§27. Three Dimensional MD-MC Hybrid Simulation for Tungsten Fuzzy Nanostructure Formation

Ito, A.M., Oda, Y., Takayama, A., Nakamura, H., Yajima, M.,
Tamura, T., Kobayashi, R., Ogata, S. (Nagoya Institute of Thechnology),
Ohno, N., Kajita, S. (Nagoya Univ.),
Takamura, S. (Aichi Institute of Thechnology),
Murashima, T. (Tohoku Univ.),
Yoshimoto, Y. (Univ. Tokyo),
Saito, S. (Kushiro Nat'l College of Technology),
Miyamoto, M. (Shimane Univ.)

Tungsten materials are used for the divertor plate in fusion reactors because tungsten materials have high melting point, high thermal conductivity, low sputtering yield, and low tritium retention. However, one problem is that helium plasma irradiation generates nano-bubbles and fuzzy nanostructures [1] on the surface of tungsten materials. The nano-bubbles and the fuzzy nanostructure eliminate the above good properties of tungsten materials as plasma facing materials. The purpose of this work is to research theoretically the formation mechanisms of the nano-bubbles and fuzzy nanostructures under the helium plasma irradiation. Simulation methods and coeds has been developed to carry out multi-scale analysis for the formation of nano-bubbles and fuzzy nanostructure. Furthermore, these methods and codes can be used for general plasma-wall/material interaction (PWI/PMI) phenomena.

The formation process of the nano-bubble and fuzzy nanostructure is classified into the four step processes [2], helium penetration process, helium diffusion and agglomeration process, bubble growth process, and fuzzy nanostructure growth process. Those processes have been calculated by using, the binary collision approximation (BCA), the density functional theory (DFT), the molecular dynamics (MD, the kinetic Monte-Carlo (KMC) has been used. In particular, the MD-MC hybrid simulation had been developed to represent the growth process of a fuzzy nanostructure [2,3].

We advanced the research of the MD-MC hybrid simulation in the point which the simulation result is corresponding to realistic fuzzy nanostructure or not. Then, the growth speed of the fuzzy nanostructure was compared with the experimental result. Figure 1 shows the mean square of height of fuzzy nanostructure during the MD-MC hybrid simulation. From this figure, the mean square of height increased proportionally to fluence of helium atoms. This fact agrees with the experimental result that the height of the fuzzy nanostructure increases proportionally to the square root of irradiation time [4,5]. Thus, the validity of the MD-MC hybrid simulation was confirmed.

The above MD-MC hybrid simulation was performed in the semi-two dimensional system where the simulation is performed in the three dimensional space, and but the side of the simulation box in the y-direction is set to 7.85 Å. In the present work, the MD-MC hybrid simulation is extended into the simulation in full three dimensional (3D) system. Figure 2 shows a simulation snapshot in the MD-MC hybrid simulation in the full 3D system. The early structure of the fuzzy nanostructure was generated by being pushed from the helium bubbles. Thus, MD-MC hybrid simulation had been successfully represented the formation process of fuzzy nanostructures.

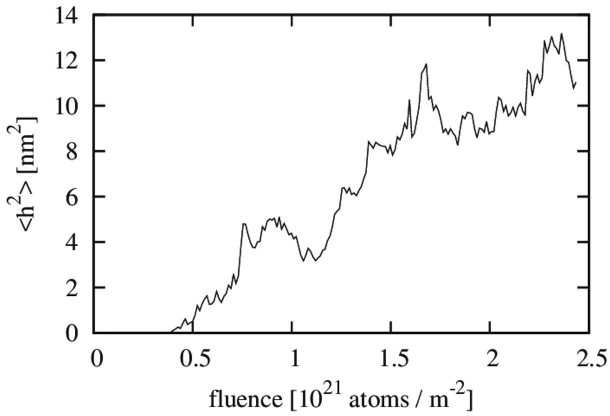

Fig. 1. the mean square of height of fuzzy nanostructure as a function of the elapsed time. The simulation was performed at temperature T = 2000 K, flux $\phi = 1.4 \times 10^{22}$ $m^{-2}s^{-1}$, diffusivity $D = 1.32 \times 10^{-11}$ m^2 s^{-1}.

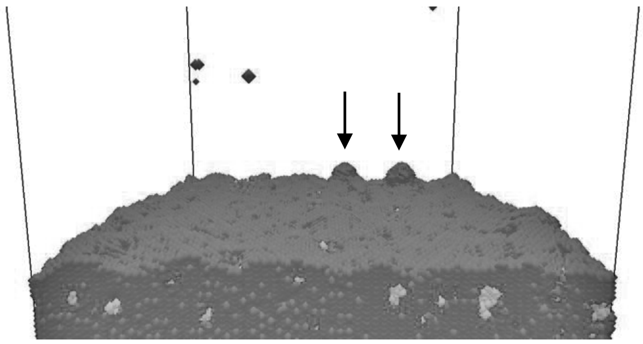

Fig. 2. the early phase of fuzzy formation process simulated by the MD-MC hybrid simulation in the full 3D system. The dark and light gray spheres indicate the tungsten and helium atoms, respectively.

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2) Ito, A. M., et al.: J. Nucl. Mater. **463** (2015) 109-115.
3) Ito, A. M., et al.: Nucl. Fusion **55** (2015) 73013.
4) Baldwin, M.J., and Doerner, R.P.: Nucl. Fusion **48** (2008) 035001.
5) Noiri, Y., Kajita, S., and Ohno, N. J. Nucl. Mater. **463** (2015) 285-288.