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A Compton scattering study of $Na_{0.75}CoO_2$

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The discovery of superconductivity in $Na_xCoO_2 \cdot yH_2O$(x~0.35, y=1.3) has brought about extensive and intensive research on the layered sodium cobalt oxyhydrate and its host compounds because of their unusual magnetic, thermodynamic and transport properties. An unconventional scenario for electron-pairing mechanism is possible associated with the structural and magnetic instabilities and the frustrated triangular Co lattice. First-principles band-structure calculations predict a nesting property of the Fermi surface that suggests strong antiferromagnetic spin fluctuation in connection with its superconductivity. However, angle-resolved photoelectron spectroscopy studies have reported that the theoretically predicted, hole pockets near the K points are absent in the host compound, Na_xCoO_2. In order to settle this controversial situation, we have initiated a collaborative work that determines the Fermi surface of Na_xCoO_2 using the high-resolution Compton scattering technique. This is the first report of this work.

A single crystal of $Na_{0.7}CoO_2$ was grown by the flux method. Compton profile measurements were performed at the BL08W beamline. The incident x-ray energy was 115 keV, and the overall momentum resolution was 0.12 atomic units. The sample was kept at 30 K in order to reduce the thermal effect on Fermi surface signatures. The data were collected along four different directions lying on the a-b plane. The Compton profiles were obtained from the raw data by the standard data-processing.

Figure 1 shows the anisotropy in the Compton profiles. Significant differences are clearly observed, although the amplitudes are small. Detailed analyses are in progress.

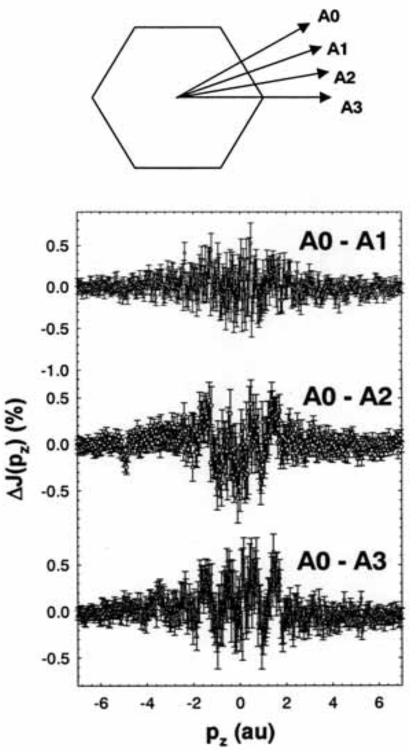

Fig.1 Anisotropy in Compton profiles

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Structure of High Pressure Low Temperature Ices

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The hydrogen bonds linking the water molecules are known to give rise to a rich variety of stable and metastable phases of H_2O under specific temperature and pressure conditions (Fig.1). The phase diagram of H_2O in the literature at temperatures below 50K is however still mostly unknown. Based on inelastic x-ray scattering of the near oxygen K-edge structure of ices at 0.25GPa and low temperatures down to 4K at the Taiwan Beamline BL12XU, we have obtained spectroscopic evidence suggesting a possible new phase of ice at temperature between 4 and 50 K [1]. Structural characterization using x-ray diffraction will provide the most direct information to confirm this finding.

We report the results of a preliminary x-ray diffraction experiment carried out at the high-pressure diffraction beamline BL10XU (Fig.2). The measurements were performed on pure water compressed to 0.26GPa using a diamond anvil cell (DAC) with stainless steel membrane, and cooled using a custom built cryostat available on the beamline. The lowest temperature attainable was ~20K. The pressure was measured in situ by Ruby fluorescence, whereas the temperature was determined by taking average of the readings from two thermal couples attached respectively to the top and bottom of the DAC. The uncertainty of the temperature of the sample was estimated to be less than 10 K.

Diffraction patterns were taken through the diamonds at a wavelength of 0.49738Å at several temperatures as shown in Fig.2. Contributions from the diamonds have been removed. One can see at 245K the sample is still in amorphous state whereas according to the phase diagram we should reach ice III. This suggests supercooling of the sample due to the fast cooling speed in the experiment. At lower temperatures, crystalline features appear with small variations in the intensity and width of the features. Further study is planned.

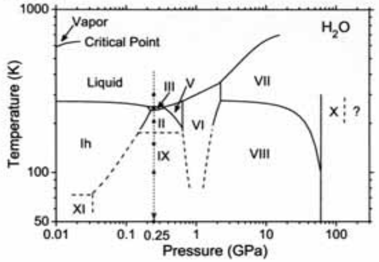

Fig. 1 Phase diagram of H_2O

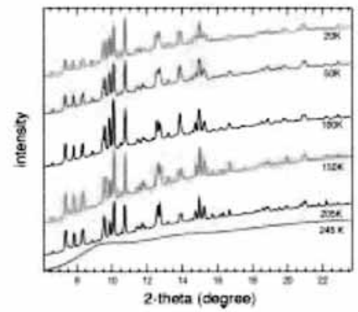

Fig. 2. X-ray diffraction patterns of H_2O at 0.26 GPa and various temperatures.

[1] Y.Q. Cai, H.-K. Mao, P.C. Chow, J.S. Tse, Y. Ma, S. Patchkovskii, J.F. Shu, V. Struzhkin, R.J. Hemley, H. Ishii, C.C. Chen, I. Jarrige, C.T. Chen, S.R. Shieh, E.P. Huang, and C.C. Kao, Phy. Rev. Lett. **94**, 025502 (2005).

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