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§14. Simulation Approach to Understanding Phenomena Occurring in Plasma Facing Materials

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We have investigated influences of plasma irradiation on plasma facing materials, such as sputtering or nano-structure formation, by use of simulations with atomic scale. The principal target was a material composed of carbon and hydrogen isotopes, and it was simulated by molecular dynamics (MD) with Brenner's reactive empirical bond order (REBO) potential, binary collision approximation (BCA), or a BCA-MD hybrid model. In the present study, simulation target material is extended to metallic materials such as tungsten. In order to understand phenomena occurring in plasma facing materials of metallic elements, first-principles calculations are carried out and potential model for MD simulation are also developed.

First-principles calculations are carried out with the 'OpenMX' code package, which is designed for nano-scale material simulations based on density functional theories (DFT), developed by Dr. Ozaki at Japan Advanced Institute of Science and Technology[1]. We improve the code package to accelerate computation speed. The improvement enable us to calculate more wide configurational and parametric space.

Systems where noble gas atoms, such as helium, are trapped within a tungsten monovacancy are considered. In the first-principles calculations, the generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional is used for exchange-correlation potential. Linear combinations of pseudo-atomic localized orbitals, norm-conserving pseudo-potentials, and projector expansions are employed for core Coulomb potential. The 'OpenMX' uses numerical pseudo-atomic orbitals (PAOs) as basis function to expand one-particle Kohn-Sham wave functions. We employ the 3 s-, 2 p-, 2 d-, and 1 f-state radial functions with cut-off radius of 7.0 a.u. for tungsten, and the 2 s-, 2 p- and 1 d-state radial functions with cut-off radius of 8.0 a.u. for helium. The Brillouin zone with $6\times6\times6$ **k**-points sampling using the Monkhorst-Pack method is employed.

The lattice constant is obtained by minimizing the cohesive energy E_c, and is 3.172 Å in the present calculation parameter set. We employ a lattice constant of 3.172 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 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.

Figure 1 depicts calculated values of the binding energy E_B as a function of the number of helium atoms trapped within a tungsten monovacancy. When the binding energy E_B takes a negative value, the configuration is less stable than the configuration whose number of trapped He atoms is less by one. It is inferred from Fig. 1 that a tungsten monovacancy can contain at least nine helium atoms. That is, helium has a property that it tend to gather in a tungsten monovacancy rather than stay as an interstitial atom. This tendency may be related to helium bubble generation, which will lead to nano-structure formation.

First-principles calculations require high computation cost, thus it is hard to be applied to a system having wide spatial scale. Moreover it is limited to a steady and ground state. Molecular dynamics (MD) or kinetic Monte Carlo (kMC) simulation is suitable for a wide scale system and can treat dynamics or kinetics. A potential model to tungsten-helium-argon coexistence system required for MD simulation has been developed with first-principle calculation in the present study. Preparation of MD simulation and development of kMC simulation code is progressing, and they will be carried out in the next fiscal year.

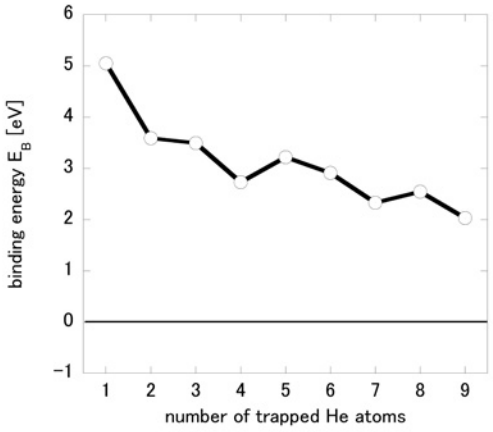

Fig. 1: Binding energy as function of the number of He atom trapped within a W monovacancy[2].

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

2) 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.