A Model of Grain Boundary Sliding during Deformation

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Abstract—A model of slip at grain boundaries is proposed based on the concept of local melting of the grain boundary under intense external influence and by analogy with ultrathin lubrication. A discontinuous regime of slip along the grain boundaries similar to the stick−slip process in thin lubricants is described.

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Superplasticity (SP) is one of the intriguing properties of a large class of solids and had long attracted the attention of researchers [1, 2]. Different theoretical models are used to explicate the principles of its realization [3−6]. Many of them are based on the concept of a slip along grain boundaries (GBs) [1−3]. One of the directions in which SP theory is being developed is based on the idea of melting GBs under intense external action [4, 7]. This concept was experimentally confirmed in [8−11]. In this case, the GB can be considered as an ultrathin lubricant [12, 13] separating adjacent grains, in which case we can ignore complicating factors such as the finite size of the grains and the effect of triple junctions. Different modes of slip are observed in thin lubricants, including the regime of intermittent stick−slip during the process of dry friction. Provided that, in the area of grain boundaries, shear melting occurs as a result of heat exchange with the volume of grains, solidification of the lubricant is possible. Periodic repetition of this process leads to an intermittent process of sliding.

That it is possible for grain boundaries to be in a molten state has not yet to be proved, as there are currently no measurements or estimates of the entropy of the grain boundaries (see the detailed discussion of the problem in [7]). The existing evidence of the absence of GB melting is based on principles of equilibrium thermodynamics. However, we must keep in mind that the presence of thermodynamic equilibrium melting in the absence of external influences may be problematic. At the same time, melting of the grain boundaries can occur in the presence of intense external influences, such as intense plastic deformation (IPD) or superplastic flow. The system as a whole proves to be in

this case in a highly nonequilibrium state, and GB melting can proceed by the mechanism of shear melting [12, 13]. This means that, in the initial state, the borders cannot be in a molten state, but will move to the state of shear melting in the process of deformation.

The well-known and experimentally observed effects on bicrystals may be considered another argument in favor of these ideas [2, 7]. The interfaces between them can be thought of as ideally flat and endless grain boundaries. Similarly to lubricants, they slide as is observed for a periodic stick−slip—"long cycles in which the velocity of the slip decreases to almost zero before it rises again" [7]. When GBs are being melted, the stationary states in which the system is located are not real thermodynamic phases, but represent kinetic modes of friction, so there may be several stationary states. In this case, one cannot speak of solid and liquid phases, but of solid- and liquidlike ones.

To describe the state of GBs, we use the parameter f, which has the physical meaning of the excess volume resulting from the chaotic structure of the solid in the process of melting. In contrast to the order parameter, which is widely used to describe the process of solid−liquid transition, the parameter f increases with increasing total internal energy in such a transition.

To describe the interface in a bicrystal as a GB model, we apply the approach developed in [12, 13]. We write the expansion for the density of free energy of the solid under external loading taking into account

the contributions from the elastic components of shear strain ε_{ij}^e and temperature T in the form

$$\Phi = \frac{1}{2}\lambda(\varepsilon_{ii}^e) + \mu(\varepsilon_{ij}^e)^2 - \varphi_0 f + \frac{1}{2}\varphi_1 f^2 - \frac{1}{3}\varphi_2 f^3 + \frac{1}{4}\varphi_3 f^4, \quad (1)$$

where λ and μ are the elastic modules of the material; φ_0, φ_1, φ_2, and φ_3 are the expansion coefficients; and ε_{ii}^e and $(\varepsilon_{ij}^e)^2 = \varepsilon_{ij}^e \varepsilon_{jj}^e$ are the first and the second invariants of the strain tensor. Since the free energy should not depend on the choice of the coordinate system, it must be expressed in terms of the invariants of the strain tensor. Coefficient φ_0 corresponding to the lowest degree of f depends in its turn on the invariants of this tensor and on the temperature of GBs as controlling parameters

$$\varphi_0 = \varphi_0^* + \frac{1}{2}\bar{\lambda}(\varepsilon_{ii}^e)^2 + \bar{\mu}(\varepsilon_{ij}^e)^2 + \alpha T. \quad (2)$$

Here, $\bar{\lambda}$ and $\bar{\mu}$ are the "defects" of the elastic modules in the region of the GBs associated with the existence of free volume f and α is a new coefficient of expansion. The stress that appears in the GBs is given by

$$\sigma_{ij}^e \equiv \frac{\partial \Phi}{\partial \varepsilon_{ij}^e} = \lambda \varepsilon_{ii}^e \delta_{ij} + 2\mu \varepsilon_{ij}^e + (\bar{\lambda}\varepsilon_{ii}^e \delta_{ij} + 2\bar{\mu}\varepsilon_{ij}^e)f. \quad (3)$$

Let us write the evolution equation for the nonequilibrium parameter f in the Landau–Khalatnikov form:

$$\frac{\partial f}{\partial t} = -\gamma_f \frac{\partial \Phi}{\partial f}, \quad (4)$$

where γ_f is the kinetic coefficient.

