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Molecular Dynamics and Density Functional Simulations of Tungsten Nanostructure Formation by Helium Plasma Irradiation

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The tungsten nanostructure induced by helium plasma irradiation had been found by the experimental researches for the plasma facing materials in fusion reactors. For the generation of the tungsten nanostructure, it is concerned about the decrease of the maximum allowable heat load and the erosion by arcing on the surface. To clear these problem, we had researched on the formation mechanisms of the tungsten nanostructure by using molecular dynamics(MD), density functional theory(DFT), and any other simulation methods.
The diffusion and agglomeration of helium in tungsten material were investigated by DFT calculation. As a result, the binding energy of helium atoms at interstitial site is about 1.5 eV comparable to that at mono-vacancy, about 2.5 eV[1]. This reason is that the electron density in the region around the interstitial site trapping a noble gas atom decreases and then this region also becomes new trap site for the other noble gas atoms[2]. The migration barrier energy of a helium atom in tungsten material is third part of that of a hydrogen atom. Moreover, the migration barrier energies of helium dimer and trimer at an interstitial site are much smaller than that of single helium atom. These facts imply that helium atoms can be spontaneously agglomerated at interstitial site.
The nanostructure formation on the surface was calculated by MD using developed high accuracy potential model[3]. According to our simulation result, the tungsten nanostructure formation proceeds as follows: The growth of helium bubbles generated the foam structure of tungsten which means nano-walls separating the helium bubbles. Simultaneously, the foam structure in the region close to the surface was lifted up by the helium bubble swelling in the bulk region. Strictly speaking, the foam structure created by the MD is not fuzzy fibered and then the MD is considered as early formation phase of tungsten nanostructure. We suggest that the foam structure changes to porous structures due to the bursting of helium bubbles and it can transform to the fuzzy structure by the surface diffusion.

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Author: Mr ITO, Atsushi (Japan)

Presenter: Mr ITO, Atsushi (Japan)

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