot{\varepsilon}$ are components of rate-of-strain deviator, $\dot{\varepsilon} = \frac{1}{3} \dot{\varepsilon}_{ij} \delta_{ij}$.

Taking into account (4), (5), the inequality (3) modified to the local shape will be as follows:

$$\begin{aligned} &(1 - f_\rho) \left[\left(\sigma_{ij}^v - \frac{\partial F^v}{\partial (\varepsilon_{ij}^v - \delta_{ij} \dot{\varepsilon}^v)} \right) (\dot{\varepsilon}_{ij}^v - \delta_{ij} \dot{\varepsilon}^v) + (\sigma_{ij}^v - \frac{\partial F^v}{\partial \varepsilon^v}) \delta_{ij} \dot{\varepsilon}^v \right] + \\ &+ f_\rho \left[\left(\sigma_{ij}^w - \frac{\partial F^w}{\partial (\varepsilon_{ij}^w - \delta_{ij} \varepsilon^w)} \right) (\dot{\varepsilon}_{ij}^w - \delta_{ij} \dot{\varepsilon}^w) + \left(\sigma_{ij}^w - \frac{\partial F^w}{\partial \varepsilon^w} \right) \delta_{ij} \dot{\varepsilon}^w \right] + S^{loc} \dot{T} + \\ &+ F_{\Omega_i} [f_\rho \Delta w_i - (1 - f_\rho) v_i]_i - [q_l - \rho c \Delta w_l \Delta T] \Delta T_{,l} \frac{1}{T} \geq 0. \end{aligned} \tag{6}$$

As far as, according to (6), the following defining relations are true

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$$\sigma_{ij}^{v} = \frac{\partial F^{v}}{\partial(\varepsilon_{ij}^{v} - \delta_{ij}\varepsilon^{v})} + \frac{\partial F^{v}}{\partial \varepsilon^{v}}\delta_{ij}, \quad \sigma_{ij}^{w} = \frac{\partial F^{w}}{\partial(\varepsilon_{ij}^{w} - \delta_{ij}\varepsilon^{w})} + \frac{\partial F^{w}}{\partial \varepsilon^{w}}\delta_{ij}$$

and inequality $-[q_l - \rho c \Delta w_l \Delta T]\Delta T_{,l}\dfrac{1}{T} \geq 0$ leads to implementation of heat-transfer law

$$q_l = -\lambda \Delta T_{,l} + \rho c \Delta w_l \Delta T\,, \tag{7}$$

then correspondence (10) is performed identically, if

$$P_D = F_{\Omega_i}\ [f_\rho \Delta w_i - (1 - f_\rho) v_i] \geq 0, \tag{8}$$

where P_D is a power dissipation function connected with expenditure of energy for structure formation caused by relative (over the field of velocities Δw_i) movement of grain boundaries.

Taking into account fulfillment of inequality (8), we can write expanding of F_{Ω_i} in series: $F_{\Omega_i} = \sum_{n=1}^{N} b_n [f_\rho \Delta w_i - (1 - f_\rho) v_i]^{2n-1}, n \in N$, from which, considering the first member of the line when n=1, it follows that:

$$F_{\Omega_i} = b\ [f_\rho \Delta w_i - (1 - f_\rho) v_i], \tag{9}$$

Free energy F is a scalar value of the invariant of state of rate of deformation and temperature. After finding values of partial derivatives of F at thermodynamic equilibrium point $(0,0,0,0,T)$ as characteristics of the material properties, which is equivalent to Taylor's serial expansion coefficients similar to (6), we will find defining relations for the deformed polycrystalline medium:

$$\sigma_{ij}^{v} = 2\frac{\mu_{\Sigma}^{v}}{\dot{\varepsilon}_2^{v}}\dot{\varepsilon}_{ij}^{v} + (\mu_{\Omega}^{v}\dot{\varepsilon}^{v} - v_m^{v}\Delta T_{,t} + \sigma^{v})\delta_{ij}, \ \sigma^{v} = \frac{1}{3}\sigma_{ij}^{v}\delta_{ij}, \ \dot{\varepsilon}^{v} = \frac{1}{3}\dot{\varepsilon}_{ij}^{v}\delta_{ij}$$

$$\sigma_{ij}^{w} = 2\frac{\mu_{\Sigma}^{w}}{\dot{\varepsilon}_2^{w}}\dot{\varepsilon}_{ij}^{w} + (\mu_{\Omega}^{w}\dot{\varepsilon}^{w} - v_m^{w}\Delta T_{,t} + \sigma^{w})\delta_{ij}, \ \sigma^{w} = \frac{1}{3}\sigma_{ij}^{w}\delta_{ij}, \dot{\varepsilon}^{v} = \frac{1}{3}\dot{\varepsilon}_{ij}^{v}\delta_{ij}$$

