

Binary-collision-approximation simulation for noble gas irradiation onto plasma facing materials

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Abstract. A number of experiments show that helium plasma constructs filament (fuzz) structures whose diameter is in nanometer-scale on the tungsten material under the suitable experimental condition. In this paper, binary-collision-approximation-based simulation is performed to reveal the mechanism and the conditions of fuzz formation of tungsten material under plasma irradiation. The irradiation of the plasma of hydrogen, deuterium, and tritium, and also the plasma of noble gas such as helium, neon, and argon atoms are investigated. The possibility of fuzz formation is discussed on the simulation result of penetration depth of the incident atoms.

1. Introduction

Tungsten material is one of promising candidates for divertor plates in nuclear fusion reactors. Bubble formation [1, 2] is observed on the surface of the tungsten material which is irradiated by helium plasma. Furthermore, a number of experiments show that helium plasma constructs filament (fuzz) structures [3, 4] whose diameter is in nanometer-scale on the tungsten material under the suitable condition (i.e., material temperature of 1,000-2,000 K and incident energy of 20-100 eV). The formation of these structures does not only decrease the thermal conductivity of the material, but also enhances the tolerance in cracking and the radiation efficiency. It also causes reduction of sputtering yield.

As shown in fig. 1, it is inferred that the formation of fuzz structure consists of the following three elementary processes: Penetration process of incident atoms; Diffusion of the incident atoms and trapping by vacancies; Formation and aggregation processes of bubbles of the incident atoms. In this paper, 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 [5]. The fuzz structure is not observed under other noble gas plasma irradiation except helium plasma [6]. We review the result of our previous study at first. The irradiation of hydrogen isotope onto tungsten material is also the key issue

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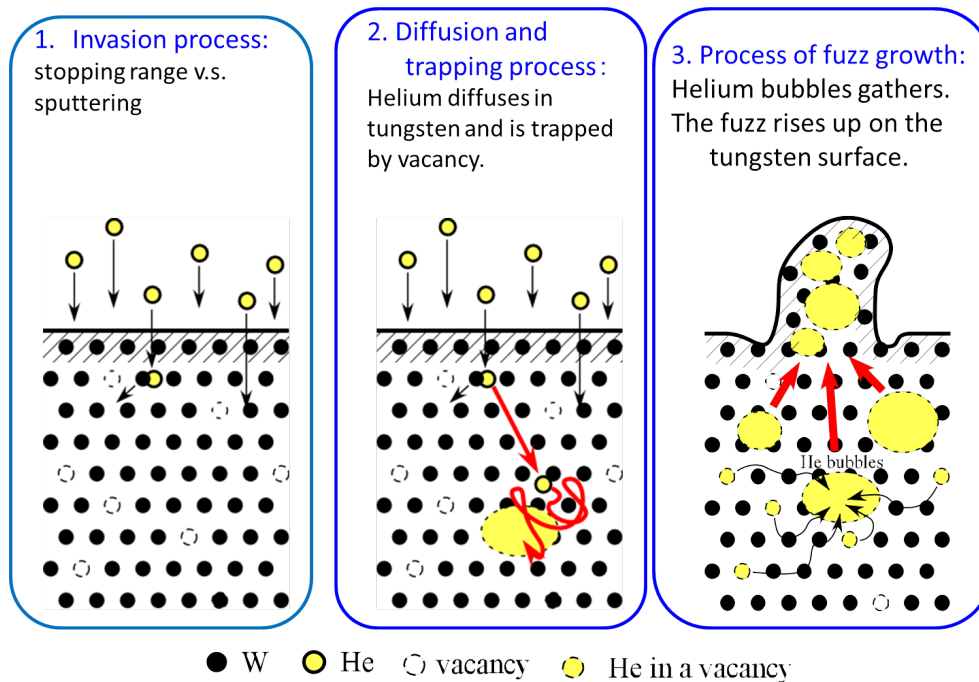


Figure 1. Outlook chart of the fuzz formation process.

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 is strongly depends on the structure of the target material. Therefore, the penetration depth for amorphous and bcc crystalline structure is carefully investigated in this paper.

2. Simulation Model

BCA simulation is performed by ACVT (atomic collision in any structured target) code [7, 8]. 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 scattering angle of the projectile and the recoil atom at each binary collision is obtained analytically in a two-body interatomic potential. In ACVT code, the Moliere approximation to the Thomas-Fermi potential is employed.

BCA simulation is performed for two types of tungsten structure, i.e., amorphous and bcc crystalline structure. 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.

3. Simulation Result

Figure 2 shows the incident energy dependence of the sputtering yield and the mean depth of penetration in the case of He, Ne, and Ar injection. The solid and dashed lines denote the results in the case 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 compared with that of amorphous structure when incident energy is larger than threshold energies (i.e., approximately 20 eV, 100 eV, and 160 eV for He, Ne, and Ar, respectively). It is found that the difference of the profiles is caused by channeling effect.

