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X-ray Studies on Dynamical Phase Transition of Charge-Density-Wave superlattice in $K_{0.3}MoO_3$

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By means of electron-phonon interactions, the electron density $n(\vec{r})$ of a one dimensional material in its ground state has a small sinusoidal component superimposed on its normal distribution:

$$n(\vec{r}) = n_0[1 + p\cos(\vec{q}\cdot\vec{r} + \phi)],$$

where p, ϕ, and q stand for the fractional amplitude, phase, and wave vector, respectively. This is so-called charge-density-wave (CDW). The structural modulation can be easily observed by x-ray diffraction of CDW satellite reflection when the sample is at a temperature lower than the Peierls transition temperature. CDW materials suffer nonlinearity in conductivity, which rises abruptly at an applied electric field close to some thresholds E_T. It is believed that CDW undergoes a dynamical phase transition as the applied electric fields approach and exceed the threshold, from a pinned/creeping state to a moving state.

The incommensurately modulated structure of the isostructural blue bronze $K_{0.3}MoO_3$ with modulated wave vectors $\vec{q} = m(0.748\vec{b}^* + 0.5\vec{c}^*)$ at T<180K, where m is an integer, has been determined by x-ray diffraction. If we consider a transformation of lattice-A=a, B=b, C=2c, we will get $\vec{q} = 0.748m\vec{b}^*$. Therefore the indices of reflections [h,k,l,m] can be transformed to [H=h, K=k, L=2l+m]. Major structure modulations only appear along $\vec{b}^*$. The additional electron density distribution could also be affected by applied E-fields. Our main purpose is to observe structural information such as the correlation length with applied E-fields along $\vec{b}^*$.

Fig. 1 shows σ -V curves at different temperatures. The threshold voltage was higher at lower temperature. We performed reciprocal vector scans (q-scans) of the CDW satellite peak [13 0.748 -6.5] at several voltages. Some data are shown in Fig. 2. There was no obvious change of FWHM below the threshold voltage. However, we observed that the peak seemed split into two parts near the threshold voltage. This might be a sign that CDW exhibited two domains with slightly different q values. It may be an evidence for CDW plastic flows.

Besides, electrical hysteresis was observed in this sample. The hysteresis effect was enhanced in the presence of x-rays, and currents jumped more abruptly around the threshold. The later phenomenon may be an indication of photo-induced effect. See Fig. 3.

Fig. 1

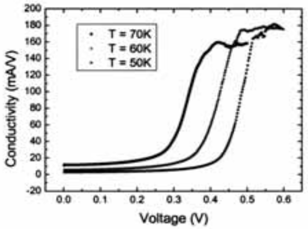


Fig. 2

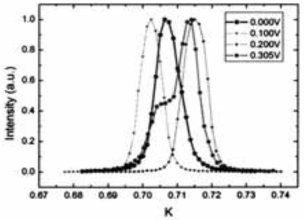
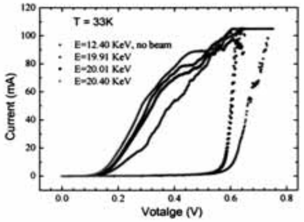


Fig. 3



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Pressure-induced valence change of the thulium in TmTe

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The valence state of Tm in TmTe is divalent. It was shown by compressibility to undergo a transition from 2+ to 3+ as the pressure is increased from 2 to 6 GPa. Nevertheless, no spectroscopic measurement of the Tm valency in TmTe as a function of pressure has been reported so far. We hereby report for the first time on the investigation of the electronic structure of Tm in TmTe and the quantitative determination of its valency for pressures up to 10.6 GPa by resonant inelastic x-ray scattering (RIXS) derived techniques : X-ray Absorption Spectroscopy in the Partial Fluorescence Yield (PFY-XAS) and Resonant X-ray Emission Spectroscopy (RXES), working at the Tm *LIII* edge.

The complete series of PFY-XAS spectra are fitted using two asymmetric peak functions accounting for the transitions towards the 2+ and 3+ 5d states and two arctangent functions representing the 2+ and 3+ continuum excitations. The fit of the spectrum obtained at a pressure of 5.7 GPa is presented in figure 1 as an example. The valencies inferred from the fit of the PFY-XAS spectra are plotted in figure 2.

The Tm valency remains unchanged up to 3 GPa, and then increases through two distinct regimes (regions II and III). In the decompression mode, a pseudo-plateau is observed (region IV), which may be due to the phase transition taking place from 8.2 GPa. Then, the valency decreases through two distinct regimes (region V and VI), whose decreasing rates are comparable respectively to the increasing rates of the regions III and II. This interestingly divides the hysteresis into two regions, above and below a valency of 2.4.

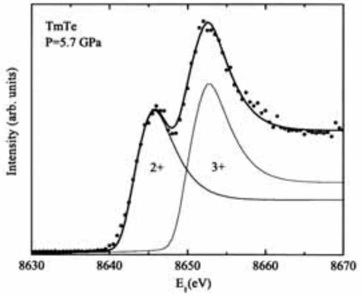

Figure 1 : PFY-XAS spectrum obtained at P=5.7 GPa and its deconvolution into pure 2+ and 3+ components.

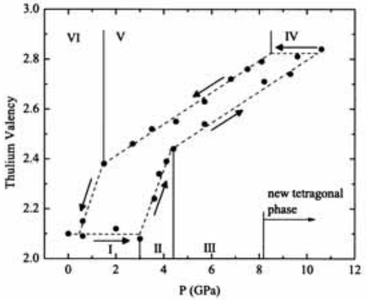

Figure 2 : Pressure dependence of the thulium valency in TmTe as a function of pressure. The valency is estimated by PFY-XAS. The dashed line is guide to the eye.