$$\mu_{\Sigma}^{w} = \mu_{\Sigma_0}^{w} + \eta^{w}\dot{\varepsilon}_{2cp}{}^{w},$$
$$\mu_{\Sigma}^{v} = \mu_{\Sigma_0}^{v} + \frac{f_\rho}{1 - f_\rho}\mu\,, \tag{10}$$
$$v_m^{v} = \mu_{\Omega}^{v}\alpha_m^{v}, \quad v_m^{w} = \mu_{\Omega}^{w}\alpha_m^{w}$$

where $\dfrac{\mu_{\Sigma}^{v}}{\dot{\varepsilon}_2^{v}}, \dfrac{\mu_{\Sigma}^{w}}{\dot{\varepsilon}_2^{w}}$ are shear moduli for continual and grain boundaries constituents $\mu_{\Sigma_0}^{v} = \left(\dfrac{\partial^2 F^{v}(0,0,0,0,T)}{\partial \dot{\varepsilon}_2^{v}\partial t}\right), \mu_{\Sigma_0}^{w} = \left(\dfrac{\partial^2 F^{w}(0,0,0,0,T)}{\partial \dot{\varepsilon}_2^{w}\partial t}\right)$;

$$\mu_{\Omega}^{v} = \frac{\partial^2 F^{v}(0,0,0,0,T)}{(\partial \dot{\varepsilon}_1^{v})^2}, \mu_{\Omega}^{w} = \frac{\partial^2 F^{v}(0,0,0,0,T)}{(\partial \dot{\varepsilon}_1^{w})^2}$$

are moduli of volume elasticity for corresponding constituents of the medium; $\dot{\varepsilon}_{2cp}^{w}$ is an invariant corresponding to the deformation rate intensity which is average for the deformation process.

Coefficients v_m^{v}, v_m^{w} from (10), describing thermophysical properties of the deformed medium constituents are defined with the help of relations

$$v_m^{v} = \frac{C_{\sigma}^{v} - C_{\Omega}^{v}}{3\alpha_m^{v}T}, \quad v_m^{w} = \frac{C_{\sigma}^{w} - C_{\Omega}^{w}}{3\alpha_m^{w}T} \tag{11}$$

Power dissipation, connected with thermophysical restructuring, is determined by internal forces capacity and change of heat flow inside of volume and passage of heat via its surface, which follows from the correspondence (4) for substantial derivative of the internal energy $\dot{U}$:

$$T\dot{S}^{\text{лок}} = 3[(1-f_\rho)v_m^{v}\dot{\varepsilon}^{v} + f_\rho v_m^{w}\dot{\varepsilon}^{w})]T + c_{\Omega}\dot{T} = F_{\Omega_i}[f_\rho \Delta w_i - (1-f_\rho)v_i] - q_{i,i} + \rho c \Delta T_{,i}\Delta w_i$$

The last correspondence together with (11) and heat-transfer law (7) lead to a generalized equation for heat transfer in a polycrystalline medium:

$$\lambda\nabla^2 T + F_{\Omega_i}[f_\rho \Delta w_i - (1-f_\rho)v_i] = c_{\Omega}\dot{T} + f_\rho\frac{c_{\sigma}^{w} - c_{\Omega}^{w}}{\alpha_m^{w}}\dot{\varepsilon}^{w} + (1-f_\rho)\frac{c_{\sigma}^{v} - c_{\Omega}^{v}}{\alpha_m^{v}}\dot{\varepsilon}^{v} \tag{12}$$

We can calculate the coefficient b from the polycrystalline medium motion law in the form (13) after analyzing (12) in stationary conditions of isothermic restraint at grain boundaries:

$$b = (-1)^{n}\frac{(c_{\sigma}^{w} - c_{\Omega}^{w})\Delta T_{,t}}{(f_{\rho}^{w} \cdot \Delta w_i)^2}\,, \tag{13}$$

where n defines average direction of grain size change under dynamical recrystallization $(n = 0 \text{ - grain is increasing, } n = 1 \text{ - grain is decreasing})$.

Taking into account (13) and the fact that main volume of the deformed continuous medium falls on the continual constituent, and the structure formation coefficient f_ρ is of quantum nature, heat-transfer equation equals to the system:

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$$\lambda\nabla^2\square T = c_\Omega \square \dot{T} + \frac{c_\sigma^v - c_\Omega^v}{\alpha_m^v}\dot{\varepsilon}^v - \text{ inside of grain}$$
$$(-1)^n \frac{(f_\rho^w \cdot \Delta w_i - (1-f_\rho^w)v_i)^2}{(f_\rho^w \cdot \Delta w_i)^2}\delta_{ii}\square T_{,t} = \frac{\dot{\varepsilon}^w}{\alpha_m^v} \text{ - in local domain at grain} \tag{14}$$

We will find the coefficient of heat migration of grain boundaries α_m^w using the phenomenological approach and supposing that grain size is proportional to the function describing diffusion:

$$\alpha_m^w(T) = \alpha_{T_н}\left[\exp\left(\frac{Q}{R}\left(\frac{1}{T_н} - \frac{1}{T}\right)\right)\right]^{a_1}, \tag{15}$$

where Q is a self-diffusion activation energy, R is a universal gas constant, $\alpha_{T_н}$, a_1 are constant coefficients.