In both cases of amorphous and bcc crystalline structure, the mean depth of He is larger than that of Ne and Ar. Even if the target material has polycrystalline tungsten which has the mixed structure of amorphous and bcc crystal structure, it is expected that He can penetrate to deeper position than Ne and Ar. For the fuzz formation, it is important that incident atoms penetrate deeply enough (more than a few nanometer) with lower incident energy than sputtering threshold energy (i.e., 100 eV, 35 eV, and 33 eV for He, Ne, and Ar, respectively). It is concluded that the fuzz structure is more easily formed by He irradiation than that of Ne or Ar. And the simulation result supports Yajima's experimental results [6].

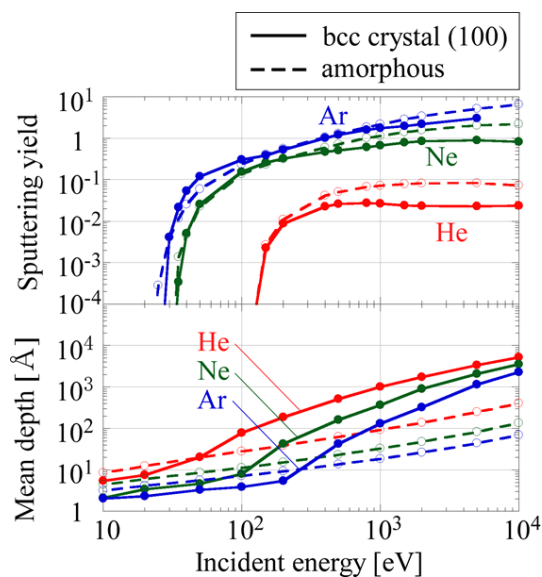


Figure 2. Incident energy dependence of the sputtering yield and the mean depth of penetration in the case of He, Ne, and Ar injection.

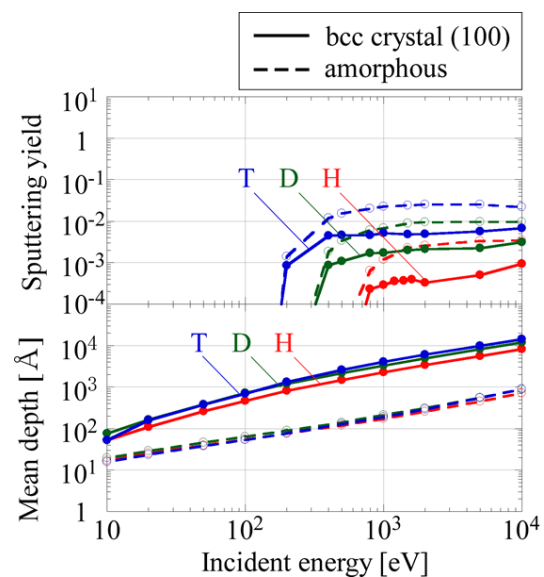


Figure 3. Incident energy dependence of the sputtering yield and the mean depth of penetration in the case of H, D, and T injection.

Figure 3 shows the incident energy dependence of the sputtering yield and the mean depth of penetration in the case of H, D, and T injection. The sputtering threshold energies of H, D, and T are larger than the case of He, Ne, and Ar. It is because the scattering cross-section of H, D, and T is shorter than that of He, Ne, and Ar. The average energy transfer to tungsten atom from H, D, and T is also lower than that from He, Ne, and Ar because the mass ratio of H, D, and T to tungsten atom is low. Because of the same reason, the mean depth of H, D, and T is larger than that of He, Ne, and Ar. Therefore, it is concluded that the H, D, and T has the ability to form the fuzz structure as He as a manner of penetration depth. However, the fuzz formation by irradiation of H, D, and T has not been observed experimentally. For the further

discussion of the possibility of fuzz formation, it is necessary to investigate of the diffusion and trapping process of the incident atoms by vacancies.

4. Summary

The mean depth strongly depends on atomic species and the structure of the target material. However, in both cases of amorphous and bcc crystalline structure, the mean depth of He is larger than that of Ne and Ar. For the fuzz formation, it is important that incident atoms penetrate deeply enough (more than a few nanometer) with lower incident energy than sputtering threshold energy (i.e., 100 eV, 35 eV, and 33 eV for He, Ne, and Ar, respectively). It is concluded that the fuzz structure is more easily formed by He irradiation than that of Ne or Ar. The probability of fuzz formation under H, D, and T plasma irradiation is also investigated in a manner of the penetration depth. The depth of H, D, and T is larger than that of He, Ne, and Ar. H, D, and T is possible to reach deep place under the sputtering threshold energy. For the further discussion of the possibility of fuzz formation, it is necessary to investigate of the diffusion and trapping process of the incident atoms by vacancies.

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