

### Charge Density Study by Powder X-ray Diffraction

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The experimental period is from Oct. 4th to Oct. 9th. The main purpose of this time is to calibrate the zero shift of angle and to collect the low temperature data of KNiF<sub>3</sub> and other complexes for charge density analysis because the previous experiment on KNiF<sub>3</sub>, carried out on Oct. 16 in 2002, was indicated the structure factors (  $h+k+l = \text{odd}$  ) affected by TDS<sup>1</sup> ( Temperature Diffuse Scattering ). Thus, the low temperature experiment is necessary for charge density analysis.

We set up the powder end station and aligned it on Oct. 4th. However, the Storage Ring had been out of operation since 10:30am on Oct. 5th as a result of vacuum leakage. On Oct. 6th, an announcement of beamtime available was on Oct. 9th. Thus, we stayed one more day in order to collect the data. Whereas the final beamtime available was at 10:00pm on Oct. 9th and the light source was not stable until 4:00am on Oct. 10th. We took use of the available beamtime from 4:00am to 3:00pm to realign the powder station, but no time to collect any data. Although there was no data obtained this time, the powder end station still must be modified because the optical table is the first time to install in the hutch. First of all is that there must be installed a motor to precisely adjust the height of the optical table. The second is to install a motor to precisely adjust the height of collimeter. Finally, a more serious concern is the possibility to always install the powder station in the

Beamline. If not, users always have to spend one or two days to setup and align the powder station.

#### Reference

1. Hsu, I.-J. Ph. D. Thesis, NTU, 2003.

### The Quasi-one-dimensional Oxide Conductor K<sub>0.3</sub>MoO<sub>3</sub> Studies by X-ray Absorption Spectroscopy

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The quasi-one-dimensional transition-metal oxide K<sub>0.3</sub>MoO<sub>3</sub>, known as blue bronze, which exhibits quasi-one-dimensional electron transport and metal-semiconductor transition due to charge density wave (CDW) at 180K.<sup>(1)</sup> The basic unit of the blue bronze K<sub>0.3</sub>MoO<sub>3</sub> is a cluster of ten distorted MoO<sub>6</sub> octahedral interlocking by edge-sharing to give a Mo<sub>10</sub>O<sub>30</sub> unit and monoclinic in structure. There are three K<sup>+</sup> ions, known as valence electrons are incorporated in each cluster. Low-dimensional metals often possess electronic instabilities toward a metal-insulator transition, which occurs when the Fermi surfaces of their partially filled bands are nested. When an electric field is applied to the CDW, it can slide relative to the lattice, and the lattice atoms oscillate back and forth, producing a traveling potential, which produces current due to movement of conduction electrons.<sup>(2)</sup>

The normalized extended x-ray absorption fine structure (EXAFS) oscillations  $\chi(k)$  are weighted by  $k^3$  for Mo K-edge, and the corresponding Fourier transforms (FTs) of the  $k^3$  data for K<sub>0.3</sub>MoO<sub>3</sub> at different temperature (T) and applied voltages (E) are shown in Figs. 1 and 2, respectively. From those FTs spectra we can obtain the local atomic structure of K<sub>0.3</sub>MoO<sub>3</sub>. The first peak (labeled A) of all spectra (Fig. 1) have almost the same peak position, heights and full widths at the half maximum except the spectra of T=300K. The first peak of the spectrum at T=300K in Fig. 1 appears to a small shift to shorter radial distance and an addition small shoulder appears, shown with a vertical bar. Moreover, the peaks labeled B and C in Fig. 1 at distant larger than ~2 Å differ significantly and can be attributed to differences in the average environment in farther away shells. In Fig. 2 the first peaks labeled D and the two peaks E, F at a distant larger than ~2 Å of the FTs of the  $k^3$  data and are similar to each other. Those peaks have same position and full widths at the half maximum, and almost the same heights, suggesting that the overall atomic structure in farther away shells are similar at different applied voltages (E) at T=100K.

<sup>(1)</sup> *Low Dimensional Electronic Properties of Molybdenum Bronzes and Oxides*, edited by C. Schlenker (Kluwer, Dordrecht, 1989).  
<sup>(2)</sup> R. E. Thome, *Physics Today* **49**, 42 (1996).

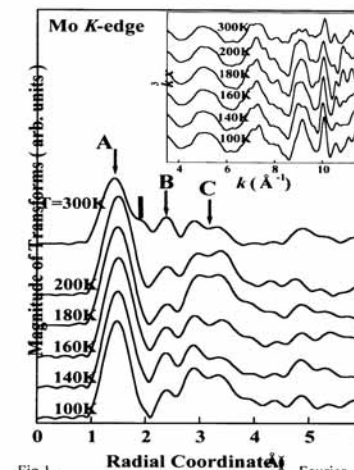


Fig.1. Fourier-transformed EXAFS spectra at Mo K-edge with various temperature (T). The inset represents the Mo K-edge EXAFS oscillation  $k^3$  data.

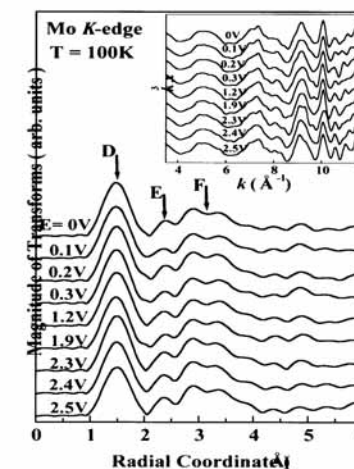


Fig.2. Fourier-transformed EXAFS spectra at Mo K-edge with various applied voltages (E). The inset represents the Mo K-edge EXAFS oscillation  $k^3$  data.