§17. Molecular Dynamics for Bursting of Helium Bubble on Tungsten Surfaces

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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 [1-3] 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 can be explained by the four step process which is composed of the penetration of helium, the diffusion and aggregation of helium, the growth of helium bubble, and the growth of fuzzy nano-structure. Some of numerical simulation works relate to these four step process have been performed by using binary collision approximation (BCA), and density functional theory (DFT), molecular dynamics (MD), and kinetic Monte-Carlo (KMC). As the third step process, we should treat the dynamics of helium bubble in sub-micro meter scale. The present work, we had investigated the "bursting" of the helium bubble with in the tungsten surface.

As an important preparation for this purpose, we made the potential model for tungsten and noble gas system using the downfolding method [4]. 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 system was developed [5].

The behaviors of a helium bubble observed in the present MD simulations are classified into the following three cases. The first case is the standing process that the helium atoms are kept within the initial helium bubble region. The second case is the expanding process that the helium atoms pushed out the tungsten atoms and the helium bubble region was extended. The third case is the bursting process that the helium atoms escaped from the surface as shown in Fig.1. From the animation of the MD simulation, it is understand that the size of tunnel for the helium atoms to pass through the surface is roughly the diameter of one tungsten atoms. When these slight tunnel is created once, all helium atoms can escape through the tunnel.

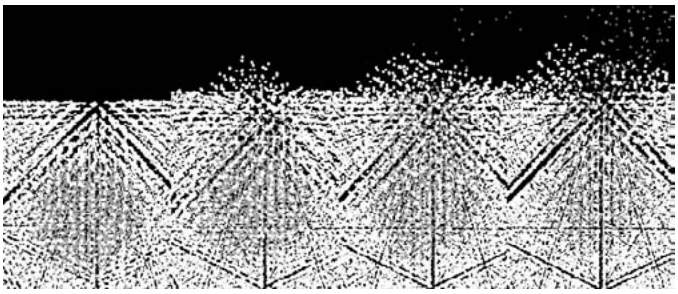

Fig. 1. The simulation result of the bursting of helium bubble on the surface.

As the result of the present MD simulation from the statistical viewpoint, the dependency of the helium bubble behaviors on the temperature T and the ratio of the number of initial helium atoms to the number of vacancy corresponding to the initial helium region He/Vac were calculated in this MD simulation. It is understand that when the temperature T and He/Vac increase are high, the helium bubble shows bursting behavior. When the thickness between the surface and helium bubble becomes wide, the threshold of He/Vac to start bring about the bursting process becomes high.

By the MD simulation, we can estimate the pressure in the helium babble. The pressure can be defined from the position, momentum and forces of atoms. The results of the simulation indicate that a helium bubble with a radius of 1.0 nm needs a high pressure of several tens of GPa to burst near the surface and to expand the bubble structures under the surface to the scale of ten nanometers. Moreover, from the viewpoint of dynamics, the results of the MD simulation expects that the concavities and convexities observed on the surface in the early stage of the formation of a tungsten fuzzy nano-structure are caused by the bursting of the helium bubble.

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