International Journal of Plasticity 60 (2014) 58–70

Contents lists available at ScienceDirect

International Journal of Plasticity

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

Simulations of dislocation mobility in magnesium from first principles

Ilgyou Shin [a], Emily A. Carter [b,*]

[a] Department of Chemistry, Princeton University, Princeton, NJ 08544-1009, United States
[b] Department of Mechanical and Aerospace Engineering, Program in Applied and Computational Mathematics, and Andlinger Center for Energy and the Environment, Princeton University, Princeton, NJ 08544-5263, United States

ARTICLE INFO

Article history:
Received 29 September 2013
Received in final revised form 31 March 2014
Available online 18 April 2014

Keywords:
A. Dislocations
A. Ductility
B. Metallic material
C. Optimization
C. Density functional theory

ABSTRACT

The strength and ductility of metals are governed by the motion of dislocations, which is quantified by the Peierls stress (σ_p). We use orbital-free density functional theory (OFDFT) to characterize the motion of $\frac{1}{3}\langle 11\bar{2}0\rangle$ dislocations on the basal $\{0001\}$ and prismatic $\{1\bar{1}00\}$ planes in hexagonal-close-packed magnesium (Mg) in order to understand its deformation mechanisms. We predict σ_p values of edge dislocations on the basal and prismatic planes to be 0.6 and 35.4 MPa, respectively. The presence of stable stacking faults only on the basal plane produces partial dislocation splitting, which significantly lowers σ_p for basal dislocations. Our atomic scale simulations reveal that dislocation mobility is strongly correlated with the number of core atoms moving collectively. OFDFT σ_p results are in excellent agreement with experiments (~0.5 and 39.2 MPa), further validating OFDFT as an independent and predictive tool for simulating plastic behavior in main group metals at the mesoscale with first principles' accuracy.

1. Introduction

In order to lower fuel consumption, reduce emissions, and improve vehicle performance, the automobile industry has strived to reduce vehicle weight by replacing denser materials, not only steels and cast irons but even Al alloys, with lighter weight materials. Because of Mg's low density (1.74 g/cm^3) as well as its abundance, high specific strength, and stiffness (Mordike and Ebert, 2001; Agnew, 2004; Doege and Droeder, 2003; Nyberg et al., 2008), Mg alloys are considered among the most promising materials for reducing weight. The use of Mg alloys has grown over the past couple of decades but is still limited to an average of 10–12 lbs. in an average 3360 lbs. vehicle, which is only ~0.3% (Magnesium, 2006; Materials Technologies, 2010). Mg's minimal deployment to date is mainly attributable to its limited ductility. According to the von Mises criterion (von Mises and Angew, 1928), at least five independent slip systems are required for a general homogeneous deformation of a polycrystalline material. Since the hexagonal-close-packed (HCP) structure that Mg adopts under ambient conditions has only two independent primary slip systems, its ductility is limited (Oppedal et al., 2012).

In order to improve Mg's ductility for broader industrial use, we must understand its plastic deformation mechanisms. These mechanisms in metals are mainly governed by atomic-scale motion of dislocations (Hirth and Lothe, 1982). Their mobility is quantified by the Peierls stress (σ_p), which is the minimum external stress required to move a stationary

* Corresponding author. Tel.: +1 6092585391; fax: +1 6092585877.
E-mail address: eac@princeton.edu (E.A. Carter).

http://dx.doi.org/10.1016/j.ijplas.2014.04.002
0749-6419/

dislocation irreversibly at 0 K. Unfortunately, *in situ* measurements of the atomic-scale motion of dislocations are not yet possible. Therefore, reliable theoretical modeling is needed to probe dislocation motion.

Among theoretical techniques, the embedded atom method (EAM) (Daw and Baskes, 1983; Daw and Baskes, 1984) has been the most widely used means to simulate dislocation motion and to evaluate σ_p in metals because of its computational efficiency. Although it has achieved many successes, EAM in general cannot be considered an independent, predictive tool because EAM potentials are not fully transferable, i.e., their accuracy can suffer when applied to environments that differ significantly from those in which they were originally fit. For example, EAM predicts stacking fault energies (SFEs) and dislocation core structures less accurately than quantum mechanics (QM) methods do (Yasi et al., 2009; Shin and Carter, 2011) (for Mg) and (Shin et al., 2009; Hung and Carter, 2011) (for Al). By contrast, first principles QM methods, such as Kohn–Sham density functional theory (KSDFT) (Hohenberg and Kohn, 1964; Kohn and Sham, 1965), provide a predictive, non-empirical approach for studying metal properties. However, despite its moderate computational cost, routine calculations on several thousand metal atoms (generally required for simulating dislocation motion) are still prohibitively expensive.

