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ON MACROKINETICS UNDER DYNAMIC SUPERPLASTICITY

D.A. Kitaeva[1*], **Ya.I. Rudaev**[2]

[1]Peter the Great St.Petersburg Polytechnic University, St.Petersburg, 29 Politechnicheskaya str., 195251, Russia

[2]Kyrgyz-Russian Slavic University, Bishkek, 44 Kiev str., 720000, Kyrgyzstan

*e-mail: kitaeva_da@spbstu.ru

Abstract. The experimental study of deformation behavior of group industrial aluminum alloys in the broad temperature and high-speed ranges led to creation of the mathematical model for the case of simple tensile and compression, establishing the relationship between stress, temperature and kinetic variables, and responding to analytically formulated conditions of transition to superplastic state. Within synergetic conceptions we will choose the potential function in the form of assembling catastrophe from conditions of qualitative identity of the experimental data. It is added by the kinetic equations for the control parameter and inner state parameters. The given ratios are acceptable for the description of concrete regularities of deformation when the function of material sensitivity to the structural transformations is expressed. Basic model use allow to research nonequilibrium system reaction to behavior of thermodynamic response functions – the specific heat and entropy – and to establish implementations features of the irreversible indistinct phase transitions observed in the conditions of dynamic superplasticity for aluminum alloys.

Keywords: aluminum alloys; specific heat; entropy; superplasticity.

1. Introduction

According to [1], we suppose that macrokinetics carries out researches related to evolutionary type transformations at all hierarchical levels in nonequilibrium systems. Therefore in macrokinetics various transformations in their interrelations with simultaneous mass transfer processes, variability of a structural state with hierarchy of systems and their mechanical properties taken into account.

The given reasoning follows that it is necessary to use nonequilibrium statistical mechanics methods for the analysis of structural and phase transitions of dynamic type, for example, in relation to superplasticity effect [2].

It is observed [3] that superplastic properties' exhibiting is answered for by the mechanism of sliding along grain boundaries as predominant over other mass transfer forms. Implementation of this mechanism is facilitated by fine-grained structure formation at the preliminary stage (structural or micrograin superplasticity) or during heating and deformation processes (dynamic superplasticity). In other words, superplasticity of dynamic type can occure in materials in any initial state from cast to deformed [2]. In essence, during the heating and deformation the initial structure is transferred into the one ready for superplasticity. The mentioned above changes are caused by the superposition of deformation rates and structural and phase transitions of evolutionary type in the open nonequilibrium systems [4-6]. In particular, for commercial aluminum alloys such irreversible transition is dynamic recrystallization [7,8] resulting in grain shattering and equiaxial fine-grained structure. Model which adequately represents the accumulated experimental and generalized in [2] data from positions of deformable solid mechanics is summed up in works [2,6,9]. The

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model describes deformation behavior of aluminum alloys not only in case of superplasticity, but also in the boundary fields of thermoplasticity and high-temperature creep.

Basic model [2,6,9] use allows to research nonequilibrium system reaction to behavior of thermodynamic response functions – the specific heat and entropy – and to establish development aspects of irreversible indistinct phase transitions [10-12] observed under the conditions of dynamic superplasticity for aluminum alloys. The immediate data of specific heat change which are carried out, for example, for classical superplastic alloy Zn-22%Al [13] confirm compliance of optimum superplasticity temperature to specific heat peak.

Making association of deformation process with metal flow, that has irreversible structural and phase transition of indistinct type at one of the stages, the continuity of entropy and specific heat functions is priori assumed [15,16].

2. Dynamic model

The classical description [17] of the determined approach of phase transitions includes introduction of the potential functions $\Phi(\eta,\beta)$, where η – order parameter, β – control parameter.

