Contribution ID: **159** Type: **Poster**

Structural change of amorphous ice with warming

Tuesday 9 January 2018 12:35 (1h 30m)

Water exists as amorphous ice in interstellar molecular clouds. Because molecules undergo chemical evolutions through various processes on amorphous ice, the structure and properties of amorphous ice is one of the important factors govern the chemical evolutions of organic molecules in the universe. Amorphous ice is formed by various methods; vapor deposition of water on cold substrates under vacuum, droplet quenching of liquid water, pressurization of crystalline ice Ih, and matrix sublimation method [1]. The formation process of the deposition method is similar to the situation of amorphous ice formation in interstellar molecular clouds. The amorphous ice is mainly classified into two types: low-density amorphous (LDA) and high-density amorphous (HDA) ice, although the structure and properties dependent on formation conditions and thermal history. In the present study, to investigate the structural change of amorphous ice with warming, we measured infrared spectra and performed molecular dynamics (MD) calculations.

Amorphous ice was prepared with vapor deposition of distilled and degassed water on a substrate of oxygen-free copper at 42 K. The total pressure in the vacuum chamber was kept at about 3.5 × 10−5 Pa during the deposition. After the deposition of amorphous ice, the substrate was warmed to 180 K with a rate of 2 K/min. The IR spectra were measured using Shimadzu IRPrestage-21 at 2 K intervals during warming.

Because several peaks exit in the IR spectra in the region of the O–H stretching band (2800–4000 cm−1), the peak positions were analyzed by fitting the data using five Gaussian functions. For four modes in the lower wave numbers are assigned to the in-phase mode of the O–H symmetric stretching, TO and LO modes of the O–H asymmetric stretching, and out-of-phase mode of the O–H symmetric stretching [2]. The mode at the highest wave number is assigned to less coupled H2O [3]. The result shows that the vibrational frequency of the five modes discontinuously change at around 110 K. To analyze the detailed structural change without effects of thermal expansion and pore collapse, the IR spectra of the annealed samples at a temperature in 50 – 150 K were measured. The result shows that the vibrational frequencies of the five peaks significantly change at around 80 –120 K. This indicates that the HDA ice is transformed into LDA ice via few types of intermediate structures in 80 –120 K. The existence of the intermediate structures was also confirmed from the MD result.

References
[1] A. Kouchi, T. Hama, Y. Kimura, H. Hidaka, R. Escribano, N. Watanabe, 2016, Chem. Phys. Lett., 658, 287.
[2] E. Whalley, 1997, Can. J. Chem., 55, 3429.
[3] A. Givan and A. Loewenschuss, C. J. Nielsen, 1997, J. Phys. Chem., 101, 8696.

Significance statement

To investigate the structural change of amorphous ice with warming, we measured infrared spectra and performed molecular dynamics calculations. The result show the HDA ice is transformed into LDA ice via few types of intermediate structures.

Author: Mr KINJO, Akimichi (Department of Applied Chemistry, Meiji University, Japan)

Co-authors: Mr NETSU, Rentaro (Department of Applied Chemistry, Meiji University, Japan); Prof. IKEDA--FUKAZAWA, Tomoko (Dpartment of Applied Chemistry, Meiji University, Japan); Mr KUMAGAI, Yu (Department of Applied Chemistry, Meiji University, Japan)

Presenter: Mr KINJO, Akimichi (Department of Applied Chemistry, Meiji University, Japan)

Session Classification: Poster & Lunch