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The growth of tungsten fuzzy nanostructure by BCA-MD-KMC multi-hybrid simulation

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The fuzzy nanostructure, which is a fiber form nanostructure on a tungsten surface, is generated from helium plasma irradiation onto the tungsten surfaces [1,2]. This formation phenomenon was found from the experimental researches on the plasma-wall interaction for the tungsten divertor plates of a magnetic confinement fusion reactor. Helium is the ash of the D-T fusion reaction. In fact, the fuzzy nanostructures are actually formed in the Large Helical Device (LHD) [3]. I Concern due to fuzzy nanostructure generation is the occurrence of arcing and microcracks in the material [4], enhancing tritium retention [5], and decreasing the thermal conductivity of the divertor plates [6].

For the fusion reactor, we should suppress the generation of the fuzzy nanostructure. On the other hand, in the viewpoint of plasma application, we should enhance the growth of similar nanostructures on the other metals. In both purposes, we need to elucidate the formation mechanism of the fuzzy nanostructure.

In general, the phenomena of plasma material interactions are classifies into processing which include etching and erosion, and deposition. However, the mechanism of fuzzy nanostructure formation is considered neither because the kinetic energy of the helium ions is lower than sputtering threshold energy. Key phenomenon is helium bubble formation in a tungsten material. The size of the helium bubble is several nanometer or more. In experiments, the fuzzy formation occurs after the helium bubble formation. 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]. 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 [10,11].

However, important experimental fact is the fuzzy nanostructure formation occurs after the total helium fluence reaches 10^{24} m^{-2}, which is called incubation fluence. This fluence cannot be possibly achieved by using MD with the irradiation flux of 10^{22} $m^{-2}s^{-1}$ corresponding to that in actual experimental device NAGDIS-II (Nagoya Divertor Simulator-II). If the irradiation flux is set higher in simulation, the competition with the diffusion speed of helium atoms in the tungsten material becomes unreal and then the place at which helium bubbles form becomes shallow.

In order to represent the formation process of fuzzy nanostructure in simulation, it is necessary to achieve high incubation fluence while keeping low flux equivalent to the experiments. For this purpose, we has developed hybrid simulation approach. In the MD-MC hybrid simulation [12,13], the diffusion of the helium atoms in the material is solved by the random walk of the Monte-Carlo (MC) method, and the deformation of the tungsten material is solved by the MD. The MD-MC in the two dimensional system achieved the fluence of 0.5 x 10^{22} m^{-2} (0.5 s) under the flux of 10^{22} $m^{-2}s^{-1}$. However, the realistic fuzzy growth was not confirmed.

In the present work, the MD-MC hybrid simulation was advanced to the BCA-MD-KMC triple hybrid simulation [14]. In addition to the diffusion process of helium atoms and the deformation process of tungsten material, the incident process of helium ions are solved by binary collision application (BCA). Moreover, because the MC algorism for the diffusion process of helium atoms was changed into the kinetic Monte-Carlo (KMC), simulation speed becomes faster than the MD-MC. The BCA-MD-KMC in the three dimensional system achieved the fluence of 10^{24} m^{-2} (100 s) under the flux of 10^{22} $m^{-2}s^{-1}$. As a result, it was demonstrated that the fuzzy nanostructure grows up to several ten nanometer.

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