The potential function in the form of assemblage catastrophe [18] with account for external field effect is chosen from condition of qualitative identity to the experimental data [2,6,9].

$$\Phi(\eta,\beta)=\frac{1}{4}m_0\eta^4+\frac{1}{2}\beta(\xi)\eta^2-q\eta\,. \tag{1}$$

Here we have

$$q=\frac{\sigma}{\sigma^*}-1;\quad \eta=\frac{\dot{\varepsilon}}{\dot{\varepsilon}^*}-1;\quad \xi=\frac{\theta-\theta_c^m}{\theta_c^v-\theta_c^m}, \tag{2}$$

where σ is a flow stress; $\dot{\varepsilon}$ is a strain rate; $\beta=\beta(\xi)$ is the control parameter; $\xi=\left(\theta-\theta_c^m\right)/\left(\theta_c^v-\theta_c^m\right)$ is the specified temperature; m_0 is a material constant; $\sigma^*(\xi)$ and $\dot{\varepsilon}^*(\xi)$ are inner alternating state parameters; θ is the absolute temperature; θ_c^m and θ_c^v are lower and upper limits of thermal superplasticity range.

Concept of the function (1) as Morse function [19] let us insist that for $\beta>0$ $\left(\xi\notin(0;1)\right)$ there are no structural changes in the material being deformed. Condition $\beta<0$ $\left(\xi\in(0;1)\right)$ corresponds to structurally unstable state of the system. In transient states there are equations $\beta(0)=\beta(1)=0$.

Order parameter η has the following bounds:

– for structural transformation field $\left[\dot{\varepsilon}\in\left(\dot{\varepsilon}_c^m,\dot{\varepsilon}_c^v\right)\right]$

$$\eta\le\left|\left(-\frac{\beta}{m_0}\right)^{1/2}\right|; \tag{3}$$

– for superplasticity realization effect

$$\eta\le\left|\left(-\frac{\beta}{3m_0}\right)^{1/2}\right|. \tag{4}$$

Since control parameter β is introduced as time independent, an equation of autonomous type is used to describe its evolution

$$\frac{d\beta}{dt}=f\left(\beta\right), \tag{5}$$

where $f\left(\beta\right)$ is named [2,20] function of material sensitivity to the structural transformations for which it was received

$$f\left(\beta\right)=\frac{4\left(\mu-1\right)}{\alpha\left(\mu+1\right)}\left[\Gamma\left(\beta\right)-\frac{1}{2}\right], \tag{6}$$

besides for function $\Gamma\left(\beta\right)$, that is for $\beta<0$ $\left(\xi\in\left(0;1\right)\right)$ a phase transformation efficiency degree, we have

$$\Gamma\left(\beta\right)=\left(1-\beta\right)^{-\alpha}\cdot\frac{1+\mu}{2}\cdot\frac{2\xi-1}{1+\mu\left(2\xi-1\right)^2}+\frac{1}{2}, \tag{7}$$

α and μ are material constants.

Evolutions of alternative internal parameters correspond to equations

$$\frac{d\ln\sigma^*}{dt}=A_0\left(\beta-\beta_0\right)^n;\qquad \frac{d\ln\dot{\varepsilon}^*}{dt}=B_0\left(\beta-\beta_0\right)^{n_1}\frac{d\beta}{dt}, \tag{8}$$

where A_0, B_0, n, n_1 are constant parameters; $\beta=\beta_0$ is the minimum value of control parameter corresponding to the midpoint of superplasticity thermal range.

Equilibrium condition of system is determined by potential function minimization (1) with respect to order parameter. Then

$$q=m_0\eta^3+\beta\left(\xi\right)\eta\,. \tag{9}$$

Thus the model establishing the relationship between stress, temperature and kinematic variables for cases of simple extension and compression including superplasticity ranges was suggested. At that state equation has final form (9) and contains evolution equation for control parameter (5) and internal state parameters (8). The ratios mentioned can be used for descriptions of aluminum alloys deformation patterns when the function of material sensitivity to structural transformations can be definitely determined (6), (7).

3. Phase transitions

Let us compare the hypothesize models with the basic provisions of the classical phase transitions Landau’s theory [21].

Various theories of the critical phenomena face the necessity to formulate the analytical apparatus allowing describing nonanalytical behavior of thermodynamic quantities in critical points [19].

One of results of the phase transitions Landau’s theory is existence of thermodynamic function which is analytic by the arguments at the critical temperature point of $\theta=\theta_c$. It assumes to be fair that thermodynamic properties have to be determined with the help of free energy which is accepted as function of the system condition in thermal balance.

In [21] it is shown that entropy function as the first derivative of free energy with respect to temperature has no discontinuity. At the same time, values of specific heat which is derivative of entropy with respect to temperature at the approach to the critical temperature point are not identical at the left and on the right. This result corresponds to the theory of second order phase transitions. Because of the continuity of entropy function phase transition is considered to be continuous.

