Atomistic Simulation of Hydrogen Diffusion in Titanium.

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Summary

Study of the behavior of hydrogen in metals and alloys. The study is based on classical molecular dynamics (MD) and density functional theory (DFT) calculations.

Study of the behavior of hydrogen in metals and alloys is of great importance due to the practical uses of hydrogen-metal systems for absorption of nuclear radiation, in neutron sources, for storage of hydrogen, or as catalyzers. This work is devoted to atomistic simulation of hydrogen diffusion in titanium hydrides and the effect of stresses and lattice defects on diffusivity.

The study is based on classical molecular dynamics (MD) and density functional theory (DFT) calculations. LAMMPS [1] is involved for molecular dynamics simulations and VASP [2, 3] as a density-functional code.

The energies of hydrogen at different sites in hcp, bcc and fcc titanium are calculated within DFT approach. The results indicate that a single hydrogen in hcp Ti has a lowest energy in the octahedral position and then, with a small difference, in tetrahedral. Estimated vibration frequencies of hydrogen in different structures can be identified in the experimental data from inelastic neutron scattering [4]. Taking into account the assignment thus made one can conclude that both octahedral and tetrahedral sites are occupied in hcp Ti at 600 K.

In a classical molecular dynamics interatomic interactions in titanium are described within embedded atom method approach. Hydrogen-metal potential is produced by means of force matching method, taking into account stability of basic Ti-H crystalline structures (calculated within DFT approach). The applicability of different potentials for the description of hydrogen-metal systems is discussed. Diffusion coefficients of hydrogen are estimated from the simulations for different temperatures and hydrogen concentrations in titanium and titanium hydrides. Corresponding migration energies are evaluated and compared with estimates from DFT and experimental data. The structure of radiation defects in titanium-hydrogen system is obtained from the MD simulations of ion irradiation within primary knocked atom approach. The influence of the radiation defects on hydrogen diffusivity is estimated.

[1] S. J. Plimpton, “Fast Parallel Algorithms for Short-Range Molecular Dynamics,” *J Comp Phys*, **117**, 1–19 (1995).

[2] G. Kresse and J. Hafner, *Phys. Rev*. **B 4**7, 558(R) (1993).

[3] G. Kresse and J. Furthmuller, *Phys. Rev*. **B 54**, 11169 (1996).

[4] R. Hempelmann, D. Richter, and B. Stritzker, *J. Phys. F: Met. Phys*. **12**, 79 (1982).