2002A3004 -LD –np BL10XU

The Development of Experimental Techniques for Charge Density Studies under High-Pressure.

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For charge density study of crystalline materials, it is essential to collect a precise x-ray diffraction data. In order to observe charge density under high pressure, the X-ray data is usually measured by using the Diamond Anvil Cell (DAC).

It has been well known that DAC diffraction experiment has some difficulties for reliable X-ray diffraction data measurement since DAC limits the observable diffraction angle and only a small amount of sample can be sealed in DAC. However, a high energy, high brilliance and high efficiency beam emanating from the undulator at BL10XU in SPring-8 has advantage to collect an accurate diffraction data from a DAC experiment.

The high-energy beam allows us to collect much more Bragg reflections when the diffraction angle is limited by DAC. In addition, the effects of absorption and diffraction of Diamond become less serious. The drawback is the difficulty to obtain homogeneous intensity of Debye-Scherrer ring. The requirement of granularity of the powder sample becomes very severe. And, the use of flat imaging plates as detectors requires a correction for oblique incidence of the diffracted beam on the plate. The purpose of this study is to overcome the difficulties and establish a structure analysis for charge density study under high pressure at BL10XU.

We have examined and solved the following problems up to now.

1. Satisfactory homogeneity of Debye-Scherrer ring intensities, which is absolutely needed for an accurate structure analysis.
2. Influence on the intensity recording reliability due to fast fading property of IP.
3. Correction of reflection intensities recorded on flat imaging plates.

As for 1 and 2, we found that one of the most efficient ways is to measure the data in horizontal diffraction area with the DAC oscillating system as shown in Fig.1. The problem 3 was examined by comparing the observed intensities measured by the curved IP(BL02B2) and flat IP(BL10XU) for the same sample, CeO_2. Consequently, we concluded that the reflection intensities recorded on the flat IP can be corrected by the Zalwski s formalis[1)].

Fig.1 shows the data correction process of $Cs_2Au_2Br_6$ powder data(2.2GPa) on polarization effect and absorption correction on flat IP. The processed data was analyzed by Rietveld method as shown in Fig.2. The charge density study by the MEM/Rietveld method is now in progress.

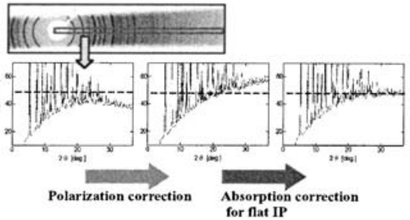

Fig.1 The process of data correction

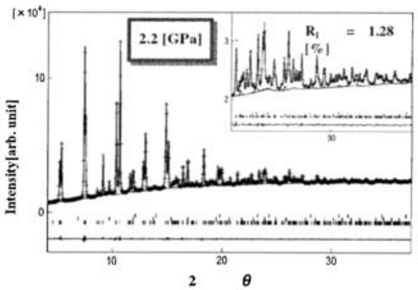

Fig.2 The Rietveld fitting result of $Cs_2Au_2Br_6$.

1) J.Zaleski *et al.* : J. Appl. Cryst (1998). **31**, 302-304

2002A0046-ND3-np BL011XU

Study of Phonon Anomalies near T_c in Perovskite-related Oxides with Colossal Magnetoresistance

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In several itinerant ferromagnet materials having the metal-to-insulator transition in their phase diagram, the anomalous behavior of the phonon frequencies was known to occur near the magnetic-ordering transition. In the same temperature region, an external field applied to the material allows to reduce its resistance by tens of percent. From the phonon density of states (DOS), it is interesting to obtain the information on the role of the spin-phonon coupling in the colossal magnetoresistance (CMR) effect.

Phonon DOS were determined from the nuclear resonant inelastic scattering (NIS) spectra in a series of perovskite-related oxides. The oxides $Sr_2FeCoO_{6-\delta}$ and $BaSrFeCoO_{6-\delta}$ selected for this study were subjected to the high-isostatic-pressure (HIP) treatment in oxygen at 8.8 MPa and 570°C. NIS spectra were measured at the beam line BL11XU of the SPring-8 storage ring, operated in the timing mode C (11-bunch train ×29). The assembly of nested asymmetric Si(511) and Si(975) channel-cut monochromators allowed to narrow the bandwidth down to 2.5 meV.

We observed a narrowing of the bands in the phonon densities of states at cooling across the temperature of ferromagnetic transition, where the charge transport coherence sets in. Clearly, the phonon bands in the DOS become better separated from each other below T_c as shown in Fig. 1.

The phonon DOS in a number of ^{57}Fe-doped manganites, cobaltites and ruthenates were also obtained at room temperature.

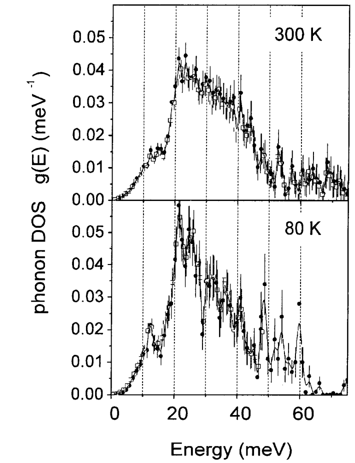

Fig. 1. Phonon DOS in $BaSrFeCoO_{6-\delta}$ at indicated temperatures. The ^{57}Fe enrichment is 20%.

The features at 15 and 24 meV in the ^{57}Fe partial DOS of $La_{0.7}Sr_{0.3}Mn_{0.99}{}^{57}Fe_{0.01}O_3$ coincided in energy with the features observed in generalized DOS derived from neutron inelastic scattering spectra.

We have also obtained the DOS in brownmillerite $SrCaFeCoO_5$, in which the "chemical pressure" effect of Ca prevent the incorporation of extra-oxygens. While the perovskites $Sr_2FeCoO_{6-\delta}$ and $SrBaFeCoO_{6-\delta}$ show the lowest-energy peak at 13 to 15 meV, the brownmillerite shows the DOS peak at 8 meV. The peak at the energy of 8 meV results in the strong decrease of the Lamb-Mössbauer factor for brownmillerites relative to the perovskites.