§13. Molecular Dynamics Simulation Research on Helium Bubble Behavior in Tungsten Material

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Fuzzy nano-structures on tungsten surfaces are generated by the bombardment of helium ions. This phenomenon was found from the experimental researches[1,2] for the interaction between plasma and the inside walls of the nuclear fusion reactors. The tungsten nano-structure is also interesting for plasma application. The formation process of the tungsten nano-structure is as follows: first the nano-scale bubbles, which are called helium bubble, are created in a surface, and next fuzzy fibers which are sub-micro meter in diameter grow perpendicularly to the surface. This process differs from the deposition, in which source atoms are supplied as injected molecules onto surface, and the processing, in which the injected particles scrape the surface along a mask film. In the formation process of the tungsten nano-structure, injected helium ions are not source and the surface is not scraped. Our purpose is to clarify the mechanisms of formation of the tungsten nano-structure. We consider that the formation process of the tungsten nano-structure should be classified into three step processes which are the penetration of helium, the diffusion and aggregation of helium, and the growth to the fuzzy nano-structure. We had investigated these three step processes by using binary collision approximation (BCA),[3] and density functional theory (DFT),[4] and molecular dynamics (MD), respectively.

As the third step process, we should treat the dynamics in sub-micro meter scale for the growth from the bubble structure to the fuzzy nano-structure within surface region. We have tackled to reproduce the growth to the fuzzy nano-structure by MD. As one case of growth of the fuzzy nano-structure, we examined Krasheninnikov's model,[5] in which the growth of the fuzzy structure was explained by the viscosity of metal in a macroscopic viewpoint, by using MD simulation. Accordingly, we researched the behavior of the nano-meter scale helium bubble in the tungsten material.

As an important preparation for this purpose, we made the potential model for tungsten and noble gas system using the downfolding method[6]. In the downfolding method, the parameters in the function of potential model were optimized to reduce the difference between the energy of potential model and that calculated by DFT. By this way, the potential model for tungsten-helium-argon system was developed. In relation to this, by using the downfolding method, we developed the potential model for carbon system which can treat graphite-diamond transition under the high pressure environment[7]. The transition pressure of 15 GPa agrees with the experimental reports[8].

The calculation of DFT is executed by using "open source package for material explorer (OpenMX)" code.[9-11] The OpenMX code was developed by Dr. Ozaki and we had tackled the turning of this code for the super computer "Plasma Simulator" in NIFS, Japan and "IFERC-CSC" in Rokkasho, Japan. The parts of our turning points were formally adopted by the original OpenMX code. Through the latest version of the OpenMX code, our tuning points are also contributing to the activities of material science and "K-computer" in Kobe, Japan. The use of the DFT is important for the research of plasma facing material for nuclear fusion. Especially, it is necessary for the investigation of metal, such as tungsten material, to calculate detail electronic property in quantum mechanics by using DFT. By the cooperation of Dr. Ozaki and OpenMX code, the numerical simulation technic of Plasma-Wall Interaction group in Numerical Simulation Research Project is enhanced.

Here, as the behavior of the helium bubble in tungsten material, the extension of size of the helium bubble by the high pressure of helium atoms, and the bursting of helium bubble, which is the escape of the helium atoms from the surfaces of tungsten (See Fig.1). This MD simulation implies that the temperature of 1000K or more is needed for helium bubble to extend it and to burst.

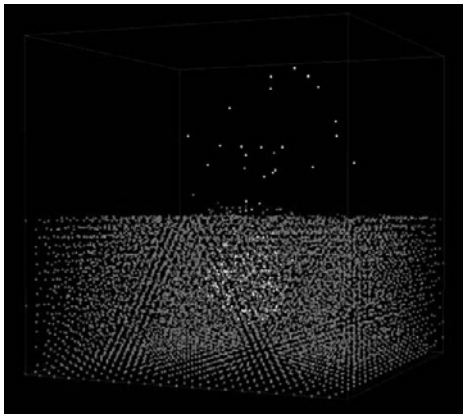

Fig. 1: the bursting of helium bubble on the surface of tungsten in the MD simulation.

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