赤外分光法によるアモルファス氷の表面構造の解析
Analyses of surface structure of amorphous ice using infrared spectroscopy

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In interstellar molecular clouds, water molecules deposit on dust grains, and forms amorphous ice. The amorphous ice includes various molecules such as CO, CO_2, NH_3, CH_4, H_2CO, and so on. These molecules undergo chemical evolutions to organic molecules through various processes. Because the deposited amorphous ice has a large surface area due to its uneven structure, the surface of amorphous ice has an important role for chemical evolutions of included molecules in molecular clouds [1].
Structure of amorphous ice depends on formation condition [2], and has been mainly classified by density into two types: low-density amorphous (LDA) and high-density amorphous (HDA) ice. The densities of the LDA and HDA ice are 0.94 ±0.03 and 1.1 ±0.1 g cm^{-3}, respectively. Although there are various studies for structures and properties of amorphous ice in bulk states, only a few studies have been reported for surface. In the present study, the surface structure of amorphous ice was analyzed by measurements of infrared (IR) spectra for thin film of vapor-deposited amorphous ice.
Amorphous ice was prepared with vapor deposition of distilled and degassed water on a substrate of oxygen-free copper at 43 K. The deposition rate was controlled to be a value in range of 0.02–0.61 nm/min. The inner pressure of the vacuum chamber during the deposition was about 5.0 $\times 10^{-5}$ Pa. The IR spectra were measured using Shimadzu IRPrestage-21.
The spectral features change with deposition. According to the assignments of IR spectra for amorphous ice [3], the O–H stretching vibration band observed in 2800–4000 cm^{-1} was decomposed into three vibration modes (i.e., in-phase and out-of-phase modes of symmetric stretching, and asymmetric stretching mode). From the variations of the wave number of the out-of-phase mode, the variations in water structure of amorphous ice were analyzed.
The result shows that the wave number of the out-of-phase mode increases as the thickness of the amorphous ice increases, and gradually approaches a constant value of 3480 cm^{-1}. From the observed variations, the thickness of the surface layer is estimated to be around 20 nm. Furthermore, the wave numbers of the surface layer and bulk state are estimated to be 3420 and 3480 cm^{-1}, respectively. Because these values are close to those for HDA and LDA ice [4], the internal part of the sample is confirmed to be HDA ice. For the surface layer, the density is smaller than that of the internal part. Therefore, it is supposed that the structure is a close representation of LDA ice. Furthermore, it was found that the surface structure of the amorphous ice depends on deposition rate. From the results, we discuss the structure and dynamics of amorphous ice surface.
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