Hydrogen storage in Palladium nanoparticles

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ABSTRACT

Understanding the transport of hydrogen within metals is crucial for the advancement of energy storage and the mitigation of hydrogen embrittlement. Using palladium nanoparticles as a model, recent experimental studies have revealed several highly nonlinear phenomena that occur over a long period of time (up to hours), including avalanching strain dynamics, phase boundary propagation and lattice misorientation during phase transformation. The time scale of these phenomena is beyond the capability of established atomistic models e.g., transition state theory based accelerated molecular dynamics. In this talk, we present the application of a new model, referred to as diffusive molecular dynamics [1, 2], to simulating long-term diffusive mass transport at atomistic length scale. Specifically, we present several large-scale simulations of hydrogen diffusion in perfect and defective palladium nanoparticles, which are designed to capture the mechanisms of both hydrogen diffusion and lattice deformation. We show that when the ambient hydrogen pressure is sufficiently high, the palladium-hydrogen reaction features the nucleation of a new phase at the corners of the nanoparticle, and hydrogen diffuses inwards in the form of phase boundary propagation. During phase transformation, there is large lattice deformation on the phase boundary, and the time history of the new phase fraction follows a characteristic sigmoidal profile. Moreover, we investigate how crystal defects affect hydrogen absorption process.

REFERENCES

[1] X. Sun, M.P. Ariza, M. Ortiz, K. Wang, Journal of the Mechanics and Physics of Solids, 125: 360-383, 2019.

[2] G. Venturini, K. Wang, I. Romero, M.P. Ariza, M. Ortiz, Journal of the Mechanics and Physics of Solids, 73: 242-268, 2014.