**Structural transitions of amorphous ice during heating**

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In molecular clouds, elements such as hydrogen, oxygen, carbon, and nitrogen deposit on dust grains, and are transformed into amorphous $H_2O$ ice and other various molecules. Because the molecules undergo chemical evolutions through various processes on amorphous ice, the amorphous ice has an important role for the chemical evolutions in the universe. Vapor deposition method is often used for formation of amorphous ice, because deposition process is similar to the situation of amorphous ice formation in the universe. When water vapor is deposited at a low temperature, high density amorphous ice (HDA) ice is formed [1]. HDA ice is transforms into low density amorphous (LDA) ice with warming. However, the phase transition dynamics is less conclusive because the structure of deposited amorphous ice depends on various factors; deposited temperature, growth velocity, impurities, thermal history after deposition, and so on. To investigate the effects of deposition temperature on phase transition dynamics, we analyzed sublimation and structural changes of water with heating process using mass spectrometry and infra-red (IR) spectroscopy.

Amorphous ice was prepared with vapor deposition of distilled and degassed water on a substrate of oxygen-free copper at 42–100 K. The total pressure in the vacuum chamber was about $2.0 \times 10^{-4}$ Pa during the deposition. After deposition of amorphous ice, the substrate was warmed to 180 K at a rate of 2 K/min. The IR spectra were measured using Shimadzu IRPrestage-21 at 2 K intervals during warming. The mass spectra were measured by Pfeiffer QME220.

From the analyses of mass spectra, the four steps of gas desorption was observed in the temperature range of 42–140 K. For the sample from deposition at 42 K, for instance, the observed gas-desorption temperatures are 70, 100, 110 and 126 K. The desorption temperature decreases as the deposition temperature increases. From the temperature dependence of wave number of O–H stretching modes in IR spectra, the crystallization point to cubic ice (Ic) and transition point from Ic to hexagonal ice (Ih) are confirmed to be around 145 and 175 K, respectively. Thus, the present result suggests that the five types of amorphous phases exist in the temperature range of 42–140 K. The first phase at <~70 K and the second phase at ~70 < $T$ < ~100 K are assigned to HDA and LDA ice, respectively [1]. The fifth phase at > 126 K is probably attributed to a precursor of ice Ic due to glass transition of water [2]. The precursor exists because the crystallization to ice Ic is inhibited. For the third and fourth phases observed at ~100 < $T$ < ~126 K, the assignments are less conclusive. However, the gas desorption observed in this temperature range may be due to a collapse of pore structures, because wave number of the O–H stretching mode in IR spectra increases with warming. This indicates the strength of hydrogen bonds increases as the temperature rise.

## References

[1] A. H. Narten, C. G. Venkatesh, and S. A. Rice, 1976, J. Chem. Phys. 64, 1106.
[2] P. Jenniskens, and D. F. Blake, 1996, ApJ 473, 1104.