§11. BCA Simulation on Noble-gases-absorptivity of Tungsten Fuzz Structure

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1. Introduction

Tungsten fuzz structure is one of the phenonema which attracts attention in the fusion science[1]. In the previous work, we showed the absorptivity as well as the penetration depth and sputtering yield which are basic information to reveal the fuzz formation of tungsten[2]. In this calculation, we used a binary corrison approximation (BCA) to solve scattering phenomena between tungsten atoms and injected atoms, i.e., noble gas atoms. The BCA simulation is performed by AC∀T (atomic collision in any structured target) code[3-5].

In this report, to focus on the target structure, we consider the crystal structure of tungsten whose surfaces are (100), (110) and (111). It is well-known that irradiated atoms can enter the crystal more deeply than the amorphous structure, because "channeling phenomena" occurs in the crystal[4]. Moreover, we treat the simplified fuzz structure in BCA simulaiton, to compare with crystals.

2. Simulation methods and results

The algorithm of the simulation is the same as the previous paper [1,5]. The BCA simulation is performed by AC∀T (atomic collision in any structured target) code [3]. As the tungsten target, we adopted the five types, that is, BCC crystals with (100), (110) and (111) surfaces, the simplified fuzz structure and an amorphous structure.

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) 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.

In Fig.1, the absorptivity of He, Ne, Ar, for each tungsten structure is plotted. From this figure, it is found that the absorptivity depends on the target structure, quantitatively.

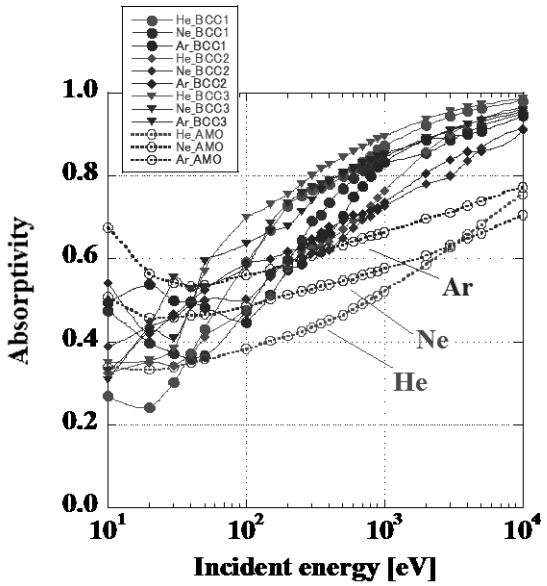

Fig. 1 Absorptivity of He, Ne, Ar for tungsten targets, i.e., amorphous, BCC crystals with (100), (110), (111) surfaces.

In the case of amorphous structure, the absorptivity becomes lower than other crystal structures for all gases. The reason of this dependence is as follows: When the gases are injected, "channeling" phenomena occur in the tungsten crystal. On the other hand, if tungsten target has amorphous structure, gas-atom cannot invade into the tungsten target because the atom is collided with tungsten atoms more frequently than in the tungsten crystals. Thus, the gas is absorbed by amorphous tungsten less than by the crystal ones. The above intuitive investigation is confirmed with the results of BCA simulation.

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