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Dislocation modeling in bcc lithium: A comparison between continuum and atomistic predictions in the modified embedded atoms method

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ABSTRACT

In this study, the modified embedded-atom method (MEAM) was applied to compare the predictions of dislocation core properties obtained by molecular statics with the continuum predictions obtained in the framework of the simplified 1D-Peierls–Nabarro model. To this end, a set of four fictive Li potentials in the MEAM framework was proposed with the condition that all four potentials reproduce the same elastic constants, the same transition energies between bcc and fcc crystal structures, and between bcc and hcp crystal structures, while the unstable stacking fault energy on the plane {110} in the direction $<111>$ was varied around the value predicted by first-principles. Within these potentials, direct atomistic calculations were performed to evaluate dislocation core properties such as dislocation half width and Peierls stress and the results were compared with continuum predictions. We found that the trends predicted by the Peierls–Nabarro model, i.e. (i) a decrease of the dislocation half width with increasing unstable stacking fault energy, and (ii) an increase of the Peierls stress with increasing the magnitude of the unstable stacking fault energy, were recovered using atomic calculations in the MEAM framework. Moreover, the magnitude of the dislocation half width and the Peierls stress calculated in the MEAM framework are in good agreement with the Peierls–Nabarro predictions when the dislocation half width is determined using a generic strategy. Specifically, the dislocation half width is defined as the distance for which the disregistery is included between *b/4* and *3b/4*. It was, therefore, demonstrated herein that the set of fictive potentials could be parameterized in the MEAM framework to validate or to disprove the continuum theory using atomistic methods.

1. Introduction

The strength and ductility of metals are governed by the nature of the dislocation core. Once the dislocation core properties are established at the atomic scale, scale-bridging strategies may be applied to transfer information from the lower length scale up to the engineering scale to predict the material's inelastic behavior [1,2,26,49]. From the literature, two strategies are commonly used to predict dislocation core properties. In the first strategy, dislocation core properties are directly modeled at the atomistic scale using semi-empirical potentials. This approach was extensively used over the years to gain information on the dislocation mobility in pure materials ([25] and references therein; [66,18,67]), and to identify the effect of solute atoms on the dislocation core properties ([29,38,50,57] and references therein). In the second strategy, the full atomistic analysis is avoided and a hierarchical multiscale approach is employed instead. The multiscale approach consists in combining the γ-surface obtained from atomistic calculations with a continuum dislocation-based model; the Peierls–Nabarro (PN) model [58,59] is considered to be an efficient framework to predict dislocation core properties using γ-surfaces derived from either first-principles or semi-empirical models [10,21]. Recently, Tsuru et al. [62] applied this multiscale approach to reveal the softening effect of solute atoms of yttrium in magnesium. Within the same approach, Moitra et al. [45] revealed the influence of nine solute elements on the formability of magnesium alloys. Even though Moitra et al. [45] only considered $<\mathbf{a}>$ dislocations in their analysis, they demonstrated that solute atoms of Ce, Gd, Ca, and Zr could improve the formability of magnesium alloys.

While the two strategies were applied extensively to reveal dislocation core properties in pure materials and in alloys, only a few number of comparative studies in which predictions obtained from full atomistic calculations and predictions derived from PN analyses have been carried out over the last two decades. Zhou et al. [69] performed atomistic calculations using a force law

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derived from the universal binding-energy relation to evaluate the dislocation core structure. In agreement with a PN model, their data revealed the dependence of the dislocation core width on the Peierls stress. However, the atomistic predictions of the Peierls stress were overestimated in their case by nearly four orders of magnitude compared the PN predictions. Lu et al. [40] examined the relation between the dislocation core properties (energetics, core width, and Peierls stress) and the dislocation character in aluminum using a semidiscrete variational Peierls–Nabarro model [41]. To model the interfacial restoring stress in the PN model, Lu et al. [40] used the generalized stacking fault energy curves obtained either from first-principles or in the framework of the embedded-atom method (EAM) of Ercolessi and Adams [15]. A perfect match was found between their predictions of the Peierls stress for the screw and the 60° dislocations and the data reported by Bulatov et al. [8] and obtained by performing the full atomistic computation using the same Al-EAM potential. Unlike Lu et al. [40] who demonstrated the reliability of the PN model as a function of the dislocation character, the objective of this work is to demonstrate that the modified embedded-atom method (MEAM) can be used to validate or to disprove the dislocation-based theory. To reach this goal, a set of four fictive potentials is derived in the MEAM framework. These four potentials are constructed to reproduce similar physical, thermal, and mechanical properties, apart from the unstable stacking fault energy that is varied around a reference value derived from first-principles. Using the four fictive potentials, the generalized stacking fault energy curves are calculated, and used in a PN model to predict the evolution of the dislocation width, and the corresponding Peierls stress, as a function of the unstable stacking fault energy. In parallel, the full atomistic calculations are performed using the four fictive MEAM potentials to measure the dislocation half width, and the Peierls stress, as a function of the unstable stacking fault energy. In the end, the predictions obtained with the two strategies are compared against each other to demonstrate the ability of the MEAM potential to validate the dislocation-based theory.

