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Atomistic Modelling of Desorption of Hydrogen isotopes from Tungsten Surface and Diffusion in Cu and Fe Metal
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Abstract

Atomistic understanding about the interactions of H, D and T with tungsten (W) is of importance in nuclear fusion where deuterium (D) and tritium (T) is used as fuel. The dissociation and desorption kinetics of H isotopes on W(100) were carried out by evaluating energy barriers using DFT followed by HTST. The rate constants for adsorption and desorption of hydrogen isotopic molecules were evaluated using HTST. The rate constant for reassociation of H2 from W surface was calculated to be much slower than the rate of dissociation of H2 molecule from W(100) surface. The desorption rate of heavier T is slower than that of D and H in the case of W surface. Further, fracture energy of W surface with increase in the coverage of H is evaluated to account for hydrogen embrittlement.
Copper (Cu) and Cu alloys are considered to be the most promising candidates for heat sink materials (HSM) in fusion reactors because of high thermal conductivity, mechanical strength and good radiation resistance. Hydrogen isotopes can substantially influence the microstructure and mechanical properties of Cu, and limit the lifetime of Cu–HSM. It will be worthwhile to understand the interaction of H isotopes with Cu using DFT. Here, the interaction and dynamical behaviours of hydrogen isotopes in fcc Cu have been studied employing plane wave based DFT. Nudge elastic band methods have been used to determine the activation energy barrier whereas phonon calculations are performed to investigate the isotope effects. The dissociation pathway for H2 isotopic molecules on Cu(100) surface was established on bridge and hollow positions using DFT. The bridge path has lower barrier energy for dissociation and reassociation for H2 isotopes compared to hollow path. The adsorption of H isotopes on bridge position is found to be stable compared to top and hollow position in the case of Cu(100) surface. Further, the hydrogen isotope absorption in the tetrahedral interstitial void is found to be less stable than octahedral void of bulk Cu. In addition, the surface to subsurface diffusion (absorption of hydrogen isotopes on surface) of H isotopes was established on Cu(100) surface. Further, the activation barriers for the diffusion of H from octahedral (o) to nearby tetrahedral (t) site, t- to nearby t-site, and o- to o-site were evaluated using NEB method. From the energy barriers, it is evident that the diffusion of H through o-o site happens via t-site. The diffusion, permeability and solubility values were predicted for H isotopes in Cu and compared with available experimental values.
Additionally, the diffusion of H atom in bulk bcc Fe was determined using embedded atom model (EAM) potential and corroborated with experimental results.

References
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