Oxygen K-edge in vanadium oxides: simulations and experiments

C Hébert [1], M Willinger , D S Su [2], P Pongratz [1], P Schattschneider [1], R Schlögl [2]

[1] Institut für Festkörper Physik, Technische Universität Wien, Wiedner Hauptstrasse 8-10 1040 Wien, Austria
[2] Department of Inorganic Chemistry, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Abstract

Abstract: Band-structure (BS) calculations of the density of states (DOS) using the full potential augmented plane waves code WIEN97 were performed on the four single-valence vanadium oxides VO, V_2O_3, VO_2 and V_2O_5. The DOS are discussed with respect to the distortions of the VO_6 octahedra, the oxidation states of vanadium and the orbital hybridisations of oxygen atoms. The simulated oxygen K-edge fine structures (ELNES) calculated with the TELNES program were compared with experimental results obtained by electron energy-loss spectrometry (EELS), showing good agreement. We show that changes in the fine structures of the investigated vanadium oxides mainly result from changes in the O-p DOS and not from the shift of the DOS according to a rigid band model.