The equation that determines relative velocity V of shear in the rubbing bicrystals and emerging elastic shear strain ε_{ij}^e in GBs has the form [12, 13]

$$\tau_\varepsilon \frac{d\varepsilon_{ij}^e}{dt} = -\varepsilon_{ij}^e + \frac{V\tau_\varepsilon}{h}, \quad (5)$$

where τ_ε is the Maxwell relaxation time of the internal stresses and h is the thickness of the GBs. The system of kinetic equations (4) and (5) can be used to study the kinetics of GB melting.

In this model, in accordance with the experimental data, we have chosen the normal stress value $n = -7 \times 10^5$ Pa (stress n is clearly implicit in the definition of the first invariant ε_{ii}^e [12, 13]) and the following values for the constants of the theory: $\lambda = 2 \times 10^{11}$ Pa, $\bar{\lambda} = 10^8$ Pa, $\mu = 4.2 \times 10^{11}$ Pa, $\bar{\mu} = 4 \times 10^{11}$ Pa, $\varphi_0^* = 5$ J/m^3, $\varphi_1 = 1100$ J/m^3, $\varphi_2 = 2700$ J/m^3, $\varphi_3 = 2070$ J/m^3, $\alpha = 0.16$ J K^{-1}/m^3, $h = 10^{-9}$ m, $\gamma_f = 1$ Pa^{-1} s^{-1}, and $\tau_\varepsilon = 10^{-8}$ s.
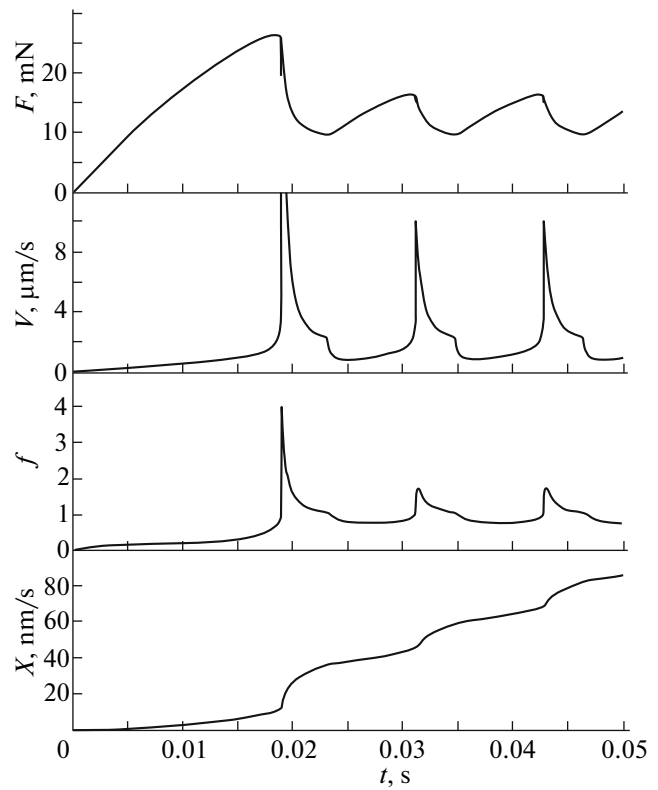
Dependences of frictional force F, relative shear velocity V, and values of f and coordinate X on time t for the parameters $M = 10^{-3}$ kg, $K = 10^6$ N/m, $k = 2.5 \times 10^5$ Pa s$^{1/3}$, $\gamma = -2/3$, $A = 3 \times 10^{-9}$ m^2, $T = 700$ K, and $V_0 = 2$ μm/s.

The expression for the friction force between the grains with the presence of a viscoelastic GB between them is given by [12, 13]

$$F = \left[\tau + k\left(\frac{V}{h}\right)^{\gamma+1}\right]A, \quad (6)$$

where A is the area of the touching surfaces, k and γ are the phenomenological parameters that determine the viscosity properties of the GB, and $\tau = \sigma_{ij}^e$ is the shear stress that is determined by Eq. (3) at $i \neq j$.

The equation of motion of the chosen grains is given by [12, 13]

$$M\frac{d^2 X}{dt^2} = K(V_0 t - X) - F, \quad (7)$$

where M and X are the equivalent mass and coordinate of the grain under consideration, K is the stiffness coefficient that appears due to elastic properties of the grains, and V_0 is the velocity of relative displacement in a pair of rubbing grains [12, 13].

When f reaches a critical value, the GB melts and parameter f abruptly increases. The GB then again begins to solidify owing to the diminishing relative velocity of the friction surfaces, dX/dt. When the GB is completely solidified, elastic stresses τ appear, with

a subsequent increase in them again leading to an increase in the parameter f, and the process is repeated again. In accordance with this, all characteristics periodically change: frictional force F, velocity V, and displacement X (see figure). As a result, a regime of a stick–slip melting (solidifying) GB sets in. Note that, with increasing velocity V_0, the frequency of the stick–slip cycles first increases due to a more rapid establishment of the critical value f. In line with this, the GB melts quickly and, for the given period of time, a large number of cycles of melting/solidification occur. With even greater increase of velocity V_0, the frequency of the peaks of dependence $F(t)$ decreases again due to appearing extended kinetic domains [12,13].

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