Regular article

Thermodynamic dislocation theory of adiabatic shear banding in steel

K.C. Le [a,*], T.M. Tran [a], J.S. Langer [b]

[a] Lehrstuhl für Mechanik - Materialtheorie, Ruhr-Universität Bochum, D-44780 Bochum, Germany
[b] Department of Physics, University of California, Santa Barbara, CA 93106-9530, USA

ARTICLE INFO

ABSTRACT

The statistical-thermodynamic dislocation theory developed in our earlier studies is used here in an analysis of the experimental observations of adiabatic shear banding in steel by Marchand and Duffy (1988). Employing only a small set of physics-based parameters, we are able to explain experimental stress-strain curves, including yielding transitions and strain hardening, over wide ranges of temperatures and strain rates. We make a simple model of weak notch-like perturbations that, when driven hard enough, trigger shear banding instabilities that are quantitatively in agreement with those seen in the experiments.

© 2018 Elsevier Ltd. All rights reserved.

Our purpose here is to use the statistical-thermodynamic dislocation theory developed in Refs. [1–7] to analyze the classic observations of adiabatic shear banding (ASB) by Marchand and Duffy (MD) [8]. The latter authors made stress-strain measurements over a range of substantially different temperatures and shear rates using thin steel tubes bonded to torsional Kolsky bars. They observed ASB formation at high shear rates and low temperatures. Specifically, they observed abrupt stress drops, large increases of temperature in emerging narrow bands, and strong strain localization leading to crack formation and failure. (See also Ref. [9] for a review of the existing literature on this topic.) Our challenge is to predict those behaviors quantitatively using a realistic physics-based theory.

Our new ability to interpret data of the kind published in MD [8] is related to the fact that the statistical thermodynamic dislocation theory is able to predict nonequilibrium behaviors that previously had been beyond the reach of conventional phenomenological methods in this field. These behaviors include strain hardening [1,2], steady-state stresses over exceedingly wide ranges of strain rates [1], Hall-Petch effects [5], thermal softening during deformation [6], yielding transitions between elastic and plastic responses [3,5], and – most importantly for present purposes – the competition between thermal and mechanical effects that produces shear banding instabilities [4,7].

By definition, "adiabatic" shear banding is a thermal effect. It happens when the heat generated at a hot spot is unable to flow away from that spot as fast as new heat is being generated there, thus initiating a runaway instability. These thermal effects were missing in the early versions of the thermodynamic dislocation theory, which were based on data for copper as shown, for example, in Refs. [10,11]. There, the thermal conductivity is large enough that heat generation can be neglected and no appreciable thermal softening occurs. However, typical stress-strain curves such as the ones shown for aluminum and steel in Refs. [12,13] and discussed by us in Ref. [6] exhibit thermal softening at large strain rates even without undergoing ASB. When ASB does occur, temperatures within the band may increase by hundreds of degrees or more, and thermal forces become one of the principal driving mechanisms. In order to demonstrate the possibility of ASB formation theoretically, one of us [3,4] studied an artificial model with all the same mechanical parameters as copper but with substantially reduced thermal conductivity and an enhanced thermal conversion coefficient. We will have to be more realistic than this in our analyses of the MD data. Specifically, we will need to deduce from the MD data a longer list of both mechanical and thermal parameters for their steel alloy than was needed for copper.

The thermodynamic dislocation theory is based on two unconventional hypotheses. The first of these is that, under nonequilibrium conditions, the atomically slow configurational degrees of freedom of deforming solids are characterized by an effective disorder temperature that differs from the ordinary kinetic-vibrational temperature. Both of these temperatures are thermodynamically well defined variables whose equations of motion determine the irreversible

---

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

behaviors of these systems. The second hypothesis is that entanglement of dislocations is the overwhelmingly dominant cause of resistance to deformation in the materials considered here. It is these two hypotheses that have led to the successfully predictive theory mentioned above. A recent, more complete discussion of this theory can be found in Ref. [7].

As in Ref. [4], we consider a strip of polycrystalline material, of width 2W, driven in simple shear in the x direction at constant velocities V_x and $-V_x$ at its top and bottom edges respectively. The total strain rate is $V_x/W \equiv Q/\tau_0$, where $\tau_0 \approx 10^{-12}$ s is an arbitrarily chosen microscopic time scale that we use in order to express rates as meaningful dimensionless quantities. In order to observe shear localization, we look at spatial variations in the y direction, perpendicular to the x axis.

