The Role of Dielectric Breakdown in the Formation of Water Molecules in Lunar Regolith. Z. Huang[1], K. Nomura[2], J. Wang[1],(ziyuhuan@usc.edu , josephjw@usc.edu) [1]Department of Astronautical Engineering, University of Southern California, Los Angeles, CA, 90089 [2]Collaboratory for Advanced Computing and Simulations, Department of Chemical Engineering and Materials Science, Department of Physics and Astronomy, and Department of Computer Science, University of Southern California, Los Angeles, CA, 90089

Introduction

While the existence of water and OH molecules in lunar regolith have been confirmed by observations, the mechanism underlying the formation of those molecules is still under debate. Several recent studies have suggested that solar wind proton implantation as a major source for hydrogen in the formation of OH/H_2O. As the lunar surface is electrically charged, previous studies have studied the effects of surface charging on solar wind proton implementation. Multiple models [1] [2] showed that the water distribution detected by M^3[3] matches well with the characteristics of solar wind particle dynamics around lunar surface. The observation from M^3 [4] also provides a direct evidence for the accumulation of water in the permanently shadowed regions (PSRs) where the surface can be charged to an extremely large electric potential [5].

The paper focuses on the role of deep dielectric charging in the formation of OH/H_2O from implemented solar wind protons. Galactic cosmic rays (GCR) and solar energetic particles (SEP) can penetrate into the lunar regolith layer. SEPs deposited inside the regolith layer may stay for days or weeks before they are dissipated [6]. The charge deposited in the regolith layer can build up a strong electric field. Once the electric field exceeds the threshold, it will trigger electrostatic discharge (ESD) of the regolith. We hypothesize that ESD breaks down the lunar regolith and generates oxygen ions. These oxygen ions recombine with the implemented proton to from OH and H_2O molecules. This paper presents a simulation study of this process.

Deep Dielectric Charging Calculation

We first calculate deep dielectric charging by SEP on the lunar surface. Utilizing the JPL proton fluence model[7], the electric field in the regolith layer for a given SEP event is calculated from[8]:

$$\nabla \cdot E = -\nabla^2 \Phi = \frac{\rho}{\varepsilon_0}$$
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (J_R + J_C)$$

where the J_R in the second equation is the incident radiation current density, and the J_C is the conduction current density. For a typical SEP event, we find the electric field inside the lunar regolith layer will reach $10^6 - 10^8$ V/m, which generally exceed the threshold for dielectric breakdown. A more general model with the statistics of SEP events will be given in this paper.

Molecular Dynamics Simulation

We next carry out Molecular Dynamic (MD) simulation to study the breakdown process. The MD simulation utilizes the results from deep dielectric charging as input. In the simulation, we approximate a lunar regolith grain as a silica (SiO_2) nanoparticle. The MD model used is RXMD [9][10], which simulates the dynamics of atoms under electric field. MD simulations are carried out for different nanoparticle sizes and temperatures to simulate the breakdown processes under various environmental conditions. Preliminary results are shown in Figure 1.

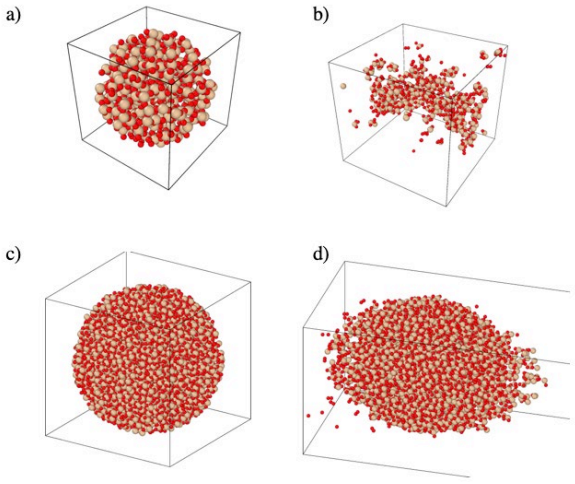

Figure 1 – RXMD simulation of the silica nanoparticle breakdown process under strong electric field. a) and b): dielectric breakdown of a silica nanoparticle with a radius of 50Å. c) and d): dielectric breakdown of a silica nanoparticle with a radius of 500Å. In both simulations, the temperature is 300 K and the initial electric field is 1V/Å. The yellow particles represent silicon atoms and the red particles represent oxygen atoms. The oxygen ions broken away from the silica can be seen in b) and d).

Summary

We propose a new hypothesis that the origin of water molecule in lunar regolith. Deep dielectric charging and molecular dynamics simulation are used to simulate the breakdown process of the regolith and the formation process of the water molecule. This model may also explain the abundant distribution of water in PSRs. The PSRs experience more dielectric breakdown events from GCR and SEP since the regolith in PSRs has longer discharging timescale [11].

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