## §24. Binary-collision-approximation Simulation for Noble Gas Irradiation onto Tungsten

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To find plasma facing materials (PFM), which must endure a plasma irradiation, is one of the important issues in order to realize the nuclear fusion reactor. Tungsten material is one of the candidates of PFMs. However, bubble or nano-structure formation in tungsten is observed under the irradiation of helium onto the tungsten surfaces. This structure appears not only in tungsten but also in other materials, e.g., iron. The nano-structure weakens mechanical strength and increases the tritium retention. Therefore it is better to avoid the nano-structure formation in PFM. To achieve this aim, it is necessary to reveal the mechanism of the nanostructure formation in PFM under helium gas irradiation [1-4]. Intuitively, the nano-structure formation is regarded as the phenomenon composed of the invasion of helium gas into PFM, the difussion of helium in PFM and the transformaiotn of PFM material.

It is inferred that the formation of fuzz structure consists of the following three elementary processes[5]: Penetration process of incident atoms; Diffusion of the incident atoms and trapping by vacancies; Formation and aggregation processes of bubbles of the incident atoms. Therefore, binary-collision-approximation-based simulation is performed to reveal the mechanism and the conditions of fuzz formation of tungsten material under plasma irradiation, as the first step of investigation. The penetration depth of helium, neon, and argon gases were investigated in our previous study [6]. The fuzz structure is not observed under other noble gas plasma irradiation except helium plasma [7]. We review the result of our previous study first. The irradiation of hydrogen isotope onto tungsten material is also the key issue for the nuclear fusion device. After the review of the study of the noble gas irradiation, the case of the irradiation of hydrogen, deuterium, and tritium plasma is discussed. The penetration depth strongly depends on the structure of the target material. Therefore, the penetration depth for amorphous and bcc crystalline structure is carefully investigated.

BCA simulation is performed by AC ∀ T (atomic collision in any structured target) code [7]. In BCA simulation, multi-body interactions in a material approximate to consecutive two-body interactions between a projectile atom and the nearest neighbor atom. The size of the target material is set to 47:47 Å long, 47:47 Å wide, and 9998:24 Å deep. The z-axis of the simulation box is set parallel to the edge of the target material whose length is 9998:2 Å. Periodic boundary conditions are used in the x- and y-directions. The lattice constant of bcc crystal is set to 3.16 Å. Amorphous structure is formed by distributing tungsten atoms randomly. The density of amorphous structure is set to the same as the density of bcc crystal. The temperature of the tungsten materials is set to 0 K. Helium (He), neon (Ne), argon (Ar), hydrogen (H), deuterium (D), tritium (T) atoms are injected into these tungsten materials. The mean depth of penetration of incident atoms for 10,000 injections is calculated for constant incident energy from 10 eV to 10 keV. The x- and y-coordinates of the starting positions of the incident atoms are set randomly. The incident angle is set to parallel to the z-axis, i.e., perpendicular to (100) surface in the case of bcc crystal. To calculate the mean depth, the target material is refreshed to the initial perfect crystal before each injection.

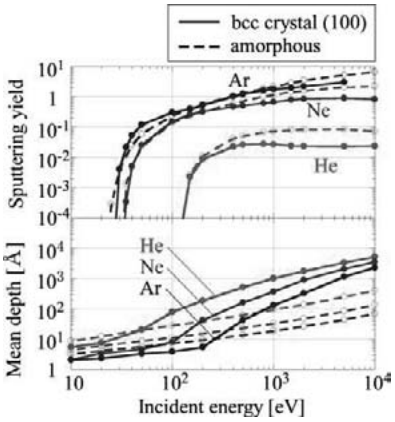


Fig. 1. Photoshop of miter bend. Grooves are engraved in the inside of miter bend. The width, the depth and the pitch of grooves are 1.0 mm, 0.76 mm, and 1.3 mm, respectively.

Figure 1 shows the incident energy dependence of the sputtering yield and the mean depth of penetration in the cases of He, Ne, or Ar injection. The solid and dashed lines denote the results in the cases of bcc crystalline and amorphous structure, respectively. The mean depth strongly depends on atomic species and the structure of the target material. In the case of amorphous structure, the mean depth is almost proportional to the square root of incident energy. The mean depth in the case of bcc crystalline structure has a different profile in contrast with that of amorphous structure when incident energy is larger than threshold energies. It is found that the difference of the profiles is caused by channeling effect.

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