

	承認日 Date of Approval 2014/12/26 承認者 Approver Takanori Hattori 提出日 Date of Report 2014/12/26
課題番号 Project No. 2014A0119 実験課題名 Title of experiment A study of the structure of aqueous NaCl solution under high pressure 実験責任者名 Name of principal investigator Toshio Yamaguchi 所属 Affiliation Fukuoka University	装置責任者 Name of responsible person Takanori Hattori 装置名 Name of Instrument/(BL No.) BL-11 (PLANET) 実施日 Date of Experiment 26 April 2014 – 1 May 2014

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)
 Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.
Water, H ₂ O Deuterium, D ₂ O Sodium chloride, NaCl

2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。) Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.
<p>The sample solutions are 2.825 mol/L NaCl in D₂O and D₂O/H₂O mixture. These sample were prepared in the applicant's laboratory of Fukuoka University. An Al cell was used. These sample were measured on PLANET at BL 11 of J-PARC MLF. High pressure were generated by a cubic anvil installed at PLANET. The empty cell and vanadium standard were also measured. The total diffraction data were corrected for background and empty cell and normalized by using the data of vanadium standard. (Figure 1) The structure factor thus obtained was corrected for the recoil effect by using a six-order polynomial function and subjected to EPSR modelling (Figure 2). The agreement between the experiment and EPSR fit is satisfactory. We plan to test another method to correct the recoil effect by using nullH₂O data where the scattering length of H is zero by mixing H₂O and D₂O to a required amount. All the measured structure factors are subjected to EPSR modelling to extract the partial structure factor, the partial pair correlation functions, coordination number, and spatial density functions (3D structure) of the present aqueous solution to reveal the effect of pressure on the ion hydration, in particular, the orientation of water molecules around the ion, and the solvent water structure.</p>

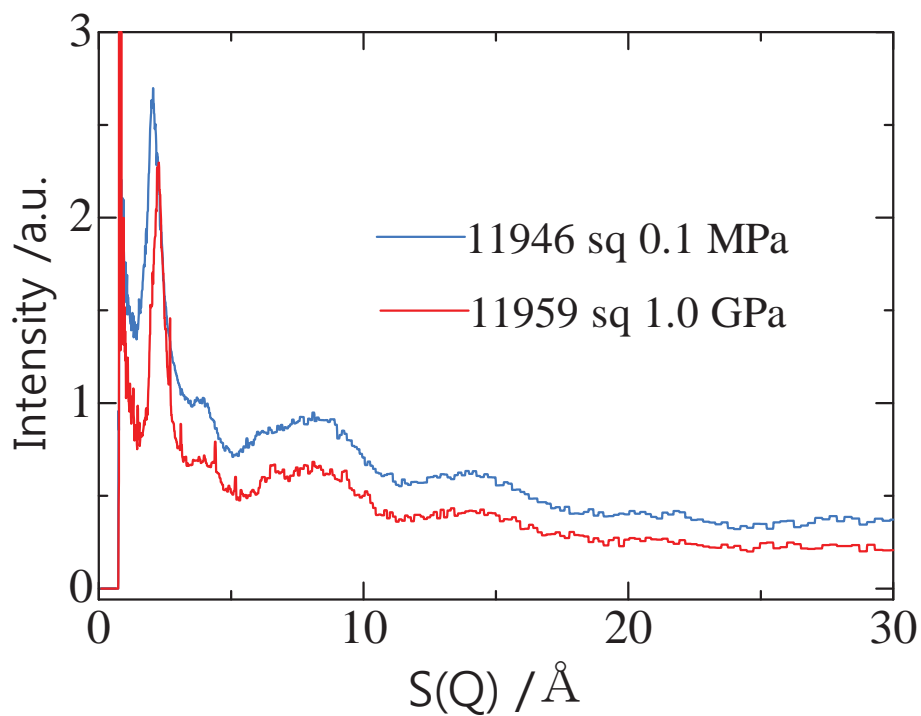


Figure.1 Diffraction spectra of NaCl solution at 0.1 MPa and 1.0 GPa

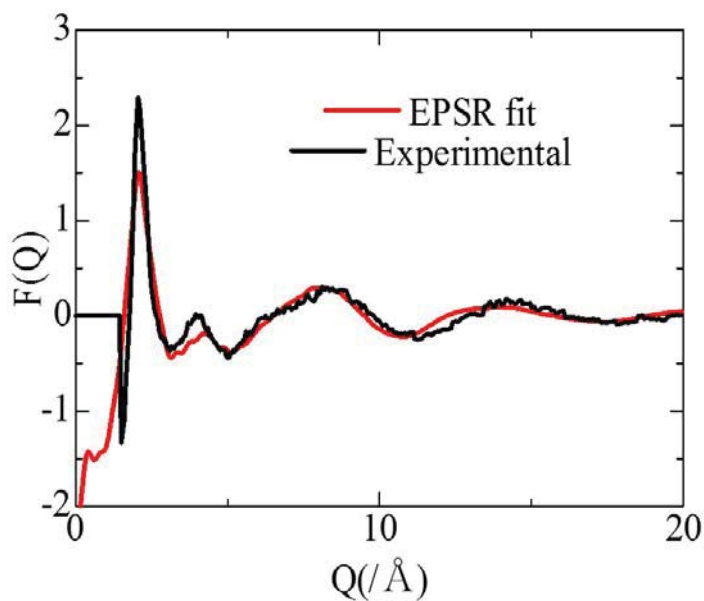


Figure 2. Structure factors of a 3 m NaCl-D2O solution at 298 K/0.1 MPa measured on PLANET