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On structural and phase transitions in aluminum alloys

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Abstract. Mathematical modelling of behavior of group of the industrial aluminum alloys with initial varying grain size structure showing superplastic properties in certain temperature and strain rate ranges is presented. It is known that the structural superplasticity is connected with facilitated by fine-grained structure formation (1...10 microns) at the preliminary stage. However, for realization of superplasticity of “dynamic type” there has to be a replacement of an initial varying grain size structure state of material with another, ready for superplasticity. Therefore the used definition “the dynamic superplasticity” reflects consecutive change of states which happens in material with initial varying grain size structure under the changing temperature-rate conditions: initial varying grain size → equiaxed fine-grained structure (4...7 microns) formed under the temperature-rate conditions of superplasticity → coarse-grained at further increase in strain rate. These changes are caused by simultaneous action of deformation rates and structural (phase) transitions of evolutionary type in open nonequilibrium systems. In particular, for the considered commercial aluminum alloys with initial varying grain size structure such irreversible transition is dynamic recrystallization. The association of deformation process with metal flow that has irreversible structural and phase transition of indistinct type at one of the stages, allows using synergetic approach. The mathematical model formulated from positions of solid mechanics 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.

1. Introduction

As a result of complex experimental research [1,2] of constructional materials properties different features in the temperature-rate course of change of the measured values which are treated as structural and phase transitions are established. Research of models, theories, hypotheses resulting in creation of the general, universal ratios suitable for the description of such transitions in hierarchy of structural states is hardly possible [3-5].

It is convenient to consider specifics of ideas about structural and phase transformations of the material systems which are far from thermodynamic balance, in particular, from macrokinetic positions [6]. At such approach [7] various phase transformations are studied in their interrelation with simultaneous processes of mass transfer, variability of a structural state with account for hierarchy of mechanical properties. In compliance with stated above we will consider the analysis of structural and phase transitions of dynamic type which take place during the realization of superplasticity effect [8].



Superplasticity is considered as a specific state of a polycrystalline material, which undergoes plastic deformation at a low stress and has the fine-grained structure having formed at a preliminary stage (structural superplasticity) or during heating and subsequent deformation (dynamic superplasticity) [9].

Note that both types of superplasticity are characterized by the predominance of grain-boundary sliding over other mass-transfer mechanisms [10]. Obviously, for the dynamic superplasticity effect to occur, an initial (deformed or ascast) structural state should change into another one to be capable of superplasticity. These changes are due to a coherent superposition of strain rates and structural (phase) transitions of the evolutionary type in open nonequilibrium systems [11].

It is obvious that the dynamic superplasticity occurs under the conditions of indistinct phase transition [12-14] and therefore it is reasonable to observe the behavior of response functions which are defined subject to analytical expression of thermodynamic potential density is specified. To the mentioned functions one could refer entropy and specific heat, first of all. The immediate data of specific heat change which are carried out, for example, for classical superplastic alloy Zn-22%Al [15] 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.

2. Formulation of the problem

During macrokinetic explanation [16] of high-temperature deformation processes in the wide temperature-rate ranges including intervals of superplasticity effect realization it is expedient to decide upon methods of nonequilibrium statistical mechanics. In [17] an opportunity on the basis of stationary solutions of the Fokker-Planck's equation to determine close analogies between phase transitions that take place under thermal balance conditions and some transitions in nonequilibrium systems is shown.

Using the dynamic model [6,9] we will consider a problem of quantitative assessment of the specified analogy existence reality.

3. Dynamic model

Model which adequately represents the accumulated experimental and generalized in [1,2] data from positions of deformable solid mechanics is summed up in [6,9]. The 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.

The model [6,9] 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 and contains evolution equation for control parameter and internal state parameters. 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.

4. Specific heat

When determining specific heat c_p within the dynamic model [6,9] it is necessary to consider dependence of parameters not only on kinematic variables, but also on temperature.

The calculation of specific heat will be made by formula [18]

$$c_p = -\theta \left(\partial^2 F / \partial \theta^2 \right), \quad (1)$$

where free energy F is defined by dependence

$$F = \bar{\Phi} k_B \theta. \quad (2)$$

Here $\bar{\Phi}$ is the thermodynamic potential density; k_B is the Boltzmann's constant; θ is the temperature.

Diagrams for specific heat $c_p = c_p(\xi)$ on figure 1 are calculated for the deformed aluminum AlMg-5 ($\alpha = 0.54$; $\mu = 1.08$; $m_0 = 0.33$; $A_0 = -1.77$) and AlCuMg0.5 not annealed ($\alpha = 0.5$; $\mu = 1.2$; $m_0 = 0.3965$; $A_0 = -1.78$) alloys. Here α , μ , m_0 , A_0 are material constants; $\xi = (\theta - \theta_c^m) / (\theta_c^v - \theta_c^m)$ is the reduced temperature; θ_c^m , θ_c^v are the upper and lower temperatures (K), respectively, that bound the thermal range of superplasticity [6,9].

