ESRF	**Experiment title:** Low-energy excitations in V2O3	**Experiment number:** HE-2451
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Report:

An experiment to study the low-energy electronic excitations in V_2O_3 was performed at beamline ID16. The purpose of the experiment was to observe the low-lying *dd* excitations and their difference in the metallic phase and the insulating phase which is obtained by doping with Cr (2.8%). The *dd* excitations take place within the 3*d* band and are in general very weak in optical spectroscopy, but can be studied by inelastic scattering of electrons or x-rays. In the x-ray regime the experiments are typically done either in resonant inelastic x-ray scattering (RIXS) or non-resonant IXS (NRIXS). V_2O_3 has not been studied extensively with hard-xray RIXS because the V K edge has an awkwardly low energy (5.5 keV) and also because the analysers for that energy are difficult to produce. We performed the experiment in NRIXS where the incident photon energy and analyser configuration can be chosen freely. The spectrometer was based on the recently developed design utilising dispersion compensation; the analyser crystal was cross-grooved Si(nnn) crystal with a focal distance of 1 m. The x-rays were monochromatised by a combination of Si(111) premonochromator and a Si(nnn) channel-cut postmonochromator. The reflection order of the channel-cut and the analyser crystals were the same, and both worked close to backscattering conditions in order to reach best possible energy resolution. The final resolution was 50 meV with reflection order $n = 4$ (photon energy 7.9 keV).

The samples were single crystals of $V_{2-x}Cr_xO_3$ with dopings $x = 0$ and x=2.8%, corresponding to the metallic and an insulating phase, respectively. The spectra were taken with momentum transfer vector **q** along the hexagonal c-axis. All measurements were done in room temperature. Before the actual high-resolution measurement, we measured also the main volume plasmon of both samples with low resolution (1.5 eV), shown in Figure 1 left panel for the pure sample. There was, within experimental accuracy, no difference between the metallic and insulating phase in the low-resolution spectra. Next we changed energy resolution to 250 meV which helped us to aim for the high-resolution measurement. Figure 1 middle panel for the doped sample, compared to the low-resolution measurement for $q = 2.3$ Å^{-1}. There was a clearly observed 3-eV feature which increases in intensity with increasing momentum transfer due to its non-dipole character. The spectrum at $q = 3.2$ Å^{-1} also reveals a broad structure developing at about 8 eV which could be related to charge-transfer excitation. Also here no large differences were found between the metallic and the insulating phase. More interesting is the data taken of the 3-eV excitation with 50 meV resolution. It exists in both insulating and metallic phases. In the metallic phase the peak was found at 2.72 eV, and in the insulating phase at 2.87 eV. The insulating phase peak is broader and has a slight low-energy shoulder, although it is difficult to quantify it due to weak count rate and resulting large statistical errorbar. Nevertheless, theoretical studies are being currently pursued to be compared with the experimental results. We are very much interested to continue the experiments in other phases and samples of vanadium oxides since this experiment proves the feasibility of such studies in high-resolution NRIXS.

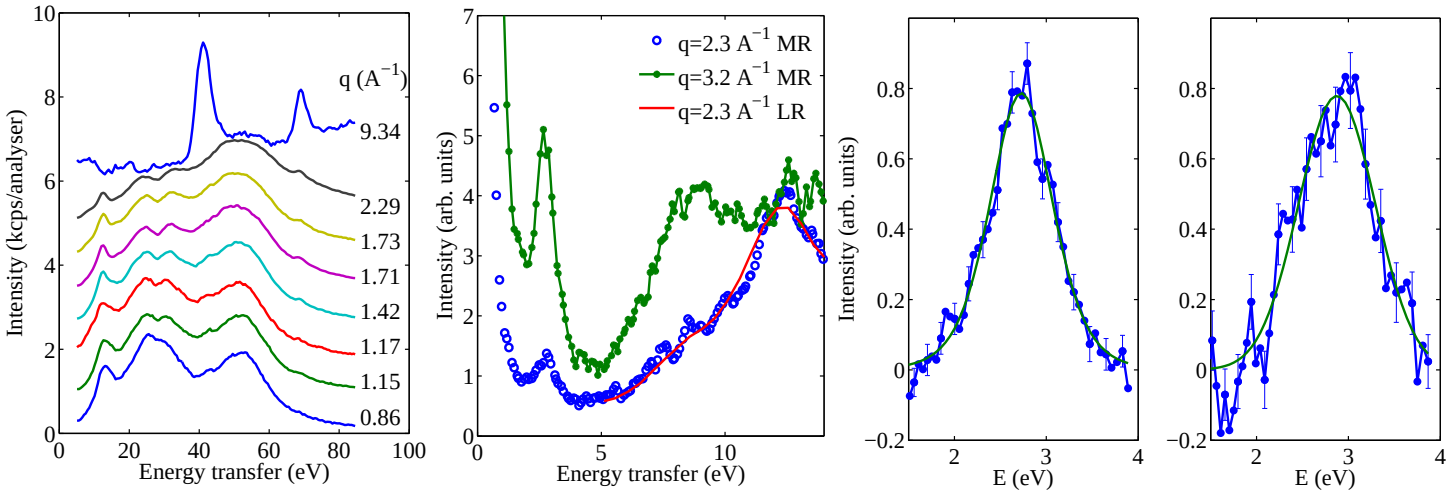

Figure 1. Left panel: Low-resolution spectra (1.5 eV) of the volume plasmon and electron-hole excitations of pure V_2O_3 in room temperature. Second panel from left: Medium-resolution spectra (250 meV) for the Cr-doped sample compared to a low-resolution spectrum. Third panel from left: 3-eV excitation measured with 50 meV resolution in the metallic sample. Last panel on right: Same as before but from insulating sample. The two last plots also include a fit of a Voigt function to the data.