

## Molecular Dynamics Simulation Approach to Plasma-Wall Interaction

プラズマ壁相互作用の分子動力学シミュレーション研究

Atsushi M. Ito<sup>1</sup>, Seiki Saito<sup>2</sup>, Arimichi Takayama<sup>1</sup>, Sachio Yonemura<sup>2</sup>, and Hiroaki Nakamura<sup>1,2</sup>

伊藤 篤史<sup>1</sup>, 斎藤 誠紀<sup>2</sup>, 高山 有道<sup>1</sup>, 米村 幸朗<sup>2</sup>, 中村 浩章<sup>1,2</sup>

1) National Institute for Fusion Science, 322-6 Oroshi-cho, Toki 509-5292, Japan.

2) Graduate School of Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan.

1) 核融合科学研究所 〒509-5292 岐阜県土岐市下石町322-6

2) 名古屋大学大学院 工学研究科 〒464-8602 愛知県名古屋市不老町

In the investigation of integrated simulation for plasma-wall interaction (PWI) to evaluate tritium retention and exhaust, the role of molecular dynamics (MD) simulation was to clear the mechanism of chemical sputtering. The results of the MD simulations implied that the chemical sputtering is composite phenomenon of "chemical desorption" and "thermal desorption" processes. The former is the molecular detachment by using not only incident energy but also adsorption energy of incident atoms and ions. The latter means that molecules are thermally desorbed from local fragile structures created by amorphization, i.e. chemical erosion. In this paper, furthermore, new extensions of PWI simulation are introduced.

### 1. Introduction

In the "tritium science and technology for fusion reactor" project, the Ohya simulation group has developed an integrated simulation code for PWI in order to estimate accurately tritium retention and exhaust in fusion reactors. The key point of this integrated simulation code was how to connect different models of scrap-off layer (SOL)/divertor plasma and plasma facing material (PFM). Here, the EDDY<sup>[1]</sup> based on binary collision approximation (BCA) was employed as a simulation code for the particle dynamics in PFM because the BCA can be quickly executed. The effect of chemical sputtering, which cannot be treated by the BCA, was compensated with the parameters evaluated by the MD. However, when the project started, the chemical sputtering was not well understood. Therefore, the first goal of the MD was to clarify the mechanism of the chemical sputtering.

In the present paper, at first the chemical sputtering is explained with the result of the MD. Next, new extensions of the MD and BCA for future problem of PFM are introduced.

### 2. Understanding of the Chemical Sputtering

The word of "chemical sputtering" had been used as meaning of the molecular desorption from PFM which cannot be explained by physical sputtering. Researches with the MD made progress in understanding the chemical sputtering. As a result, the chemical sputtering can be classified into the following two processes.

The first process is that atoms on a PFM surface are desorbed by chemical reaction with an incident hydrogen atom/ion in a short time of pico-second.

In this "chemical desorption process", although the incident energy is lower than displacement energy, the atoms on a PFM surface can be detached by adding energy generated from the adsorption of an incident particle onto the surface, which is called adsorption energy. The chemical desorption process can be clearly explained by the MD in which an hydrogen atom was injected onto a diamond (111) surface<sup>[2]</sup>. On the diamond (111) surface, atoms or molecules are sputtered if an incident energy was higher than 5 eV. Figure 1 shows the ratio of species of the sputtered atoms and molecules. From this figure, it is understood that the CH molecule is mainly desorbed for incident energy of lower than 20 eV, while the C atom is dominantly sputtered in higher incident energy. Moreover, from many simulations varying incident position, it was found that the incident position causing the CH desorption corresponds to that causing the adsorption of the incident hydrogen atom. This fact confirms the expectation that hydrocarbon molecules are generated by the chemical desorption mainly whereas the physical sputtering means to knock out a single atom by high energy incidence.

It is expected that the chemical desorption process easily occurs in also the surface of amorphous graphite. However, we has difficulty in understanding that the chemical desorption process hardly occurs in the center region of a surface of "graphene" because the structure of the graphene is too stable to be sputtered by low energy incidence of an hydrogen atom<sup>[3,4]</sup>.

Desorption from graphitic materials, which are composed of the graphenes, e.g. carbon fiber composite (CFC), is explained by the second process in a long time. Through incident and

adsorption energies are not enough to detach hydrocarbon molecules from the surface of the graphene, they are enough to reconnect covalent bonds. Namely, the graphitic material is amorphized by the chemical reaction with the incident hydrogen atoms/ions, which is called chemical erosion. By the chemical erosion, local fragile structures are generated with the increase of the H/C ratio. The hydrocarbon molecules are detached from the local fragile structure by using thermal energy during long time vibration, which is called "thermal desorption process" here.

