Structural Analysis of Supercritical Water.

Y.Ohmasa, Y.Kajihara, H.Kouno, Y.Hiejima, A.Chiba and M.Yao*
Department of Physics, Graduate School of Science, Kyoto Univ.

I. Introduction

Water in supercritical state has recently attracted much attention. In the supercritical state, density of the system can be easily controlled from liquid-like one to gas-like one by changing pressure. In the present experiment, we have carried out X-ray diffraction study of liquid water at 1bar 25C and at 1bar 50C as a test for the high pressure and high temperature experiments

II. Experimental

We carried out X-ray diffraction study of liquid water at 1bar 25C and at 1bar 50C on the BL-04B1 at SPring-8. The strage ring was operated at 8GeV with 20mA during the present experiment. White X-ray up to 150keV was generated by the bending magnet. The X-ray beam was collimated to 0.2 × 0.2mm^2 using the horizontal and vertical tungsten slits located at the upper stream.

We tested two kinds of sample cell, one was made of BN, and the other was made of SUS. The BN cell had a cylindrical shape with OD 4mm and ID 3mm, OD 5mm and ID 4mm or OD 7mm and ID 6mm. The incident X-ray was perpendicular to the axis of the cylinder. The SUS cell also had a cylindrical shape, but the incident X-ray was parallel to the axis of the cylinder. The sample thickness in the SUS cell was 10mm or 0.8mm. As windows for the SUS cell, we used single crystalline sapphire, whose thickness was 0.24mm. The sample cell was surrounded by a nichrome heater. The sample assembly was mounted on the horizontal goniometer fixed on XZ stage.

The intensity of the scattered X-ray was measured with a Ge solid state detector.
The measurements were made by the transmitting mode.

III. Results and Discussion

In Fig.1, we show scattered X-ray profile from the empty SUS cell with sapphire window. From the figure we can see that there is no Bragg peak from the sapphire window, which indicate that the Bragg reflections are out of direction of the detector. The broad background is mainly due to Compton scattering from sapphire. From these data, we can determine energy profile of the incident X-ray beam.

In Fig.1, X-ray profile scattered from water in the cell is shown. The thickness of the sample was 10mm. The signal is much stronger than that from the empty cell. By subtracting back ground scattering such as incoherent scattering from the cell and water from the signal, we can get interference function S(Q) of water.

These data provide useful information for the X-ray diffraction experiments under high pressure and high temperature.

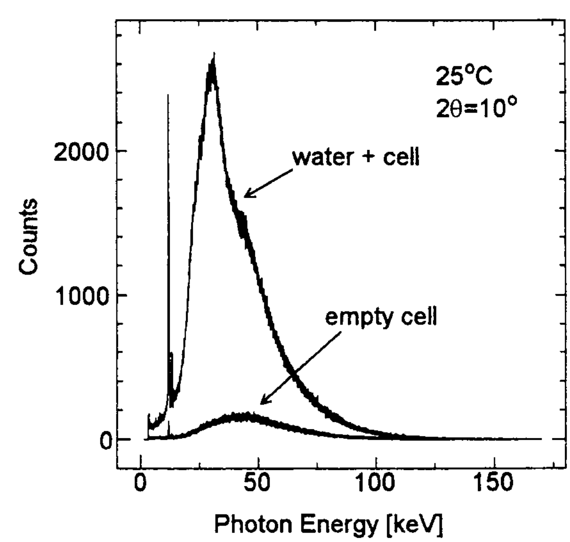

Fig.1 scattered X-ray profile from the empty SUS cell with sapphire window, and from water in the cell.