フォルステライトガラス–アモルファス氷界面の構造とダイナミクス
Structure and dynamics of 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 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 coexisting molecules on the structure and properties of forsterite glass. To investigate the structure and dynamics of interface between forsterite glass and amorphous ice, molecular dynamics (MD) calculations were performed.

The MD calculations were performed using an atom-atom potential model with MXDORTO program [3]. The potential parameters were empirically determined by constraining the structure to reproduce the experimental results of density, thermal expansion coefficient, and bulk modulus [4, 5]. A fundamental orthorhombic cell consisting of 1176 Mg_2SiO_4 with two-dimensional periodic boundary conditions was used. The glass structure was prepared by quenching the liquid phase from 3000 to 10 K with 2 K/fs in rate. Then, an amorphous ice layer with 9–1580 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 using NTP ensemble with constant area for the surface directions. The pressure was maintained at 0.1 MPa.

The result shows that the atomic displacement parameter (ADP) of each atomic species in forsterite (i.e., Mg, Si, and O) in the interface decreases as the number of H_2O molecules increases. For the forsterite glass without water adsorption, the ADP values of the surface layer are higher than those of internal part due to existence of dangling bonds in the surface layer [6]. To investigate the mechanisms of ADP decrease observed in the interface with amorphous ice, the structure of interface between forsterite glass and amorphous ice was analyzed. The result shows that MgO_xH_y units exist in the interface due to formation of covalent bonds between Mg and O in H_2O. The amplitude of thermal vibration of Mg decreases as the coordination number increases. The present results have important implications for the role of forsterite glass in chemical evolutions in the universe.

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