Diffusion of a single H atom in the tungsten bulk

Sabine Morisset[1,2], Alain Allouche[2]

[1]*Laboratoire de Physique des Interactions Ioniques et Moléculaires CNRS/ Université Aix-Marseille, UMR 7345, Marseille, France*
[2]*Institut des Sciences Moléculaires d'Orsay, CNRS/ Université Paris-Sud, UMR 8214, Orsay, France*
sabine.morisset@u-psud.fr

The study of the diffusion of the H atom in the tungsten (W) bulk is particularly interesting for thermonuclear fusion. Thermonuclear fusion aims to produce energy through the interaction between deuterium (D) and tritium (T) atoms. The interaction of the (D/T) plasma with the walls of a thermonuclear reactor induces retention and diffusion of hydrogen isotopes in the walls. In the case of the future reactor ITER (International Thermonuclear Experimental Reactor), the retention of H and particularly T will cause safety problems.

In this work, the dynamics of H atom diffusion in the W bulk is studied in the sudden approximation where the vibrational period of W atoms is smaller than the diffusion time: the W atoms have no time to follow the motion of the H atom. In this approximation, the interaction potential and the diffusion barrier of the H atom in W are calculated using the Density Functional Theory (DFT). Two interstitials diffusion sites are found: the tetrahedral and the octahedral sites. The diffusion coefficient is calculated as a function of the H atom energy using a time dependant dynamics method: the wavepacket propagation method. In the sudden approximation, two cases are considered: the adiabatic approximation where two degrees of freedom are taken into account (2D), and the case where the H atom can freely move in the W bulk (3D). Our results show that at small energies the H atom can diffuse by tunnel effect. Moreover at high energies the adiabatic approximation reproduces the same behavior as the 3D case. Our results are also compared to previous theoretical works [1,2] based on the transition state theory. This statistical method only takes into account the minimal diffusion barrier between consecutive tetrahedral sites, neglecting octahedral sites. Our dynamics calculations show that H atom diffusion through octahedral sites is not negligible.

References:

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