

Dissolution process of forsterite coexisting with interstitial water

Y. Kobayashi, T. Ikeda-Fukazawa

Department of Applied Chemistry, Meiji University, Japan

Inclusions of liquid water have been found in the samples collected from the carbonaceous asteroid Ryugu [1]. Though the origin of water is not conclusive, the deposited ice on mineral dust grains in interstellar molecular clouds could be a potential cause. In interstellar molecular clouds, mineral dust grains are covered with amorphous ice mantles [2]. The major component of the mineral dust grains is forsterite (Mg_2SiO_4) in glassy state [3], which is considered to undergo a mineral evolution through various processes to be a crystalline state in planets. Although most water molecules desorb from the mineral grains with heating during the formation of protoplanetary disk, residues can be confined in the grain boundaries as an interstitial water. The interstitial water of forsterite has unique properties. Kubo et al. [4] found that the interstitial water of glassy forsterite has higher density than that of ordinary water and exists as liquid state at high temperatures above the boiling point. However, the mechanisms of the structural change of the interstitial water have not yet been well understood. In this study, molecular dynamics (MD) calculations were performed to investigate the effects of thickness of water layer on structure of interstitial water and forsterite.

MD calculations were performed using the MXDORTO program developed by Kawamura [5]. Fundamental orthorhombic cells consisting of 484–3311 H_2O and 1176 Mg_2SiO_4 (forsterite in crystalline or glassy states) were used as the initial structures. The thicknesses of water layer d between the forsterite phases were controlled with the number of H_2O to be 1–6 nm at the initial structure. The MD code was run with an NTP ensemble at 280–670 K. The pressure was kept at 0.1 MPa. The structure was analyzed using the equilibrated states. For the comparison, the pure water system consisting of 360 H_2O was also calculated.

Dissolutions of Mg and Si from the glassy forsterite toward interstitial water were observed at temperatures above 280 K for the system with $d > 1$ nm. The dissolved Mg exists as MgO_6H_x unit and forms $\text{Mg}(\text{OH})_2$ crystal by collisions of the MgO_6H_x units in water layer [4]. The dissolved Si maintained tetrahedral SiO_4 structure due to the strong Si–O bond.

For crystalline forsterite, in contrast, no dissolution of Mg and Si was observed at temperatures below 610 K. Only Mg dissolved at temperatures above 630 K for the system with $d < 1.5$ nm. The dissolution of Mg generates a defect on the surface of crystalline forsterite. The distortion of structure around the defects might promote an additional dissolution of Mg. The dissolution occurs for the systems with $d < 1.5$ nm, because the density of water increases as the thickness of the water layer decreases. The result suggests that the dense structure of interstitial water has an effect to enhance the decomposition of crystalline forsterite. Since the number of dissolved Mg was extremely small, the formation of $\text{Mg}(\text{OH})_2$ crystal was not observed in the calculation period of the present study (3.0 ns).

References

- [1] T. Nakamura et al., 2023, *Science* 379, 8671.
- [2] J. M. Greenberg & J. I. Hage, 1990, *ApJ* 361, 260.
- [3] T. Henning, 2010, *Annu. Rev. Astron. Astrophys.* 48, 1.
- [4] A. Kubo, J. Nishizawa, & T. Ikeda-Fukazawa, 2022, *Chem. Phys. Lett.* 805, 139932.
- [5] K. Kawamura, MXDORTO, 1996, Japan Chemistry Program Exchange 029.