Abstract

With the advent of reliable mathematical models and simulation techniques, a multi-scale modeling approach that spans several length and time scales is a promising approach in investigating and elucidating various crystal properties and phenomena. Dislocation core properties especially their core structure and related properties are integral components and key ingredients in the computational framework employed in exploring such crystal phenomena. Various analytical and computational approaches have been employed to estimate the core structures of line defects and understand their impacts on properties. Nevertheless, a meticulous assessment of the existing body of research uncovers that even in relatively simple systems, the line defects can behave in a peculiar and unfamiliar fashion. The core structures of dislocations contributing to such phenomena have remained unclear. In this dissertation, several such uncharted aspects within dislocation theory are identified and efforts are made to shed light on these unexplored areas. In particular, three specific phenomena have been identified, where the techniques of mathematical modeling and atomistic simulations are shown to render fundamental insights.

To estimate the core structure and related properties of dislocation, elucidate their implications, a systematic workflow is employed involving multiple sophisticated modeling and simulation techniques. These include molecular static and dynamics simulations, kinetic Monte Carlo simulations, atomistically informed continuum models, and optimization techniques such as Bayesian optimization and conjugate gradient. LAMMPS simulator is utilized to carry out atomistic simulations, while OVITO visualization software is used for post-processing. Moreover, this dissertation integrates in-house MATLAB codes tailored to address specific mathematical models pertinent to the research.

The dissertation commences by estimating the core-structure and Peierls stress of twinning dislocations in four fcc metals. The study employs atomistically informed semi-discrete variational Peierls-Nabarro (SVPN) framework in computing these core properties. Besides investigating the conventional route of twinning, the study examines the newly discovered twinning route i.e., alternate-shear mechanism, commonly observed in high stacking fault fcc metals, and maneuvers a method to compute core structure and Peierls stress of twinning dislocations. The work also highlights the importance of incorporating the correction terms into the SVPN model to estimate reliable results and therefore motivate further studies to integrate these inputs in the multi-scale

framework.

The second study elevates the primary investigation to a more complex alloy system, implementing the SVPN framework to estimate the core properties. Nevertheless, the study primarily focuses on critically analyzing the representative-atom methods and emphasizes the applicability and transferability of such potentials in reproducing these properties. In particular, the dissociated dislocations and twinning partials in TWIP steel have been investigated thoroughly employing the framework of the SVPN in conjunction with meta-atom potential. The pioneering work underscores the significance of statistical length scale, which is an inherent feature of the representative-atom method. The proposed critical length scale exceeds the obtained core-widths, consequently impacting the Peierls stress values as well. Therefore, it urges a cautious interpretation of the results obtained through the use of these potentials and might lead to misleading results when used in the multi-scale models.

Unlike the first two segments of investigations, the third study emphasizes the implications of core-structure rather than the core-structure itself. The work considers V-Al alloy system, a potential prospective material in several applications pertinent to hydrogen production and storage. The work highlights the effect of local composition variation due to the Al atom on the core-structure of edge dislocation and further probes the link between the core-structure and pipe diffusion of hydrogen in the alloy. The results from the multi-scale models clearly demonstrate the trapping of hydrogen atom in the edge dislocation due to the solute atoms, thereby decreasing diffusivity. As shown in Chapter 6 of the dissertation, the quantitative influence of alloying on pipe diffusivity is found to be drastically different than on bulk diffusivity. This work attempts to resolve the ambiguity outlined in prior studies concerning the impact of dislocations on hydrogen diffusion in V-Al alloys.

This thesis essentially focus on estimating the dislocation core properties and their implications on various physical effects in crystalline solids, thereby enhancing our knowledge of material properties. Future research directions resulting from this work include extending the work to higher-scale models like the dislocation dynamics simulations, and investigating pipe diffusion in screw dislocation due to local variation of core structure.

Keywords: Atomistic simulations; Peierls-Nabarro model; Dislocation core; Deformation twinning; TWIP steel; meta-atom potential; V-Al alloy; hydrogen diffusion; kinetic Monte Carlo; Nudged elastic band; Bayesian optimization.