Effects of Adsorbed H_2O amorphous ice on Surface Structure of Forsterite Glass

A. Kubo, J. Nishizawa, and T. Ikeda-Fukazawa

Department of Applied Chemistry, Meiji University, Japan

Forsterite (Mg_2SiO_4) glass exists as dust grains in interstellar molecular clouds and young stellar objects [1]. In interstellar molecular clouds, elements such as hydrogen, oxygen, carbon, and nitrogen deposit on 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 molecular adsorption on the structure and properties of forsterite glass [3]. To investigate the adsorption process of H_2O and the effect of adsorption on surface structure of forsterite glass, molecular dynamics (MD) calculations were performed.

The MD calculations were performed using an atom-atom potential model with MXDORTO program [4]. The potential parameters for forsterite were empirically determined by constraining the structure to reproduce the experimental results of density, thermal expansion coefficient, and bulk modulus [5]. For H_2O, KAWAMURA potential model was used [6]. A fundamental orthorhombic cell consisting of 2400 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. The quenched glass was warmed to 300 K with the same rate, and 2682 H_2O were adsorbed on the glass. Then, the system was quenched to 10 K with 2 K/fs, and structures were analyzed at 10 K. The MD code was run with NTV ensemble.

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 with adsorption of H_2O amorphous ice. For the forsterite glass without water adsorption, the ADP values of the surface layer were higher than those of internal part due to existence of dangling bonds in the surface layer. To investigate the mechanisms of ADP decrease observed in the interface with amorphous ice, the coordination number of the magnesium atoms was analyzed. The result shows that the coordination number in the interface layer increases with adsorption of H_2O amorphous ice, because new covalent bonds are formed with the adsorbed H_2O molecules. The decrease in the ADP values observed in the interface is resulted from the variation of the coordination number. The mean Mg–O length of the newly formed covalent bonds is 0.256 nm, and is slightly longer than that in the MgO_x units in the forsterite glass without water adsorption (i.e., 0.238 nm). Due to the formation of covalent bonds with H_2O molecules, MgO_xH_2 units exist as an intermediate state in the interface with forsterite glass and amorphous ice. The present results have important implications for the role of forsterite glass in chemical evolutions in the universe.

References

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