Let's present the second equation in (14) in the differential form

$$d\varepsilon_{ii}^w = (-1)^n \alpha_m^w \left(1 - \frac{1-f_\rho^w}{f_\rho^w f_{ii}}\right)^2 dT, \quad f_{ii} = \frac{\square w_i}{v_i}$$ and

replace differentials with finite increments, and after transformations we will obtain the system of equations describing the process of dynamical recrystallization during grain size change in the direction of axis i from d_0 to d_i.

$$\frac{d_i - d_0}{d_0} = (-1)^n a_0 \cdot \alpha_m^w \cdot (T - T_\varepsilon)\cdot k_i;\ k_i = \left(1 - a_2(\dot{\varepsilon}_2^v)^{a_\Sigma}\right)^2 = \left(1 - \frac{1-f_\rho^w}{f_\rho^w f_{ii}}\right)^2, f_{ii} = f_0 k_{\varepsilon i},$$
$$\text{when } d_i = d_{cp}\ \ f_0 = f_{cp}, k_{\varepsilon i} = 1,\ f_{cp} = (f_{cp})_0\left(\frac{\dot{\varepsilon}_2^v}{(\dot{\varepsilon}_2^v)_0}\right)^{-a_\Sigma}, \alpha_m^w = \alpha_{T=273}\left[\exp\left(\frac{Q}{R}\left(\frac{1}{273} - \frac{1}{T_\varepsilon}\right)\right)\right]^{a_1}, \tag{16}$$

where unknown coefficients a_1, a_Σ and $a_0 = (f_{cp})_0(1 - f_\rho^w)$, $a_2 = \dfrac{1-f_\rho^w}{f_\rho^w (f_{cp})_0 k_{\varepsilon i}}(\dot{\varepsilon}_{2\varepsilon}^v)^{-a_\Sigma}$ are found experimentally with the help of dynamical recrystallization diagrams; T, T_ε are current temperature and some reference temperature found experimentally.

To define coefficients of connection between linkage parameters of movement of polycrystalline medium and its microstructure let's state functional relations between field parameters describing grain boundaries migration and microstructure geometrical parameters which can be found by means of optical metallography. Let's put 12 coefficients of connection with the form $\Delta w_i = \Theta(v_i)$: $f_{ii} = \dfrac{\Delta w_i}{v_i}$ - 3 coefficients,

$f_{ii}' = f_{ii,i}\dfrac{v_i}{v_{i,i}} + f_{ii},\ f_{ij}' = f_{ii,j}\dfrac{v_i}{v_{i,j}} + f_{ii}$ - 9 coefficients, where $f_{ii,i} = f_{ii}\left(\dfrac{\Delta w_{i,i}}{\Delta w_i} - \dfrac{v_{i,i}}{v_i}\right), f_{ii,j} = f_{ii}\left(\dfrac{\Delta w_{i,j}}{\Delta w_i} - \dfrac{v_{i,j}}{v_i}\right)$, then:

$$\dot{\varepsilon}_{ii}^w = f_{ii}'\dot{\varepsilon}_{ii}^v,\ \dot{\varepsilon}_{ij}^w = \frac{1}{2}(f_{ij}' v_{i,j} + f_{ji}' v_{j,i}) \tag{17}$$

Let's introduce some functions ψ_i, ψ_{ij}, such that the following will be performed: $\dfrac{\Delta w_{i,i}}{\Delta w_i} = \dfrac{v_{i,i}}{v_i} + \dfrac{\psi_i}{v_i},\ \dfrac{\Delta w_{i,j}}{\Delta w_i} = \dfrac{v_{i,j}}{v_i} + \dfrac{\psi_{ij}}{v_i}$, then if $f_{ij}' = f_{ji}'$ the following relations are true:

$$\dot{\varepsilon}_{ii}^w = f_{ii}(\dot{\varepsilon}_{ii}^v + \psi_i),\ \dot{\varepsilon}_{ij}^w = f_{ii}\left(1 + \frac{\psi_{ij}}{v_{i,j}}\right)\dot{\varepsilon}_{ij}^v,\ \psi_{ij} = v_{i,j}\left[\frac{f_{jj}}{f_{ii}}\left(1 + \frac{\psi_{ji}}{v_{j,i}}\right) - 1\right] \tag{18}$$

If, for example, we put $\psi_{ij} = 0$, which is equal to $\psi_{ji} = 0$, then we will obtain:

$$\dot{\varepsilon}_{ij}^w = f_{ii}\dot{\varepsilon}_{ij}^v, \quad \dot{\varepsilon}_{ji}^w = f_{jj}\dot{\varepsilon}_{ji}^v \tag{19}$$

