Molecular dynamics simulation for dehydration of phyllosilicate of Ryugu

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The Hayabusa2 spacecraft, which was launched by the Japan Aerospace Exploration Agency (JAXA), conducted in situ observations of the near-Earth asteroid (162173) Ryugu [1-3]. Through these observations, the near-infrared spectrometer (NIRS3) equipped in Hayabusa2 detected a ∼2.7 μm absorption band in the reflectance spectrum [2]. This wavelength (∼2.7 μm) of the absorption band corresponds to the O–H stretching vibration mode. Thus, it was revealed that Ryugu has phyllosilicate such as serpentine and saponite [1, 2]. NIRS3 also observed the ∼2.7 μm absorption band inside an artificial crater (~1 m subsurface) [4]. The absorption depth at the subsurface was found to be deeper than that of the surface [4]. Thus, the amount of OH is reduced at the surface. This tendency was also indicated by several laboratory analyses of Ryugu samples [5-7]. The absorption depth of the samples was about twice as large as that observed through remote sensing.

One probable cause of this discrepancy of the absorption depth is space weathering [8]. Space weathering is defined as the gradual alteration of materials by outer space environment such as micrometeoroid bombardment and solar wind irradiation [9]. Laboratory experiments using laser pulse have revealed that micrometeoroids can cause dehydration of phyllosilicate [10].

Experiment is one of the most important methods to reveal the mechanism of space weathering. However, chemical changes for dehydration occur within a picosecond (~10^{-12} second) of time scale, which is too short to observe detailed atomic interactions in laboratory. To understand chemical interactions between atoms, molecular dynamic (MD) simulation can be useful. Recently, reactive MD simulations for dehydration by micrometeoroid bombardment were performed [11]. In these simulations, ~2nm sized dust particles with 20 km of impact velocity dissociated ~200 O-H bonds in serpentine. A part of the dissociated O and H atoms initially connected to Mg generated Si-OH and H_2O, which can be an offset of the dehydration (OH reduction). Although the timescale of the simulation is limited to 1 ps due to small calculation domain, the MD simulations showed that micrometeoroid bombardment can cause dehydration of phyllosilicate of Ryugu. Here, I introduce these MD simulation results. In addition, we are now conducting MD simulations for nano phase iron ($npFe^0$) with olivine structure. Nano phase iron is observed lunar grains, which has been indicated to be caused by space weathering. Although the results are still preliminary, the simulations for micrometeoroids impact to olivine will also be introduced briefly.

References

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