Vacancy dissociation in body-centered cubic screw dislocation cores

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ABSTRACT

The interaction between screw dislocations and vacancies in body-centered cubic metals is investigated using molecular dynamics simulations. For thirteen different classical interatomic potentials, materials properties relating to vacancies, dislocations, and the interaction between the two are evaluated. The potentials include six for iron, two for molybdenum, and five for tantalum, and they are a mix of embedded atom method (EAM), modified embedded atom method (MEAM), and angular dependent potential (ADP) styles. A previously unknown behavior was identified during the interaction simulations. Out of the thirteen potentials investigated, ten predict a vacancy on the dislocation core to no longer remain as a discrete point defect, but rather to dissociate along the dislocation line. The structure of the dissociation is dependent on the potential and is characterized here. As this vacancy dissociation alters the core structure of the dislocation, it may prove to be a new mechanism for dislocation pinning and pipe diffusion.

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1. Introduction

The mechanical properties of metals are intimately tied to the nature of the dislocations within the material, and how those dislocations interact with other types of defects. In particular, point defects can alter the slip nature of dislocations resulting in softening or hardening of the material, and self-point defects (vacancies and self-interstitial atoms) allow for dislocations with edge components to climb. This interaction is coupled in the sense that the presence of dislocations also alters the diffusion of the point defects. Dislocations can serve as sinks for point defects, and diffusion along dislocation lines is different than in the bulk material (pipe diffusion) [1].

Despite the importance of defect interactions, experimental measurements of behaviors and mechanisms at the relevant scales are limited. Computational tools and models can thus provide insight not easily obtained experimentally. Atomic scale calculations have been used for decades to investigate the structures, motions and interactions of point defects and dislocations. Multiple studies have performed molecular statics calculations of the vacancy formation energy near the dislocation core [2–11]. Maps of the formation energy versus position have been compared to elasticity models [2,5], used to estimate a vacancy trap energy and radius [5,10], and used as the foundation for modeling the

vacancy diffusion pathway in and around the dislocation core using a variety of techniques [7,9,10,12,13]. A hybrid quantum-classical investigation revealed that the core reconstruction influences the interaction energy close to the dislocation core [11]. Density functional theory (DFT) calculations of impurity interstitials in body-centered cubic (bcc) iron revealed that the impurities alter the stable screw dislocation core [14].

The power of classical atomistic simulations is that they allow for the prediction of materials properties and behaviors that require both an atomistic description as well as length and time scales far beyond what can be achieved with quantum-based atomic calculations. The limitation is that their empirical nature means that the predictions obtained can be strongly potential-dependent, especially for behaviors that were not explicitly fit to. This is particularly relevant for the investigation here as, while most metallic potentials are fit with vacancy properties in mind, only a few so far have explicitly considered dislocation behaviors, and none have been fit to produce specific dislocation-vacancy interactions. Because of this, it is necessary to consider the predictions of multiple potentials, and to show how each of those potentials predicts not only the dislocation-vacancy interaction, but also the more basic properties of the isolated defects.

In this paper, we investigate the interaction of the bcc screw dislocation with vacancies using thirteen different classical interatomic potentials. The basic formation energies and structures for the isolated defects are calculated and compared. Static dislocation-vacancy interaction maps are computed showing the

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strength of the dislocation-vacancy interaction as a function of the radial vector from the dislocation core to the vacancy's position. In investigating the size-dependence of the dislocation-vacancy interaction energies on the periodic z-dimension, it was revealed that a number of potentials predict the vacancy to dissociate along the dislocation line. This dissociation is characterized for all of the potentials.

2. Calculation methods

In order to differentiate the various interatomic potentials used here, we follow the convention used on the National Institute of Standards and Technology's Interatomic Potential Repository website. The name for each potential is composed by combining the publication year, first author's last name and initials, and short description of the model. The six potentials of iron used are 1997--Ackland-G-J--Fe [15], 2003--Mendelev-M-I--Fe-2 [16], 2003--Mendelev-M-I--Fe-5 [16], 2004--Zhou-X-W--Fe [17], 2006--Chamati-H--2006--Fe [18], and 2012--Proville-L--Fe [19]. The two potentials of molybdenum used are 2004--Zhou-X-W--Mo [17] and 2012--Park-H--Mo [20]. And, the five potentials of tantalum used are 2003--Li-Y-H--Ta [21], 2004--Zhou-X-W--Ta [17], 2013--Ravelo-R--Ta-1 [22], 2013--Ravelo-R--Ta-2 [22], and 2015--Purja-Pun-G-P--Ta [23]. All of these potentials are embedded atom method (EAM) potentials [24] with the exception of 2012--Park-H--Mo being a modified embedded atom method (MEAM) potential [25] and 2015--Purja-Pun-G-P--Ta being an angular dependent (ADP) potential [26].

