

Structure and diffusion dynamics of forsterite and its interstitial water

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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 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] showed that the interstitial water of glassy forsterite has high density than that of ordinary water. However, the mechanisms of the changes in the structure and properties have not yet been understood. In this study, molecular dynamics (MD) calculations were performed to investigate the effects of thickness of water layer on diffusive properties and structures of interstitial water of forsterite. In addition, the effects of interstitial water on the diffusive properties of the coexisting forsterite were also investigated.

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 of forsterite-water systems. The thicknesses of water layer between the forsterite phases were controlled with the number of H_2O to be 1–6 nm. The MD code was run with an NTP ensemble for 2.0 ns at 280–470 K. The pressure was kept at 0.1 MPa. The structure and diffusive properties were analyzed using the equilibrated structures. To compare the results, the calculations were performed using a pure water consisting of 360 H_2O .

The results showed that the density of water increases as the thickness of the water layer decreases at the thickness of $< \sim 2$ nm. The density becomes almost constant when the thickness is larger than ~ 2 nm. The mean number of hydrogen bonds of the high-density state is larger than that of pure water. Furthermore, it was found that the self-diffusion coefficient of water molecules decreases as the thickness of the water layer decreases. A similar trend was observed for the interstitial water of crystalline forsterite. The results suggest that the effects of the structurization of water in the interface with forsterite glass [6] propagate to the layer.

To investigate the effects of interstitial water on the structure and properties of forsterite phases, the coordination structure and atomic displacement parameter (ADP) as a measure of the amplitude of thermal vibration of Mg atoms were analyzed. The result showed that the ADP value of Mg decreases as the thickness of the water layer decreases even in the internal part of forsterite, although the coordination number of Mg is almost constant. The decrease in ADP of Mg can be related to the decrease in the self-diffusion coefficients of interstitial water. Due to a restriction from the structured water in the interface, the thermal vibrations of the atoms in the forsterite are hindered.

[1] T. Nakamura *et al.*, *Science* (in press). 10.1126/science.abn8671.

[2] J.M. Greenberg, J.I. Hage, *Astrophys. J.* **361** (1990) 260.

[3] T. Henning, *Annu. Rev. Astron. Astrophys.* **48** (2010) 1.

[4] A. Kubo, J. Nishizawa, T. Ikeda-Fukazawa, *Chem. Phys. Lett.* **805** (2022) 139932.

- [5] K. Kawamura, MXDORTO, Japan Chemistry Program Exchange **029** (1996).
- [6] A. Kubo, J. Nishizawa, T. Ikeda-Fukazawa, *Chem. Phys. Lett.* **760** (2020) 138028.

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