The local, elastic plus plastic strain rate is $\dot{\varepsilon}(y) = dv_x/dy$, where v_x is the material velocity in the x direction. This motion is driven by a time-dependent, spatially uniform, shear stress σ. Because the overall shear rate is constant, we can replace the time t by the accumulated total shear strain, say ε, so that $\tau_0 \partial/\partial t \to Q \partial/\partial\varepsilon$. Then we denote the dimensionless, y-dependent plastic strain rate by $q(y,\varepsilon) \equiv \tau_0 \dot{\varepsilon}^{pl}(y,\varepsilon)$.

The internal state variables that describe this system are the areal density of dislocations ρ, the effective temperature $\tilde{\chi}$ (in units of a characteristic dislocation energy e_D), and the ordinary temperature $\tilde{\theta}$ (in units of the pinning temperature $T_P = e_P/k_B$, where e_P is the pinning energy defined below). We define $\rho \equiv \tilde{\rho}/a^2$, where a is the average spacing between dislocations in the limit of infinite $\tilde{\chi}$, which is a length of the order of tens of atomic spacings. Note that $a/\sqrt{\tilde{\rho}}$ is the average distance between dislocations. All three of these dimensionless quantities $\tilde{\rho}$, $\tilde{\chi}$, and $\tilde{\theta}$ are functions of y and ε.

The central, dislocation-specific ingredient of this analysis is the thermally activated depinning formula for the dimensionless plastic strain rate q as a function of the stress magnitude σ:

$$q(\varepsilon) = \sqrt{\tilde{\rho}} \, \exp\left[-\frac{1}{\tilde{\theta}} \, e^{-\sigma/\sigma_T(\tilde{\rho})} \right]. \tag{1}$$

This is an Orowan relation of the form $q = \rho \, b \, v \, \tau_0$, where b is the length of the Burgers vector, and v is the speed of the dislocations given by the distance between them multiplied by the rate at which they are depinned from each other. Without loss of generality, we have absorbed the ratio b/a into the definition of τ_0. The depinning rate is approximated here by the activation term in Eq. (1), in which the energy barrier e_P (implicit in the scaling of $\tilde{\theta}$) is reduced by the stress dependent factor $e^{-\sigma/\sigma_T(\tilde{\rho})}$. Here, $\sigma_T(\tilde{\rho}) = \mu_T \sqrt{\tilde{\rho}}$ is the Taylor stress, given by the shear modulus μ multiplied by the strain $(b'/a)\sqrt{\tilde{\rho}}$, that is, by the ratio of a small depinning length b' to the distance between dislocations. Then define $\mu_T \equiv r \mu$, where the dimensionless ratio $r = b'/a$ is a system-specific geometrical constant.

The pinning energy e_P is large, of the order of electron volts, so that $\tilde{\theta}$ is very small. As a result, $q(\varepsilon)$ is an extremely rapidly varying function of σ and $\tilde{\theta}$. This strongly nonlinear behavior is the key to understanding yielding transitions and shear banding as well as many other important features of polycrystalline plasticity. In what follows, we shall see that this temperature sensitivity of the plastic strain rate is the key to understanding important aspects of the thermomechanical behavior. Moreover, the extremely slow variation of the flow stress as a function of strain rate discussed in Refs. [1,7] is the converse of the extremely rapid variation of q as a function of σ in Eq. (1). This can be seen by rewriting Eq. (1) in the form

$$\sigma = \sigma_T(\tilde{\rho}) \, \nu\left(\tilde{\theta}, \tilde{\rho}, q\right); \quad \nu\left(\tilde{\theta}, \tilde{\rho}, q\right) \equiv \ln\left(\frac{1}{\tilde{\theta}}\right) - \ln\left[\ln\left(\frac{\sqrt{\tilde{\rho}}}{q}\right)\right]. \tag{2}$$

Thus, the flow stress is equal to the Taylor stress multiplied by a slowly varying function of temperature, dislocation density and strain rate, consistent with a wide range of experimental observations.

