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Molecular Dynamics Simulation Study of Helium Diffusion in Tungsten Materials

タングステン材料中ヘリウム拡散挙動の分子動力学シミュレーション

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Diffusion property of helium in tungsten containing defects such as vacancies and grain boundary is investigated by use of both DFT calculation and MD simulation. DFT calculations are carried out with the "OpenMX" code package and PBE-GGA functional. MD simulations are performed with a potential model developed by the downfolding method. Grain boundary is modeled by coincidence site lattice (Σ3, Σ5).

1. Introduction

Tungsten is one of the most promising materials for a plasma facing material of inside walls in forthcoming magnetic confinement nuclear fusion reactors. In the surface of plasma facing materials, high concentrations of hydrogen, hydrogen isotopes and helium can build up and interact with the materials. These interactions will induce changes in the surface morphology and the bulk microstructure and thus in the mechanical properties. Therefore, the mechanical properties and the structural strength of tungsten under exposure to plasma irradiation have been intensively investigated both experimentally and theoretically [1-9].

In our previous work [8], the binding energies of mixed helium and hydrogen clusters consisted of interstitially trapped atoms in bcc tungsten are evaluated by first-principles calculations based on density functional theories (DFT). It is shown that helium-rich interstitially-trapped clusters have the positive binding energies and the low electron-density region expand as the number of helium in the cluster increase as shown in Fig. 1. These results indicate that the helium-rich interstitially trapped clusters can act as a trapping site for hydrogen, and interstitially trapped helium interrupts or disturbs the hydrogen diffusion in tungsten.

In the present study, diffusion property of helium in tungsten containing defects such as vacancies and grain boundary is investigated by use of both DFT calculation and molecular dynamics (MD) simulation, whose potential model is developed by the downfolding method [10].

Diffusion property of hydrogen in tungsten and effect of helium onto hydrogen diffusion are important to clarify in order for nuclear fusion reactor engineering. As these require construction of a reliable potential model which can treat mixture of hydrogen, helium, and tungsten, they remain future works.

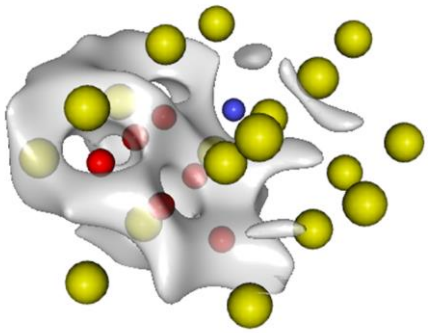

Fig.1. Optimized atomic configurations and the low electron-density isosurfaces for the system containing 6-He and 1-H atoms obtained by a DFT calculation. The yellow, red, and blue spheres represent W, He, H atoms, respectively. The isosurfaces indicate 0.036 electrons a.u.$^{-3}$, representing low electron density region. Helium atoms are relaxed at tetrahedral sites on a plane.

2. Simulation Model

2.1 *DFT calculation*

DFT calculations in this study are carried out with the "OpenMX" code package [11]. The generalized gradient approximation with Perdew -Burke-Ernzerhof functional [12] is used for the exchange-correlation potential. Linear combinations of pseudo-atomic localized orbitals [13,14], norm -conserving pseudo-potentials [15], and projector expansions [16] are employed for core Coulomb potential. All the calculations are carried out at

constant volume with the atomic positions in the supercell fully relaxed with use of the Broyden -Fletcher-Goldfarb-Shanno method [17-20].

2.2 *MD simulation*

MD simulations in this study are performed with a potential model for tungsten and helium system developed by the downfolding method, where potential function is optimized by comparison with various data of structure and energy obtained by DFT calculations [10]. The temperature of the simulation system is controlled by Nosé-Poincaré thermostat. The periodic boundary condition in *x*-, *y*-, and *z*-direction is employed.

