§18. First-principles Investigations of Hydrogen-helium Atoms Interstitially-trapped in Tungsten

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First-principles calculations of the binding energies[1] of hydrogen-helium atoms interstitially-trapped in tungsten are carried out 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[2].

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 exchange-correlation potential and norm-conserving pseudo-potentials and pseudo-atomic localized basis functions are employed for core Coulomb potential. The Brillouin zone with $4 \times 4 \times 4$ **k**-points sampling using the Monkhorst-Pack method is employed.

In this study, total energies are calculated for a body-cubic-center (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 $E[\mathrm{W}_{128}\mathrm{H}_m\mathrm{He}_n]$.

The lattice constant is obtained by minimizing the cohesive energy E_c, and is 3.186 Å in the present calculation parameter set. We employ a lattice constant of 3.186 Å for present calculations, although this value is slightly large than that in the literature, 3.165 Å (at 298K).

Iterative calculations of self-consistent field (SCF) convergence and molecular dynamics (MD) according to the resulting force are performed, and a relaxation state is obtained. For the geometry optimization, the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method is employed. 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.

Solution energies of hydrogen and helium against tungsten are evaluated as -1.46 eV and 6.17 eV, respectively. This means that hydrogen is fusible in tungsten, meanwhile helium is hardly-soluble.

Figures 1 and 2 depict the total binding energies E_B evaluated in this study as a function of the number of helium and hydrogen atoms interstitially-trapped in tungsten, respectively. It is inferred from these figures that interstitially-trapped helium atoms have a tendency to gather in tungsten once they are trapped. On the other hand, though hydrogen is easy to solve in tungsten, interstitially-trapped hydrogen hardly form a cluster. They, however, can gather in tungsten with the help of interstitially-trapped helium. This result indicates that diffusion of helium in tungsten can be disturbed and that hydrogen retention in tungsten may be enhanced.

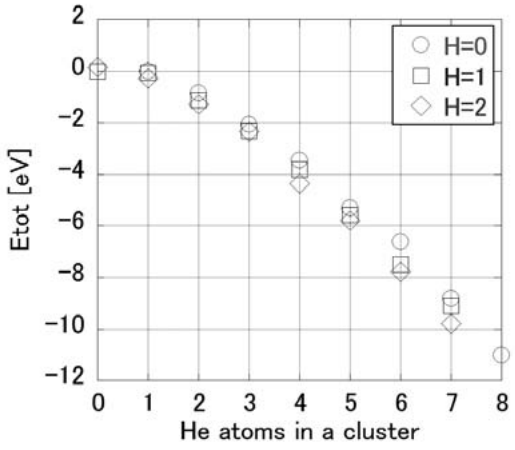

Fig. 1: Total binding energy as a function of the number of interstitially-trapped He atom.

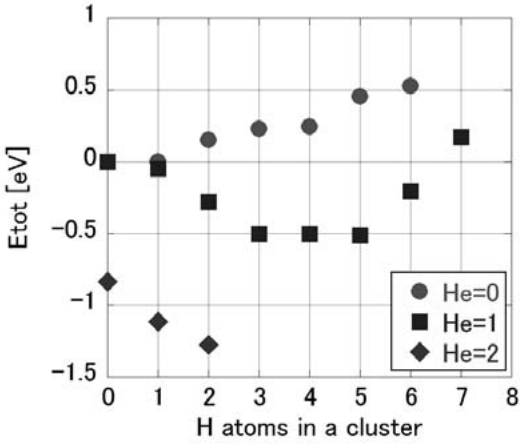

Fig. 2: Total binding energy as a function of the number of interstitially-trapped H atom.

1) A. Takayama, A. M. Ito, et al., *"First-principles Investigation on Trapping on Multiple Helium Atoms within a Tungsten Monovacancy"*, Jpn. J. Appl. Phys., (2013) vol. 52, 01AL03.

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