Contribution ID: **73** Type: **not specified**

Permeation and Solubility of Hydrogen Isotopes in Chromium (Cr) and Iron (Fe) Metal: Ab-initio Theoretical Studies

Tuesday, 5 October 2021 10:00 (30 minutes)

Steel, a widely used structural stuff contains iron and chromium as important elements. It is of fundamental as well as technological importance to understand the behaviour of hydrogen isotopes with Fe and Cr metal to derive an appropriate material for arresting the permeation of H isotopes through metal structure. As such the interaction and dynamical behaviours of hydrogen isotopes in bcc Cr lattice have been studied employing projector augmented wave function enabled DFT with dispersion correction. Nudge elastic band method was applied to evaluate the energy barrier. The frozen phonon calculations were performed to calculate the zero point energy and isotope effects. The dissociative surface adsorption of hydrogen was predicted to be exothermic, whereas surface to sub-surface and bulk absorption was found to be endothermic but the vacancy induced absorption energy for H atom in bulk Cr was found to be exothermic. The diffusion of H atom from one tetrahedral to the adjacent tetrahedral hole was established to be the most preferred jump mode. The permeability coefficients, solubility and rate constants follow the order: H>D>T. The computed values of permeability and solubility of H in Cr was in reasonable agreement with the experimental results. Further, the temperature-dependent diffusion of interstitial H, D, and T in pure Fe were computed using transition state theory. The temperature effect was incorporated by considering thermal expansion of lattice. The coefficient of thermal expansion, free energy of activation and jump factor for diffusion were obtained from activation energy and phonon calculations. The experimentally observed higher diffusion of hydrogen at low temperature compared to high temperature can plausibly be explained by Wigner+hTST analysis with temperature correction. Further, surface fracture energy of Fe metal with increased hydrogen coverage was evaluated using ab-initio surface energy in conjunction with Born-Haber thermodynamic cycle to account for hydrogen embrittlement. The present topic will cover our recent ab initio findings on permeation and solubility of hydrogen isotopes in metal relevant to fusion reactor.

1. A. Boda, S. Bajania, Sk. Musharaf Ali, K. T. Shenoy, S. Mohan, Chemisorption, Diffusion and Permeation of Hydrogen Isotopes in bcc Bulk Cr and Cr(100) Surface: First-Principles DFT Simulations, J. Nu. Materials, 2021, 543, 152538.
2. A. Boda, Sk. Musharaf Ali, Abinitio studies on permeation and solubility of hydrogen isotopes in Iron (Fe), Tungsten (W) and Chromium (Cr), 20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods " International Centre for Theoretical Physics, February, Trieste, Italy, 23-25, 2021.

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Session Classification: Atomistic Modelling