Comparison of ELNES and NEXAFS of vanadium oxide V_2O_5 with different spectral resolution

D.S. Su*, M. Hävecker*, A. Knop-Gericke*, R. Mayer*, C. Hebert**, R. Schlögl*

*Department of Inorganic Chemistry, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, D-14195 Berlin, Germany
**Institut für Angewandte und Technische Physik, Technische Universität Wien, Wiedner Hauptstraße 8-10, A-1040 Wien, Austria

Electron energy-loss spectrometer (EELS) on a transmission electron microscope (TEM) exhibit the advantages of high lateral resolution and on-line structure determination by the facilities of electron diffraction and high-resolution imaging. However, EELS usually suffers under the bad energy-resolution (ca.1 eV on TEM with field emission gun). Recently, many efforts have been made to increase the energy resolution; the most promising way is the development of a monochromator selecting electrons with monoenergy. In the present work, we give a comparison of ELNES (energy-loss near edge structure) , measured with an energy resolution of 1 eV, with NEXAFS (near edge X-ray absorption fine structure), extracted from X-ray absorption spectrum (XAS) with an energy-resolution of 0.08 eV.

The EELS measurements were performed on a Philip CM 200 FEG TEM using the GATAN GIF 100 imaging filter, recorded in diffraction mode with a collection angle of 3.5 *mrad*. V_2O_5 single crystals were used. Spectra were recorded with the electron beam parallel to the c-axis (perpendicular to the layer plan). XAS experiments were carried out at the undulator beam line UE/56-2 PGM-1 at the third generation synchrotron radiation facility BESSY in Berlin [1]. The data were collected in the total electron yield mode under vacuum conditions. V_2O_5 single crystal was fixed on an alumina sample holder by a double adhesive conductive tape.

Fig. 1 shows the ELNES and NEXAFS of V_2O_5, characterised by the V *L*-edges at above 519 and 526 eV, and the O *K*-edge at above 530 eV. Due to the high energy-resolution, the more detailed spectral feature in V L_3 NEXAFS become evident, and a drastic increase of the t_{2g}* peak at the O *K*-edge is visible. The t_{2g}* and e_g* splitting is clearly better resolved in NEXAFS than in ELNES. Fig. 2 shows in an enlarged diagram of the V L_3 edge fine structures measured with 1 eV and 0.08 eV resolution. While the upper spectrum shows only a slight shoulder at 516.5 eV, the lower spectrum can be decomposed into 6 resonances. Empirically, a linear relationship between the 6 resonances and the V-O bond length in the VO_6 octahedron was established [2]. Theoretical interpretation of V L_3 and O *K* fine structure, which now becomes possible due to the high energy resolution, will be discussed using the band-structure calculations.

Acknowledgement
The work at FHI is supported by the Deutsche Forschungsgemeinschaft SFB 546.

Reference
1. K.J.S. Sawhney, F. Senf, M. Scheer, F. Schäfer, J. Bahrdt, A. Gaupp, and W. Gudat, Nucl. Instru. Meth. A 390 (1997) 395
2. M. Hävecker, A. Knop-Gericke, R. Mayer, M. Fait, H. Bluhm, and R. Schlögl, to be published

