Electron Density Distribution Analysis of Pressure-Induced s-d Transition of Cesium by MEM

Yasuo OHISHI(1213)*, Masaki TAKATA(3167)[1], Ken-ichi TAKEMURA[2], Nozomu HAMAYA(1229)[3] and Osamu SHIMOMURA(1202)

SPring-8, Mikazuki, Sayo, Hyogo 679-5198, Japan
Department of Material Science, Shimane University, Matsue 690, Japan[1]
National Institute for Researches in Inorganic Materials, Ibaraki 305, Japan[2]
Department of Physics Ochanomizu University, Tokyo 112, Japan[3]

In the pressure range form atmosphere to 10GPa, metallic cesium undergoes five structural phase transitions(phase I ~ VI), which structure changes from bcc to fcc I, II to tetragonal I, II and to hcp(?). The isostructural electronic transition (fcc I > fcc II) is well known as s-d transition[1,2]. In order to investigate the nature of s-d transition in Cs, it is very important to observe their electron density distributions at each phase.

In this case, MEM[3] (maximum entropy method) is the best method to produce the electron density distribution using a high-pressure x-ray powder diffraction data.

This work included the installation of MEM analysis system and the test experiments for BL10XU.

1. Experiment and results

DAC (diamond anvil cell) contained the powdered Cs was assembled in the glove box with great cares against moisture and oxygen in the air. The melting point of Cs at atmospheric pressure is 29℃. In order to keep off grain growth, we wanted to do this high-pressure experiment under low temperature condition. But we could not do that at room temperature, because the installation of cryostat system on BL10XU station was not complete at our machine-time.

X-ray energy is 24.80keV (wavelength is 0.0500nm, the third harmonics when IDgap is 12.98mm). X-ray diffraction detector was imaging plate(R-AXIS IV, 0.10mm resolution, 300×300mm area size). The exposure time was 10 minutes.

High-pressure experiments were done from 1.4GPa to 10.7GPa. The x-ray diffraction profile changes were observed whenever the phase transitions (bcc > fcc > tetra. > hcp) were occurred.

However, in x-ray diffraction patterns there were many spots by preferred orientation in the sample. This preferred orientation would be not only caused by grain growth, caused by the high-grade resolution of this beamline.

Anyway, it was difficult to carry out MEM analysis using such spot-like profiles in phase I, II and III, so the electron density distribution maps were not carried out in this experiment.

Above the phase IV, the diffraction profile became to a smooth line shape from spotty profile, because the drops in the sample were broken by large volume change under the transformation. This fact gave a hint to get a good x-ray diffraction profiles for delicate MEM analysis.

2. MEM analysis in BL10XU

The combination system of Rietveld refinement and MEM analysis were installed on free-BSD in one of the PCs at BL10XU. Every user of SPring-8 can utilize this system.

The test high-pressure experiments were done for the YBCO system at BL10XU. The high-resolution x-ray powder diffraction data were observed, and were be able to bring electron density distribution maps by MEM.

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