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Density Functional Theoretical Simulation of Hydrogen Behaviour in Fe-Cr Binary System: Impact of Chromium Content

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Abinitio atomistic modeling nowadays is used to simulate hydrogen diffusion, permeation, and interactions with Fe-Cr alloys, providing critical insights into material behavior and embrittlement mechanisms. Thus, the interaction and dynamical behaviours of hydrogen isotopes in bcc Fe-Cr lattice have been studied employing plane wave based density functional theory. The lattice volume and cohesive energy are calculated with variation in the Cr content of bulk Fe. A positive and negative deviations are obtained with variation in the Cr content in the case of lattice volume compared to the values of Vegard's law of mixing of solid solutions.

Nudge elastic band methods have been used to determine the activation energy barrier and phonon calculations are performed to investigate the isotope effects. The absorption energy is calculated for H in tetrahedral void with variation in the Cr content of bulk Fe. An increase in the endothermicity is obtained with increase in the Cr content. Further, the effect of Cr content on the diffusion, permeation and solubility of H in Fe-Cr system was studied. From the calculated values it is observed that the diffusion and permeation values found to be decreased with increase in the Cr content as per the experimental observation. The effect of isotopes on the diffusion, permeation and solubility of H isotopes in Fe-Cr system was studied. From the calculated values it is observed that the diffusion and permeation are higher for lighter isotope H compared to D and T. This observation is in line with the experimental observation.

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