Owing to its highly specific mechanical behavior, lithium (Li) is considered in this study. Unlike other bcc metals, the plasticity of Li has a characteristic signature similar to the one of sodium [20]. For both elements, lithium and sodium, the dependence of the critical resolved shear stress on the temperature is not as strong as for other unary metals crystallized with a bcc crystal structure, and, based on TEM observations, the kink pairs mechanism as a rate controlling process was ruled out at low temperature [20]. A theory of stress-induced martensitic nuclei acting as obstacles to dislocation motion was derived from experimental observations to explain the lack of a temperature dependence of the critical resolved shear stress [54]. However, no numerical validation of the theory derived from experimental data was performed until today. Therefore, if one is able to control one individual bulk property at a time in a semi-empirical framework, then the use of molecular statics or dynamics in the framework of (semi)-empirical potentials can be envisioned to clarify the origin of the specific deformation behavior of Li single crystals, and in particular, to validate the postulated mechanism that triggers the stress-induced martensitic transformation. For this reason, the possibility of developing fictive, but accurate, (semi)-empirical potentials is required to understand the nature of the plastic deformation in Li single crystals. Furthermore, Li is of high interest in industrial applications. For example, it was experimentally shown, that the presence of solute atoms of Li enhances non-planar deformation, independently of the temperature, by decreasing the stress for cross-slip [63]. Moreover, the addition of Li in magnesium alloys was found to improve the ductility and the formability of the Mg alloys [46,68]. Even though bulk properties are not considered when Li is employed as an alloying element to improve ductility and formability of an alloy, before a cross-potential is developed one must ensure that the pure component potentials yield sufficiently accurate predictions of materials properties. In this work, the main focus of the study is on dislocation modeling even though the surface energy of different orientations is used to check non-bulk properties.

In this manuscript, the MEAM framework is reviewed in Section 2 with a special focus on introducing the MEAM parameters rather than reviewing all equations. The methodology to calculate dislocation core properties is presented in Section 3, in addition to the procedure used to parameterize the set of the four fictive Li-MEAM potentials. Numerical results, as well as their comparison with continuum predictions are reported and discussed in Section 4. Concluding remarks and envisioned future studies are given in Section 5. It should be noted that, in this study, the 1D Peierls–Nabarro (PN) model reviewed by Bulatov and Cai [9] is considered.

2. Interatomic potential

Over the years, the modified embedded-atom method, proposed by Baskes [3], was successfully applied to metals and covalent materials [35,4,55]. The original framework, in which interactions only up to the first nearest neighbor are considered, was improved by Lee et al. [36] to take into account the interactions up to second nearest neighbors. The second nearest neighbor formulation of the MEAM (2NN MEAM) model was then successfully applied to model single elements [30,37,67], binary systems [22,27,31,32], and ternary systems [17]. A number of these potentials were recently used to perform large-scale atomistic simulations to (i) identify the microscopic mechanisms involved during void growth [24], (ii) reveal the nature of the screw $<\mathbf{a}>$ dislocation core structure in Ti [18], (iii) understand the nature of the brittle to ductile transition in the MEAM framework [33], and (iv) identify the mechanism of dislocation bypass in Mg–Al alloys [23,39]. For simplicity, both abbreviations MEAM and 2NN MEAM refer to the second nearest neighbors modified embedded-atom method. The objective of this section is not to recall the theoretical formulation of the MEAM framework, but to introduce the parameters of the model that need to be correlated with experimental or first-principles data.

In the 2NN MEAM, the total energy E of a system of atoms is approximated as the sum of the atomic energies, i.e.

$$E = \sum_i \left(F(\bar{\rho}_i) + \frac{1}{2} \sum_{i \neq j} \Phi(r_{ij}) \right) \tag{1}$$

where $\phi(r_{ij})$ is a pair potential. The embedding function $F(\bar{\rho})$ is taken as

$$F(\bar{\rho}) = AE_c \frac{\bar{\rho}}{\rho_0} \ln\left(\frac{\bar{\rho}}{\rho_0}\right) \tag{2}$$

where A is an adjustable parameter, E_c is the cohesive energy, and ρ_0 is a scaling parameter. Unlike the original embedded-atom method, where the electron density is assumed to be spherically symmetric, MEAM assumes that the background electron density at a specific site is a function of the angle dependent *partial electron densities*,

$$\bar{\rho} = \rho^{(0)} \exp(\Gamma/2) \tag{3}$$

with

$$\Gamma = \sum_{h=1}^{3} t^{(h)} \left[\rho^{(h)}/\rho^{(0)}\right]^2 \tag{4}$$