Physical meaning of the value ψ_i is illustrated by Figure-1, where $f_{ii}\psi_i$ is deformation $\dot{\varepsilon}_{ii}^w$ rate step due to grain division after reaching critical value $(\dot{\varepsilon}_{ii}^w)_{кр}$. Approximating (fitting) curve is defined by the relation:

$$\dot{\varepsilon}_{ii}^w = f_0 k_{\varepsilon i}\dot{\varepsilon}_{ii}^v, \tag{20}$$

where

$k_{\varepsilon i}$ is a coefficient of grain boundaries structure sensitivity towards deformation intensity. Let's define coefficients $k_{\varepsilon i}$ in such a way that they could be found via grain size change in three projections.

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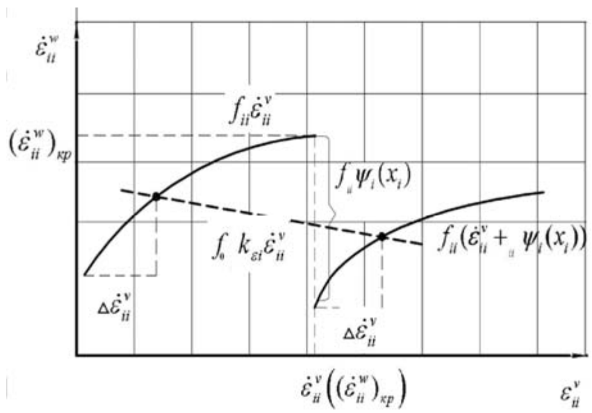

Figure-1. Dependence of $\dot{\varepsilon}_{ii}^{w}$ on $\dot{\varepsilon}_{ii}^{v}$ considering recrystallization: solid line - recrystallization true curve; dashed line - approximating relation.

Let it be

$$k_{\varepsilon i}=(1+\operatorname{sgn}(\varepsilon_{ii}^{v})(k_{jj}^{i}-\frac{\dot{\varepsilon}_{jj}^{v}}{\dot{\varepsilon}_{ii}^{v}})),$$

$$k_{\varepsilon i}=(1+\operatorname{sgn}(\varepsilon_{ii}^{v})(k_{kk}^{i}-\frac{\dot{\varepsilon}_{kk}^{v}}{\dot{\varepsilon}_{ii}^{v}}))$$, then for 3-dimensional deformation we will have:

$$k_{ll}^{m\neq l}=\begin{pmatrix}0 & k_{jj}^{i} & k_{kk}^{i}\\ k_{ii}^{j} & 0 & k_{kk}^{j}\\ k_{ii}^{k} & k_{jj}^{k} & 0\end{pmatrix}\text{ - coefficient matrix,} \tag{21}$$

$$k_{ll}^{m\neq l}-\frac{\dot{\varepsilon}_{ll}^{v}}{\dot{\varepsilon}_{mm\neq ll}^{v}}=k_{pp\neq ll}^{m\neq p}-\frac{\dot{\varepsilon}_{pp}^{v}}{\dot{\varepsilon}_{mm\neq pp}^{v}}\text{ - coefficientconnectionequations.}$$

For plane deformation state:

$$\dot{\varepsilon}_{ii}^{w}=f_0 k_{\varepsilon i}\dot{\varepsilon}_{ii}^{v}=f_0\left(1+\operatorname{sgn}(\dot{\varepsilon}_{ij}^{v})k\right)\dot{\varepsilon}_{ii}^{v} \tag{22}$$

The condition of constancy of volume of the grain with sizes along the axes d_i, d_j, d_k : $d_{cp}^{3}=d_i d_j d_k$ and dynamical recrystallization equation in the form (16) lead to the relation:

$$\left(1-\alpha_T\left(1-\frac{1-f_{\rho}^{w}}{f_{\rho}^{w}f_{cp}}\right)^{2}\right)^{3}=\prod_{l=i,j,k}\left(1-\alpha_T\left(1-\frac{1-f_{\rho}^{w}}{f_{\rho}^{w}f_{ll}}\right)^{2}\right), \tag{23}$$

where $\alpha_T=(f_{cp})_0\cdot(1-f_{\rho}^{w})\cdot\alpha_m^{w}\cdot(T-T_{\varepsilon})$

In total we have 7 unknown values (6 coefficients $k_{ll}^{m\neq l}$ and 1 coefficient f_0). They are connected by 4 relations: 3 equations (21) and sizes connection equation (23). Therefore, to define unknown coefficients we need 3 orthogonal planes of microstructure shear, which pass through unit vectors i, j, k.

As a result, we found linear functional relations connecting deformation rates $\dot{\varepsilon}_{ii}^{w}$ of grain boundaries and $\dot{\varepsilon}_{ii}^{v}$ continual constituents of the deformed polycrystalline medium via coefficients $k_{ll}^{m\neq l}$, defined according to microstructure parameters.

