Electronic and atomic structures of the nanomaterials, quasicrystal, epitaxial magnetic trilayer, ABO_3-type perovskite, quasi-one-dimensional oxide conductor, and carbon-related materials

(The Quasi-one-dimensional Oxide Conductor $K_{0.3}MoO_3$ studied by X-ray Absorption Spectroscopy)

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The quasi-one-dimensional transition-metal oxide $K_{0.3}MoO_3$, known as blue bronze, which exhibits quasi-one-dimensional electron transport and metal–semiconductor transition due to charge density wave (CDW) at 180K.[1] 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.[2]

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 $k^3\chi$ data for $K_{0.3}MoO_3$ at various temperature (**T**) in b-axis (010) and applied voltages (**V**) are shown in Figs. 1-2, respectively. Due to quasi-one-dimensional electron transport property of the sample $K_{0.3}MoO_3$ we also performed Mo K-edge in d-axis (102) to investigate the dependence of local atomic structure of different crystallographic axis at various temperature (**T**). From these FTs spectra we can obtain the local atomic structure of $K_{0.3}MoO_3$. The first four peaks labeled $\mathbf{A_1}$, $\mathbf{B_1}$, $\mathbf{C_1}$ and $\mathbf{D_1}$ in Fig. 1 and $\mathbf{A_2}$, $\mathbf{B_2}$, $\mathbf{C_2}$ and $\mathbf{D_2}$ in Fig. 3 appear to have roughly the same peak position, though they have different heights and full widths at the half maximum. Moreover, the other peaks in Figs. 1 and 3 at distant larger than ~4 Å differ considerably and can be attributed to differences in the average environment in farther away shells. In contrast the peaks $\mathbf{A_2}$, $\mathbf{B_2}$, $\mathbf{C_2}$ and $\mathbf{D_2}$ in Fig. 2 of the FTs of the $k^3\chi$ data and the peaks at distant large than ~4 Å are more or less similar to each other, having the same position and full widths at the half maximum, and almost the same height, suggest that the overall atomic structure in the nearby as well as farther away shells are similar at different applied voltages (**V**) at T=100K.

[1] *Low Dimensional Electronic Properties of Molybdenum Bronzes and Oxides*, edited by C. Schlenker (Kluwer, Dordrecht, 1989).

[2] R. E. Thorne, Physics Today **49**, 42 (1996).

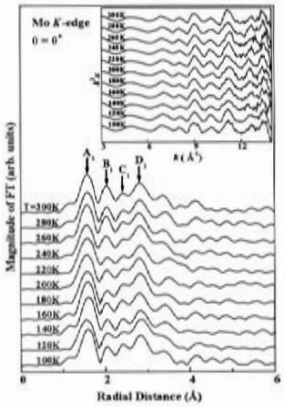

Fig. 1. Fourier-transformed EXAFS spectra at Mo K-edge in b-axis with various temperature (**T**). The inset represents the Mo K-edge EXAFS oscillation $k^3\chi$ data.

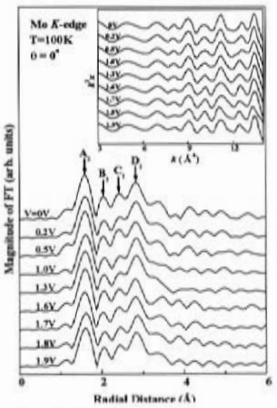

Fig. 2. Fourier-transformed EXAFS spectra at Mo K-edge in b-axis with various applied voltages (**V**). The inset represents the Mo K-edge EXAFS oscillation $k^3\chi$ data.

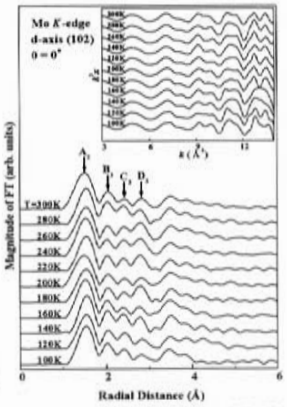

Fig. 3 Fourier-transformed EXAFS spectra at Mo K-edge in d-axis with various temperature (**T**). The inset represents the Mo K-edge EXAFS oscillation $k^3\chi$ data.

Solving the X-ray phase problem for macromolecular crystals, thin films, and less-ordered systems with high-resolution X-ray optics and intense X-ray sources

(Phase Determination of CDW material: $K_{0.3}MoO_3$ with Transport Measurement)

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The incommensurately modulated structure of the isostructural blue bronze of $K_{0.3}MoO_3$ with modulation wavevector $\mathbf{q}=\mathbf{a}^*+0.748\mathbf{b}^*+0.5\mathbf{c}^*$ at 100K has been determined by X-ray diffraction. And the transition at 180K is a Peierls transition leading to an incommensurate semiconducting charge-density-wave state. From the theoretical model, as a result of the electron-phonon interaction, the electronic ground state of CDW is given by $n(\vec{r}) = n_0[1 + p\cos(\vec{q}\cdot\vec{r} + \phi)]$, where the n_0 is the undistorted electron density, p the distorted amplitude, $\vec{q}$ the wave vector of the CDW, and ϕ the phase. It has been demonstrated that the phase ϕ governs the propagation of the CDW and is responsible for the occurrence of the unusual physical phenomena such as the memory effects, nonlinear electrical conduction, and sliding behavior. It is well known that this kind of structure modulation can be easily observed by measuring the satellite reflections of CDW while the temperature is below 180K. For analyzing the systematic extinctions, we need to consider a transformation of lattice: $A=a$, $B=b$, $C=2c$ giving $\mathbf{q}=0.748\mathbf{b}^*$. The indices of the reflections, $hklm$, are transformed to $H=h$, $K=k$, $L=2l+m$. Therefore the modulation wavevector appears along $\mathbf{b}^*$ only. By virtue of the variation of the electron density distribution when applying electric field along $\mathbf{b}^*$, multiple diffraction along the azimuthal scans of a CDW reflection is possible to determine the collective phases of CDW. The experiment of multiple diffraction and 2-wave intensity distribution of (13 0.75 -6.5) in q-space were done in order to observe if the collective phases of CDW change with varying applied electric field, and to study the relation between the x ray scattering and the collective phase of CDW. The asymmetric profiles of the azimuthal scans along the primary reflection (13 0.75 -6.5) with different voltage driven along b* (or different current driven) are as follows. In the fig. 1, it shows the multiple diffraction profile with the varying electric field. We can see the triplet phase change roughly around 30mA to 70mA. Fig. 2 shows the I-V curve corresponding to different temperature. Apparently, the triplet phases change with varying the applied electric field around the second flat regime of I-V curve before CDW is destroyed. By means of data fitting, according to a model of multiple diffraction result from the interference effect between the CDW modulation and the host lattice, the collective phases of CDW are therefore determined.

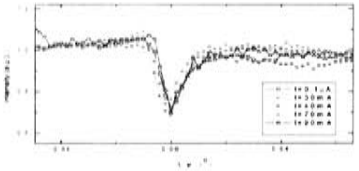

FIG 1

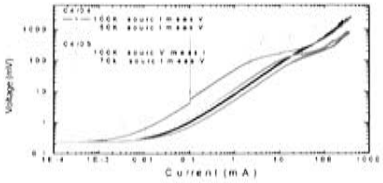

FIG2