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Dislocation motion in tungsten: Atomistic input to discrete dislocation simulations

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ABSTRACT

A computational framework for the discrete dislocation dynamics simulation of body-centered cubic (*bcc*) metals which incorporates atomistic simulation results is developed here on the example of tungsten. Mobility rules for the a/2⟨111⟩ screw dislocations are based on the kink-pair mechanism. The fundamental physical quantity controlling the kink-pair nucleation, the stress-dependent activation enthalpy, is obtained by fitting the line-tension model to atomistic data extending the approach by Gröger et al. (2008a,b) and Gröger and Vitek (2008c). In agreement with atomistic simulation, kink-pair nucleation is assumed to occur only on {110} planes. It is demonstrated that slip of the crystal along high-index planes like {112} which is often observed in experiments is obtained by the glide of the dislocation on two or more {110} planes. It is shown that such an atomistic based description of the dislocation mobility provides a physical basis to naturally explain many experimentally observed phenomena in *bcc* metals like the tension–compression asymmetry, the orientation dependence of loading, temperature dependence of yield stress and the crystallography of slip.

1. Introduction

Since the early studies of plastic flow in α-iron by Taylor and Elam (1926), it has been known that slip in body-centered cubic (*bcc*) metals occurs by sliding along crystallographic planes parallel to the ⟨111⟩ direction. Their early observations, combined with later experimental evidence confirmed that yielding in *bcc* metals does not obey the well-known Schmid law (Schmid and Boas, 1935) used to describe the plastic flow of face-centered cubic (*fcc*) metals. An implication of this law is that there exists a well defined critical resolved shear stress (CRSS) to initiate plastic flow that is independent of the orientation of applied loading and the sense of shearing on a crystallographic plane and that is not affected by components of the stress tensor other than the resolved shear stress (Duesbery, 1986). Accordingly, plastic flow is expected to initiate on the plane having the highest resolved shear stress. However, many experiments on various *bcc* metals (Christian, 1983) have revealed that these metals display features like the temperature and strain-rate dependence of yield and flow stresses. Fracture experiments on tungsten single crystals (Riedle et al., 1996; Gumbsch et al., 1998; Gumbsch, 2003) also show that the fracture toughness and the brittle to ductile transition are both directly correlated with the temperature and strain rate dependent changes of dislocation mobility (Hartmaier and Gumbsch, 2005). Single crystal deformation experiments in *bcc* metals (Christian, 1983) generally show a tension–compression asymmetry, and/or a twinning-antitwinning

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asymmetry which all clearly contradict the Schmid law and are, therefore, referred to as non-Schmid behavior. Low-temperature experiments in tension and compression on high-purity single crystals of niobium (Duesbery and Foxall, 1969; Bolton and Taylor, 1972) and molybdenum (Jeffcoat et al., 1976; Matsui et al., 1976) have further shown that for some orientations, the plastic flow occurs on planes that are not the most highly stressed. This phenomenon is known as anomalous slip.

The non-planar spreading of the dislocation core of screw dislocations in *bcc* metals, first proposed by Hirsch (1960), provides an explanation for the large Peierls stresses in these materials and the orientation dependence of the CRSS. The importance of dislocation core structure and dislocation core effects on the mechanical properties of different metals has been emphasized in the review by Vitek (1992). Most importantly core effects lead to a temperature dependence of the flow stress due to the overcoming of the intrinsic energy barriers, the Peierls barriers, by the kink-pair nucleation mechanism (Seeger, 1956; Dorn and Rajnak, 1964).

Atomistic investigations of an isolated a/2⟨111⟩ screw dislocation in molybdenum and tungsten (Ito and Vitek, 2001) revealed that the dislocation core and hence the Peierls barrier is strongly affected by the shear stresses parallel to the slip direction acting in a different plane of the corresponding ⟨111⟩ zone than the slip plane, and the shear stresses perpendicular to the slip direction. These components are non-glide stresses. The latter do not exert any direct glide force on the dislocation but break the symmetry of the dislocation core and thus promote slip on the {110} plane into which the dislocation core is predominantly extended (Gröger et al., 2008a). It is important to note that other stress components than these two shear stresses do not play any major role (Ito and Vitek, 2001).