For large-scale simulations of dislocation motion, orbital-free density functional theory (OFDFT) (Wang and Carter, 2000) can offer first principles predictions with much faster calculations than KSDFT. OFDFT is a transferable, first principles QM method that approximates KSDFT while scaling quasilinearly (*NlnN*) (Hung and Carter, 2009). Unlike KSDFT, OFDFT relies on the electron density as the sole variable, based on the first Hohenberg–Kohn theorem (Hohenberg and Kohn, 1964) that proves the electron density uniquely determines the ground state properties of a many-electron system. Consequently, the degrees of freedom are reduced from $3N$ in KSDFT (N KS orbitals for N electrons) to 3 spatial coordinates in OFDFT. This reduction dramatically lowers the overall computational time. Hence, a sufficient number of atoms (10^3–10^4) needed to simulate dislocations can be explicitly treated with QM accuracy at moderate computational cost within OFDFT (Hung and Carter, 2009).

Increased speed comes at the potential sacrifice of accuracy because of two approximate terms used in OFDFT beyond the usual electron exchange–correlation (XC) functional in the total energy functional. These are a kinetic energy density functional (KEDF) and a local pseudopotential (LPP) that are respectively used to evaluate the non-interacting electron kinetic energy and the ion (screened nucleus) – valence electron interaction energy, respectively. With state-of-the-art nonlocal KEDFs (Wang and Teter, 1992; Foley and Madden, 1996; Wang et al., 1999) and transferable bulk-derived local pseudopotentials (BLPPs) (Huang and Carter, 2008), OFDFT accurately describes many fundamental properties of main group metals with comparable accuracy to KSDFT (e.g., equilibrium volumes, relative phase stabilities, elastic constants, and SFEs (Shin and Carter, 2011; Shin et al., 2009; Jesson and Madden, 2000; Carling and Carter, 2003; Gonzalez et al., 2006)). In addition, a number of large-scale simulations for complex mechanical phenomena of such metals have been successfully studied with OFDFT (e.g., liquid metal properties (Jesson and Madden, 2000), grain boundary motion (Watson and Madden, 1998), crack propagation (Hung and Carter, 2011), and dislocation structure and mobility (Shin and Carter, 2011; Shin and Carter, 2013)), lending credence to its use in what follows.

In the present work, we calculate σ_ps of $\frac{1}{3}\langle 11\bar{2}0\rangle$ edge and screw dislocations on basal $\{0001\}$ and prismatic $\{1\bar{1}00\}$ slip planes in HCP Mg from OFDFT atomic simulations. Such dislocation motions have also been studied with EAM atomic simulations (Yasi et al., 2009; Groh et al., 2009) using Sun et al.'s potential (Sun et al., 2006). This EAM potential was fitted to crystal, liquid, and melting properties of Mg, but also to sets of *ab initio* forces using the force matching method (Ercolessi and Adams, 1994). Although this EAM potential is widely used and considered to be the most accurate one to date for Mg plasticity simulations, it still exhibits quantitative and even qualitative errors in its predicted SFE surfaces for Mg (Yasi et al., 2009; Shin and Carter, 2011). Hence, this potential is expected to produce incorrect predictions for dislocation behavior, e.g., spurious cross-slip of a screw dislocation from the basal to prismatic plane may occur (Shin and Carter, 2011). (Other Mg EAM potentials are also available, e.g., Zhou et al. (2001), designed to simulate specific systems, but most Mg plasticity simulations have employed Sun et al. (2006) or Liu et al. (1996) EAM potentials, with the former showing clear improvement over the latter for Mg dislocation simulations (Yasi et al., 2009).) By contrast, KSDFT accurately predicts Mg SFE surfaces, but its high computational cost hinders its use in direct atomic simulations of dislocation motion. Therefore, an additional theory and its attendant assumptions have been used to extract σ_ps from KSDFT SFE calculations (Uesugi et al., 2003). In this work, we perform direct atomic simulations using OFDFT to obtain first principles predictions of Mg σ_ps. OFDFT very accurately reproduces KSDFT predictions for Mg SFE surfaces (Shin and Carter, 2011), which implies that OFDFT should calculate σ_ps of HCP Mg with comparable accuracy to KSDFT. The OFDFT calculations presented below allows us to quantitatively compare unstable SFEs (slip barriers for a perfect crystal) and Peierls energies (energy barriers for dislocation motion) of the basal (primary) and prismatic (secondary) slip systems. These comparisons elucidate the microscopic mechanisms of slip in Mg, how dislocations control material deformation in different slip systems, and offer an atomic scale view into its lack of ductility.

Finally, we note that the computational cost of OFDFT, while orders of magnitude less than KSDFT, is still sufficiently high that simulations of a number of complex processes of plasticity such as the interaction of dislocations with grain boundaries (Wang et al., 2014) and texture evolution in a polycrystal from deformation in single crystals (Homayonifar and Mosler, 2011; Lim et al., 2011), remain beyond reach. Therefore, we foresee EAM persisting for now as the method of choice for dealing with such complicated plastic processes. However, DFT methods can contribute to improving EAM potentials by sophisticated parameterization. For example, Peng et al. have used OFDFT-calculated bulk properties of aluminum to more precisely rescale the force-matching EAM potential (Peng et al., 2008, 2010). Although we did not suggest a new EAM potential in this paper, we expect that our first principles OFDFT calculations of dislocation properties can provide meaningful