§11. First Principles Investigation on Trapping of Multiple Helium Atoms within a Tungsten Mono-vacancy

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First-principles calculations of the binding energies between helium atoms and mono-vacancies of tungsten are performed with the 'OpenMX' code package, which is designed for nano-scale material simulations based on density functional theories (DFT). 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.

Total energies are calculated for a body-cubic-center (bcc) supercell composed of 54 tungsten atoms ($3 \times 3 \times 3 \times 2$) $E[\mathrm{W}_{54}]$, a supercell of 53 atoms with mono-vacancy $E[\mathrm{W}_{53}\mathrm{V}_1]$, and supercells with n helium atoms trapped within the mono-vacancy $E[\mathrm{W}_{53}\mathrm{V}_1\mathrm{He}_n]$. The Brillouin zone with $6\times6\times6$ **k**-points sampling using the Monkhorst-Pack method is employed.

The 'OpenMX' uses numerical pseudo-atomic orbitals (PAOs) as basis function to expand one-particle Kohn-Sham wave functions. We employ the 2 s-state, 2 p-state, 1 d-state, and 1 f-state radial functions with cut-off radius of 8.0 a.u. for tungsten, and the 2 s-state, 1 p-state, and 1 d-state radial functions with cut-off radius of 6.0 a.u. for helium.

Cohesive energy E_c of tungsten is estimated by

$$E_\mathrm{c} = E(\mathrm{W}) - E(\mathrm{W}_{54})/54, \qquad (1)$$

where $E(\mathrm{W})$ is the energy of isolated tungsten atom. The lattice constant is obtained by minimizing E_c, and is 3.220 Å in the present calculation parameter set. We employ lattice constant of 3.220 Å for present calculations, although this value is rather large compared to a literature data, 3.165 Å (at 298K). In this case, E_c of 8.92 eV is obtained, which is comparable to an experimental observation. Parameters used for present calculations are summarized in the table I.

Binding energies of helium atoms trapped within the mono-vacancy are given by

$$E_\mathrm{B}^{n\leftarrow(n-1)} = E[\mathrm{W}_{53}\mathrm{V}_1\mathrm{He}_{n-1}] + E[\mathrm{W}_{54}\mathrm{He}_1] - E[\mathrm{W}_{53}\mathrm{V}_1\mathrm{He}_n] - E[\mathrm{W}_{54}], \qquad (2)$$

where $E[\textit{configuration}]$ is a total energy of the given configuration.

In order to search stable configurations with single and multiple helium atoms trapped in a mono-vacancy, samples consisted of octahedral-site (O-site) or tetrahedral-site (T-site) helium atom(s) and mono-vacancy tungsten are prepared. Iterative calculations of self-consistent field (SCF) convergence and molecular dynamics (MD) according to the resulting force are performed, and we obtain a relaxation state. The final state of sample with the lowest total energy for each sample of the same number of 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, eq. (2).

Table I: Parameters for calculation

target material	tungsten bcc
supercell	$3 \times 3 \times 3$
	(54 lattice points)
lattice constant	3.220 Å
k-grids	$6 \times 6 \times 6$
PAOs	W 8.0-s2p2d1f1
	He 6.0-s2p1d1

Figure 1 depicts calculated values of the binding energy E_B as a function of the number of helium atoms trapped within a tungsten mono-vacancy, defined in eq.(2). The binding energy gradually decreases as the number of the trapped He atoms increases, steeply drops at 7 trapped He, and then recovers. When a binding energy E_B takes negative value, the configuration is less stable than the configuration whose tungsten is less by one. It is inferred that tungsten mono-vacancy can contain at least 6 helium atoms from Fig. 1. In the case of 6 helium trapped within the tungsten mono-vacancy, the 6 mono-vacancy-trapped helium atoms form octahedral configuration. He atoms are tightly bounded around a mono-vacancy located at center of W cube, and make a kind of cluster structure. The formation of this cluster structure may be related to helium bubble generation.

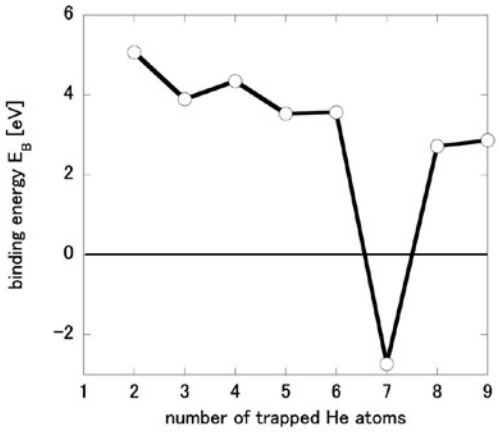

Fig. 1: Binding energy as function of the number of He atom trapped within a W mono-vacancy.