2.3 *Model of Grain Boundary*

Coincidence site lattice (CSL) [21] with lower index (such as Σ3 and Σ5) is employed as a model of grain boundary. Figure 2 depicts the grain boundary modeled by Σ5 CSL. All of the tungsten atoms positions are relaxed with DFT calculation before MD simulation.

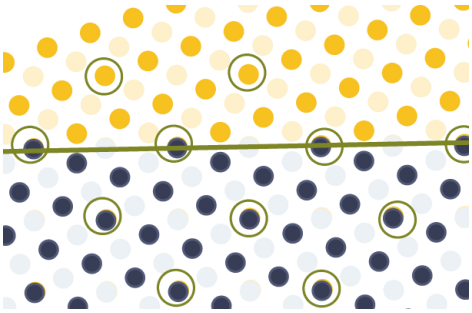

Fig.2. A model of grain boundary constructed by coincidence site lattice (CSL) Σ5. Blue and orange solid circles represent tungsten atoms of two distinguished (001) crystal layers aligned on paper. Light blue and light orange solid circles show tungsten atoms located on the surface next to paper. Green line and open circles show the grain boundary and coincidence sites, respectively. The crystal layer represented orange circles is rotated around [001] axis with an angle of 36.87 degree.

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References

[1] Y. Ueda, M. Fukumoto, J. Yoshida, Y. Ohtsuka, R. Akiyoshi, H. Iwakiri, N. Yoshida: J. Nucl. Mater. **386-388** (2009) 725.
[2] S. Kajita, W. Sakaguchi, N. Ohno, N. Yoshida and T. Saeki: Nuclear Fusion **49** (2009) 095005.
[3] C. S. Becquart, C. Domain: J. Nucl. Mater. **386-388** (2009) 109.
[4] B. Jiang, F. R. Wan, and W. T. Geng: Phys. Rev B **81** (2010) 134112.
[5] A. Takayama, A. M. Ito, S. Saito, N. Ohno, H. Nakamura: Jpn. J. Appl. Phys. **52** (2013) 01AL03.
[6] T. Tamura, R. Kobayashi, S. Ogata, A. M. Ito: Model. Sim. Mater. Sci. Eng. **22** (2014) 015002.
[7] Y. Oda, A. M. Ito, A. Takayama, H. Nakamura: Plasma Fusion Res. **9** (2014) 340117.
[8] A. Takayama, A. M. Ito, Y. Oda, H. Nakamura: submitted to J. Nucl. Mater.
[9] A. M. Ito, A. Takayama, Y. Oda, T. Tamura, R. Kobayashi, T. Hattori, S. Ogata, N. Ohno, S. Kajita, M. Yajima, Y. Noiri, Y. Yoshimoto, S. Saito, S. Takamura, T. Murashima, M. Miyamoto, H. Nakamura: submitted to J. Nucl. Mater.
[10] A. M. Ito, Y. Yoshimoto, S. Saito, A. Takayama, H. Nakamura: Phys. Scr. **T159** (2014) 014062.
[11] OpenMX web-site: http://www.openmx-square.org/
[12] J. P. Perdew, K. Burke, M. Ernzerhof: Phys. Rev. Lett. **77** (1996) 3865.
[13] T. Ozaki: Phys. Rev. B **67** (2003) 155108.
[14] T. Ozaki, H. Kino: Phys. Rev. B **69** (2004) 195113.
[15] I. Morrison, D. M. Bylander, L. Kleinman: Phys. Rev. B **47** (1993) 6728.
[16] T. Ozaki, H. Kino: Phys. Rev. B **72** (2005) 045121.
[17] C. G. Broyden: J. Inst. Math. Appl. **6** (1970) 76.
[18] R. Fletcher: Comput. J. **13** (1970) 317.
[19] D. Goldrarb: Math. Comp. **24** (1970) 23.
[20] D. F. Shanno: Math. Comp. **24** (1970) 647.
[21] K. Maeda, S. Takeuchi: *Physics of Crystal Defects* (Shokabo, Tokyo, 2011; in Japanese), Chap.6, p.178.