Diffusion mechanisms of H^+ in interface between forsterite glass and amorphous ice

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Forsterite (Mg_2SiO_4) glass exists as dust grains in interstellar molecular clouds [1]. In interstellar molecular clouds, elements such as hydrogen, oxygen, carbon, and nitrogen deposit on the dust grains, and form various molecules (e.g., H_2O, CO, CO_2, NH_3, CH_4, H_2CO, CH_3OH, and so on) [2]. These molecules undergo chemical evolutions to organic molecules through various processes on the surface of the dust grains [2]. The structure of forsterite glass is one of the important factors governing the chemical evolutions in interstellar molecular clouds. However, there are few studies for effects of molecular adsorption on the structure and properties of forsterite glass [3]. To investigate the diffusion mechanisms of proton, we performed molecular dynamics calculations of forsterite glass with amorphous ice, molecular dynamics (MD) calculations were performed.

The MD calculations were performed using an atom-atom potential model with MXDORTO program [4]. The potential parameters were empirically determined by constraining the structure to reproduce the experimental results of density, thermal expansion coefficient, and bulk modulus for forsterite crystal and ice polymorphs [5,6]. A fundamental orthorhombic cell consisting of 1176 Mg_2SiO_4 with two-dimensional periodic boundary conditions was used as the initial structure. The glass structure was prepared by quenching the liquid phase from 3000 to 10 K with 2 K/fs in rate. Then, amorphous ice layer with 3311 H_2O, which was prepared by quenching a liquid phase from 290 to 10 K, was adsorbed on the glass surface. The MD code was run with NTP ensemble in a temperature range of 10–300 K at 0.1 MPa.

The result shows that the coordination number of Mg in the forsterite-ice interface is larger than that of forsterite surface without water phase. At temperatures above 200 K, furthermore, a decomposition phenomenon of H_2O molecule to hydroxide and hydrogen ions was observed. From an observation of the trajectories of the ions, the diffusion mechanism was analyzed. The result shows that the hydrogen ion diffuses in the internal part of forsterite glass via repeated formation and decomposition of MgO_xH_y or SiO_4H_z structures. No diffusion was observed for the hydroxide ion, because the hydroxide ion becomes a stable state due to formation of covalent bonds with Mg or Si in forsterite. The diffusion processes have important implications for chemical evolution in interstellar spaces.

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