In the MD, this thermal desorption process can be observed by using thermostat method[5]. The MD with the Langevin thermostat showed the dominant molecular species emitted by the thermal desorption process was hydrogen rich hydrocarbon molecules such as CH<sub>4</sub> and CH<sub>3</sub>, and their sputtering yields agreed with experimental results[6] in the dependence on surface temperature. The important prediction from the MD is that almost all hydrocarbon was detached in a state of CH residue firstly and then it grew to CH<sub>4</sub> while drifting in the void region of eroded amorphous carbon. Direct detachment in the state of CH<sub>4</sub> and CH<sub>3</sub>, which has been considered as a main process for a number of years, hardly occurred. Moreover, the quantum chemical calculation result that the state of CH<sub>2</sub> residue is unstable in formation energy[7] supports this prediction from the MD.

In this manner, "chemical sputtering" we has been called is classified into the chemical desorption process in a short time and the thermal desorption process in a long time. The deference between the chemical and thermal desorption processes is that in the former process, the desorbed hydrocarbon molecule is accompanied by the last incident hydrogen atom.

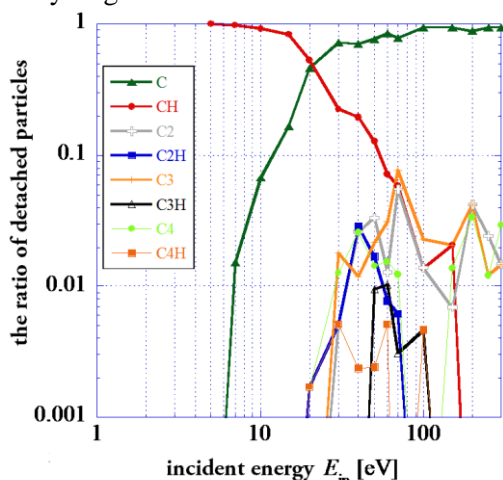


Fig.1. The ratio of species of the sputtered atom and molecules from the diamond (111) surface as a function of the incident energy of an hydrogen atom.

### 3. Development of New Simulation Methods

The problems about the PFM cannot be solved only by the current simulation codes. Therefore, we have developed theory and simulation methods, where we stick to atomic dynamics.

One of developed methods for high energy incidence is modified BCA code AC $\nabla$ T[8] which can deal with arbitrary material structure, while the original ACAT[9] and ACOCT[10] codes can treat only random (not amorphous) and crystal structures, respectively. Using the AC $\nabla$ T code, amorphization from a crystalline material by the continuous injection of atoms and ions can be simulated[11].

Furthermore, we have developed BCA-MD hybrid simulation code[12] in which while the kinetic energy is high, atomic trajectory is quickly calculated by the AC $\nabla$ T, and after the kinetic energy becomes low, region around cascade particles is locally simulated by the MD. The BCA-MD hybrid code enables to treat chemical and physical processes in micro- scale PFM.

### 4. Summary

By the MD simulation, the chemical sputtering is clarified as combination phenomena of the chemical desorption and thermal desorption processes. In order to achieve nuclear fusion, new simulation methods for the PWI and PFM problems should continue to be developed.

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### References

- [1] K. Ohya, Phys. Scripta T124 (2006) 70.
- [2] S. Y., S. S., A. M. I., A. T., H. N., 30th JSST Annual Conference. October 22-23, 2011, Tokyo, Japan, 86.
- [3] A. I., H. N. and A. T., JPSJ **77** (2008) 114602.
- [4] S. S., A. M. I. and H. N. J. Appl. Phys. in press.
- [5] A. I., K. O., K. I. and H. N., Contrib. Plasma Phys. **50** (2010) 464-469.
- [6] B. V. Mech, A. A. Haasz and J.W. Davis, J. Nucl. Mater. **241-243** (1997) 1147.
- [7] Y. Zempo and M. Tanaka, Newsletter of NIFS (Feb. 2004)
- [8] A. T., S. S., A. M. I., T. K. and H. N., JJAP **50** (2011) 01AB03.
- [9] Y. Yamamura and Y. Mizuno, IPPJ-AM-40, Inst. Plasma Physics, Nagoya University (1985).
- [10] Y. Yamamura and W. Takeuchi, Nucl. Instr. Meth. **B29** (1987) 461.
- [11] S. S., A. T., A. M. I., H. N., 30th JSST Annual Conference. October 22-23, 2011, Tokyo, Japan, 86.
- [12] S. S., A. M. I., A. T., T. K. and H. N., J. Nucl. Mater. **415** (2011) S208-S211.