Thus, Landau's theory describes phase transitions in equilibrium systems inadequately. At the point of phase transition specific heat and, apparently, other physical quantities have the features described by critical indicators. The theory, for this reason, won't be agreed with experimental data. The ordinary opinion on it consists in inadequate accounting of fluctuations [19]. For the studied phenomenon it is considered that the critical point of $\theta = \theta_c$ corresponds to the peak of superplasticity [14,16]. At the same time we won't forget that Landau's theory is true for the systems which are in thermal balance. It is clear, that real phase transition is indistinct and thermodynamic functions of response are continuous. Such fact is characteristic for the systems which are far from thermodynamic balance and is considered at the model (1)-(9).

We will consider the analysis of nonequilibrium system to which it is possible as it was already mentioned above, to refer the material having superplasticity as one of deformation stages.

Let us consider the reaction of nonequilibrium system to the behavior similar to ruptures of specific heat, following from the theory of second order phase transitions.

We will characterize kinematics of a plastic flow by order parameter η, and a measure of this action by the value η^2. According to [19], for the average value η^2 we have

$$\left\langle \eta^2 \right\rangle = \frac{\int \eta^2 \exp\left(-\bar{\Phi}\right) d\eta}{\int \exp\left(-\bar{\Phi}\right) d\eta}, \tag{10}$$

where $\bar{\Phi}$ is the thermodynamic potential density, besides

$$\bar{\Phi} = \frac{F}{k_B \theta}, \tag{11}$$

and F is the free energy, k_B is the Boltzmann's constant.

Identifying thermodynamic potential density with potential function (1), we will receive for η^2:

$$\eta^2 = 2\frac{\partial \Phi}{\partial \beta}. \tag{12}$$

Having substituted (12) in (10), we will have

$$\frac{1}{2}\left\langle \eta^2 \right\rangle = \frac{\int \frac{\partial \mathrm{E}}{\partial \beta} \exp\left(-\Phi\right) d\eta}{\int \exp\left(-\Phi\right) d\eta}. \tag{13}$$

The last expression is equivalent to the following

$$\frac{1}{2}\left\langle \eta^2 \right\rangle = -\frac{\partial}{\partial \beta} \ln \int \exp\left(-\Phi\right) d\eta. \tag{14}$$

In calculating of integral in (14) we suppose that the function $\exp\left(-\Phi\right)$ has acuity with a maximum at $\eta = \bar{\eta}$. This assumption [19] allows to considering the situation called under second order phase transition as symmetry distortion.

We will decompose an exponent under the integral (14) for the minimum value Φ leaving only quadratic terms. We have

$$\Phi = \Phi\left(\bar{\eta}\right) + \frac{1}{2}\Phi''\left(\bar{\eta}\right)\left(\eta - \bar{\eta}\right)^2. \tag{15}$$

Having substituted (15) in (14), we will receive

$$\frac{1}{2}\left\langle \bar{\eta}^2 \right\rangle = -\frac{\partial}{\partial \beta} \ln \left\{ \int \exp\left[-\Phi\left(\bar{\eta}\right) - \frac{1}{2}\Phi''\left(\bar{\eta}\right)\left(\eta - \bar{\eta}\right)^2 \right] \right\} d\eta. \tag{16}$$

After evaluation of the integrals in (16) we will present the final result in the form:

$$\left\langle \eta^2 \right\rangle = \bar{\eta}^2 + \frac{1}{3m_0 \bar{\eta}^2 + \beta}. \tag{17}$$

It can be seen that the dependence (17) is reasonable under the condition:

$$\bar{\eta} = \mp\left(\frac{\beta}{3m_0}\right)^{1/2}. \tag{18}$$

Thus, it is shown that the probabilistic value of order parameter (18), corresponding to the specific heat peak, and, therefore, to the optimum temperature for superplasticity effect, doesn't go beyond the bounds determined by dependence (4).

4. Specific heat

When determining specific heat within ratios (1)–(9) it is necessary to consider dependence of parameters not only on kinematic variables, but also on temperature.