Performing the calculations in a high-throughput manner was further supported by the iprPy Python-based framework (source code available at https://github.com/usnistgov/iprPy). This framework was developed as part of the NIST Interatomic Potential Repository project to assist in evaluating and comparing how different interatomic potentials predict a variety of basic materials properties. The atomman Python package (source code available at https://github.com/usnistgov/atomman) was used as a wrapper for the LAMMPS molecular dynamics software [27,28] by preparing atomic systems, constructing LAMMPS input scripts, executing LAMMPS, and performing post-run analysis of the simulation results. Embedding the simulations in Python is advantageous as it creates a complete record of the calculation process which supports sharing the calculation code for verification and knowledge transfer. Additionally, atomman treats LAMMPS potentials as modular entries making it easier to perform the same simulations with multiple potentials.

Lattice and elastic constants were calculated using the refine_structure calculation in iprPy. This routine starts with an initial guess for the lattice constants of a structure. System-wide pressures are evaluated statically using LAMMPS for both the initial system as well as for small strains (1×10^{-5}). The elastic constants of the system are obtained by comparing changes in stress (pressure) to changes in strain, and a new lattice parameter guess is obtained by assuming linear elasticity and extrapolating to the lattice dimensions associated with zero pressure. The calculation then iterates until the lattice parameters converge.

The iprPy calculation point_defect_static was used to compute the vacancy formation energy. Perfect systems are constructed using the refined lattice constant values, then an atom is deleted and the local atomic positions are allowed to relax to a force tolerance of 1×10^{-8} eV/Å. The formation energy is obtained as the change in energy of the system with the addition of the vacancy minus the per-atom cohesive energy of the perfect system. This is repeated for supercells ranging from $3 \times 3 \times 3$ to $10 \times 10 \times 10$, and final values are obtained by plotting the formation energy

versus the inverse number of atoms and extrapolating to infinite atoms.

Dislocations were investigated using dislocation monopole systems. Initially, a perfect bcc block of atoms was constructed with Cartesian axes corresponding to the crystallographic axes of $[[\bar{1}\,2\,\bar{1}], [\bar{1}\,0\,1], [1\,1\,1]]$. The dimensions of the atomic block are $48a\sqrt{6} \times 80a\sqrt{2} \times Z$, where a is the cubic lattice constant and Z varies with different simulations. Z is always a multiple of $2b$, where b is the magnitude of the $a/2[1\,1\,1]$ Burgers vector.

A dislocation parallel to the z-axis was created by adding to the atom positions the displacements associated with the Eshelby anisotropic elasticity solution [29] for a perfectly straight dislocation. The anisotropic elasticity solution was obtained using the Stroh method [30–32] code contained in atomman.

The system is divided into two regions: an active region defined by the volume within a cylinder parallel to the z-axis, and a non-active region defined as the remaining volume of the system. The atoms in the non-active region remain fixed at the positions associated with the anisotropic displacement solution while the atoms in the active region are relaxed using energy minimization. The radius of the active region is defined such that the non-active region is always at least $3a$ thick, i.e. $r_{active} = a(20\sqrt{2} - 3) \approx 25.284a$. The atoms in the active region were relaxed by performing 10,000 Nose-Hoover NVT integrations at 100 K, followed by 1000 NVT integrations with the temperature linearly scaling down to 0.01 K, and finally performing a minimization to a force tolerance of 1×10^{-5} eV/Å.

The Peierls barrier was evaluated using nudged elastic band (NEB) calculations [33,34]. Two dislocation monopole systems with Z thickness of $2b$ are constructed in which the dislocations are one periodic distance apart along the $(\bar{1}\,0\,1)$ slip plane. The NEB calculation identifies the low energy transition pathway between the two initial end states giving the non-kinked slip barrier of the dislocation.

The interaction of the dislocation with a vacancy was examined by performing multiple simulations where a single atom at radial position, **r**, from the dislocation core's xy position was removed from the relaxed dislocation monopole system, and the system was relaxed to a force tolerance of 1×10^{-5} eV/Å. The formation energy of the vacancy near the dislocation core, $E_f(\mathbf{r})$, was then obtained by comparing the energy of the dislocation system before and after the vacancy was added. Finally, the dislocation-vacancy interaction (DVI) energy, E_{DVI}, is taken to be the vacancy formation energy relative to the bulk formation energy, E_f^0,

$$E_{DVI}(\mathbf{r}) = E_f(\mathbf{r}) - E_f^0 \tag{1}$$

3. Results and discussion

3.1. Basic properties

The lattice constants, elastic constants, cohesive energy, vacancy formation energy, dislocation core structure and Peierls barrier shape results are summarized in Table 1. These basic properties of the perfect crystal and the isolated defects of interest all influence how the defects move and interact with each other. The bulk crystal and vacancy property values can be directly compared to experimental measurements.

Across the potentials of the same element we see that the bulk property values tend to be similar, with most differences due to the potentials fitting these values precisely to different reference values. The only unexplained outlier is that the lattice constant for the 2012--Proville-L--Fe potential is noticeably smaller than the other iron potentials. There is more variation across the vacancy