Comparison of ELNES and NEXAFS of vanadium oxide V$_2$O$_5$ with different spectral resolution


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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$_2$O$_5$ 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$_2$O$_5$ single crystal was fixed on an alumina sample holder by a double adhesive conductive tape.

Fig. 1 shows the ELNES and NEXAFS of V$_2$O$_5$, characterised by the V L$_3$-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.

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

Fig. 2 (left) $V_L3$-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.