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Thermally-activated non-Schmid glide of screw dislocations in W using atomistically-informed kinetic Monte Carlo simulations

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ABSTRACT

Thermally-activated $1/2\langle 111\rangle$ screw dislocation motion is the controlling plastic mechanism at low temperatures in body-centered cubic (bcc) crystals. Dislocation motion proceeds by nucleation and propagation of atomic-sized kink pairs in close-packed planes. The atomistic character of kink pairs can be studied using techniques such as molecular dynamics (MD). However, MD's natural inability to properly sample thermally-activated processes as well as to capture $\{110\}$ screw dislocation glide calls for the development of other methods capable of overcoming these limitations. Here we develop a kinetic Monte Carlo (kMC) approach to study single screw dislocation dynamics from room temperature to $0.5T_m$ and at stresses $0 < \sigma < 0.9\sigma_P$, where T_m and σ_P are the melting point and the Peierls stress. The method is entirely parameterized with atomistic simulations using an embedded atom potential for tungsten. To increase the physical fidelity of our simulations, we calculate the deviations from Schmid's law prescribed by the interatomic potential used and we study single dislocation kinetics using both projections. We calculate dislocation velocities as a function of stress, temperature, and dislocation line length. We find that considering non-Schmid effects has a strong influence on both the magnitude of the velocities and the trajectories followed by the dislocation. We finish by condensing all the calculated data into effective stress and temperature dependent mobilities to be used in more homogenized numerical methods.

1. Introduction

$1/2\langle 111\rangle$ screw dislocations are the main carriers of plasticity in body-centered cubic (bcc) single crystals. Experimentally, bcc slip is seen to occur on $\{110\}$, $\{112\}$, and $\{123\}$ planes, or any combination thereof. To determine the slip plane for a general stress state, Schmid's law is used, which states that glide on a given slip system commences when the resolved shear stress on that system, the Schmid stress, reaches a critical value (Schmid and Boas, 1935). This law is known to break down in bcc metals, which has great implications on the overall plastic flow and deformation behavior in these systems. Experimentally, *non-Schmid* behavior is well documented in the literature going back several decades (Sestak and

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Zarubova, 1965; Sherwood et al., 1967; Zwiesele and Diehle, 1979; Christian, 1983; Pichl, 2002),[1] and its reasons have been thoroughly investigated. First, as Vitek and co-workers have noted (Duesbery and Vitek, 1998; Ito and Vitek, 2001), slip planes in bcc crystals do not display mirror symmetry (a common characteristic of planes belonging to the ⟨111⟩ zone), and so the sign of the applied stress does matter to determine the critical stress. This is most often referred to as the *twinning–antitwinning asymmetry*. Second, studies using accurate atomistic methods (semi empirical interatomic potentials and density functional theory calculations) have shown that stress components that are not collinear with the Burgers vector $\boldsymbol{b}$ couple with the core structure of screw dislocations resulting also in anomalous slip (Bulatov et al., 1999; Woodward and Rao, 2001; Gröger and Vitek, 2005; Chaussidon et al., 2006).

Although effective corrections that reflect deviations from Schmid law have been implemented in crystal plasticity models, and their effects assessed at the level of grain deformation (Dao et al., 1996; Vitek et al., 2004; Gröger and Vitek, 2005; Yalcinkaya et al., 2008; Wang and Beyerlein, 2011; Lim et al., 2013; Chen et al., 2013; Soare, 2014), there is no model establishing the fundamental impact of non-Schmid behavior on single screw dislocation motion. Molecular dynamics (MD) simulations naturally include non-Schmid effects as part of the simulated dynamics of screw dislocations (Gilbert et al., 2011; Cereceda et al., 2013). However, it is exceedingly difficult to separate these effects from the bundle of processes (and artifacts) brought about by size and time limitations inherent to MD simulations. In addition, screw dislocation motion proceeds by way of the nucleation and sideward relaxation of so-called *kink pairs* in a broad stress and temperature range. Kink pair nucleation may be regarded as a rare event occurring on a periodic energy substrate known as the *Peierls potential*. MD's inability to sample these events accurately often leads to overdriven dynamics and unrealistically high dislocation velocities (Cereceda et al., 2013).

