X-RAY STRUCTURE ANALYSES OF AIR HYDRATES IN A DEEP ICE CORE FROM DYE 3, GREENLAND (Abstract)

by

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ABSTRACT

Clathrate hydrate inclusions of various shapes and sizes were first found by Shoji and Langway (1982) in ice cores from a depth greater than 1280 m at Dye 3, Greenland. Although we have assigned clathrate guest molecules to $\rm O_2$ and $\rm N_2$ by observing Raman spectra of the hydrates in a core from 1501 m depth (Nakahara and others, in press), it has not been determined whether the crystal structure of the hydrate is structure I or structure II.

Using the 4-circle diffractometer in the High Brilliance X-ray Laboratory at Hokkaido University, many reflections from the hydrate crystals were identified. Applying extinction rules for cubic crystals, the space group of the hydrate was determined as Fd3m, which corresponded to structure II. The average lattice parameter for a unit cell obtained from three samples was 17.21 Å, and this also supports structure II. Structure II was also found with artificial air hydrates by the method of neutron diffraction (Davidson and others 1984).

The density of the hydrate was calculated for various combinations of the occupancy of the two types of cage by

guest molecules (in a composition ratio of $N_2:O_2=(1.5\,2.0):1$ as determined from Raman intensity). A reasonable value of the density 950 kg m⁻³ was obtained when only the 12-hedrons were occupied. Therefore it was concluded that the air molecules were trapped only in 12-hedrons which formed the structure II hydrate with 16-hedrons.

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