Let's analyze 3 coefficients f_{ii}, obtained from the dynamical recrystallization equation, describing connection between $\dot{\varepsilon}_{ij}^{w}, \Delta w_i, f_{ii}$ (correlations (18)-(22)) and also describing correlations (10). As a result, after substituting these relations into (3) we obtain 6 equations of deformed polycrystalline medium motion in the form (24):

$$\mu_{\Sigma}^{v}\nabla^{2}v_i+\sigma_{,i}^{v}-\mu_{\Omega}^{v}\alpha_m^{v}\Box T_{,ti}+F_{\Omega_i}-\rho(1-f_{\rho})v_{i,t}=0,$$

$$\mu_{\Sigma}^{w}\nabla^{2}(f_{ii}v_i)+\frac{\mu_{\Omega}^{w}}{3}((f_{ii,i}v_i+f_{ii}v_{i,i})\delta_{ij})_{,i}+\sigma_{,i}^{w}-\mu_{\Omega}^{w}\alpha_m^{w}\Box T_{,ti}-F_{\Omega_i}-\rho(f_{\rho}+\delta\Omega_0)f_{ii}v_{i,t}=0\,, \tag{24}$$

where $f_{ii,i}=f_{ii}\dfrac{\psi_i(x_i)}{v_i}$ and according to (18), (20) $\psi_i=\left(\dfrac{f_0}{f_{ii}}k_{\varepsilon i}-1\right)\dfrac{\dot{\varepsilon}_{ii}^{v}}{v_i}$.

With some approximation we can accept that average pressure is equal for both constituents of the medium $\sigma_{,i}^{v}\approx\sigma_{,i}^{w}=\sigma_{,i}$, then (24) will have the following form:

$$\mu_{\Sigma}^{v}\nabla^{2}v_i+\sigma_{,i}^{v}-\mu_{\Omega}^{v}\alpha_m^{v}\Box T_{,ti}+F_{\Omega_i}-\rho(1-f_{\rho})v_{i,t}=0,$$

$$\mu_{\Sigma}^{w}\nabla^{2}(f_{ii}v_i)+\mu_{\Omega}^{w}\left(\frac{1}{3}f_0 k_{\varepsilon i,i}\delta_{ij}-\alpha_m^{w}\Box T_{,ti}\right)+\sigma_{,i}-F_{\Omega_i}-\rho(f_{\rho}+\delta\Omega_0)f_{ii}v_{i,t}=0 \tag{25}$$

Thus, 6 equations (25) connect 3 unknown constituents of the medium flow rate v_i, 3 unknown values of hydrostatic pressure gradient $\sigma_{,i}$, 3 constituents of structure formation internal force $F_{\Omega_i}=b_i[f_{\rho}f_{ii}-(1-f_{\rho})]v_i$, $b_i=(-1)^{n}\dfrac{(c_{\sigma}-c_{\Omega})\Delta T_{,t}}{(f_{\rho}^{w}\cdot f_{ii}v_i)^{2}}$ and, if ignoring heat passage from local volume for high

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rates of deformation, law of transformation of plastic deformation energy into heat energy $\square T_{,t} = k_T^v \dot{\varepsilon}_2^v$.

Calculations and experimental part

The most difficult task in finding invariables appearing in the motion equations (25) is to find a coefficient of shear modulus for grain boundaries μ_Σ^w. As an example let's take hot deformation of titanium alloy BT9. Value μ_Σ^w for BT9 is estimated on the basis of coefficients found according to the dynamical recrystallization model in the form (16) [9]. The dynamical recrystallization model according to (16) is visually presented in Figure-2. Models were obtained under a priori accepted values of coefficients n=1, a_0= 0.001. Calculated coefficients and statistics corresponding to them are shown in Table-1.

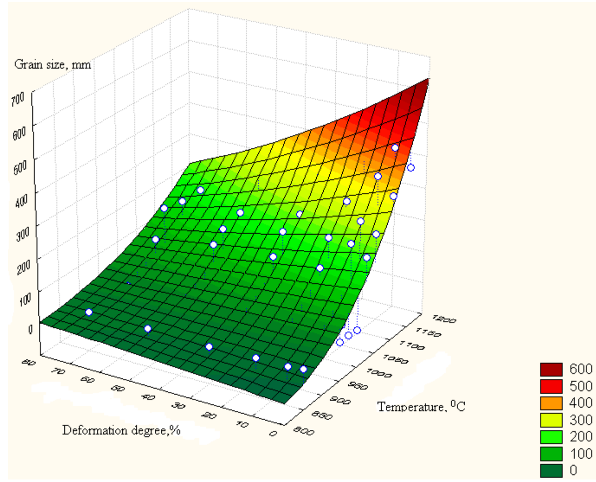

Figure-2. Dynamical recrystallization surface (mathematic model visualization) and experimentally obtained points for hot slump of titanium alloy BT9.

