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Dislocation mediated plastic flow in aluminum: Comparison between theory and experiment

K.C. Le*, T.M. Tran

Lehrstuhl für Mechanik - Materialtheorie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

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ABSTRACT

The theory of dislocation mediated plastic flow proposed by Langer, Bouchbinder, and Lookman is applied to compute the stress-strain curve of aluminum over a wide range of temperatures and strain rates. The parameter identification by the least squares method is provided leading to the excellent agreement with experiment.

1. Introduction

Langer, Bouchbinder, and Lookman (2010) have proposed recently the theory of dislocation mediated plastic flow in metals and alloys, termed LBL-theory for short (see also Langer, 2015, 2016). The main feature distinguishing it from all other standard theories of plastic flow is the decomposition of the system crystal containing dislocations into configurational and kinetic-vibrational subsystems. The configurational degrees of freedom describe the relatively slow, i.e. infrequent, atomic rearrangements that are associated with the irreversible movement of dislocations as opposed to the kinetic-vibrational degrees of freedom describing the fast vibrations of the atoms in the lattice. In view of these two different time scales, the configurational entropy and temperature characterizing the slow atomic rearrangements due to dislocations should be introduced in addition to the kinetic-vibrational entropy and temperature. Based on the principles of thermodynamics and several plausible arguments these authors proposed the system of equations governing the plastic flow of metals and alloys. They used these equations to simulate the stress-strain curve for copper over fifteen decades of strain rate, and for temperatures between room temperature and about one third of the melting temperature. It turns out that only one fitting parameter is required to get the full agreement with the experiment conducted in Follansbee and Kocks (1988) over a wide range of temperatures and strain rates. The successfulness of LBL-theory poses the legitimate question of its applicability in the most general case, and, if not, its limit of validity. Langer (2016) wrote: “One way to do that will be to repeat the analyses of Langer, Bouchbinder, and Lookman (2010) and Langer (2015) using other sets of experimental data, measured for different kinds of materials under different driving conditions”. The aim of this short communication is to simulate the stress-strain curves for pure aluminum at different strain rates and different temperatures using the LBL-theory. We identify the parameters involved in the LBL-theory by minimizing the sum of squares of the differences between the solution and the experimentally measured stresses. The comparison with the experiments conducted by

* Corresponding author.
E-mail address: chau.le@rub.de (K.C. Le).

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Shi, McLaren, Sellars, Shahani, and Bolingbroke (1997) and Chen, Stout, Kocks, MacEwen, and Beaudoin (1998) shows again excellent agreement confirming the applicability of LBL-theory to aluminum.

2. Governing equations

Let us present the governing equations of LBL-theory in the form

$$\frac{d\sigma}{d\epsilon} = \mu\left[1 - \frac{\tilde{q}(\sigma,\tilde{\rho})}{\tilde{q}_0}\right], \tag{1}$$

$$\frac{d\tilde{\chi}}{d\epsilon} = \mathcal{K}\sigma\,\frac{\tilde{q}(\sigma,\tilde{\rho})}{\tilde{q}_0}\left[1 - \frac{\tilde{\chi}}{\tilde{\chi}^{ss}(\tilde{q})}\right], \tag{2}$$

and

$$\frac{d\tilde{\rho}}{d\epsilon} = \frac{\mathcal{K}_\rho\sigma}{\tilde{v}(T,\tilde{\rho},\tilde{q}_0)^2}\,\frac{\tilde{q}(\sigma,\tilde{\rho})}{\tilde{q}_0}\left[1 - \frac{\tilde{\rho}}{\tilde{\rho}^{ss}(\tilde{\chi})}\right]. \tag{3}$$

