Molecular dynamics simulations on behavior of hydrogen isotopes interacting with vacancy-type defect clusters in bcc-Fe

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Long-term tritium retention would determine with the wall lifetime the future steady-state reactors availability. Requirements related to tritium retention are causing a shift from carbon-based materials to high Z metal-based materials. Among candidates materials for plasma-facing components, tungsten based ones are thought to be promising due to their good thermal properties and low sputtering rate. However, knowledge on tritium retention in tungsten is still limited.

Hydrogen isotope retention in tungsten is related to trapping phenomena in vacancies. Previous studies based on ab-initio calculations gave a highlight to hydrogen segregation mechanisms at the vicinity of a monovacancy in structures of bcc-iron [1] and tungsten [2] and potential accumulation patterns in the case of vacancy clusterization. The computing limitations in terms of simulation duration time and box size of density-functional theory (DFT) calculations encourage the shift to a molecular dynamics based investigation for the behavior of clusters of hydrogen-vacancy complex in such structures. As a preliminary step, this behavior was studied in α-iron, which like tungsten, is a bcc metal and has a negative solution energy of hydrogen, with a recently developed set of interatomic potentials based on DFT calculations [3]. The solution energy and diffusion barrier of hydrogen isotopes existing in defect-free systems were evaluated. The results obtained were compared to those previously obtained from DFT calculations in order to assess the reliability and the limitations of the potential used for the study. Subsequently, interaction energies between hydrogen atoms and vacancy clusters were calculated as a function of the number of vacancies contained in a cluster. The probable vacancy cluster configurations were investigated in order to verify the extrapolations derived from DFT calculations [1].

[1] Tateyama Y., Ohno T., Phys. rev. B67, 174105, 2003
[2] Liu Y.L. et al., Phys. Rev. B79, 172103, 2009
[3] Ramasubramianiam A., Itakura M., Carter. E.A., Phys. rev. B79, 174101, 2009