Table-1. Design coefficients of the dynamical recrystallization mathematic model.

Titanium alloy BT9. $a_3 = 1$, $\alpha_{T\varepsilon} = 0{,}9 \cdot 10^{-5}$, $\frac{Q}{R}$=38,7·10³ **K, initial grain size -** d_0 **=20 µm. The model's confidence level - 90 %**			
a_1	0.141	0.00097	145.541
a_2	0.565	0.09272	6.095
T_ε	1191.465	16.4696	55.767

Value of shear modulus μ_Σ^v for the continual constituent can be found in reference data or in experimental data. In our case deformation proceeds under high temperatures T_0=1223K, when yield limit is determined by temperature factor, in this case it is $\mu_\Sigma^v = \frac{\sigma_s}{3}$=18.3MPa [10].

Using value of μ_Σ^v, and also Hall-Petch law [11-13], let's estimate the shear modulus μ_Σ^w for the grain boundaries constituent.

Plastic deformation local power is estimated via expression $(1-f_\rho)\sigma_2^v\dot{\varepsilon}_2^v + f_\rho\sigma_2^w\dot{\varepsilon}_2^w$, and usually during the process of deformation, under conditions of all-around non-uniform compression, grain is atomized. Even during large deformation, grain is atomized to a certain limit under permanent increase of plastic deformation power; therefore, for local volume at grain boundaries the following inequality is true:

$(1-f_\rho^w)\sigma_2^v\dot{\varepsilon}_2^v \geq f_\rho^w\sigma_2^w\dot{\varepsilon}_2^w$ or $(1-f_\rho^w)\mu_\Sigma^v \cdot (\dot{\varepsilon}_2^v)^2 \geq f_\rho^w\mu_\Sigma^w \cdot (\dot{\varepsilon}_2^w)^2$, from which we obtain an upper estimate:

$$\mu_\Sigma^w \leq \mu_\Sigma^v \frac{1-f_\rho^w}{f_\rho^w}\left(\frac{\dot{\varepsilon}_2^v(v_i)}{\dot{\varepsilon}_2^w(v_i, f_{ii})}\right)^2 \quad (24)$$

Let's estimate the ratio $\frac{\dot{\varepsilon}_2^v}{\dot{\varepsilon}_2^w}$ in (25). For this purpose, to simplify computations, let's take a plastically deformed state for which $v_3 \equiv 0, \dot{\varepsilon}_{11} = -\dot{\varepsilon}_{22}$, and besides, according to (22) the following is performed:

$$\dot{\varepsilon}_{ij}^w = f_0 k_{\varepsilon i}\dot{\varepsilon}_{ij}^v, \quad (25)$$

where $k_{\varepsilon 1} = 1 + k,\ k_{\varepsilon 2} = 1 - k$

Accordingly, for intensities of deformation rates of continual and grain boundaries constituents we have the following relations:

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$$\dot{\varepsilon}_2^v = \frac{2}{\sqrt{3}}\left((\dot{\varepsilon}_{11}^v)^2 + 2(\dot{\varepsilon}_{12}^v)^2\right)^{1/2}, \tag{26}$$

$$\begin{aligned}\dot{\varepsilon}_2^w &= \frac{\sqrt{2}}{3} f_0\left(2k_{\varepsilon 1}k_{\varepsilon 2}(\dot{\varepsilon}_{11}^v)^2 + 2(k_{\varepsilon 1}{}^2 + k_{\varepsilon 2}{}^2)(\dot{\varepsilon}_{11}^v)^2 + 6(k_{\varepsilon 1}{}^2 + k_{\varepsilon 2}{}^2)(\dot{\varepsilon}_{12}^v)^2\right)^{1/2} = \\ &= \frac{\sqrt{2}}{3} f_0\left(4(\dot{\varepsilon}_{11}^v)^2 + 2(1+k^2)\left[(\dot{\varepsilon}_{11}^v)^2 + 6(\dot{\varepsilon}_{12}^v)^2\right]\right)^{1/2} \geq \sqrt{2} f_0 \dot{\varepsilon}_2^v\end{aligned} \tag{27}$$

Then the upper estimate (24) of shear modulus μ_Σ^w in this case will be as follows:

$$\mu_\Sigma^w < \mu_\Sigma^v \frac{1 - f_\rho^w}{2 f_\rho^w (f_0)^2} \tag{28}$$

Sizes of an α-phase of a grain, obtained under high-speed extrusion of workpieces of blades made from titanium alloy BT9 [14] (Table-2):

Table-2. Parameters of microstructure of titanium alloy BT9.

