Abstract Submitted
for the GEC13 Meeting of
The American Physical Society

Molecular dynamics simulation analysis of ion irradiation effects on plasma-liquid interface[1] YUDAI MINAGAWA, NAOKI SHIRAI, SATOSHI UCHIDA, FUMIYOSHI TOCHIKUBO, Tokyo Metropolitan University — Nonthermal atmospheric plasmas are used in a wide range of fields because the high-density plasma can be easily irradiated to various substances such as solid, liquid, biological object and so on. On the other hand, the mechanisms of physical and chemical phenomena at the plasma-liquid interface are not well understood yet. To investigate the effects of ion impact from plasma on water surface, we analyzed behavior of liquid water by classical molecular dynamics simulation. Simulation system consists of an irradiation particle in gas phase and 2000 water molecules in liquid phase. O^+ ion with 10 eV or 100 eV was impinged on the water surface. Ion impact induced increasing water temperature and ejection of water molecules. The averaged number of evaporated water molecules by ion impact is 0.6 molecules at 10 eV and 7.0 molecules at 100 eV. The maximum ion penetration depth was 1.14 nm at 10 eV and 2.75 nm at 100 eV. Ion entering into water disturbs the stable hydrogen bonding configurations between water molecules and gives energy to water molecules. Some water molecules rotated and moved by ion interaction impact on other water molecules one after another. When the water molecule near the surface received strongly repulsive force, it released into gas phase.

[1]This work was supported financially in part by a Grant-in-Aid for Scientific Research on Innovation Areas (No21110007) from MEXT, Japan.

Yudai Minagawa
Tokyo Metropolitan University

Date submitted: 14 Jun 2013 Electronic form version 1.4