The equation of motion for the scaled dislocation density $\tilde{\rho}$ describes energy flow. It says that some fraction of the power delivered to the system by external driving is converted into the energy of dislocations, and that that energy is dissipated according to a detailed-balance analysis involving the effective temperature $\tilde{\chi}$. This equation is:

$$\frac{\partial\tilde{\rho}}{\partial\varepsilon} = \kappa_1 \, \frac{\sigma \, q}{\nu\left(\tilde{\theta},\tilde{\rho},Q\right)^2 \mu_T \, Q} \left[1 - \frac{\tilde{\rho}}{\tilde{\rho}_{ss}(\tilde{\chi})} \right], \tag{3}$$

where $\tilde{\rho}_{ss}(\tilde{\chi}) = e^{-1/\tilde{\chi}}$ is the steady-state value of $\tilde{\rho}$ at given $\tilde{\chi}$. The coefficient κ_1 is an energy conversion factor that, according to arguments presented in Refs. [1,4] and [7], should be approximately independent of both strain rate and temperature for the situations considered here. This equation plays the role of the phenomenological "storage-recovery" equation [10]. (See Ref. [1] for a discussion of the inadequacies of the latter equation.) Here, however, Eq. (3) has been derived directly from first principles with only a single system-specific parameter κ_1 that needs to be obtained from strain-hardening data. Note that the scaled effective temperature $\tilde{\chi}$ plays an absolutely essential role in it.

The equation of motion for $\tilde{\chi}$ is a statement of the first law of thermodynamics for the configurational subsystem:

$$\frac{\partial \tilde{\chi}}{\partial\varepsilon} = \kappa_2 \, \frac{\sigma \, q}{\mu_T \, Q} \left(1 - \frac{\tilde{\chi}}{\tilde{\chi}_0} \right). \tag{4}$$

Here, $\tilde{\chi}_0$ is the steady-state value of $\tilde{\chi}$ for strain rates appreciably smaller than inverse atomic relaxation times, i.e. much smaller than τ_0^{-1}. The dimensionless factor κ_2 is inversely proportional to the effective specific heat c_{eff}. Unlike κ_1, there is no reason to believe that κ_2 is a rate-independent constant. In Ref. [5], κ_2 for copper was found to decrease from 17 to 12 when the strain rate increased by a factor of 10^6. Here, we shall assume for simplicity that κ_2 is a constant. Again, we emphasize that there is nothing phenomenological about Eq. (4); it has been derived directly from basic principles of thermodynamics. Only the parameter κ_2 needs to be determined from experiment. Even $\tilde{\chi}_0$ can be obtained to a good approximation from statistical arguments as shown in Refs. [1,7].

The equation of motion for the scaled, ordinary temperature $\tilde{\theta}$ is the usual thermal diffusion equation with a source term proportional to the input power. We assume that, of the three state variables, only $\tilde{\theta}$ diffuses in the spatial dimension y. Thus,

$$\frac{\partial\tilde{\theta}}{\partial\varepsilon} = K\left(\tilde{\theta}\right) \frac{\sigma \, q}{Q} + \frac{K_1}{Q} \frac{\partial^2\tilde{\theta}}{\partial y^2} - \frac{K_2}{Q} \left(\tilde{\theta} - \tilde{\theta}_0 \right). \tag{5}$$

Here, $K(\tilde{\theta}) = \beta/(T_P c_p \rho_d)$ is a thermal energy conversion factor, while $K_1 = k_1\tau_0/(c_p\rho_d)$ characterizes heat conduction in the axial direction of the tube. c_p is the thermal heat capacity per unit mass, ρ_d is the mass density, $0 < \beta < 1$ is a dimensionless constant known as the Taylor-Quinney factor, and k_1 is the thermal conductivity. K_2 is a thermal transport coefficient that controls how rapidly the system relaxes toward the ambient temperature T_0, that is, $\tilde{\theta} \to \tilde{\theta}_0 = T_0/T_P$. As discussed in Ref. [6], $K(\tilde{\theta})$ may be non-trivially temperature dependent. In the range of temperature under consideration, we take it to be

$$K\left(\tilde{\theta}\right) = c_0 + c_1 \, e^{-c_2/(T_P \, \tilde{\theta})}. \tag{6}$$