International Journal of Plasticity 70 (2015) 1–29

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

Analytic model of the remobilization of pinned glide dislocations from quasi-static to high strain rates

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ARTICLE INFO

Article history:
Received 8 October 2014
Received in revised form 12 December 2014
Available online 25 February 2015

Keywords:
Dislocations
Mean-first-passage-time (MFPT) theory
Constitutive behavior
Shock waves

ABSTRACT

In this paper, we construct an analytic model describing mobile-immobile dislocation intersections using a mean-first-passage-time (MFPT) framework. By applying MFPT theory to dislocation intersection, the deformation mechanics at high strain rates is more reliably described than in traditional models based on Van't Hoff-Arrhenius thermal activation. The plastic strain rate is expressed as a function of the applied stress, mobile and immobile dislocation densities, material density, and temperature. This kinetic equation is applicable at strain rates from quasi-static to rates in excess of 10^{12} s^{-1}, pressures from ambient to about 1000 GPa, and temperatures ranging from zero to the melt temperature.

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1. Introduction

Plastic constitutive models, i.e., material strength models, applicable at strain rates of roughly 10^5 s^{-1} and higher, are essential for simulations of explosively-driven systems, hypervelocity impacts, and more generally, material deformation and failure under shock wave loading. As plastic strain rates increase to 10^5 s^{-1} and above, the majority of rate-dependent plastic flow models (Seeger, 1954a,b,c, 1955b; Follansbee and Kocks, 1988; Hoge and Mukherjee, 1977; Steinberg and Lund, 1989; Zerilli and Armstrong, 1987) exhibit a progressive drop in fidelity, in some cases leading to explicit failure, because the rate-controlling intersections of non-coplanar, attractive mobile and immobile (forest) dislocations are described by Van't Hoff-Arrhenius thermal activation theory, which breaks down at high stresses. The main result of this paper, our kinetic equation, is an analytic model of mobile-immobile dislocation intersection that generalizes the standard low-strain-rate relation $\dot{\varepsilon} = \dot{\varepsilon}_0 \exp(-E(\sigma)/kT)$ up to strain rates of roughly 10^{12} s^{-1}. This equation describes the formation and dissolution of dislocation-dislocation intersection nodes and short junctions, and relates plastic strain rate to the stress, mobile and immobile dislocation densities, material density, and temperature. Our kinetic equation is applicable at plastic strain rates from quasi-static to rates of order 10^{12} s^{-1}, temperatures from zero to melt, and pressures greater than 1000 GPa. It is intended to be used in conjunction with a model for the evolution of mobile and immobile dislocation densities.

It is well known that metals and alloys exhibit a significant increase in strain rate sensitivity at rates ~10^{4-5} s^{-1}. This behavior is usually interpreted as a change in the rate-controlling mechanism from thermally-activated glide at low rates, as described by a Van't Hoff-Arrhenius equation, to dislocation drag at high rates. Conversely, our kinetic equation, predicts an increase in strain rate sensitivity at high rates by correctly accounting for the effects of thermal fluctuations at dislocation

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http://dx.doi.org/10.1016/j.ijplas.2015.01.008
0749-6419/Published by Elsevier Ltd.

intersections, i.e. in the absence of dislocation drag. Of course, at high rates ($>10^5$ s^{-1}), drag and relativistic effects must also be included to accurately model high rate material behavior.

Consider a crystal with total dislocation density ρ_{tot}, which can be decomposed into mobile and immobile (also called network or forest) components: $\rho_{tot} = \rho_m + \rho_i$. As an attractive pair of dislocations approach one another, the configuration evolves in a complex way due to the tensor interaction between the dislocations. We limit this discussion to pairwise interactions, which have been shown to predominate the work hardening process (Friedel, 1964); thus, we neglect interactions involving three or more dislocations, including multi-junction formation by dislocation intersection with a junction previously formed by pairwise intersection (Bulatov et al., 2006). When two dislocation cores are within a critical distance, the attraction is unstable, resulting in the formation of either a junction, i.e. a straight segment branching into the two reacting dislocations at both of its ends (Fig. 1(a)), or a crossed state, a single node that does not zip up to form a junction (Fig. 1(b)) (Wickham et al., 1999). Furthermore, simulations completed by Wickham et al. (1999) indicate that crossed states or dislocation nodes are formed considerably more frequently than junctions. Hence, we focus on accurately describing dislocation node (crossed-state) formation and dissolution. For a more detailed discussion on the physical origin of the crossed states see Madec et al. (2002b).

