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A phenomenological dislocation mobility law for bcc metals

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ABSTRACT

Dislocation motion in body centered cubic (bcc) metals displays a number of specific features that result in a strong temperature dependence of the flow stress, and in shear deformation asymmetries relative to the loading direction as well as crystal orientation. Here we develop a generalized dislocation mobility law in bcc metals, and demonstrate its use in discrete Dislocation Dynamics (DD) simulations of plastic flow in tungsten (W) micro pillars. We present the theoretical background for dislocation mobility as a motivating basis for the developed law. Analytical theory, molecular dynamics (MD) simulations, and experimental data are used to construct a general phenomenological description. The usefulness of the mobility law is demonstrated through its application to modeling the plastic deformation of W micro pillars. The model is consistent with experimental observations of temperature and orientation dependence of the flow stress and the corresponding dislocation microstructure.

1. Introduction

Dislocation mobility is a fundamental property of crystals that determines many characteristics of their plastic deformation. In computational multiscale methods of plastic deformation (e.g. discrete or continuum DD, crystal plasticity, continuum plasticity), dislocation mobility is modeled by a *phenomenological* law, which prescribes the dependence of the steady-state velocity of a dislocation on local parameters, such as line character, slip system, stress, temperature, and composition.

In fcc crystals, the task of formulating mobility laws is simplified by several features of close-packed $\{111\}\langle 110\rangle$ slip. First, the lattice resistance to dislocation motion is typically negligible compared to the applied force, ultimately as a consequence of the planar character of the disassociated dislocation core and the reduced magnitude of the partial Burgers vector [1,2]. Second, the planar core structure results in dislocation glide being controlled by the resolved shear stress only. Thus, dislocation motion obeys closely Schmid's postulation [3]. Third, in lieu of Neumann's principle [4], the mirror symmetry of the fcc lattice with respect to $\{110\}$ planes (i.e. planes normal to the slip direction) guarantees that the flow stress is independent of slip plane orientation and sense of shear (Fig. 1). As a consequence, dislocation glide can be considered an "atomically smooth" process, and simple mobility laws can be obtained from the condition that the mechanical force balances the dissipative friction force. In particular, for small dislocation velocity compared to the shear wave speed, the interaction of phonons with dislocations provides the main mechanism of energy dissipation, resulting in a drag force that depends linearly on the dislocation speed. The type of mobility law that emerges from these considerations typically involve a drag coefficient, which may depend on temperature and dislocation character (screw vs edge).

It bears emphasis that fcc-type mobility laws automatically satisfy Schmid's law, the empirical yield criterion formulated in the pre-dislocation era by Schmid [3,5] for close-packed metals subject to uniaxial loads. The law contains two distinct statements [6]. First, that plastic deformation initiates on the (low-index) crystallographic plane with the highest Schmid factor, when the stress resolved on that plane in the slip direction reaches a critical value. Second, that the critical value is a *constant* material parameter, known as the *critical resolved shear stress* (τ_{crss}). In particular, the τ_{crss} does not depend on orientation of the slip plane, sense of the load, and local stress state.

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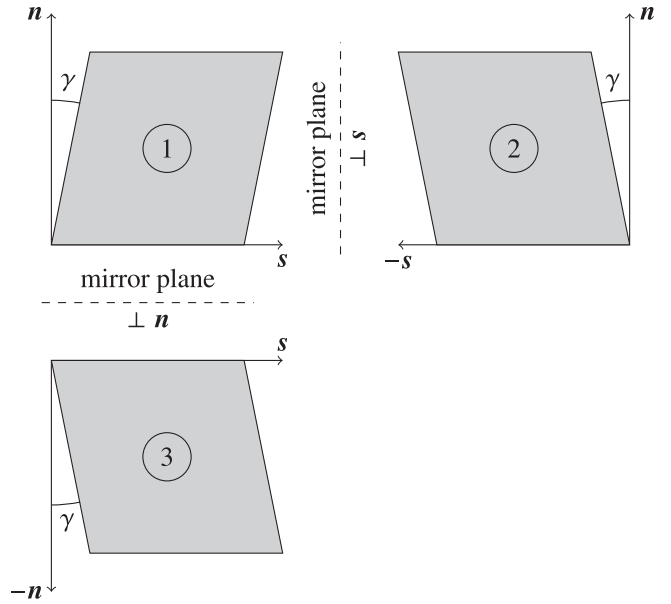

Fig. 1. Sketch of Neumann's principle in relation to the symmetry of the flow stress [26]. Crystal (1) is plastically deformed in shear with distortion $\beta_1 = \gamma \boldsymbol{s} \otimes \boldsymbol{n}$. Crystal (2) is deformed with opposite distortion $\beta_2 = \gamma(-\boldsymbol{s}) \otimes \boldsymbol{n}$, by shearing it along the opposite slip direction. If the two crystals lattices are mirror-symmetric with respect to planes perpendicular to $\boldsymbol{s}$, then the two deformed crystals are indistinguishable. This symmetry guarantees the independence of the flow stress on the sense of shear, as in the case of ⟨110⟩ slip in fcc crystals, for any slip plane of the ⟨110⟩ zone. It does *not* apply to ⟨111⟩ slip in bcc metals. Crystal (3) is also subject to the opposite distortion $\beta_3 = \gamma \boldsymbol{s} \otimes (-\boldsymbol{n})$. If the crystals lattices (1) and (3) are mirror-symmetric with respect to planes perpendicular to $\boldsymbol{n}$, then the two deformed crystals are indistinguishable from each other. This symmetry applies to {110} planes in bcc metals. Therefore ⟨111⟩{110} slip should be unaffected by the TAT asymmetry. However, recent studies [27,28] have shown that the actual trajectory of ⟨111⟩{110} screw dislocations between consecutive "easy-core" configurations bows out of {110} planes.

