Molecular Dynamics Simulation of Reaction Mechanism between Reactive Oxygen Species and Membrane Lipid Molecules in Moisture

S. Uchida[1], T. Yoshida[1], and F. Tochikubo[1]

[1] *Department of Electrical and Electronic Engineering, Graduate School of Science and Engineering, Tokyo Metropolitan University, Tokyo, Japan*

Plasma medicine is an attractive application of atmospheric pressure discharge. However, the atomic scale mechanism related to biological effects was not understood well. In the present work, reactive behavior of plasma radials with a membrane lipid in moisture was simulated using adaptive molecular dynamics. The dependence of chemical processes on radical energy was investigated. At low incident energy, oxygen atom did not penetrate to the water layer of some angstroms. The elemental reaction with water molecule produced two hydroxyl radicals, which finally changed to hydrogen peroxide. On the other hand, high energetic oxygen atom reached to phospholipid and combined with the part of choline. Then, most of incident energy dispersed in surrounding water.

1. Introduction

Medical applications of atmospheric pressure non-equilibrium plasma have been promoted on the basis of stable formation techniques. The biological responses by plasma irradiation must be initiated by the interaction between plasma radical and membrane molecule. However, the theoretical mechanism thorough the complicated reaction processes was not understood well. Recently, the structural change of stratum corneum was numerically clarified with reactive molecular dynamics [1]. In addition, surrounding water strongly affected the chemical reaction of radicals with DNA [2]. In the present work, we investigated the interaction between reactive oxygen species and membrane phospholipid in moisture using adaptive solvent molecular dynamics. The change in reaction processes on the irradiation direction and initial position of radical was also discussed.

2. Analytical method

In the present analysis, the direct contact of oxygen atom (O) to phosphatidylcholine (PC) in water was modeled as a basic interaction of plasma radical with biological membrane. The initial distance from O to PC was set to 6 Å. The incident energy of O was varied from 0 to 10 eV. The calculation time was 10 ps. The force field of each time increment was derived using a semi-empirical molecular orbital method (PM3).

3. Results and discussion

Figure 1 shows the trajectory of O at the irradiation to hydrophilic group of PC. At an incident energy of 0.1 eV, O could not penetrate deeply to water layer. The radical bound to H_2O at the vicinity of initial position. Then, two hydroxyl radicals (OH) were produced. Consequently, the direct combination of OH radicals generated H_2O_2. These are general processes between O and H_2O. On the other hand, high energetic O reached to PC. After colliding with PC, transient binding was occurred around the part of choline. The behavior was different from the dissolve process of PC in air. This result suggests that most of the incident energy of O was dispersed in the surrounding water.

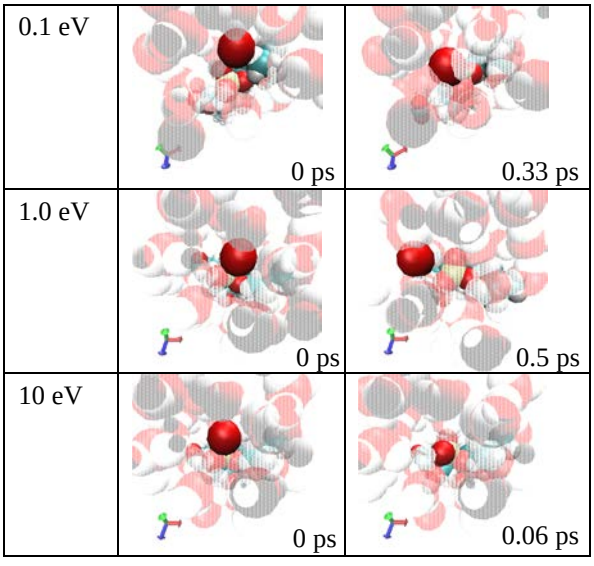

Fig1. Change in reaction processes between O and PC at different irradiation energies in water

References

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