Coefficient f_ρ^w	Coefficient f_0	Size of α -phase in initial grain, μm	Size of α -phase in grain after deformation, μm
0.92761	0.1377	4.2	2.85

Using (28), we obtain the stiffness factor upper estimate

$$\mu_\Sigma^w < 2,058 \mu_\Sigma^v \tag{29}$$

It is known that the classical Hall-Petch law describes relation between yield limit σ_s^w and average size of grain *d* of polycrystalline material:

$$\sigma_s^w = \sigma_{st} + K d^{-1/2}, \tag{30}$$

where σ_{st} is a certain friction stress necessary for glide of dislocations in a monocrystal, and K is a material constant often called "a Hall-Petch coefficient". This law is well-fulfilled for polycrystals, grains of which are of size more than 1 μm, and this good correspondence usually preserves up to a very small grain of size nearly 100 nanometers [13].

Using known Tabor's law [16] $\sigma_s = CH$, which states proportional relations between microhardness H and yield limit σ_s with proportionality coefficient C (C=0.4…0.6), let's estimate, in accordance with experimental data obtained for titanium in the work [17], value of Hall-Petch coefficient:

$K = (5...7,8)\square\sigma_s \text{ MPa} \cdot м^{1/2}$, where $\square\sigma_s$ is a microhardness increment according to the data of [17].

Therefore, if we know the estimation of $\sigma_s^w |_{d=d_0} = \sigma_0$ under grain size d_0, then we have:

$$\sigma_s^w = \sigma_0 + K(d^{-1/2} - d_0{}^{-1/2})$$

Because σ_s^w, given due to Hall-Petch correlation, determines lower value leading to yield, then the estimation of μ_Σ^w below is valid:

$$\mu_\Sigma^w > \frac{1}{3}(\sigma_0 + K(d^{-1/2} - d_0{}^{-1/2})) \tag{31}$$

On the basis of (29) and (31), we obtain boundaries for estimation of μ_Σ^w

$$\begin{gathered}(1,522...1,814)\mu_\Sigma^v < \mu_\Sigma^w < 2,058\mu_\Sigma^v \\ \mu_\Sigma^v = \frac{\sigma_s}{3}\end{gathered} \tag{32}$$

Values of coefficients ν_Ω^v and ν_Ω^w can be calculated using known data (Table-3).

Table-3. Thermophysical data for titanium alloy BT9 ([18]).

C_p, J/kg K		α_m, K[-1]		Q/R, K	a_T [Aut.]	T₀,K	ρ, kg/m³	m_a g/mole	ν_Ω^v, MPa/K (11)	ν_Ω^w MPa/K (11)
T= 273K	T= 1223K	T= 273K	T= 1223K							
530.8	633.9	8E-6	1E-5	3.87E+4	0.141	1223	4.5E+3	47.88	13.9	2.49

According to the Table data, increment of internal stress in grain border area due to deformation thermal effect will be correspondingly 13.9 and 2.49 Mpa for each 1 K of temperature increment.

CONCLUSIONS

a) We suggested a modelling method and obtained relations of state of a polycrystalline body under severe plastic deformation in the temperature range outside the phase changes area, where a body is a heterogeneous medium consisting of two interacting constituents - a continual medium and a structure of grains boundaries imbedded into this medium.
b) Equations of medium state, expressed via medium's flow rate and grain boundaries migration rate, include per-unit force of interaction of continual medium and grain boundaries, which is proportional to the rate of relative displacement of grain boundaries, and this force is determined by invariables which can be found in the dynamical recrystallization diagram.
c) On the basis of microstructure change during dynamical recrystallization (change of size of a grain or a subgrain) we can estimate parameters of the stress-strain state if we know a 2-level model including:

- defining relations between stress fields and deformations (deformation rates) and, correspondingly, the deformation hardening law;
- dependence of parameters of microstructure (size of a grain or a subgrain) on the specified field functions.

REFERENCES

[1] Hirth J., Lothe J. 1972. Dislocation theory [Text:]/ J. Hirth, J. Lothe.-Moscow.: Atomizdat. p. 598.

[2] Bergstrom Y. 1969-1970. Dislocation model for the stress-strain behaviour of polycrystalline alpha-iron with special emphasis on the variation of the densities of mobile and immobile dislocations [Text:]/ Y. Bergstrom// Mater. Sci. Eng. 5: 193-200.

[3] Bergstrom Y. 1983. The plastic deformation of metals - A dislocation model and its applicability. [Text:]/ Y. Bergstrom// Reviews on powder metallurgy and physical ceramics. 2(2, 3): 79-265.

[4] Thomas J.Ph. 2006. Mesoscale Modeling of the Recrystallization of Waspaloy and Application to the Simulation of the Ingot-Cogging Process [Text:]/ J. Ph. Thomas, S.L. Semiatin //AFRL-ML-WP-TP. 483, p. 11.

