



Incident Energy Dependence of Tungsten Fuzzy Nanostructure Growth with BCA-MD-KMC Multi-Hybrid Simulation

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The durability of the divertor plate is a critical issue for the establishment of magnetic confinement fusion reactors. Popular problems are heat load and the erosion of the surface due to sputtering. Hence, one of problems is the effect of helium plasma on a tungsten surface. The helium plasma is the ash of fusion reaction and the tungsten is the material for the divertor plate. Helium plasma irradiation induces helium nano-bubbles and fuzzy nanostructures on tungsten surfaces [1-4], even if the incident energy of helium plasma is lower than sputtering threshold energy. The fuzzy nanostructure is very brittle, so if it peels off, it becomes dust that impedes core plasma. In addition, the fuzzy nanostructure decreases the thermal conductivity of the tungsten material [5,6], the resistance of the tungsten surface decreases. Thus, the generation of the fuzzy nanostructure on the divertor plate is a key issue of the research in plasma-wall interaction. The formation and growth mechanisms of the fuzzy nanostructure have not been clarified yet.

On the other hand, the formation mechanism of the helium nanobubble, which is also generated by helium plasma irradiation, has been well clarified by simulations: The fact that helium atoms prefer to agglomerate in metal materials is confirmed by the density functional theory (DFT) for tungsten [7,8] and for several metal materials [9,10]. From molecular dynamics (MD), it was demonstrated that this helium agglomeration continues to forming the nano-scale helium bubbles and then dislocation loops are emitted from the helium bubble due to the high pressure of the helium atoms [11,12].

In experiment the fuzzy nanostructure is generated when the helium irradiation continues after the helium nano-bubble is generated. Then, the relation between the fuzzy nanostructure and the helium nanobubble has been considered. However, the total fluence of helium ion to generate the fuzzy nanostructure is 10^{24} m^{-2} , which is 100 times higher than that to generate the helium nanobubble. This gap in the fluence made the issue difficult. In order to reproduce the fuzzy nanostructure, we have promoted the development of hybrid simulations [13,14]. In the previous work, we developed the BCA-MD-KMC triple hybrid simulation [15], and then the BCA-MD-KMC triple hybrid simulation achieved 10^{24} m^{-2} in fluence. And, the incident flux is kept low at $10^{22} \text{ m}^{-2}\text{s}^{-1}$, which is comparable with an experimental condition.

As a result of the hybrid simulation, the role of the helium nanobubbles was to create nano-scale roughness on the surface by its bursting in early phase. Subsequent

growth of fuzzy fibers was caused by the transport of tungsten atoms by the sputtering by the incident helium ion and the re-deposition of the tungsten atom at the tips of the fibers. At the rough surface, the helium atom can sputter out the tungsten atom created by the helium bubble bursting even if the incident energy is lower than the threshold energy of bulk.

In the present work, we focus the process of sputtering on nano-scale roughness. This occurrence depends on the incident energy and nanoscale structures. Here, in experiment, there is an unexplained point that the incident energy of 30 eV or more is necessary for fuzzy growth [16]. Note that from the DFT calculation [8], it is clarified that the incident energy required for helium atom to penetrate into tungsten is 6 eV. In the experiment also, helium bubbles are formed in the case of incident energy higher than 6 eV. Therefore, we investigate incident energy dependence of the growth of the fuzzy nanostructure by using the BCA-MD-KMC triple hybrid simulation. And then, we discuss the threshold energy of the incident energy for growth of the fuzzy structure, that is 30 eV, in terms of the sputtering.

References

- [1] S. Takamura, et al., Plasma Fusion Res. **1**, 051 (2006).
- [2] M. J. Baldwin and D. P. Doerner, Nucl. Fusion **48**, 035001 (2008).
- [3] S. Kajita, et al., Nucl. Fusion **49**, 095005 (2009).
- [4] M. Tokitani, et al., Nucl. Mater. Energy **12**, 1358 (2017).
- [5] S. Kajita, et al., Nucl. Fusion **47**, 1358 (2007).
- [6] S. Kajita, et al., Results Phys. **6**, 877 (2016).
- [7] A. Takayama, et al., Jpn. J. Appl. Phys. **52**, 01AL03 (2013).
- [8] T. Tamura, et al. Modelling Simul. Mater. Sci. Eng. **22**, 015002 (2014)
- [9] K. Omori, et al., J. Appl. Phys. **121**, 155301 (2017).
- [10] K. Omori, et al., Nuclear Material and Energy, **16**, 226-229 (2018).
- [11] F. Sefta, et al., Nucl. Fusion **53**, 073015 (2013).
- [12] R. Kobayashi, et al., J. Nucl. Mater. **463**, 1071 (2015)
- [13] A. M. Ito, et al., J. Nucl. Mater., **463**, 109-115. (2015).
- [14] A. M. Ito, et al., Nucl. Fusion **55**, 073013 (2015).
- [15] A. M. Ito, et al., Plasma Fusion Res. **13**, 3403061 (2018).
- [16] W. Sakaguchi et al., J. Nucl. Mater. **390-391**, 1149 (2009).