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A density functional theory assessment of the clustering and migrating behaviour of He and H in tungsten

C. Domain and C.S. Becquart
LMPGM - Laboratoire de Métallurgie Physique et Génie des Matériaux, Université de Lille, UMR 8517, F-59655 Villeneuve d’Asq Cedex, France

In the near surface of plasma facing materials, high concentrations of hydrogen, hydrogen isotopes and helium can build up, which will interact with the point defects resulting from the bombardment of the surface as well as with the impurities of the materials. These interactions will induce changes in the microstructure and thus in the mechanical properties. Tungsten, because of its high melting temperature, high thermal conductivity and low sputtering erosion, is now a promising candidate for the divertor plate in ITER. We have used density functional theory based ab initio calculations and the VASP code to determine the interactions of He and H with vacancies and vacancy clusters in W. Despite the fact that for both elements the most stable site in interstitial configuration is the same: the tetrahedral site, their diffusion properties or their tendency to form clusters are completely different. The interactions of He and H in interstitial position to form clusters will be compared as well as their interactions with self interstitial W atoms. These results will be discussed in the light of experimental data.

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