ESRF	**Pressure and temperature dependence of the electronic properties of V_2O_3**	**Experiment number**: HE-2314
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Report:

V_2O_3 has been the subject of wide experimental and theoretical interest over the past decades as archetypal of electronic systems exhibiting correlation-induced Mott-Hubbard metal-insulator transitions (MIT) [1-3]. While band theory predict a pure metallic behavior in absence of correlations, V_2O_3 is known to display a rich phase diagram which involves antiferromagnetic insulating (AFI), paramagnetic metallic (PM), and paramagnetic insulating (PI) regimes. Transitions between the different phases can be induced by temperature, external pressure or chemical pressure through doping (Cr or Ti).

We present first direct spectroscopic study of the electronic structure of Cr-doped vanadium oxide through the temperature- and pressure-induced metal-insulator transitions. We have performed resonant inelastic x-ray scattering (RIXS) and near edge x-ray absorption spectroscopy (XAS) at the V K-edge of $(V_{1-x}Cr_x)_2O_3$ with x=0.011. At this doping level, the sample is stabilized in the PI phase at ambient conditions, and can be easily driven to the PM or AFI phase as a function of pressure and temperature respectively. The experiment was carried out at the ID-26 beamline at ESRF. The spectrometer was equipped with a Ge(331) analyzer and an avalanche photodiode (APD) detector, giving an overall energy resolution of about 1 eV. For pressure-dependence, the sample was crushed into fine powder and loaded in a membrane-type diamond anvil cell using silicon oil as pressure transmitting medium. Our setup allows the cell to be mounted in a liquid helium cryostat, thus giving the possibility to access low temperature / high pressure regions of the phase diagram. Pressure was measured in situ by ruby fluorescence technique.

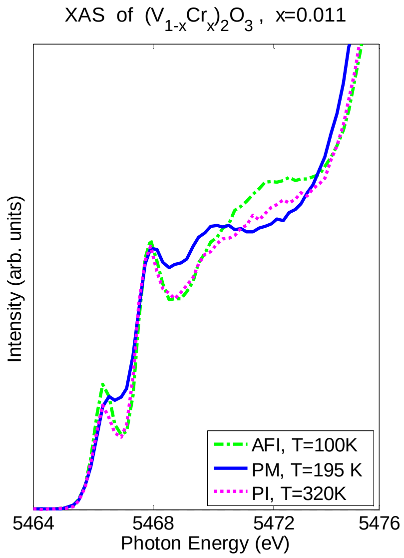

Figure 1a: V K pre-edge region in $(V_{1-x}Cr_x)_2O_3$ (x=0.011) in partial fluorescence mode as a function of temperature at room pressure.

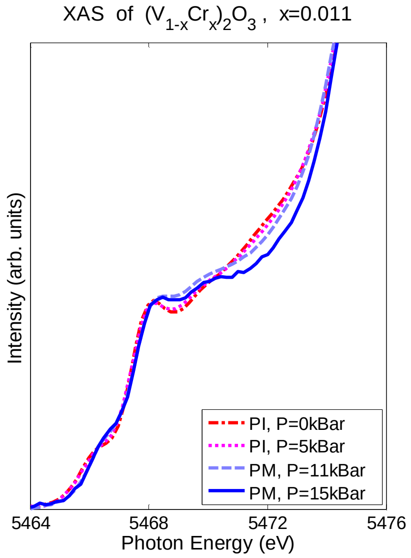

Figure 1b: V K pre-edge absorption spectra in $(V_{1-x}Cr_x)_2O_3$ (x=0.011) as a function of pressure at room temperature.

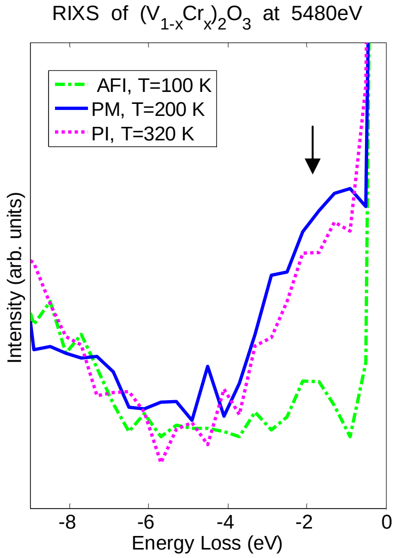

Figure 1c: Resonant inelastic x-ray scattering in $(V_{1-x}Cr_x)_2O_3$ (x=0.011) at room pressure.

Typical XAS spectra are illustrated in Figure 1a for the three phases (PI, PM, AFI) as a function of temperature at room pressure. We focus here on the pre-edge region (mainly corresponding to 1s→3d transitions) which shows the greatest sensitivity to the *d* density of states. The measurements were performed on a single crystal in reflection geometry; Absorption was acquired in the partial fluorescence yield (PFY) mode at the V Kα line. With this technique, XAS spectra with improved intrinsic resolution can be obtained, yielding an accurate picture of the electronic changes through the MIT transition. This differs from previous XAS measurements that have been carried out previously as a function of temperature [4] at the $L_{2,3}$-edges and with less emphasis onto the influence of the MIT on the electronic structure. Remarkable changes are observed in the pre-edge region between metallic and insulating regimes. Similar changes, though of smaller magnitude, could be detected by crossing the PI to PM transition upon pressure increase at room temperature (Figure 1b). The absorption spectra were here obtained in transmission mode because of the experimental constraints due to the pressure cell geometry. A comparable trend in the XAS spectra were observed while crossing the MIT phase boundary with decreasing Cr-doping level at room temperature (x=0.028 (PI), x=0.011 (PI) and x=0 (PM), results not shown here).

Finally, we have investigated the energy loss spectra by resonant inelastic x-ray scattering through the temperature-induced MIT at room pressure. The incident energy was set to ~5480 eV (i.e. in the vicinity of the white line) and we have scanned an energy range up to 10 eV from the elastic peak. The spectra show a broad feature peaking around 2 eV that grows in intensity when in the PI or PM phases (cf. Figure 1c) in addition to a structure at higher energy (~11 eV) likely associated to a plasmon excitation. The low energy excitation can be assigned to *dd*-excitations. Analysis is under way to investigate the influence of the MIT on the electronic structure.

References

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