These are three coupled ordinary differential equations of first order containing three unknowns: the stress σ, the dimensionless configurational temperature $\tilde{\chi} = \chi/e_D$ (with e_D being the formation energy of dislocations), and the dimensionless dislocation density $\tilde{\rho}(\tilde{\chi}) = a^2\rho(\chi)$, where a represents the mean distance between dislocations in the state of maximum disorder and infinite configurational temperature which is taken to be $10b$ (with b being the Burgers' vector). They must be solved in terms of the strain ϵ, whose rate $\dot{\epsilon}$ is assumed to be constant. The first equation is deduced from Hooke's law in rate form, Orowan's equation, and the kinetics of thermally activated depinning dislocations, with μ being the shear modulus, and

$$\tilde{q}(\sigma,\tilde{\rho}) = \sqrt{\tilde{\rho}}[f_P(\sigma) - f_P(-\sigma)], \quad f_P(\sigma) = \exp\left(-\frac{T_P}{T}e^{-\sigma/\sigma_T}\right).$$

In the last formula T is the kinetic-vibrational temperature, k_BT_P characterizes a depinning energy barrier, while $\sigma_T = \bar{\mu}_T\sqrt{\tilde{\rho}}$ is the Taylor stress needed for depinning. The second equation for the configurational temperature is the consequence of the first law of thermodynamics, with $\tilde{\chi}^{ss}(\tilde{q})$ being the steady-state dimensionless configurational temperature. The second term in the square brackets of the right-hand side of (2) is proportional to the rate at which heat flows from the configurational to the thermal (kinetic-vibrational) degrees of freedom. Since we are in the low strain rate regime with $\tilde{q} \ll 1$, in the numerical simulations we replace $\tilde{\chi}^{ss}(\tilde{q})$ by $\tilde{\chi}^{ss}(0) = \tilde{\chi}_0$. The third equation for the dimensionless dislocation density follows from the second law of thermodynamics and can be regarded as the equation describing the relaxation to the steady-state dislocation density $\tilde{\rho}^{ss}(\tilde{\chi}) = e^{-1/\tilde{\chi}_0}$. In this equation

$$\tilde{v}(T,\tilde{\rho},\tilde{q}) = \ln\left(\frac{T_P}{T}\right) - \ln\left[\frac{1}{2}\ln\left(\frac{\tilde{\rho}}{\tilde{q}^2}\right)\right].$$

Finally, Eqs. (1)–(3) should be complemented by the initial conditions

$$\sigma(0) = 0, \quad \tilde{\chi}(0) = \tilde{\chi}_{ini}, \quad \tilde{\rho}(0) = \tilde{\rho}_{ini}. \tag{4}$$

3. Parameter identification

In order to simulate the stress-strain curve for aluminum at different strain rates and different temperatures, we need to specify the material parameters and initial data involved in (1)–(4). First, the shear modulus as function of temperature should be taken in accordance with the empirical formula (Varshni, 1970)

$$\mu = \mu_0 - \frac{D}{\exp(T_0/T) - 1},$$

where, for pure aluminum, $\mu_0 = 28.815$ GPa, $D = 3.44$ GPa, $T_0 = 215$ K (Chen, Stout, Kocks, MacEwen, & Beaudoin, 1998). To find the steady state configurational temperature χ_0, the pinning temperature T_P, and the Taylor stress σ_T (or $\bar{\mu}_T$), assumed to be independent of the strain rate, we use three steady state flow stresses σ_i^{ss} measured in experiment at the same temperature and different strain rates (see Fig. 1) and equations (Langer, Bouchbinder, & Lookman, 2010)

$$g_i(\chi_0,T_P,\sigma_T) = \frac{\sigma_i^{ss}}{\sigma_T} - \ln\left(\frac{T_P}{T}\right) + \ln\left[\frac{1}{2}\ln\left(\frac{\tilde{\rho}^{ss}}{\tilde{q}_{0i}^2}\right)\right] = 0, \quad i = 1,2,3, \tag{5}$$

where $\tilde{\rho}^{ss} = e^{-1/\tilde{\chi}_0}$ and $\tilde{q}_{0i} = (a/b)\tau_0\dot{\epsilon}_i$ ($(a/b)\tau_0 = 10^{-12}$ s). Due to the uncertainties in the steady state stresses, we shall not fulfill Eqs. (5) exactly, but minimize instead the sum of squares

$$g(\chi_0,T_P,\sigma_T) = g_1^2 + g_2^2 + g_3^2$$