§23. Tungsten Fuzzy Nanostructure Formation by Molecular Dynamics and Monte-Carlo Hybrid Simulation

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A tungsten material is used for plasma facing material in a vacuum vessel of fusion reactors because the tungsten material has a high melting point, a high thermal conductivity, low sputtering yield, and low tritium retention. However, helium plasma irradiation generates helium bubbles and a fuzzy nanostructure on the tungsten surface[1]. The surface morphologies in nanometer scale due to the helium bubble and the fuzzy nanostructure changes the phenomena of the plasma-wall interaction on the tungsten surfaces. For instance, helium plasma irradiation reduce the occurrence of the blistering due to retained hydrogen atoms, while the helium atoms retained in tungsten material becomes the trap site of the hydrogen atoms. This complicates the estimation of tritium retention in future fusion reactors. Thus, the formation of the helium bubbles and the fuzzy nanostructure is an important problem for the fusion science.

In the present work, we had tried to clarify the formation mechanisms of the helium bubbles and fuzzy nanostructure on the surface of the tungsten material by numerical simulation. In particular, we employed the multi-scale multi-physics approach in which molecular dynamics (MD), density functional theory (DFT), binary collision approximation (BCA), and kinetic Monte-Carlo (KMC) are properly used according to the space-, time- and energy-scales of phenomena. To classify phenomena during the formation process of the helium bubbles and the fuzzy nanostructures, we proposed the four-step process[2].

The first step is the penetration process in which the competition of the penetration of helium atoms and the sputtering of the tungsten atoms during helium plasma irradiation were evaluated by using DFT and BCA. The minimum incident energy of the helium atoms to penetrate the surface is about 6.0 eV, while the maximum energy to penetrate without sputtering, i.e. the sputtering threshold energy, is 100 eV. This energy window for helium atoms are wider than neon and argon.

The second process is the diffusion and agglomeration process in which the binding energies and the migration barrier energies of helium atoms in a tungsten material were evaluated by DFT[3,4]. From the DFT calculations, it was understood that the noble gas atoms tend to assemble not only in a vacancy but also at interstitial sites in tungsten materials, and the diffusion coefficient of the helium atoms in a tungsten materials is ten times as large as the diffusion coefficient of the hydrogen atoms.

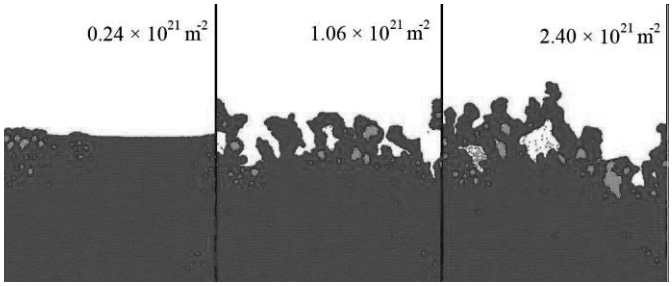

Fig. 1. The animation snapshots of the tungsten fuzzy structures calculated by the MD-MC hybrid simulation as a function of the fluence of helium atoms.

The third step is the bubble growth process in which the generation of the helium bubbles toward the size of 1 nanometer or larger in diameter was simulated by MD simulation. Empirical potential model used in the MD was developed by using downfolding method[5]. By the MD simulation, we directly observed the loop punching, which is the phenomena that the stress around the helium <111> of a tungsten lattice structure[6].

The four step is the fuzzy nanostructure growth process. The formation of the fuzzy nanostructure cannot be represented by MD or KMC. The MD cannot calculate enough time scale for the diffusion of the helium atoms, and to determine reasonable mathematical rules for the deformation of tungsten materials in the KMC was difficult. However, we successfully represented the formation process of the tungsten fuzzy nanostructure by developing the MD-MC hybrid simulation[7] as shown in Fig. 1. In the MD-MC hybrid simulation, the diffusion of the helium atoms are simulated as simple random walk in the cell data, while the deformation of the tungsten materials due to stress from helium bubbles are simulated by the MD. The growth rate of the height of the fuzzy nanostructure is proportional to the square root of elapsed time, and it agrees with experimental observation. The growth of the fuzzy structure began when the retention amount of the helium atoms is saturated. From this simulation, the formation mechanisms of the fuzzy nanostructure is considered as (1)the lift up of the surface by helium bubbles growth, (2)the creation of a concavity and a convexity by the bursting of the helium bubble, and (3)new helium bubble tends to appear at the region under the concavity.

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