Contribution ID: **27** Type: **not specified**

DFT Studies on Diffusion and Permeation of Hydrogen Isotopes in Iron (Fe) and Tungsten (W)

Monday, 23 November 2020 15:20 (20 minutes)

The fundamental understanding of H isotopes behaviour in metallic systems vis-a-vis its adsorption, absorption, diffusion and permeation is of great technological importance. This will help in controlling the hydrogen induced embrittlement and also very helpful in the selection of structural materials for reactors with minimum permeability of these gases. Steels with 9–12 wt% Cr are considered as potential structural materials in nuclear power and fusion reactors having hydrogen diffusion coefficients one order of magnitude lower than those of pure Fe. Further, Tungsten (W) has shown promise to be the most favored plasma withstanding material in nuclear fusion with deuterium (D) and tritium (T) as fuel. In order to identify a better material, atomistic understanding of the behavior of D/T with W is highly desirable. In view of that, plane wave based density functional theoretical calculations were conducted to investigate the interaction and dynamical behaviours of hydrogen isotopes in pure bcc Fe and W systems. The adsorption and dissociation pathways for hydrogen isotopes were predicted on both Fe(100) and W(100) surfaces. Further, the activation barrier energy for H atom to diffuse from one interstitial void to nearest interstitial void has been computed using nudge elastic band (NEB) method. Zero point energy was incorporated using phonon calculations to capture the isotope effects. The most favourable diffusion path of H atom was observed from one tetrahedral site to the nearest tetrahedral site in both Fe and W systems. The calculated diffusion coefficients, rate constants, permeability constants and solubility are found to be higher for H compared to its heavier isotopes D and T for W system. The calculated diffusion coefficients and permeability constants are found to be higher for lighter H compared to heavier D and T. In addition, the effect of vacancy is also studied. Further, the diffusion and permeability coefficients of H, D and T are found to be increased with increase in the temperature, which is of first of its kind prediction from DFT studies. Further, the calculated diffusion coefficients are shown to be two order of magnitude lower than Fe and thus might be the basis for considering W as plasma facing materials. The findings will be useful in modeling the behavior of tritium in Fe and W metals for which data is either scattered or least available.

1. A. Boda, Sk. M. Ali, K. T. Shenoy, S. Mohan, Adsorption, Absorption, Diffusion and Permeation of Hydrogen and Its Isotopes in bcc Bulk Fe and Fe(100) Surface: Plane Wave based Density Functional Theoretical Investigations, J. Phys. Chem. C 2019, 123, 23951-23966.
2. A. Boda and Sk. M. Ali, K. T. Shenoy, S. Mohan, Diffusion, Permeation and Solubility of Hydrogen, Deuterium and Tritium in Crystalline Tungsten: First principles DFT Simulations, Int. J. Hydrogen Energy, 2020, 45, 29095-29109.

`Future Work Plan (2021-2022)`

A. Recombination of H and its isotopes to form diatomic molecules at the surface of the collector side (Fe and W surface)
- Energy barrier for recombination of H atom using nudge elastic band (NEB) method and DFT
- Kinetics (rate constant) of recombination using TST(transition state theory) and DFT
- Effect of H coverage on the recombination and kinetics using NEB, TST and DFT
- Desorption of molecular hydrogen from the surface using NEB and DFT

B. Dissociation, adsorption, diffusion and permeation of H isotopes through bulk and surface Cr.
- Dissociation pathway of H2 molecule on the Cr surface using DFT
- Absorption H isotopes in surface and bulk Cr using DFT
- Diffusion and permeation of H isotopes through bulk and surface Cr using NEB, TST and DFT

Primary author: Dr ALI, Musharaf (Bhabha Atomic Research Centre)

Co-authors: Dr BODA, Anil (Bhabha Atomic Research Centre); Mr SHENOY, KT (Bhabha Atomic Research Centre)

Presenter: Dr ALI, Musharaf (Bhabha Atomic Research Centre)

Session Classification: Atomistic modelling II