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Energetic, Crystallographic and Diffusion Characteristics of Hydrogen Isotopes in Iron

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Energetic and crystallographic characteristics of various interstitial configurations of H atoms and their complexes with self-point defects (SIA –self-interstitial atom, vacancy) in bcc Fe have been calculated by molecular statics using Fe-H interatomic interaction potential developed by A. Ramasubramaniam et al. (Phys. Rev. B 79 (2009) 174101) and modified here and Fe-Fe matrix potential M07 developed by L. Malerba et al. (J. Nucl. Mater. 406 (2010) 19).
The most energetically favorable configuration of an interstitial H atom is tetrahedral configuration. The height of the energy barrier for H atom migration is 0.04 eV. H atom in the substitution position is unstable and shifts in the direction of the nearest octopore during the relaxation process staying at a distance of 0.024 nm from it. The resulting configuration has the highest binding energy of all the considered complexes "vacancy –H atom"(0.54 eV). The energy barriers for the jump of H atom from a vacancy to the nearest tetrapore and back are 0.47 eV and 0.05 eV, respectively. The binding energy of the most energetically favorable configuration of the considered complexes "SIA –H atom"equals 0.15 eV. The interaction energy of H atom with a SIA decreases with distance slower than in the case of interaction with a vacancy. The binding energy of H atom with an edge dislocation in <100>{001} slip system is 0.49 eV.
The binding energies of complexes "vacancy –n H atoms"(n = 1, ..., 15) have been calculated. The binding energy of H atom with the complex decreases from 0.54 eV to 0.35 eV with increasing of n from 1 to 6. The value of binding energy decreases sharply to ~0.1 eV at n > 6. One vacancy can contain up to 6 H atoms. Adding of the seventh H atom leads to the expulsion of one of the other six H atoms from the vacancy.
The temperature dependences of hydrogen isotopes diffusivities (D^H, D^D, D^T) in Fe have been calculated for the temperature range 70 –1100 K using molecular dynamics. The temperature dependencies of D^H, D^D, D^T have a parabolic form at temperatures higher than 300 K. The values of D^H, D^D, D^T are almost the same at 300 K. The isotope effect becomes stronger at higher temperature, e.g., ratios D^H/D^D and D^H/D^T at 1100 K equal 1.2 and 1.3, respectively.

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