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Simulation of Hydrogen Atom Injection into Amorphous Carbon Materials with Chemical Reaction

アモルファス炭素材への化学反応を考慮した水素照射シミュレーション

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The behavior of incident hydrogen atoms in amorphous carbon materials is investigated by particle simulation with taking both the physical and chemical reaction. The chemical reaction cannot be neglected when the kinetic energy of projectile is low because a carbon atom makes four covalent bonds. The physical sputtering is often simulated by applying binary collision approximation (BCA). However, BCA-based simulation cannot apply for the phenomena where chemical reaction is dominant. Molecular dynamics (MD) simulation with modified Brenner's reactive empirical bond order potential is possible to employ for phenomena with chemical reaction. In this paper, therefore, simulation of hydrogen injection into amorphous carbon materials is performed by BCA-MD hybrid simulation.

1. Introduction

Carbon materials are regarded as one of candidates of the divertor plate of nuclear fusion reactor because carbon material has excellent characteristics such as high melting point, low atomic number, and high thermal conductivity. However, carbon material has some problems that erosion by chemical sputtering, co-deposition of hydrogen isotope, and tritium retention in the bulk of carbon material.

The surface of divertor plate changes into amorphous structure by the irradiation of hydrogen plasmas. Moreover, carbon atoms sputtered from divertor plates and they form amorphous carbon materials on the vacuum vessel walls. Carbon and hydrocarbon redeposition onto plasma-facing components lead to long-term accumulation of large invessel tritium inventories. To achieve the steady operation of nuclear fusion device with carbon divertor, it is necessary to investigate the physical and chemical interactions between plasma and amorphous carbon materials.

In this paper, therefore, the behavior of incident hydrogen atoms in amorphous carbon materials is investigated by particle simulation with taking both the physical and chemical reaction.

2. Simulation Method

The physical sputtering is often simulated by applying binary collision approximation (BCA) [1-3]. In the BCA-based simulations, multi-body interactions between atoms in materials approximate to consecutive two-body interactions between a projectile and the nearest neighbor atom. Therefore, the BCA-based simulation is not applicable for the case where chemical reaction is dominant although the approximation significantly reduces the computation time.

Molecular dynamics (MD) simulation [4] with modified Brenner's reactive empirical bond order potential [5-6] is applicable for carbon and hydrogen system with taking chemical reaction because the MD simulation calculates multi-body interactions between atoms. However, MD simulation needs longer computation time than BCA-based simulation.

To research the motion of hydrogen atoms in carbon materials with chemical reaction in reasonable computation time, we developed hybrid simulation combining BCA-based simulation using AC∀T code [7] and MD simulation. As shown in Fig. 1, the hybrid simulation [8-9] is performed by the following way. A large material is treated by AC∀T. When the kinetic energies of atoms become lower than a threshold value, the atoms and their surrounding atoms are calculated by the MD.

3. Preparation of Amorphous Carbon Material

BCA-based simulation has often applied for Monte-Carlo simulation to obtain statistical values. In the Monte-Carlo simulation, the amorphous structure is treated as atoms placed randomly. The random structure is not applicable for the BCA-MD hybrid simulation because strong forces suddenly

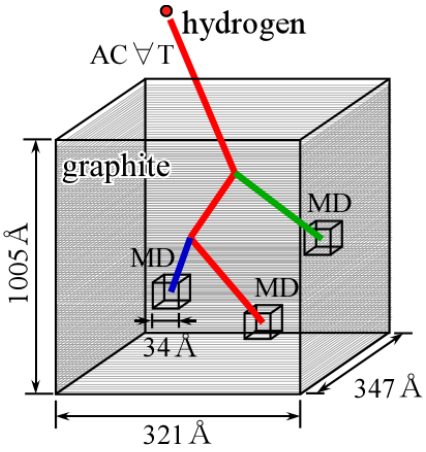

Fig.1. Schematic diagram of the BCA-MD hybrid simulation of hydrogen injection into a graphite [8].

work between atoms to reduce its potential energy when the simulation method switches from BCA to MD. For the BCA-MD hybrid simulation, therefore, it is necessary to prepare the amorphous carbon material which is in the state of local minimum of its potential energy.

We prepare a cubic amorphous carbon material whose size of 20.19Å×20.86Å×20.0Å. The cubic material has the periodic boundary in x, y and z directions. As shown in Fig. 2, a submicrometer-scale amorphous carbon material is obtained by arranging the cubic material. Figure 3 shows the preparation. The process consists of three steps. In the first step, an amorphous carbon material is obtained by carbon deposition with periodic boundary in *x* and *y* directions. In the second step, a cubic material whose size of 20.19Å×20.86Å×20.0Å is cut out from the obtained material by the first step. In the third step, the cubic material is annealed at 2400 K in a box which has periodic boundary condition in *x*, *y* and also *z* directions.

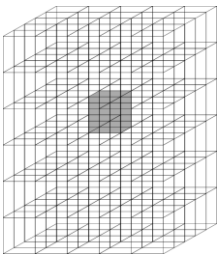

Fig.2. Amorphous material in submicrometer-scale which is divided into periodic boundary cells.

3. Research Approach

Hydrogen injection into the amorphous carbon material, which is explained in section 2, is performed by BCA-MD hybrid simulation. The ranges and reflection rates of incident hydrogen atoms are extracted from the simulation results. The sputtering yield is also investigated.

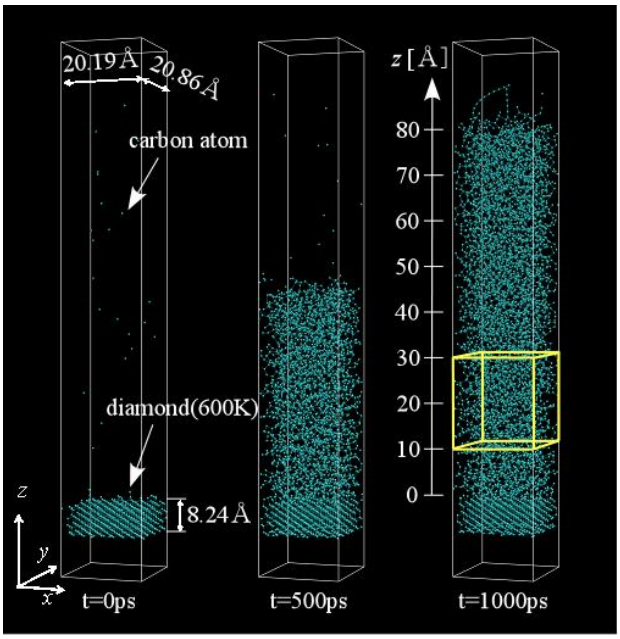

Fig.3. Simulation model for deposition [10].

Acknowledgments

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