Here, we develop a kinetic Monte Carlo (kMC) model to study thermally activated screw dislocation motion in tungsten (W). Our approach – which builds on previous works on the same topic (Lin and Chrzan, 1999; Cai et al., 2001, 2002; Deo and Srolovitz, 2002; Scarle et al., 2004; Ariza et al., 2012) – is based on the stochastic sampling of kink pair nucleation coupled with kink motion. The entire model is parameterized using dedicated atomistic simulations using a state-of-the-art interatomic potential for W (Marinica et al., 2013). Non-Schmid effects are incorporated via a dimensionless representation of the resolved shear stress, which provides the deviation from standard behavior for all the different activated slip planes. We explore the impact of these deviations on single dislocation glide and compare the results to direct MD simulations. Another novel aspect of our simulations is the inclusion of stress-assisted kink drift and kink diffusion simultaneously in our model. This quantitatively reflects the dynamic behavior observed atomistically for an isolated screw dislocation.

The paper is organized as follows. First we describe the kMC algorithm and the topological construct of screw dislocations and kink segments. We then provide a detailed account of the parameterization effort undertaken, beginning with single kink static and dynamic properties, and ending with the calculation of the non-Schmid law. In the Results section we report calculations of Schmid and non-Schmid glide as a function of stress, temperature, dislocation length, and maximum resolved shear stress (MRSS) plane. We finish with a discussion of the results and the conclusions.

2. Kinetic Monte Carlo model of thermally-activated screw dislocation motion

2.1. Physical basis

All that is required to initialize a kMC run are the total initial screw dislocation line length L, the temperature T, and the applied stress tensor $\boldsymbol{\sigma}$. In the kMC calculations, we choose a working representation of the stress tensor in its non-dimensional scalar form:

$$s = \frac{\sigma_{\mathrm{RSS}}}{\sigma_P}$$

where σ_{RSS} is the *resolved shear stress* (RSS) and σ_P is the Peierls stress. We consider two different contributions to σ_{RSS}: (i) from external sources – defined by an applied stress tensor $\boldsymbol{\sigma}$ – and (ii) from internal stresses originating from segment-segment elastic interactions. At a given dislocation segment i, the normalized resolved shear stress is:

$$s_i = \frac{\boldsymbol{t}\cdot(\boldsymbol{\sigma}+\boldsymbol{\sigma}_{int})\cdot\boldsymbol{n}}{\sigma_P} = \frac{\boldsymbol{t}\cdot\left(\boldsymbol{\sigma}+\sum_j \boldsymbol{\sigma}_{\mathrm{ij}}(r_{ij})\right)\cdot\boldsymbol{n}}{\sigma_P} \tag{1}$$

Here, $\boldsymbol{t}$ and $\boldsymbol{n}$ are unit vectors representing the slip direction and the glide plane normal, and r_{ij} is the distance between dislocation segments i and j. The calculation of $\boldsymbol{\sigma}_{ij}(r_{ij})$ is discussed in Section 2.2 but note that this definition of $\boldsymbol{\sigma}_{int}$ introduces a certain locality in s_i, hence the subindex i.

The projection of the total stress tensor on the RSS plane as in Eq. (1) is what is known as *Schmid's law*. For a straight dislocation (no internal stresses) in the coordinate system depicted in Fig. 1, the RSS is:

$$\sigma_{\mathrm{RSS}} = \sigma_{ext} = \boldsymbol{t}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{n} = -\sigma_{xz}\sin\theta + \sigma_{yz}\cos\theta \tag{2}$$

[1] Although it was first recognized as early as in the 1920s and 1930s.