An atomistic thermo-chemo-mechanical coupled model: Hydrogen storage in Mg nanowires

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Abstract

Understanding the transport of hydrogen within metallic nanomaterials is crucial for the advancement of energy storage and the mitigation of hydrogen embrittlement. Using nano-sized magnesium particles as a model, recent studies have revealed several highly nonlinear phenomena that occur over long time periods. The time scale of these phenomena is beyond the capability of established atomistic models such as molecular dynamics. In this work, we present a new approach, referred to as diffusive molecular dynamics (DMD), to the simulation of long-term diffusive mass transport at the atomic scale. The basic assumption underlying DMD is that the time scale of diffusion is much larger than that of microscopic state transitions. In terms of numerical implementation, our approach involves the numerical integration of the master equation, and the numerical solution of a highly nonlinear optimization problem at every time-step. By working with atomic fractions, the characteristic time-step size of our DMD simulations can be much larger than those based on either AMD or KMC methods. In the present work, we focus on the characterization of thermodynamic and kinetic properties of magnesium hydride nanoparticles. Modeling phase transitions of Mg/MgH2 systems introduce an additional difficulty due to the change of lattice structure. We also note that the scope of DMD is not limited to metal hydrides and a broad range of multi-species systems of practical interest suggest themselves as worthwhile foci for future studies.

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