§10. First Principles Investigation of Cluster Consisting of Hydrogen and Helium Atoms Interstitially-trapped in Tungsten

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The binding energies of mixed helium and hydrogen clusters consisted of interstitially trapped atoms in body-centered-cubic (bcc) tungsten lattice are evaluated by first-principles calculations based on density functional theories[1, 2]. Calculations are carried out on the HELIOS supercomputer system at Computational Simulation Centre of International Fusion Energy Research Centre (IFERC-CSC), Aomori, Japan, under the Broader Approach collaboration between Euratom and Japan, implemented by Fusion for Energy and JAEA and partly on the Plasma Simulator at the National Institute for Fusion Science with the 'OpenMX' code package, which is designed for nano-scale material simulations based on density functional theories (DFT) and developed by Dr. Ozaki at Japan Advanced Institute of Science and Technology[3].

The 'OpenMX' uses numerical pseudo-atomic orbitals (PAOs) as basis function to expand one-particle Kohn-Sham wave functions. The generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional is used for the exchange-correlation potential. Linear combinations of pseudo-atomic localized orbitals, norm-conserving pseudo-potentials, and projector expansions are employed for core Coulomb potential. Bcc W supercells composed of 128 tungsten atoms ($4 \times 4 \times 4$ unit cells) containing interstitial hydrogen / helium atom(s) and the Brillouin zones with $4 \times 4 \times 4$ **k**-points for sampling using the Monkhorst-Pack method are used. The equilibrium lattice parameter for the present parameter set is 3.186 Å, although this value is slightly larger than that in the literature, 3.165 Å(at 298 K). All the calculations are carried out at constant volume with the atomic positions in the supercells fully relaxed with use of the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method. The final state with the lowest total energy for each sample having the same number of hydrogen and helium atoms is regarded as the most stable state. The configurations obtained by the above mentioned method are used for the calculation of binding energy. It should be noted that in order to search for most probable configurations efficiently, not only the initial positions of interstitially trapped atoms, that is helium and / or hydrogen, but also ones of tungsten atoms are randomized.

In this study, total energies are calculated for a bcc supercell composed of 128 tungsten atoms ($4 \times 4 \times 4 \times 2$) $E[\mathrm{W}_{128}]$ and supercells with m-hydrogen and n-helium atoms interstitially-trapped in tungsten $E[\mathrm{W}_{128}\mathrm{H}_m\mathrm{He}_n]$.

Figures 1 depicts the binding energies $E^{\mathrm{bin}}[\mathrm{He}_m\mathrm{H}_{n-1}, \mathrm{H}]$ evaluated in this study as a function of the number of hydrogen atoms interstitially-trapped in tungsten. Here $E^{\mathrm{bin}}[A, B]$ is given by $E[\mathrm{W}_{128}A] + E[\mathrm{W}_{128}B] - E[\mathrm{W}_{128}AB] - E[\mathrm{W}_{128}]$.

This shows that interstitially trapped helium-hydrogen cluster can be formed even though interstitially trapped hydrogen atoms prefer not to gather. It is pointed out that helium atoms are relaxed at tetrahedral sites and align on a plane having high symmetrical structure. Since this configuration has large low electron-density regions, it is expected that hydrogen as well as helium can be interstitially trapped at a tetrahedral site near the cluster and the cluster becomes larger. As mentioned above, helium-rich interstitially-trapped cluster can act as a trapping site for hydrogen, which implies that helium interrupts or disturbs the hydrogen diffusion in tungsten. This result supports the discussion in the experimental report[4] where it is suggested that He bubble layer greatly reduces hydrogen penetration and this is a reason of simultaneous irradiation effects of He on tungsten blistering with hydrogen irradiation.

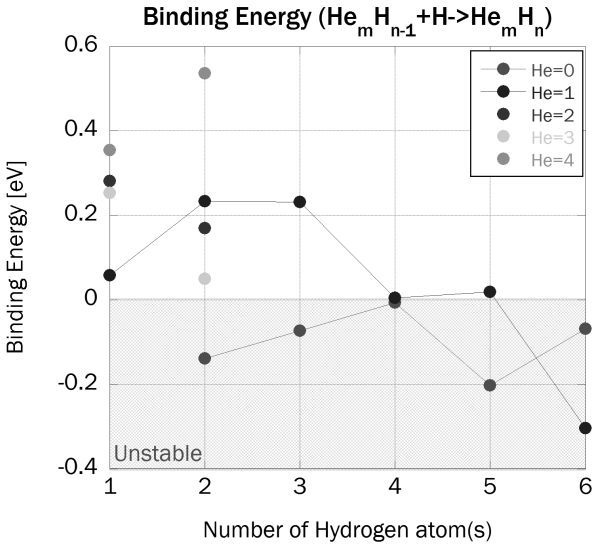

Fig. 1: Binding energies for aggregation of hydrogen atoms interstitially trapped in tungsten with helium: $\mathrm{He}_m\ \mathrm{H}_{(n-1)}$+H $\rightarrow \mathrm{He}_m\ \mathrm{H}_n$.

1) Takayama, A., Ito, A. M. et al.: Jpn. J. Appl. Phys., 52 (2013) 01AL03.

2) Takayama, A., Ito, A. M. et al.: *"First principles investigation of cluster consisting of hydrogen-helium atoms interstitially-trapped in tungsten"*, J. Nucl. Mater., in press.

3) http://www.openmx-square.org/

4) Ueda, Y. et al.: J. Nucl. Mater., 386-388 (2009) 725.