Recently, Gröger et al. (2008a) and Gröger and Vitek (2005) utilized Bond Order Potentials (BOP) for molybdenum and tungsten (Mrovec et al., 2004; Mrovec et al., 2007) to calculate the dependence of the Peierls stress on the orientation of the maximum resolved shear stress plane (MRSSP) in uniaxial loading and on the magnitude of the shear stress perpendicular to the slip direction. They found a strong twinning-antitwinning asymmetry in molybdenum but virtually none in tungsten. Additionally, the most active slip system did not systematically coincide with the most highly stressed {110}⟨111⟩ glide system but varied with both the orientation of the MRSSP and the magnitude of the shear stress perpendicular to the slip direction. Based on these results, they developed a two-dimensional Peierls potential that changes its shape in response to the non-glide stress components and orientation of the MRSSP (Gröger and Vitek, 2008c). This was utilized to develop a thermodynamic model of the dislocation glide at finite temperatures, which is based on the classical works of Seeger (1956) and Dorn and Rajnak (1964). It was thus possible to obtain physically justified flow criteria for molybdenum and tungsten that originate at the level of isolated a/2⟨111⟩ screw dislocations. By scaling the atomistically obtained stresses by a factor of roughly 3–4, this multiscale approach was shown to yield reasonable macroscopic predictions of cavitation instability and the occurrence of strain bursts in bcc metals (Gröger and Vitek, 2008c; Racherla and Bassani, 2007). However, no attempt has been made to directly employ the atomistic simulation results to study the general dislocation–dislocation interactions in these materials.

Discrete dislocation dynamics (DDD) models can provide the link between single dislocation properties, dislocation microstructure and multi-dislocation interactions, and the macroscopic response. This of course requires a physically based modeling of the mobility of screw dislocations in *bcc* metals. Screw dislocation mobility is determined from the activation enthalpy of kink-pair nucleation. Current modeling approaches in DDD are based on parametrizing the activation enthalpy of kink-pair nucleation on screw dislocations using the phenomenologically based Kocks model whose parameters are fitted to experiments (Tang et al., 1998; Naamane et al., 2010). This description remains macroscopic in nature as the activation enthalpy is a function of effective global resolved shear stress. Such a model therefore does not account for the core effects on screw dislocation mobility and is not predictive in nature. More recently Chaussidon et al. (2008) have partially incorporated non-Schmid behavior via cross-slip rules in DD simulations based on atomistic information. These rules give rise to an asymmetric glide in tension and compression loadings. Wang and Beyerlein (2011) utilize atomistic information to incorporate the effects of the non-glide components of the stress-tensor on screw dislocation mobility within the Kocks model framework.

A straightforward implementation of the atomistic information into DDD is also not feasible since the atomistic modeling has its limitations in the accessible length and time scales. Mesoscopic models such as DDD have to handle longer length and time scales, which necessitates a systematic information transfer from the atomistic scale to dislocation properties in the form of a constitutive law for the dislocation mobility, which at the same time, retains the fundamental physics.

In this article, we present an approach to transfer the results of atomistic studies to a mesoscopic DDD model which takes into account the screw dislocation core effects on dislocation mobility at the scale of DDD. The motion of each screw dislocation in DDD is governed by the local stress state along the dislocation. We start with an isolated screw dislocation and will discuss the response of this particular dislocation under different loading conditions in detail within the non-Schmid framework at various temperatures.

The approach we present here is different from a continuum description of plastic flow like that presented in Gröger et al. (2008b) and Gröger and Vitek (2008c). In such a continuum formulation the glide system, which is most easily activated, defines the inner envelope of the yield surface. In DDD simulations, the response of any given dislocation to the local stress state has to be followed. This requires a somewhat more general approach. In agreement with atomistic studies, the elementary slip planes of screw dislocations are taken as {110} planes only. The most important experimentally observed phenomena like the tension–compression asymmetry at finite temperatures (Christian, 1983) and even changes of effective slip planes with temperature will be shown to be a natural consequence of this modeling and of the incorporation of the