Japan Geoscience Union Meeting 2010
(May 23-28 2010 at Makuhari, Chiba, Japan)

SMP057-19 Room: 101 Time: May 24 10:00-10:15

Growth of ferroelectric ice XI doped with alkali metal hydroxide observed using neutron diffraction

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Ice has more than 15 crystalline phases. Ice Ih exists at pressures less than 200 MPa. Ice XI is a hydrogen-ordered phase of ice Ih, and is a thermodynamically stable structure at quite low temperatures.
Based on the numerous neutron diffraction studies for KOD-doped ice, Fukazawa et al. (2006, 200 9) proposed a hypothesis that ice XI exists in the cold space environments such as Pluto, Kuiper, Belt Objects, interstellar molecular clouds and so on. Ice XI is ferroelectric, and electrostatic force attributable to the ferroelectricity might affect the agglomeration of ice particles in space. Ice XI in space might therefore play an important role in planetary formation.
Ice XI was prepared for KOD-doped ice in the previous studies. The KOH dopant acts as a catalyst for the phase transition from ice Ih to ice XI. The OH^- ions, derived from KOH, substitute H_2O sites in the ice (Pisani et al., 1996), and increase the mobility of the protons. In order to discuss the existence of the ferroelectric ice XI in space, we need to confirm that the hydrogen ordering occurs independent of the cations from the dopants. Furthermore, nucleation and growth processes must also be studied to elucidate properties of ice XI. We must investigate the ice XI formation process in detail to estimate where and how much ice XI exists in space.
We prepared ice XI from different kinds of alkali metal hydroxide solutions with different concentrations, and measured neutron powder diffraction at JRR-3 (Japan Atomic Energy Agency, Japan) and HFIR (Oak Ridge National Laboratory, TN, USA). Rietveld analysis was carried out for the obtained diffraction patterns using a two-phase model, which includes ices Ih and XI.
The hydrogen-ordered structure in the lithium-doped ice was the same as that in the sodium-doped and potassium-doped ices. We also confirmed the optimum formation condition of ice XI for the temperature history and concentration of solution.
Furthermore, our results indicate that the phase transition from ice Ih to XI occurs in the doped ice that had once been ice XI to a notably larger degree than in the doped ice that had never transformed to ice XI. We named this phenomenon memory effect of hydrogen ordering.

Keywords: neutron diffraction, ice, planet, infrared spectroscopy, hydrogen ordering, ferroelectric