

# Infrared properties of W-doped charge-density-wave material $K_{0.3}MoO_3$

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## Abstract

The optical conductivity spectra of quasi-one dimensional compounds  $K_{0.3}Mo_{1-x}W_xO_3$  ( $x=0, 0.03$  and  $0.15$ ) have been studied over broad frequencies. While the dc resistivity measurements indicate no sign of CDW transition in heavily W-doped blue bronze, the optical conductivity spectra still show a single particle gap at around  $0.2$  eV for  $\mathbf{E}$  parallel to the chain direction. Such impurity effect challenges our understanding about the occurrence of the optical gap with the CDW transition.

*Key words:* charge-density-wave; optical conductivity; metal-insulator transition;

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A central aspect of the charge-density-wave (CDW) phase transition is the appearance of a single-particle gap, which is usually considered as a typical feature associated with CDW condensate. However, it is found that the gap, for example in  $K_{0.3}MoO_3$ , could exist at temperatures much higher than the transition temperature.[1,2] Although mean-field theory predicted that the absorption is zero for frequency less than the gap,  $2\Delta$ , and contains an inverse-square-root singularity at  $\omega=2\Delta$ ,[3] the experimental observation is quite different. The singularity is absent, and there is a substantial tail below the maximum. Some theories explain those as due to the zero-point and the thermal lattice fluctuation effects,[1,2,4] but a full understanding of these phenomena still requires more efforts in both experiments and theories. Impurities doping is an important technique for studying the mechanism of CDW. It would be very interesting to see how impurities affect the single-particle gap seen in infrared experiment. In this work, we study the pure and tungsten-doped  $K_{0.3}MoO_3$  CDW materials. The experiment seems to indicate that the observed optical gap is irrelevant to the Peierls transition.

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Pure and W-doped  $K_{0.3}MoO_3$  crystals were grown by electrolytic reduction of a molten mixture of  $K_2MoO_4$  and  $MoO_3$ . The dc conductivity was measured by a standard four-probe technique. The reflectivity data at various temperatures were collected in a Bruker 66v/s spectrometer with light polarization parallel to the chain direction in a broad frequency range from  $50$  cm $^{-1}$  to  $30000$  cm $^{-1}$ . The optical conductivity spectra were extracted from the Kramers-Kroning transformation of the reflectivity.

Figure 1 shows dc conductivity of  $K_{0.3}MoO_3$ ,  $K_{0.3}Mo_{0.97}W_{0.03}O_3$  and  $K_{0.3}Mo_{0.85}W_{0.15}O_3$ . The pure  $K_{0.3}MoO_3$  undergoes a clear metal-insulator (M-I) transition at around  $180$ K. The conductivity increases with decreasing temperature at high temperature, but decreases sharply below  $180$  K. For  $K_{0.3}Mo_{0.97}W_{0.03}O_3$ , the M-I transition occurs in a broad temperature region and the conductivity changes gradually. Therefore,  $3\%$  W doping smears the Peierls transition. Conductivity of  $K_{0.3}Mo_{0.85}W_{0.15}O_3$  decreases monotonously from room temperature to low temperature, which is a typical insulating-like behavior. In this case there is no evidence of Peierls transition and CDW is completely suppressed by  $15\%$  W impurities.

Figure 2 shows the optical conductivity spectra of

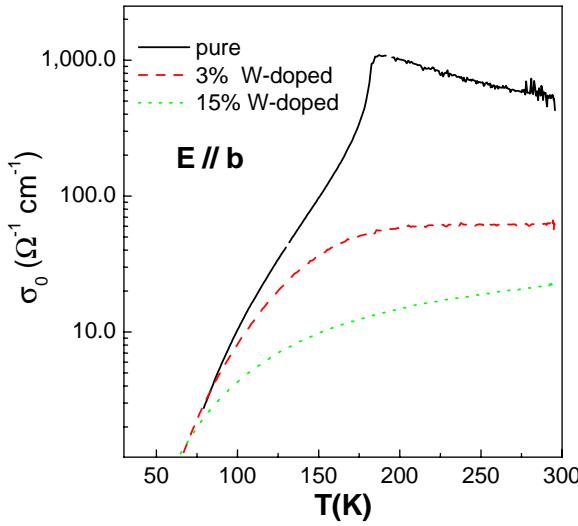


Fig. 1. The temperature-dependent dc conductivity for  $K_{0.3}MoO_3$ ,  $K_{0.3}Mo_{0.97}W_{0.03}O_3$  and  $K_{0.3}Mo_{0.85}W_{0.15}O_3$  along b-direction.

