

**MS27-2-2 In situ single-crystal neutron diffraction of a high-pressure phase of sodium chloride hydrate
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Abstract

Salt-water system has been studied from the perspectives of physical chemistry and planetary science. Its unique phenomena, such as salt-bearing ice [1,2], are found under pressured conditions, however, its phase behaviour, even possible crystalline phases, are not fully understood yet. Some salts have unique high-pressure phases, not only stacking differences of anhydrous salt, but also variation in composition ratio; e.g. MgCl₂ and MgSO₄ take unique hydration numbers under high pressure [3,4]. Sodium chloride (NaCl) is a major salt in nature. It has only one hydrate at ambient pressure: dihydrate at low temperatures [5]. Our group found its new hydrate under high pressure like the case of previously reported salt hydrates [3,4]. Its structure without the hydrogen positions was determined from single-crystal X-ray diffraction experiments. However, powder neutron diffraction techniques could not accomplish the full determination of the structure with hydrogen positions. Here, I will present the result of single-crystal neutron diffraction experiments to reveal the crystal structure of the new hydrate.

The diffraction patterns were collected at 298 K and 1.7 GPa using the Laue-TOF diffractometer at the BL18 (SENJU) beamline of the MLF J-PARC [6]. Single-crystalline specimens of the hydrate were directly grown from a NaCl saturated D₂O solution under high pressure using a newly-developed diamond anvil cell [7]. The observed diffraction patterns were analysed based on the initial structure derived from the previous diffraction experiments.

The new hydrate has a monoclinic structure with $\beta \sim 119^\circ$. It contains thirteen water molecules per pair of sodium chloride, a much larger hydration number than the other NaCl hydrate. The sodium atoms are coordinated by six water molecules forming octahedral units. The crystal structure of the hydrate consists of the hydrogen-bonding network binding the Na(D₂O)₆ octahedra, interstitial water molecules, and chlorine atoms. Considering the restriction of symmetry and stoichiometry, the water molecules are not in definitive orientations but orientationally disordered like those in ice. This is contrast to other known hydrates in which water molecules are restricted to face ionic species due to their strong electrostatic interactions. The structure with large numbers of water molecules and hydrogen-bonded structure can provide an insight to understand the structural features of salt-water systems in solid phases.

References

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