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Molecular Dynamics Simulation of Bombardment of Hydrogen Atoms on Graphite Surface

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Abstract. The new potential model of interlayer intermolecular interaction was proposed to represent "ABAB" stacking of graphite. The bombardment of hydrogen atoms on the graphite surface was investigated using molecular dynamics simulation. Before the first graphene from the surface side was broken, the hydrogen atoms caused the following processes. In the case of the incident energy of 5 eV, many hydrogen atoms were adsorbed on the front of the first graphite. In the case of the incident energy of 15 eV, almost all hydrogen atoms were reflected by the first graphene. In the case of the incident energy of 30 eV, the hydrogen atoms were adsorbed between the first and second graphenes. The radial distribution function and the animation of the MD simulation demonstrated that the graphenes were peeled off one by one, which is called graphite peeling. One C_2H_2 was generated in such chemical sputtering. But the other yielded molecules often had chain structures terminated by the hydrogen atoms. The erosion yield increased linearly with time.

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Key words: Plasma surface interaction, chemical sputtering, graphite, graphene, hydrogen atom.

1 Introduction

In the research into nuclear fusion, we deal with the plasma surface interaction (PSI) problem [1–7]. In the experiment of plasma confinement, a portion of hydrogen plasma flows into the divertor walls, which are shielded by the tiles of polycrystalline graphite or carbon fiber composite. The hydrogen plasma which has weak incident energy erodes

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these carbon tiles. This process is called chemical sputtering. The erosion produces hydrocarbon molecules, such as CH_x and C_2H_x. The hydrocarbon molecules affect the plasma confinement. The PSI has been researched using molecular dynamics simulation (MD) [8–11].

The authors have performed the MD simulation of the PSI on graphite surface using the modified Brenner reactive empirical bond order (REBO) potential [12]. From the MD simulation, it is shown that if incident energy is 5 eV, the surface of the graphite absorbs many hydrogen atoms, while if the incident energy is 15 eV, almost all of hydrogen atoms are reflected by the surface. These absorption and reflection occur on the first graphene from the surface of the graphite. This behavior appeared in the case of deuterium and tritium injection also [13]. The absorption and reflection on the first graphene layer could be explained by the MD simulation of the chemical interaction between a single hydrogen atom and a single graphene [14–16]. The MD simulation revealed that the hydrogen atom with the incident energy of more than 20 eV could penetrate the first graphene from the surface of the graphite. This penetration relates to the intercalation of the hydrogen atoms between the graphite layers. However, in the MD simulation of the graphite, the intercalation between graphite layers did not appear. To be precise, the layer structure of the graphite was broken as soon as the hydrogen atoms dived under the graphite surface. Because the incident hydrogen atoms pushed the graphite surface, covalent bonds between the first and second graphenes occur. The graphenes bound by the covalent bonds change into an amorphous structure. This was the trigger of the graphite erosion.

The above MD simulation did not include the interlayer intermolecular interaction of the graphite. If the interlayer intermolecular interaction is adopted, the above dynamics changes. However, the interlayer intermolecular interaction of the graphite has not been clarified enough. For example, the existing potential model of the interlayer intermolecular interaction for the MD simulation does not deal with "ABAB" stacking of the graphite structure. Before we look into the effect of the interlayer intermolecular interaction, we need to create a new potential model of the interlayer intermolecular interaction.

We enrich the MD simulation of the bombardment of the hydrogen atoms on the graphite surface with the interlayer intermolecular interaction. In Section 2, we denote the modified Brenner REBO potential and the potential model of the interlayer intermolecular interaction. The simulation model is described in Section 3. Simulation results are shown in Section 4 and discussed in Section 5. This paper concludes with a Section 6.

2 Potential models

2.1 Modified Brenner REBO potential model

We describe the model of Brenner reactive empirical bond order (REBO) potential [17] and our modification points. This potential model is created based on Morse potential [18], Abell potential [19] and Tersoff potential [20,21].