$K_{0.3}MoO_3$ ,  $K_{0.3}Mo_{0.97}W_{0.03}O_3$  and  $K_{0.3}Mo_{0.85}W_{0.15}O_3$  at 77 K in the polarization of  $\mathbf{E} \parallel b$ -axis. In mid-infrared region the raw reflectivity data (not shown) decreases with increasing dopant, consequently conductivity decreases with W in this region. Below 700  $\text{cm}^{-1}$ , many sharp peaks appear in reflectance and conductivity spectra of  $K_{0.3}MoO_3$ . These absorptions are assigned to the collective modes of distorted lattice vibrations being coupled with CDW condensate—so called phase-phonons.[5,1] Similar peaks also exist in the conductivity spectra of  $K_{0.3}Mo_{0.97}W_{0.03}O_3$  and  $K_{0.3}Mo_{0.85}W_{0.15}O_3$ . But the number and the amplitude of these peaks are substantially reduced. In addition, the central frequencies of those peaks are quite different from those in pure  $K_{0.3}MoO_3$ . This suggests that W impurities affect the symmetry of lattice, which result in a change of phase phonon mode.

Another striking feature is the suppression of the Low- $\omega$  spectral weight in conductivity spectrum, which gives rise to a broad maximum at  $1600 \text{ cm}^{-1}$  (0.2 eV). This absorption at 0.2 eV was assigned to the CDW single-particle gap absorption  $2\Delta$ .[1,6] Such gap feature, while being most prominent in the pure sample, still exists in the two W-doped samples and appears at the same frequency. Although the peak position is in fair agreement with the gap value estimated from the activation energy of dc conductivity measurement for the pure sample (about 0.18 eV), it is quite different for the two W-doped samples. In fact, the activated formula could not well describe the dc conductivity curve for the W-doped samples. The temperature-dependent dc conductivity has a tendency to evolve towards a logarithmic behavior at high impurity concentration. Therefore, the observed optical gap is in contradictory

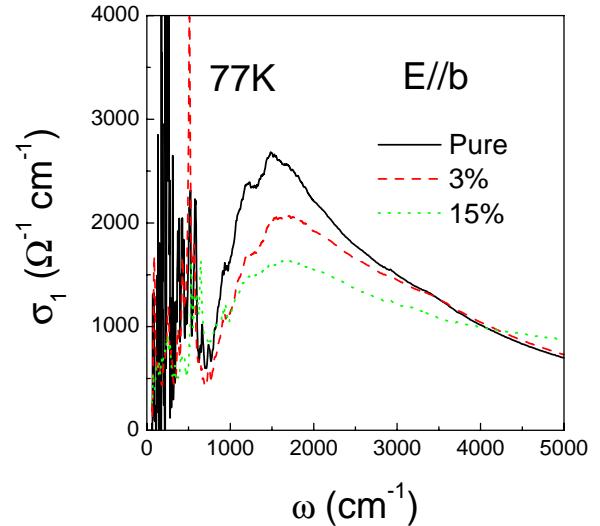


Fig. 2. The optical conductivity spectra of  $K_{0.3}MoO_3$ ,  $K_{0.3}Mo_{0.97}W_{0.03}O_3$  and  $K_{0.3}Mo_{0.85}W_{0.15}O_3$  for  $\mathbf{E} \parallel b$ -axis at 77 K.

to the dc result. Furthermore, as inferred from dc conductivity, CDW can not develop in 15% W-doped sample. Such impurity effect appears against the scenario that the occurrence of the gap is associated with the CDW transition.

In conclusion, our dc conductivity measurements reveal the suppression effect of W impurities on CDW transition in  $K_{0.3}MoO_3$ . But the optical conductivity spectra still show a single particle gap feature at around 0.2 eV for  $\mathbf{E}$  parallel to the chain direction for W-doped samples, with the shape and position quite similar to the pure  $K_{0.3}MoO_3$ . The observation indicates that the relation between the gap and CDW transition is not obvious and it needs further study.

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