At finite temperatures, atomic oscillations produce local stress fluctuations that can assist the applied stress to move mobile dislocations past short-ranged obstacles, such as forest dislocations (Friedel, 1964; Becker, 1925; Orowan, 1934a,b,c). In other words, the combination of applied stress and temperature-induced stress fluctuations can result in node dissociation. The lifetime of the node, Γ, is universally calculated on the basis of the well-known Van't Hoff-Arrhenius rate equation (Van't Hoff, 1896; Arrhenius, 1889), which originated from studies of chemical reaction rates and was first applied to dislocations by Becker (1925), Orowan (1934a,b,c), and Eyring (1936). The Van't Hoff-Arrhenius rate equation calculates the inverse of the node lifetime as

$$\Gamma^{-1} = f_a \exp\left(-\frac{E}{k_B T}\right), \tag{1}$$

where E is the activation (Gibbs free) energy, f_a is an "attempt frequency", k_B is the Boltzmann constant, and T is the temperature. Neglecting dislocation drag, the equivalent plastic strain rate, $\dot{\varepsilon}$, is directly proportional to Γ^{-1}. Intersecting mobile and immobile dislocations are in a metastable state (local potential minimum) that is separated by an energy barrier with amplitude E from the dissociated state in which the mobile dislocation is remobilized. The node oscillates around the potential minimum due to thermal noise and eventually escapes over the energy barrier after absorbing a sufficient amount of thermal energy. In other words, if the applied stress is not large enough to dissociate the node, the node can still be destroyed by thermal fluctuations. Equation (1) gives the decay rate of the metastable state due to thermal fluctuations. The calculation of such rates is the subject of reaction rate theory (Hänggi et al., 1990) which encompasses classical transition state theory (TST) (Eyring, 1935; Vineyard, 1957) and Kramer's theory for chemical reaction rates (Kramers, 1940); both lead to Equation (1) for the rate of a chemical reaction, or of plastic deformation. For an excellent account of reaction rate theory see Pollak and Talkner (2005).

Equation (1) has served as the foundation for the majority of continuum-scale models constructed by the materials science community to describe thermally-activated plastic flow (Seeger, 1954a,b,c, 1955b; Follansbee and Kocks, 1988; Hoge and Mukherjee, 1977; Steinberg and Lund, 1989; Zerilli and Armstrong, 1987; Preston et al., 2003; Langer et al., 2010; Austin and McDowell, 2011, 2012). However, the Van't Hoff-Arrhenius equation is valid only when the height of the potential barrier is large in comparison with the thermal energy: $E/k_BT >> 1$. The derivation of Equation (1) from either TST or Kramer's theory requires a separation of time scales: the time scale for escape over the barrier must be much greater than any other time scale (noise correlation time, transition time, …). In other words, the conditions for escape over the potential barrier must be quasi-stationary (to a high degree of accuracy a Maxwell-Boltzmann distribution obtains in the neighborhood of the initial minimum), meaning that there will be a very slow diffusion of particles, or dislocations, across the saddle point to another energetic minimum in comparison to other time scales. Under these assumptions, Chandrasekhar (1943) carried out a clear, elegant derivation of Equation (1) from the Smoluchowski equation over 70 years ago, a derivation which rests on the

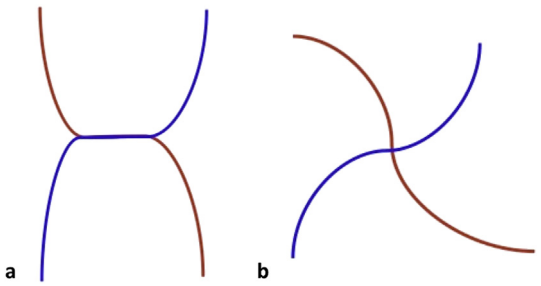

Fig. 1. Intersections of attractive mobile and immobile dislocations can result in the formation of either (a) a junction, or (b) a crossed-state or node.