Owing to the pioneering work of Taylor [7,8], it was soon recognized that bcc metals do not strictly obey Schmid's law. Early studies [9,10] revealed remarkable features common to several bcc transition metals, such as the *twinning/anti-twinning* (TAT) and the *tension/compression* (TC) asymmetries of the yield and flow stresses, macroscopically non-crystallographic slip, and a strong temperature and strain rate dependance of the flow stress.

Hirsch [11] first identified the origin of these features in the non-planar character of the core of screw dislocations, whose stress-free configuration spreads equally on equivalent low-index planes of the ⟨111⟩ zone. Several elastic, atomistic, and *ab-initio* studies followed this rationalization and shed light on the structure of screw dislocation cores in bcc metals [see [6,12–14], for a review]. Early atomistic simulations predicted an extended and degenerate (or polarized) core structure for group VB metals, while a compact and non-degenerate core was found for group VIB metals [4]. More recent electronic structure calculations, however, support the evidence that pure transition metals posses a compact and non-degenerate core structure [15]. The two most prominent aspects that stem from this particular core structure are [16,17]:

- *The temperature-dependence of the flow stress.* Because motion requires a modification of the non-planar core configuration, screw dislocations experience a high lattice resistance. As a consequence, below a certain temperature-dependent critical stress, glide of screw dislocations proceeds by way of thermally-assisted nucleation and subsequent lateral migration of kinks-pairs [18]. The rate of these two processes ultimately controls the velocity of the screw dislocation as a whole. Because kink nucleation is a thermally-activated process, the flow stress rapidly increases with decreasing temperature. Moreover, the ability of screw dislocations to proceed by kinks on different planes of the ⟨111⟩ zone may manifest in macroscopically non-planar slip, with surface slip traces showing a *pencil glide* pattern when observed along the slip direction [7,12].
- *The emergence of non-Schmid effects.* There are deviations from both statements contained in Schmid law, which in general change the condition for the onset of slip into a function of stress components other than the resolved shear stress. Originally undistinguished, two different phenomena are now recognized [4,16,19], namely the TAT asymmetry, and the TC asymmetry of the flow stress. The TAT asymmetry is an intrinsic property of the bcc lattice related to its lack of mirror symmetry with respect to planes orthogonal to the dominant ⟨111⟩ slip direction (Fig. 1). On the other hand, the TC asymmetry is due to components of the local stress other than the glide component, which influence the structure of the screw core and thus the critical conditions for dislocation motion.

Several phenomenological mobility laws have been proposed to take into account these important features, and have been used in DD simulations. Several authors [20–22] have implemented a temperature-dependent screw dislocation mobility by accounting for the thermally-activated kink-pair formation process. In similar settings, Chaussidon et al. [23] have considered a cross-slip probability influenced by the TAT orientation of the slip plane. Wang et al. [24] have proposed a mobility law with different values of the Peierls stress for [111]{112} twinning and anti-twinning dislocations. Srivastava et al. [25] account for both TAT and TC asymmetries by supplying the kink-pair activation enthalpy as a function of orientation as a lookup table compiled from atomistic calculations.

The objective of the present work is to develop an analytical mobility law for dislocation motion so as to reproduce observations and phenomena associated with plastic flow in bcc metals. The aim is to establish a procedure for accurate, yet computationally convenient description of dislocation velocity, where the influence of the applied stress state, temperature, and possibly alloying elements can be incorporated. The intended utilization of the law is in large-scale DD simulations, and in dislocation-based crystal plasticity models. To achieve our goal, we will use fundamental theory, together with experimental measurements and atomistic computer simulations (Molecular Statics, Molecular Dynamics, and First Principles) to establish a *phenomenological* law for dislocation mobility. The purpose of the theory, presented in section 2, is to guide the development of an analytical form, inspire the phenomenological description of dislocation motion, and to furnish an understanding of its physical origins. As we shall see later, the proposed law, developed in section 3 has fitting parameters obtained from detailed computer simulations, and calibrated with experimental data. We describe a *process* by which mobility parameters are established, and demonstrate the applicability of the developed mobility law in DD simulations. Since the main goal here is to allow efficient DD simulations of bcc metals, we present an application of the developed law to the study of temperature effects on the dislocation microstructure and flow stress in W micropillars in section 4. Finally, conclusions of the work and future directions are given in section 5.

2. Background theory

The Peierls stress τ_p is defined as the minimum applied shear stress needed at 0 K to move an infinitely long dislocation over the periodic misfit energy barrier of the glide plane [29,30]. τ_p is strongly dependent on the crystal lattice structure, basis atoms, and