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Atomistic Simulation Activities at Sandia
Hydrogen Materials Consortium (H-Mat)

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ABSTRACT- This presentation gives an overview of atomistic simulation efforts at Sandia within the Hydrogen Materials Compatibility consortium (H-Mat). We have been studying three types of structural materials for transportation hydrogen energy applications including low-cost Fe-C ferritic steels, austenitic stainless steels, and aluminum alloys. For Fe-C, we have constructed a Fe-C-H bond order potential that captures both ferrite-austenite-martensite transformations and the cementite structure with the correct interactions with hydrogen. These properties are essential for defining the microstructure of Fe-C steels but are challenging to capture by interatomic potentials. We then use this potential in molecular dynamics and Monte Carlo simulations to study hydrogen populations in various microstructures and hydrogen effects on decohesion energies of various interfaces. For austenitic stainless steels, we have developed an Fe-Ni-Cr-H quaternary embedded atom method potential that captures trends of ferrite-austenite stability, stacking fault energies, and H-metal interaction energies. This advances the field because no quaternary potentials currently exist in the literature and previous Fe-Ni-Cr ternary potentials in the literature do not ensure stable austenite structures. We have used the potential to study dislocation mobility laws in stainless steels, hydrogen effects on stacking fault energy, and slip band intersection mechanisms. For aluminum alloys, we have developed an Al-Cu-H ternary bond order potential that captures aluminum stacking fault energy, and Al_2Cu compound and H_2 gas phases. This also advances the field as no ternary potentials exist in the literature and no binary Al-Cu potentials in the literature capture the Al_2Cu compound phases effectively. We also demonstrated that time-averaged molecular dynamics can be used to calculate converged hydrogen Cottrell atmosphere around dislocations. This is significant as Cottrell atmosphere formation has never been studied in detail before with full atomistic resolution, enabling direct evaluation of theoretical predictions of atmosphere strengthening and solute drag. Many results of our simulations have begun to reveal phenomena seen in experiments. We will discuss details on how these results may help explain experimental observations.

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