20aC-2-1

Formation Processes of Tungsten Nano-structures Induced by Helium Plasma
ヘリウムプラズマ誘起タングステンナノ構造の形成過程の解明

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In the present paper, the formation mechanisms of the tungsten fuzzy nanostructure which is induced by exposure to helium plasma were explained by numerical simulations. We proposed the four-step process of formation of the tungsten fuzzy nanostructures which is composed of the penetration process, the diffusion and agglomeration process, the bubble growth process and the fuzzy nanostructure growth process. The first to third step processes of the four-step process were investigated by using binary collision approximation, density functional theory and molecular dynamics, respectively. In the fourth step, newly developed molecular dynamics and Monte-Carlo hybrid simulation has successfully reproduced the early formation process of tungsten fuzzy nanostructure.

1. Introduction

For the purposes of long-term use of tungsten diverter walls, it is necessary to suppress the surface deterioration due to the helium ash which induces the formations of helium bubbles and tungsten fuzzy nanostructures[1]. However, the formation mechanisms of the tungsten fuzzy nanostructure were not well understood. We have researched the formation mechanisms of the tungsten fuzzy nanostructure by using numerical simulation. This work is cross-disciplinary study between plasma, fusion and material sciences.

2. Four-step Process

The formation process of the tungsten fuzzy nanostructure is classified into the following processes.

2.1 *Penetration process*

The first step is the penetration process of irradiated helium ions into tungsten surfaces. In particular, the competition between the penetration of helium atoms and the sputtering of tungsten surfaces is important factor.

The sputtering threshold energy can be calculated by the binary collision approximation (BCA)[2]. The lower limit of the incident energy for penetration is assumed as the solution energy which was calculated by the density functional theory (DFT)[3].

By comparison of the spattering threshold energy and the solution energy between, it is understood that the energy range for penetration without causing sputtering is wide in terms of hydrogen and helium plasmas, while the energy range for

penetration without causing sputtering is narrow in terms of neon and argon helium plasmas.

2.2 *Diffusion and agglomeration process*

The second step is the diffusion and agglomeration process of helium atoms in tungsten material.

First, to confirmed the possibility of helium agglomeration, the binding energies at a mono-vacancy and an interstitial site were calculated by DFT[3-8]. By the DFT calculations results expect that although the agglomeration of hydrogen atoms is limited, the agglomeration of helium, neon and argon atoms are unlimited at the both of a mono-vacancy and an interstitial site.

Next, to compare the speed of diffusion, the migration barrier energies on the path from a tetra-site to the next tetra-site were calculated by DFT[3]. As a result, the migration barrier energy of helium is one-third of that of hydrogen. From these facts, we suggest that helium diffuses faster than hydrogen in tungsten material. In addition, although they have larger atomic radius, the migration barrier energies of neon and argon were similar to that of hydrogen.

Thus, noble gas atoms can quickly nucleate.

2.3 *Bubble growth process*

The third step is bubble growth process. The growth of helium bubbles which have 1 nm or more in radius was confirmed by molecular dynamics (MD) simulation. The potential model for helium-tungsten system[9] was developed by using the downfolding method[10], which can optimize potential function by comparison with structure and energy data calculated by DFT.

Moreover, the phenomenon called loop-punching was observed in our MD simulation[11]. We revealed that the loop-punching is the release of dislocation loops from helium bubbles. In other word, the strain of tungsten atoms around growing helium bubbles is released as a dislocation loop. When the dislocation loop stops, the region around the dislocation loop becomes a new nucleation site of helium bubbles.

2.4 *Fuzzy nanostructure growth process*

The fourth step is fuzzy structure growth process. To reproduce the fuzzy nanostructure formation by existing simulation methods is difficult because the fuzzy structure formation depends on the multi-scale and multi-physical mechanisms.

Here, we develop new hybrid simulation between MD and Monte-Carlo (MC), where we call the MD-MC hybrid simulation[12,13]. In the MD-MC hybrid simulation, the diffusion process of injected helium atoms, which is long time scale phenomenon, is simulated by MC as a random walk in a tungsten material, and the deformations of the tungsten material and helium bubbles are simulated by MD with realistic atomic interaction potential. As the time is developed, the MC phase and MD phase are cycled.

As a result, the early formation process of the tungsten fuzzy nanostructure was successfully reproduced by the MD-MC hybrid simulation (see Fig.1), where the simulation was performed in pseudo-3D (2D like) system. Now, we are engaged in the full-3D simulation, and we are planning to compare the fractal dimension of surface structure, which had been already measured by the experiment as 2.2 to 2.6[14].

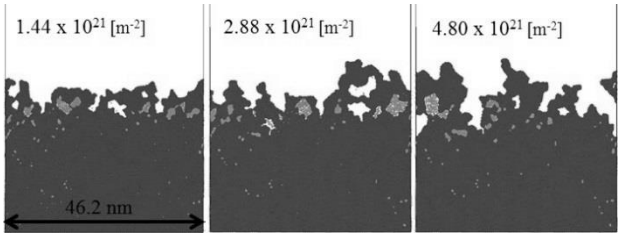

Fig.1. Tungsten fuzzy nanostructure formation calculated by the MD-MC hybrid simulation.

Acknowledgments

We would like thank to Dr. N. Yoshida, Dr. Y. Ueda, Dr. M. Tokitani and Dr. H. T. Lee for helpful discussions. Our work was supported by the NINS Program for Cross-Disciplinary Study and JSPS KAKENHI 23710135 and 25249132. Numerical simulations were carried out by using the Plasma Simulator at the NIFS and the HELIOS at the IFERC-CSC under BA, Euratom and Japan, JAEA.

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