A Novel Deformation-Diffusion Coupled Computational Model for Hydrogen Diffusion in Nanomaterials

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ABSTRACT

Physics-based modelling and predictive simulation of hydrogen diffusion in solid nanomaterials has been a focal area of research, with important engineering applications including hydrogen embrittlement and hydrogen storage. This problem is characterized by an atomic deformation-diffusion process on a length scale of Angstroms and a time scale of femtoseconds. However, the properties and behaviors of interest in real-world applications are usually characterized by a relatively slow evolution on the scale of seconds to hours. This scale is beyond the time window of conventional atomistic computational models such as molecular dynamics (MD) and transition state theory based accelerated MD. The vast disparity of time scale poses a formidable challenge in theoretical and computational material science.

In this talk, we will present a novel, deformation-diffusion coupled computational model based on the non-equilibrium statistical mechanics proposed in Ref. [1], which allows long-term simulation of hydrogen absorption and desorption at atomic scale. Specifically, we will present a carefully designed trial Hamiltonian in order to construct our meanfield based approximation, then apply it to investigate the palladium-hydrogen (Pd-H) system. We combine this meanfield model with an experimentally calibrated empirical discrete kinetic model. This combination in practice defines the evolution of H atomic fractions and lattice constants, which facilitates the characterization of the deformation-diffusion process of H over both space and time. We will present a partitioned numerical algorithm that couples the meanfield statistical mechanics and the discrete kinetics. This work is an extension of Refs. [2] and [3] to deformation-diffusion coupled analysis. Using an embedded atom method (EAM), we validate our model by comparison with the results from experiments and analytic solutions in both equilibrium and dynamic cases. Then we predict the deformation-diffusion coupled features of H diffusion in both perfect and defective Pd nanocubes.

REFERENCES

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