Accepting the system of the equations (1)–(9) as initial, the calculation of specific heat will be made by formula [19]:

$$c_p = -\theta\left(\frac{\partial^2 F}{\partial \theta^2}\right). \tag{19}$$

Assuming that free energy F is defined by dependence (11) and considering ratios (1)–(9), we will have:

$$c_p = a_0(\xi) + a_1(\xi)\eta + a_2(\xi)\eta^2 + a_3(\xi)\eta^3 + a_4(\xi)\eta^4. \tag{20}$$

Here

$$a_0(\xi) = \left(\frac{\theta}{\Delta\theta_c}\right)^2 \cdot \frac{d\ln\sigma^*}{d\xi}\cdot\frac{d\ln\dot{\varepsilon}^*}{d\xi};$$

$$\begin{aligned} a_1(\xi) = {} & \left(\frac{\theta}{\Delta\theta_c}\right)\left(-2\frac{d\ln\sigma^*}{d\xi}\right) + \left(\frac{\theta}{\Delta\theta_c}\right)^2\left(-\frac{d\beta}{d\xi}\cdot\frac{d\ln\dot{\varepsilon}^*}{d\xi} + \frac{d\ln\sigma^*}{d\xi}\cdot\frac{d\ln\dot{\varepsilon}^*}{d\xi} + \right.\\ & \left. + 2\beta\frac{d\ln\sigma^*}{d\xi}\cdot\frac{d\ln\dot{\varepsilon}^*}{d\xi} - \frac{d^2\ln\sigma^*}{d\xi^2}\right); \end{aligned}$$

$$\begin{aligned} a_2(\xi) = {} & \left(\frac{\theta}{\Delta\theta_c}\right)\left(\frac{d\beta}{d\xi} - 2\beta\frac{d\ln\sigma^*}{d\xi}\right) + \left(\frac{\theta}{\Delta\theta_c}\right)^2\left(-\frac{d\beta}{d\xi}\cdot\frac{d\ln\dot{\varepsilon}^*}{d\xi} + \frac{1}{2}\frac{d^2\beta}{d\xi^2} + \right.\\ & \left. + 4m_0\frac{d\ln\sigma^*}{d\xi}\cdot\frac{d\ln\dot{\varepsilon}^*}{d\xi} + 2\beta\frac{d\ln\sigma^*}{d\xi}\cdot\frac{d\ln\dot{\varepsilon}^*}{d\xi} - \frac{d\beta}{d\xi}\cdot\frac{d\ln\sigma^*}{d\xi} - \beta\frac{d^2\ln\sigma^*}{d\xi^2}\right); \end{aligned}$$

$$a_3(\xi) = \left(\frac{\theta}{\Delta\theta_c}\right)^2\left(4m_0\frac{d\ln\sigma^*}{d\xi}\cdot\frac{d\ln\dot{\varepsilon}^*}{d\xi}\right);$$

$$a_4(\xi) = \left(\frac{\theta}{\Delta\theta_c}\right)\left(-2\frac{d\ln\sigma^*}{d\xi}\right) + \left(\frac{\theta}{\Delta\theta_c}\right)^2\left(-m_0\frac{d^2\ln\sigma^*}{d\xi^2}\right), \tag{21}$$

besides $\beta = \beta(\xi)$ is the solution of the equation:

$$(1-\beta)^{-\alpha} = 1 - \frac{1+\alpha}{2\alpha}\cdot\frac{\mu-1}{\mu}\ln\frac{1+\mu(2\xi-1)^2}{1+\mu}, \tag{22}$$

and $\Delta\theta_c = \theta_c^v - \theta_c^m$.

The specific heat for the model in the form of ratios (1)–(9) passes through the maximum in the middle of the superplasticity temperature range. The specified temperature $\xi = 0.5$ can be considered as optimum for the effect realization [22]. Therefore, the received result qualitatively coincides with the known experimental data.

5. Conclusions

The dynamic superplasticity for aluminum alloys is considered from macrokinetic positions. In the presented research the analysis of the order parameter in the form of square deviation is made. It confirms blurring and the continuity of the structural-phase transformation which is carried out under the dynamic recrystallization conditions. In particular it is found that the probability of the order parameter peak value is limited by the temperature range of superplasticity effect realization. Analytical formula for specific heat is defined with the involvement of model dependences (1)–(7) and accepted for the evolution analysis of open nonequilibrium system which models process of temperature and high-rate deformation, including superplasticity ranges.

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