	Polarization dependent X-ray absorption in V₂O₃ single crystals at the V K-edge	Experiment number: HE-2796
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Report:

Understanding metal-insulator transitions driven by electron correlations in transition metal compounds remains an unsolved problem in the physics of strongly correlated systems. Among these V oxides, and particularly vanadium dioxide and Cr-doped vanadium sesquioxide have attracted considerable interest for undergoing a metal-insulator transition at about 340K and 200K, respectively. The former presents a well known first order MIT accompanied by structural transition [1] while the later is a canonical case for Mott-Hubbard system providing an iso-structural first order MIT between two paramagnetic phases [2]. But despite several decades of theoretical and experimental investigations, a satisfactory explanation of their electronic properties still not available.

We report on a direct spectroscopic study of the electronic structure of VO_2 and Cr-doped V_2O_3 through their temperature-induced metal-insulator transitions. In order to investigate the electronic properties of these systems, we have performed a high resolution near edge x-ray absorption spectroscopy (XAS) at the V K-edge. The absorption spectra was collected in partial fluorescence yield (PFY) mode i.e. by acquiring the intensity variations of the V $K\alpha$ emission line while scanning the incident energy through the K-edge resulting in an improved intrinsic resolution compared to conventional XAS. The experiment was carried out at the BM-30B beamline at ESRF. The spectrometer was equipped with a Ge(331) analyzer borrowed from ID-26, providing an overall energy resolution of about 1 eV. The measurements were performed in reflection geometry.

In order to explore the whole phase diagram of Cr-doped vanadium sesquioxide $(V_{1-x}Cr_x)_2O_3$, we have performed PFY-XAS measurement on powder samples as a function of temperature for different doping levels x . The results are presented in Fig. 1 – the corresponding locations in the phase diagram are indicated in the inset. We have primarily focused on the pre-edge region which corresponds to both quadrupolar $1s \rightarrow 3d$ and dipolar $1s \rightarrow 4p$ transitions, the latter occurring via hybridization between $3d$ and $4p$ states. Dramatic changes are observed in the pre-edge when crossing the MIT upon doping (Fig. 1a) and temperature (Fig. 1b) changes. The spectra show barely no x -dependence in the paramagnetic insulating phase (PI), as expected from theory. In the paramagnetic metallic phase (PM), we observe a remarkable

similarity between the spectra taken at $(x=0, T=400\text{K})$ and $(x=0.011, T=300\text{K})$, $(x=0, T=300\text{K})$ and $(x=0, T=200\text{K})$, though there are intensity differences on the high energy side. In a first approach, we can conclude that the effects of temperature and Cr-doping on the pre-edge structures in the metallic phase are principally due to the distance from the MIT line in the phase diagram, which is consistent with our recent works [3].

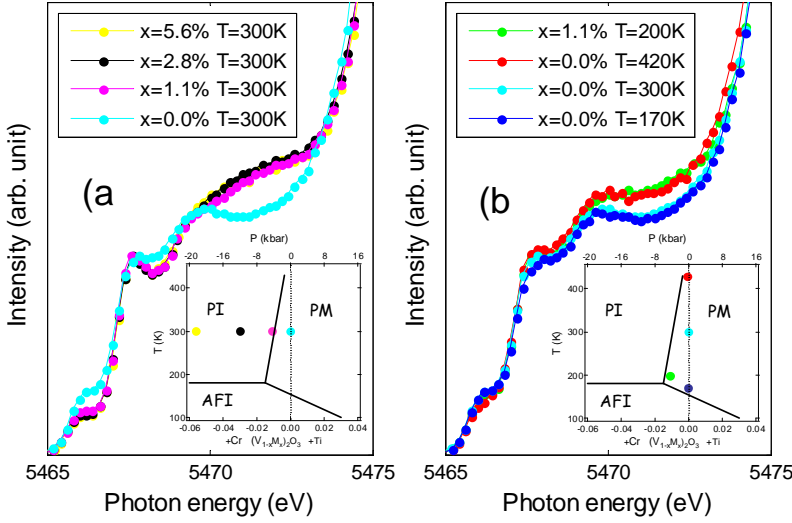


Figure 1: PFY-XAS V K pre-edge region on $(V_{1-x}Cr_x)_2O_3$ powder samples for different x values at ambient conditions (a) and for different point of temperature and doping level in the metallic phase (b).

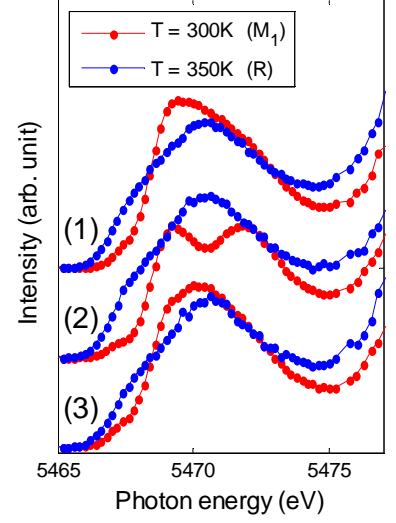


Figure 2: PFY-XAS V K pre-edge region in VO_2 single crystals for different orientations: (1) $c // \epsilon$, (2) $c \perp (\epsilon, k)$, (3) $c // k$.

As for the vanadium dioxide, we have performed polarization-dependent PFY-XAS in a single crystal. Similarly to vanadium sesquioxide, we have observed large changes in the pre-edge structures upon crossing the MIT. Fig. 2 shows the pre-edge region of the spectra when changing the orientation of the single crystal with respect to the polarization of the light. We can observe a strong angular dependence for the insulating phase (M_1). By contrast, the angular dependence is quite weak for the metallic phase (R). This result provides a new experimental evidence of an orbital switching in the $V3d$ states across the metal to insulator transition in VO_2 , as pointed out in a previous polarization-dependent x-ray absorption spectroscopy study at the V $L_{2,3}$ edges [4]. Analysis is under way to identify the pre-edge structures and thus obtain additional information on orbitals involved in the MIT.

References

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