[5] Semiatin S.L. 2004. [Text:]/ S.L. Semiatin, D.S. Weaver, P.N. Fagin, M.G. Glavicic, R.L. Goetz, N.D. Frey, R.C. Kramb, M.M. Anthony// Metal. Mater. Trans. A. 35A: 679-693.

[6] Thomas J.Ph. 2006. [Text:]/ J.Ph. Thomas, F. Montheillet, S.L. Semiatin // submitted to Metal. Mater. Trans. A.

[7] Derski W. 1978. Equations of motion of fluid-saturated porous solid. Bull. Acad. Pol. Sci., cl. IV, 26, Vol. 11.

[8] Khaimovich A.I. 2013. Equations of state of plastically deformed polycrystalline medium [E-resource:]/A.I. Khaimovich // Modern problems of science and education. (5): 11 URL: http://www.science-education.ru/111-10241 (date of reference: 03.10.2013).

[9] Khaimovich A.I. 2011. Mathematical modelling of processes of polycrystalline materials dynamical recrystallization in conditions of severe plastic deformation / A.I. Khaimovich, V.A. Mikheyev // Press-forging- Moscow. (7): 37-44.

[10] Tretyakov A.V., Trofimov G.K., Zyuzin V.I. 1974. Mechanical properties of metals and alloys in conditions of metal working process. Moscow: Metallurgy. p. 222.

[11] Carl C. Koch and J. Narayan. 2000. The Inverse Hall-Petch Effect-Fact or Artifact? MRS Proceedings, 634, B5.1.1 doi:10.1557/PROC-634-B5.1.1.

[12] Masumura R.A., Hazzledine P.M., Pande C.S. 1998. Yield stress of fine grained materials. [Text:]/ R.A. Masumura, P.M. Hazzledine, C.S. Pande// Acta Mater. 46,¹13: 4527-4534.

[13] Pande C.S., Masumura R.A., Armstrong R.W. 1993. Pile-up based Hall-Petch relation for nanoscale materials. [Text:]/ C.S. Pande, R.A. Masumura, R.W. Armstrong// Nanostruct. Mater. 2: 323-331.

[14] Shitarev L.I. 2011. Modelling of microstructure in conditions of high-velocity forming of blades made from titanium alloy BT9 /I.L. Shitarev, A.I. Khaimovich //Procuring production in machine building. Moscow: Machine building. (11): 41-44.

[15] Hall E.O. 1951. Deformation and ageing of mild steel. [Text:]/ E.O. Hall //Proc. Phys. Soc. London, ser. B. 64, 1: 747-753.

[16] Hutchings Ian M. 2009. The contributions of David Tabor to the science of indentation hardness J. Mater. Res. 24(3): 580-589.

[17] Sergueeva A.V. 2001. Advanced properties of pure titanium with ultrafine grained structure [Text:]/ A.V. Sergueeva, V.V. Stolyarov, R.Z. Valiev, A.K. Mukherjee //ScriptaMaterialia. 45: 747-752.

[18] Zinovyev V.E. 1989. Thermophysical properties of metals under high temperatures. Reference book. [Text:] / V.E. Zinovyev. Moscow: Metallurgy. p. 384.

Symbols

v_l - continual medium motion speed, $l = i, j, k$;

w_l - speed of relative motion (migration) of polycrystalline medium grain boundaries;

t - current time;

A - surface area;

Ω - volume;

f_ρ - volume coefficient of grain boundaries structure amount;

f_ρ^w - value of f_ρ in local domain at grain boundaries;

$[k_{jj}^i]$ - matrix of coefficients of sensitivity of deformed medium grain boundaries constituent's deformation to the stress-strain state form;

$f'_{ij} = \frac{w_{i,j}}{v_{i,j}}$ - relative variation of speed of grain boundaries migration in j axis direction;

α_m^v - line expansion coefficient;

α_m^w - coefficient of thermal migration of grain boundaries;

$\varepsilon_{ij}^v, \varepsilon_{ij}^w$ - components of tensor of strain of continual and grain boundaries constituents of deformed medium;

$\dot{\varepsilon}_{ij}^v, \dot{\varepsilon}_{ij}^w$ - components of tensor of rate of strain of continual and grain boundaries constituents of deformed medium;

$\sigma_{ij}^v, \sigma_{ij}^w$ - components of tensor of stress of continual and grain boundaries constituents of deformed medium;

$\dot{\varepsilon}_2^v, \dot{\varepsilon}_2^w$ - strain rate intensity for continual and grain boundaries constituents;

F_Ω - per-unit-volume power used for changing size and shape of grain;

U - internal energy;

F - Helmholtz free energy;

S - entropy;

c - thermal capacity;

c_Ω - isochoric thermal capacity;

c_σ - thermal capacity at constant pressure;

λ – thermal conductivity;

q_i [J/m^{2}c] – coordinates of heat flow vector;

k_T^v [K] - coefficient of plastic deformation energy conversion into heat energy;

T [K] - temperature;

T_0 [K] - forging temperature