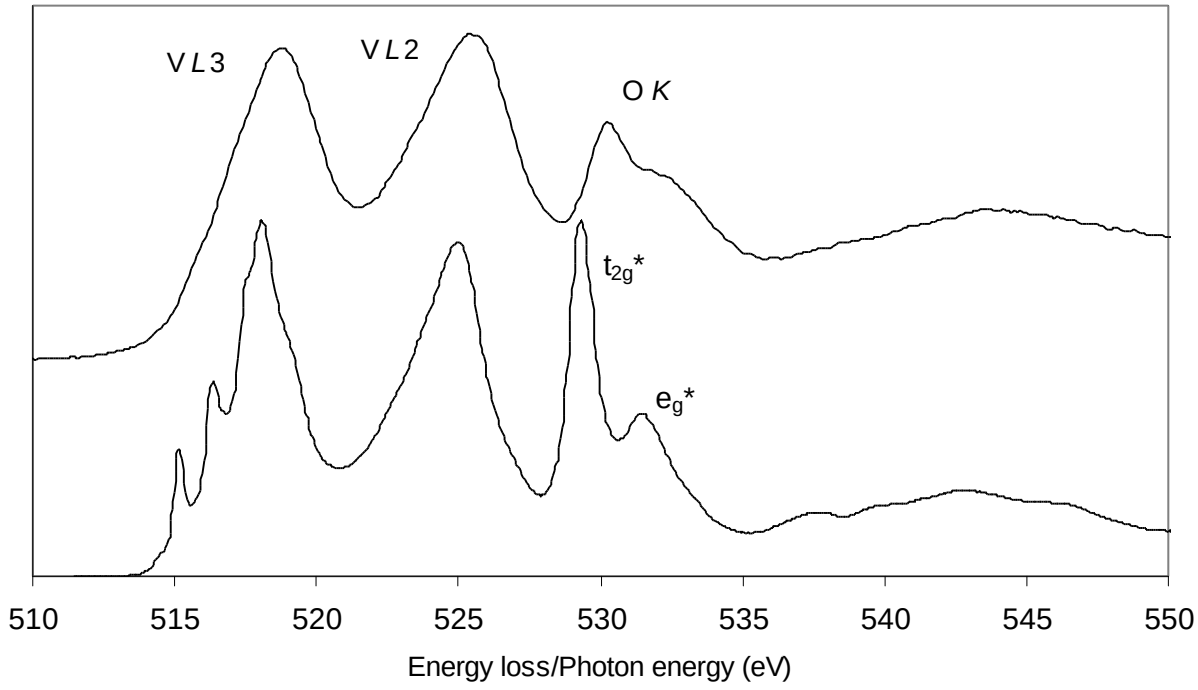

Fig. 1 (upper) ELNES and NEXAFS of V_2O_5 with an energy resolution of 1 and 0.08 eV respectively.

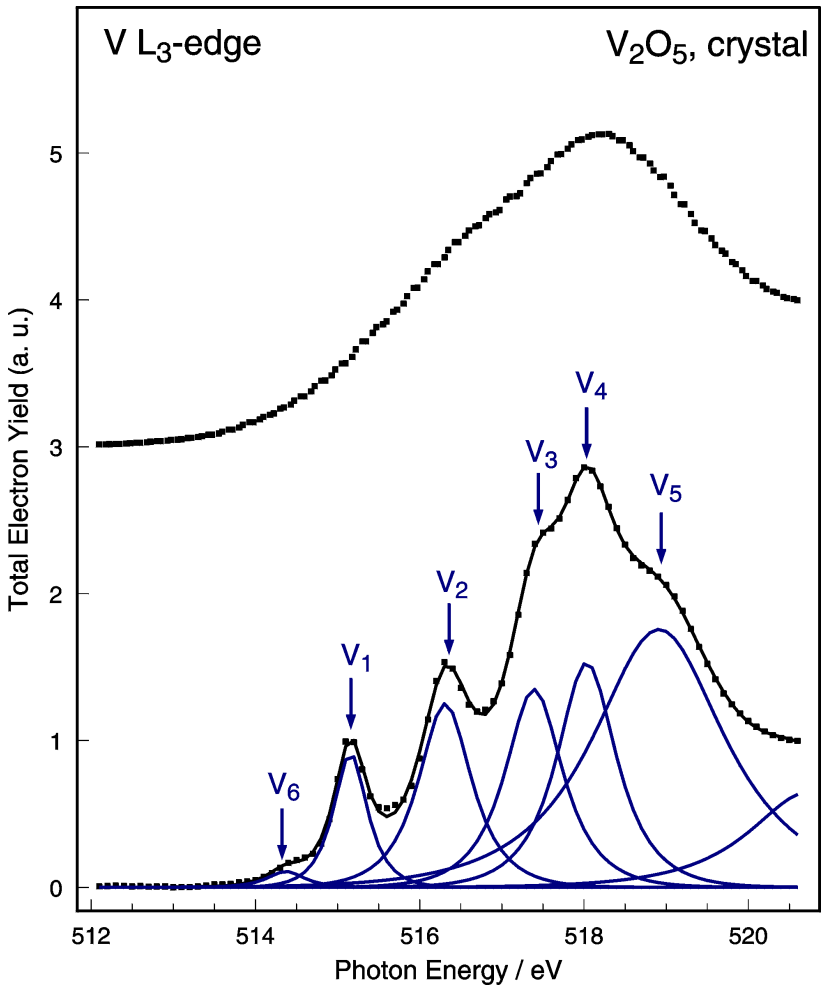

Fig. 2 (left) V L_3-edge of V_2O_5 measured with an energy resolution of 1 eV (upper) and 0.08 eV (lower), respectively.
6 resonances are obtained by deconvolution of the lower spectrum.