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タングステン中の水素・ヘリウム共存系に対する第一原理シミュレーション

First principles investigations on tungsten containing hydrogen and helium

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Tungsten is a promising element for the plasma facing material in a thermonuclear fusion reactor. Thus, enthusiastic investigations have been performed experimentally, theoretically, and computationally. It is reported that tungsten is damaged by helium irradiation and is occasionally cracked. A bubble structure called 'helium bubble' is observed in helium irradiated tungsten. Bubble itself or agglomeration of bubbles could cause cracking. Since the crack of tungsten material becomes essential issue for the use in the reactor, many tests of helium irradiation have been performed. Moreover, it was experimentally found that helium irradiation generates fuzzy structure in/on tungsten surfaces via helium bubble under the specific conditions of surface temperature, fluence, and irradiation energy [1, 2]. The fuzzy structure contains a potential for functional nanomaterial beyond the nuclear fusion research field.

Although the condition to generate bubble and fuzzy structures by helium irradiation was made clear experimentally, their formation mechanisms are not clarified. One expectation from experiments is that a key process of bubble structure creation is trap phenomenon of helium atoms into thermal vacancy of tungsten lattice structure. It, however, is found that helium atoms can be easily trapped not only within thermal vacancy but also in interstitial locations of pure tungsten crystal structure from our preliminary simulations. On the other hand, it is known that hydrogen atoms can hardly be contained in the pure tungsten crystal.

In order to clarify formation mechanisms of bubble and fuzzy structures, it is important to evaluate binding energies of helium atom(s) and hydrogen atom(s) in tungsten material. Thus we have investigated them using first principle calculation based on density functional theory (DFT) [3]. In this paper, helium atom(s) and/or hydrogen atoms(s) trapped in pure tungsten crystal of bcc structure are targeted. Binding energies of various configurations with tungsten containing both hydrogen and helium atoms obtained by first principles calculations will be given. Detailed discussion including statistical treatment, which involves finite temperature effect, will be also given.

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