Study on crystal-orientation dependence of irradiation of noble gases to tungsten by BCA approximation

二体衝突近似による希ガス照射のタングステン結晶方向依存性

<u>Hiroaki Nakamura</u>^{1,2} Seiki Saito³, Atsushi M. Ito¹, Arimichi Takayama¹ 中村浩章, 斎藤 誠紀³, 伊藤 篤史¹, 高山 有道

 ¹National Institute for Fusion Science 322-6 Oroshi-cho, Toki, 509-5292, Japan
²Department of Engineering and Science, Nagoya University, 322-6 Oroshi-cho, Toki, 509-5292, Japan
³Department of Electrical Engineering, National Institute of Technology, Kushiro College 2-32-1 Otanoshikenishi, Kushiro, Hokkaido, 084-0916, Japan
¹核融合科学研究所〒509-5292 土岐市下石町322-6
²名古屋大学〒509-5292 土岐市下石町322-6
³釧路工業高等専門学校〒084-0916 北海道釧路市大楽毛西 2-32-1

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.We pick up the first process of the fuzz structure formation, that is, the invasion process. We calculate the absorptivity of noble gases into tungsten. We use a binary collision approximation (BCA) to solve scattering phenomena between tungsten atoms and injected atoms, i.e., noble gas atoms. The BCA simulation is performed by $AC \forall T$ (atomic collision in any structured target) code. Using this code, we calculate the absorptivity as well as the penetration depth and sputtering yield which are basic information to reveal the nano-structure formation. We found that these physical quantities depend on the crystal orientation of the target tungsten.

1. Introduction

Tungsten fuzz structure is one of the phenomena which attract attention in the fusion science (Fig.1) [1]. In the last year, 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 collision approximation (BCA) to solve scattering phenomena between tungsten atoms and injected atoms, i.e., noble gas atoms. The BCA simulation is performed by $AC \forall T$ (atomic collision in any structured target) code[3-5].

In this paper, 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 simulation, to compare with crystals.

2. Binary-collision-approximation simulation

As the first approach to reveal the structure formation mechanism, we pick up the invasion process of helium into Plasma Facing Material and we developed AC \forall T (atomic collision in any structured target) code. In BCA simulation, multi-body interactions in a material approximate to consecutive two-body interactions between a projectile atom and the nearest neighbor atom. Using this code, we calculate the penetration depth and sputtering yield which are basic information to reveal the nano-structure formation.



Fig. 1 Schematic images of processes of the fuzz structure formation.

BCA simulation is performed by $AC \forall T$ code [2-4]. The scattering angle of the projectile and the recoil atom at each binary collision is obtained analytically in a two-body interatomic potential [5].

2. Simulation methods and results

The algorithum of the simulation is the same as the previous paper [1,5]. As the tungsten target, we adopted the five types, that is, BCC crystals with (100), (110) and (111) surfaces, the simplified fuzz strucutre and an amorphous structure. In Fig.2, the absorptivity of He, Ne, Ar for each tungsten strucutre is plotted. From this figure, it is found that the adsorptivity depends on the turget structure, quantitatively.



Fig. 2. Absorptivity of He, Ne, Ar for tungsten targets, i.e., amorphous, BCC crystals with (100), (110) and (111) surfaces.

Acknowledgments

This work was supported by JSPS KAKENHI Grant Numbers (24656560, 26330237), MEXT KAKENHI Grant Number (25249132), and the NIFS Collaboration Research programs (NIFS14KNTS028, NIFS13KNSS037, NIFS14KNTS030, and NIFS14KBAS016).

References

- S. Kajita, T. Saeki, Y. Hirohata, M. Yajima, N. Ohno, R. Yoshihara and N. Yoshida: Jpn. J. Appl. Phys. Vol. 50, p. 08JG01 (2011).
- [2] H. Nakamura et al, ISPlasma 2014, 06aP06.
- [3] Takayama, S. Saito, A.M. Ito, T. Kenmotsu and H. Nakamura: J. Appl. Phys. Vol. 50, p.01AB03 (2011).
- [4] S. Saito, A. Takayama, A.M. Ito and H. Nakamura: Proc. Int. Conf. Model. Simulation Technol. p.197 (2011).

[5] S. Saito, A. M. Ito, A. Takayama, and H. Nakamura: J. Nucl. Mat. Suppl. Vol. 438, p. S895 (2013).