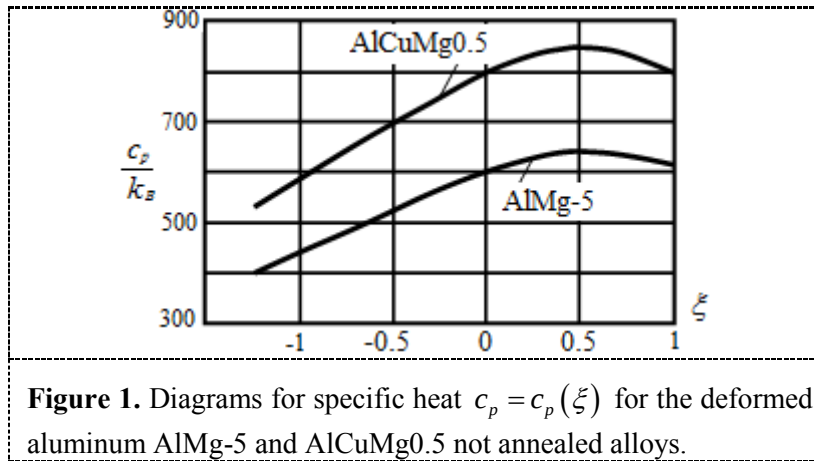


Figure 1. Diagrams for specific heat $c_p = c_p(\xi)$ for the deformed aluminum AlMg-5 and AlCuMg0.5 not annealed alloys.

From the presented diagrams it is visible that specific heat for the dynamic model 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. Therefore, the received result qualitatively coincides with the known experimental data [15].

5. Function of entropy

We will define entropy S with the help of [15] formula

$$S = -\partial F / \partial \theta. \quad (3)$$

Function of entropy $S = S(\xi)$ is presented on figure 2 for AlMg-5 and AlCuMg0.5 alloys.

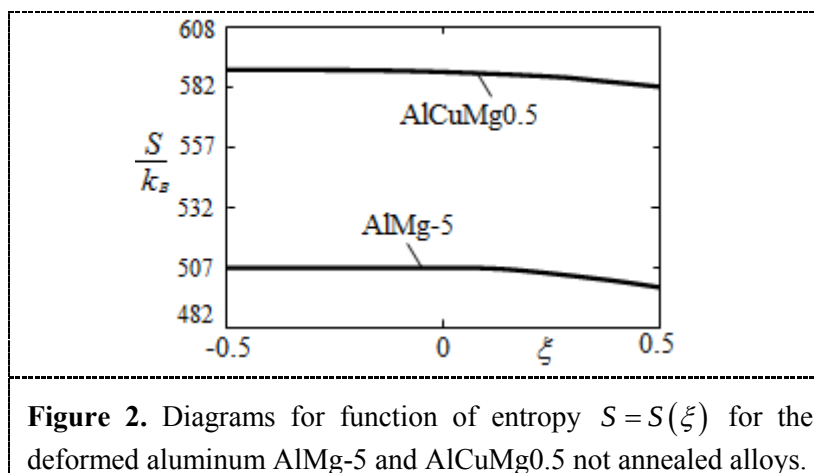


Figure 2. Diagrams for function of entropy $S = S(\xi)$ for the deformed aluminum AlMg-5 and AlCuMg0.5 not annealed alloys.

Decrease of entropy within the thermal range of superplasticity on figure 2 demonstrates transition of the dissipative structure created as a result of temperature and strain rate deformation to a new state.

As it is well-known [19], self-organization of such structures is connected with aspiration of open systems to entropy reduction under the conditions far from thermodynamic balance.

6. Conclusions

In thermal ranges to the lower value of temperature of superplasticity $\theta_c^m(\xi=0)$ there is entropy growth, and after $\theta > \theta_c^m$ entropy decreases. As it was already noted, the similar phenomenon can be explained by formation of a fine grain and considered as emergence of ordered space-time structures in open systems. It is possible to assume, judging by figure 2 that the entropy is sensitive to the size of initial grain. So for both alloys under temperature and high-rate superplasticity conditions the grain size is 4-7 microns. In the initial deformed state for AlMg-5 alloy grain didn't exceed 45 microns, and in AlCuMg0.5 alloy reached 130 microns. It results in less smooth nature of change of the function $S = S(\xi)$ for AlCuMg0.5 alloy compared to AlMg-5 alloy. Influence of the sizes of initial grain is also reflected on dependence – the specific heat of AlCuMg0.5 alloy is higher, than of AlMg-5.

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