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An atomistically-informed dislocation dynamics model for the plastic anisotropy and tension–compression asymmetry of BCC metals

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ABSTRACT

Atomistic simulations have shown that a screw dislocation in body-centered cubic (BCC) metals has a complex non-planar atomic core structure. The configuration of this core controls their motion and is affected not only by the usual resolved shear stress on the dislocation, but also by non-driving stress components. Consequences of the latter are referred to as non-Schmid effects. These atomic and micro-scale effects are the reason slip characteristics in deforming single and polycrystalline BCC metals are extremely sensitive to the direction and sense of the applied load. In this paper, we develop a three-dimensional discrete dislocation dynamics (DD) simulation model to understand the relationship between individual dislocation glide behavior and macro-scale plastic slip behavior in single crystal BCC Ta. For the first time, it is shown that non-Schmid effects on screw dislocations of both {110} and {112} slip systems must be implemented into the DD models in order to predict the strong plastic anisotropy and tension–compression asymmetry experimentally observed in the stress–strain curves of single crystal Ta. Incorporation of fundamental atomistic information is critical for developing a physics-based, predictive meso-scale DD simulation tool that can connect length/time scales and investigate the underlying mechanisms governing the deformation of BCC metals.

1. Introduction

Screw dislocations are the dominant defects in the plastic deformation of BCC metals. They have non-planar cores, which split onto several non-parallel crystallographic planes. Both atomistic and ab-initio simulations show that the configurations of screw dislocation cores spreads symmetrically onto three {110} planes (Duesbery and Vitek, 1998; Woodward and Rao, 2001). BCC lattice dislocations of edge character, on the other hand, have different core structures. For example, atomistic simulations have shown that $\frac{1}{2}\langle 111\rangle$ non-screw dislocations on {110} planes in an unstressed BCC crystal have planar cores and the configuration of their core is not sensitive to the character of the applied stress field (Yamaguchi and Vitek, 1973a,b).

The non-planar core of screw dislocations greatly influences dislocation motion under stress. The non-planar core generally leads to high Peierls stresses and drag coefficients and makes it harder for screws to glide. Compared to edge dislocations, they are far less mobile. From atomistic simulations, the Peierls stresses of non-screw dislocations are less than an order of magnitude smaller than those of screw dislocations (Duesbery and Xu, 1998). At low deformation rates, the ratio of drag coefficients of the non-screw to screw dislocations is much less than unity at about 10^{-2}–10^{-3}, while at high rates, however, the ratio draws closer to 10^{-1} (Urabe and Weertman, 1975). More importantly, atomic-scale configurations of screw dislocation cores are greatly influenced by the nature of the local stress field acting on the dislocation. Their core

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