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Simulation Study of Tungsten Materials Exposed to Helium / Neon / Argon Gas Based on Binary Collision Approximation Model

タングステン材へのヘリウム・ネオン・アルゴン入射に対する
二体衝突近似モデルによる評価

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It has been experimentally observed that nanostructured tungsten is formed due to exposure of helium plasma, and that the formation of nanostructure differs from irradiation nuclear species, for example, helium, neon, or argon. We applied a binary collision approximation (BCA) based simulation to the noble gas plasma exposure to tungsten material and found that the BCA model could qualitatively explain differences of nanostructure formation between irradiation nuclear species.

1. Introduction

Tungsten is promising for plasma-facing materials in future nuclear fusion reactors. So it has been intently investigated experimentally and theoretically. It is experimentally observed that nanostructured tungsten is formed due to exposure of helium plasma [1-3], and that the formation of nanostructure or damage on the surface differs from irradiation nuclear species, for example, helium, neon, or argon [3].

To clarify the experimental observations, we apply a binary-collision-approximation (BCA) model [4, 5] to the noble gas plasma exposure to tungsten material.

2. Simulation Model

2.1 *Binary-collision-approximation model (BCA)*

We consider solving behaviors of injected atoms into a material in atomic scale by numerical simulation. When kinetic energy of traced particles is relatively high, it is justified to simplify interactions between material elements including injected particles and reduce them to a sequence of binary collisions.

Each binary collision under a given interatomic potential can be solved analytically [4, 5]. In each collision process, momentum and energy of projectile is transferred to the collision pair of target particle. When the transferred energy is less than a given energy, which corresponds to binding energy, the target material is considered not to be flicked and the position is kept unchanged.

Furthermore, the trajectories of particles are approximated as the asymptotes of them. Thus we can obtain linkages of straight-line segments as particle trajectories. This is a basic concept of binary collision approximation (BCA) model. The BCA model is rather simple and requires less computing resources than molecular dynamics (MD) model, which solves equations of motion for all particles. By use of the BCA model, parameter surveys can be conducted.

2.2 *Simulation conditions*

We employ the BCA-based simulation code ACAT [4], which stands for atomic collisions in amorphous target. As it is indicated by the name, the ACAT code can treat only amorphous structure, not crystalline. Is should be also noted that the temperature effect of target materials is not considered and is assumed to be zero.

Amorphous tungsten is set up in a simulation domain as a target material, and a projectile of helium, neon, or argon atom is repeatedly injected into the material. Incident energy varies from 20 eV to 10 keV and incident angle is 0, that is, normal to the material surface.

For each atomic species and fixed incident energy, 10^5 trials of particle injection into the amorphous tungsten are performed. The Molière approximation to the Thomas-Fermi potential is employed as the interatomic potential.

3. Results and Discussions

A part of incident particles is reflected out of the target material, and the others remain and are distributed in the target material. Fig.1 shows the

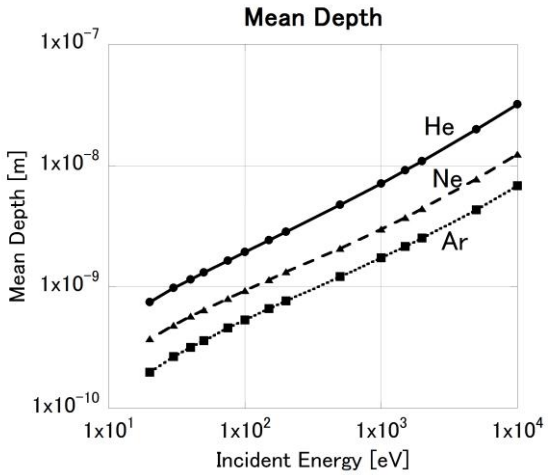

Fig.1. Dependence of mean depth of incident particles on incident energy. Solid line with circles (●), dashed line with triangles (▲), and dotted line with squares (■) indicate the cases for helium, neon, and argon injection, respectively.

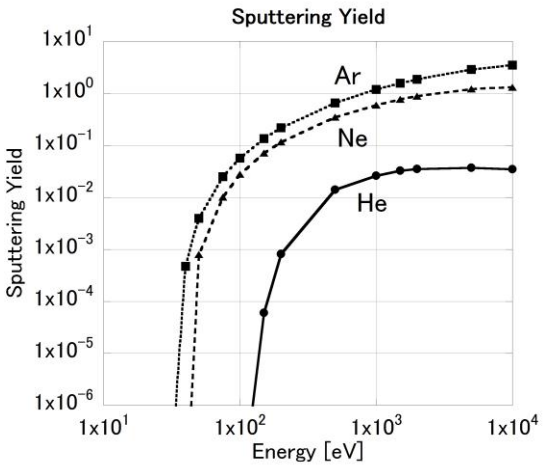

Fig.2. Sputtering yields dependence on incident energy. Meaning of the symbols is same as Fig.1.

mean depth of incident particles as a function of incident energy. It is found that the mean depth is proportional to the square root of the incident energy, which implies that mean depth is not determined by the incident energy, but by the velocity or momentum of projectiles.

Fig.2 depicts the dependence of the sputtering yields on incident energy. It is obvious that sputtering does not occur below the threshold incident energy determined for each projectile species.

In experiments [3], temperature of the target material of tungsten is kept in the range of 1000-2000 K and incident energy of projectile is in the range of 20-200 eV. In the incident energy range, sputtering does not exist, or at least, is relatively small. Fig.1 shows that the mean depth for helium injection at 20 eV is about 1 nm, which corresponds to 3 layers of tungsten crystal. On the other hand, the mean depth for neon or argon injection is 0.2-3 nm corresponding to the thickness of single layer. The depth is shallower than that of experimental results. This difference could be compensated by thermal diffusion process in target material. Furthermore, incident particles ceasing near the target material surface, whose depth corresponds to the thickness of single layer, may be escaped from the surface due to the thermal diffusion, rather than diffuse within the material. If it is the case, our simulation results could qualitatively explain experimental observations of damages on tungsten surface exposed to noble gas plasma [3], especially differences between irradiation nuclear species.

4. Conclusion

We performed binary-collision-approximation (BCA) based simulation to the noble gas plasma exposure to tungsten material. It is found that the BCA model could qualitatively explain differences of nanostructure formation between irradiation nuclear species.

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