22P002-O

Physical Action of Particle Irradiation from Atmospheric Pressure Plasma to Liquid Surface
大気圧プラズマから液体表面へ粒子照射した際の物理的作用

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Although an atmospheric-pressure glow discharge with a liquid cathode is widely studied, the phenomena at the plasma-liquid interface are not well known. In this wook, we have investigated the influence of heavy particle irradiation from plasma to liquid surface on physical phenomena by classical molecular dynamics simulation. The influences of the heavy particle impact with 10-100 eV such as sputtering and local liquid heating were studied. We found the increase in temperature of liquid and the evaporation of several molecules.

1. Introduction

In late years, the studies on generations and applications of atmospheric pressure non-thermal plasma (APNTP) have been conducted energetically. The APNTP can be irradiated to a variety of materials such as liquid and biological object in addition to the normal solid materials. When we irradiate the APNTP to liquid, the interaction at plasma-liquid interface is important. However, it is currently argued only by the analogism from experimental results. For this reason, we focus on the study of physical action at plasma-liquid interface by numerical simulation. Nikiforov investigated the plasma sputtering of water molecules from the liquid numerically[1], however, the impinging ion energy was too large as that of APNTP. Therefore, we studied influences of the impingement of low energy particles.

2.Procedure

We have carried out the numerical simulation for two cases; (i) energetic argon atom impinges on the surface of liquid argon, and (ii) energetic water molecule impinges on the surface of liquid water. Figure 1 shows geometry of molecules. In case (i) the simulation cell had a size of 29Å ×29Å ×115 Å, and in case (ii) the cell had a size of 31Å ×31Å ×62 Å. Both simulation cells contained 2000 molecules. The vacuum layers which correspond to the gas phase were adjoining the upside and downside of the simulation cell and the sides of the simulation cell were subject to periodic boundary condition. The temperature in simulation cell was adjusted for a few picoseconds by velocity scaling method [2]. A particle is placed in vacuum layer at a distance of 30 Å from the upside of liquid surface and moves to liquid surface at an initial velocity. This numerical simulation was studied by the classical molecular dynamics technique[3.4].

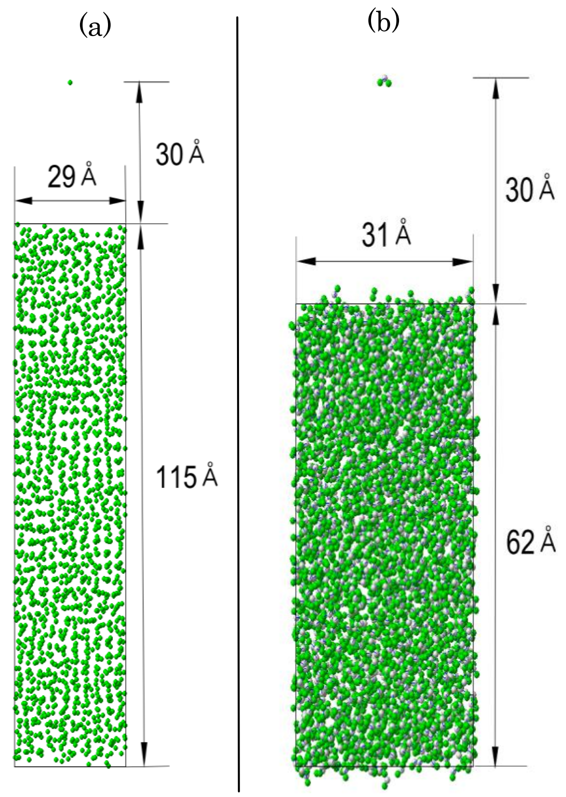


Fig.1. Geometry of the simulation cell; (a) argon and (b) water

In this work, the Lennard-Jones potential was employed as intermolecular potential function to describe the interaction between argon atoms.

Water is modeled by SPC/E-model because it was simple comparatively and properties described by it were close to those of liquid water [5].

Table I presents the initial liquid temperature and the energy of impinging particles.

Table I. Calculation condition

	Case (i)	Case (ii)
Temperature in liquids	87 K	300 K
Energy of impinging particle	10 eV	10,50,100 eV

The local heating of the liquid and the movement of molecules near the liquid surface by impact of particle were investigated.

3. Results

Figure 2 shows the configuration of water molecules at 5 ps after the impingement of the 100 eV particle. The temperature near surface increased and several molecules evaporated.

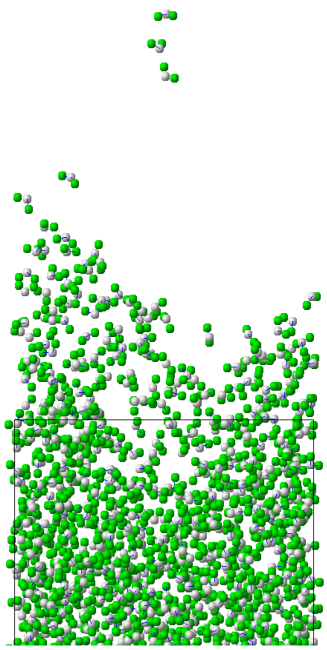
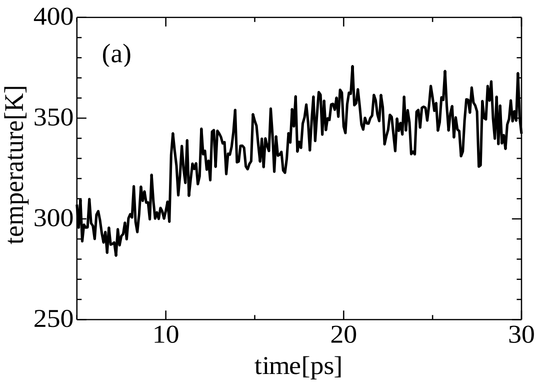


Fig.2. Configuration of water molecules at 5 ps after the impingement of the 100 eV particle.

Figure 3 presents the average temperature change in liquid water at depth in the range of 12 Å by impingement of 10 eV and 100 eV. The particle in vacuum layer started to move at 10 ps and impacted the liquid.

In case of 100 eV particle irradiation, the average temperature rose rapidly and then dropped. Similar temperature change occurred in liquid argon by the impact of 10 eV particle. In case of 10 eV particle irradiation to water surface, the average temperature rose steadily and reached a temperature of about 350 K at 10 ps after the impact of particle. The calculated results suggest that the evaporation and the temperature relaxation process strongly depend on the impinging energy of heavy particle.



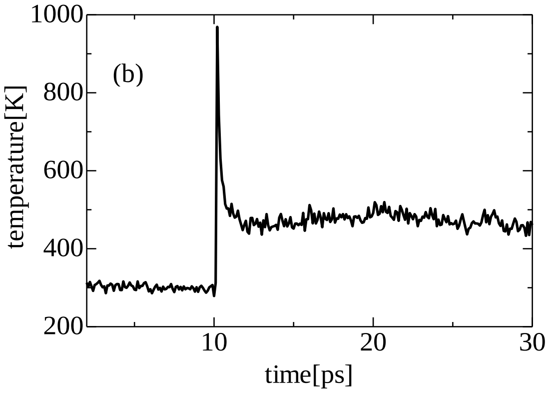


Fig.3. Temperature change of liquid in case(ii). The impinging particle energy is 10 eV for (a) and 100 eV for (b), respectively.

Acknowledgement

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