Adsorption processes of H_2O water adsorption process on forsterite surface

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Forsterite (Mg_2SiO_4) glass exists as dust grain 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 H_2O molecules forms amorphous ice on the dust grains. Thus, tThe structure of amorphous ice on forsterite glass is one of the important factors governing the chemical evolutions in interstellar molecular clouds. However, there are few studies for adsorption processes of watereffects of coexisting molecules on the structure and properties of forsterite glass. To investigate the adsorption processes structure of interface between of water on forsterite in glassy and crystalline states, and adsorbed H_2O 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 conditionsthe (010) surface was used as the forsterite crystal. The glass structure was prepared by quenching the liquid molten phase from 3000 K to 10 K with 2 K/fs in rate. Then, an amorphous ice layer with 0-100 H_2O were adsorbed on the forsterite surface. The , which was prepared by dropping H_2O molecules were introduced at intervals of 100 ps in the vacuum layer of the system with an initial from positions determined by using random numbers. The introduced H_2O molecules , wereas adsorbed on the forsterite surface with attractive interactions. The MD code was run using NTP ensemble with two-dimensional periodic boundary condition along with constant area for the forsterite surface directions. The pressure was maintained at 0.1 MPa.

The result shows that MgO_xH_y units structure are formed with H_2O adsorption exist oin the forsterite surface because the oxygen and hydrogen atoms in adsorbed H_2O molecules form covalent bonds with Mg and hydrogen bonds with O of forsterite, respectively interface due to formation of covalent bonds between Mg and O in H_2O. The arrangement of adsorbed H_2O adsorption on forsterite glass showed ruleless bondsis disorder, whereas the H_2O molecules has an order arrangement on forsterite in crystalline state. A water molecule can form oneformed 1 covalent bond with Mg atoms and two hydrogen bonds with 2 hydrogen bonds with O atoms on forsterite crystal, because the coordination number of Mg on the (010) surface of forsterite crystal(is three [5]28%). Theis result suggests that the main arrangements of the adsorbed H_2O on forsterite glass have effects on the ice structure of amorphous ice on dust grain in interstellar space is amorphousmolecular clouds. The adsorption mechanisms of H_2O molecules are important to understand not only to the origin of water terrestrial but also to the chemical evolution process of various molecules on amorphous ice in interstellar molecular clouds.

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