

Local Lattice Distortions in Al-doped V_2O_3 Measured by EXAFS

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Introduction: Although the temperature dependent metal-insulator-transition (MIT) in V_2O_3 has been intensively investigated, the relationship between changes in the physical, magnetic and electronic structure remains unclear. Previous XANES measurements of our group indicated a close relation between the local physical and electronic properties. To shed more light on this topic, we investigated changes of the crystal lattice of Al-doped V_2O_3 .

Methods and Materials: A single crystal of $(Al_{0.06}V_{0.94})_2O_3$ has been grown using reverse chemical transport. Temperature dependent Laue measurements showed the crystal to have a trigonal structure at room temperature. That symmetry was clearly broken at 77 K, indicating the transition from the paramagnetic insulating (PI) to the antiferromagnetic insulating (AFI) phase. The transition temperature has been determined by SQUID to be 155 K. Fluorescent EXAFS measurements were carried out using a closed cycle Helium refrigerator system (DISPLEX) and a fluorescent yield detector of the Lytle type¹ in the two significant crystal orientations, i.e. with the polarization vector of the photon beam parallel resp. perpendicular to the (pseudo-)hexagonal c-axis.

Results: Figure 1 (a) and (b) show spectra corrected for selfabsorption, as described elsewhere,² at 30 K and 180 K in both orientations. Apart from some damping at high k values due to the increased noise at higher temperatures, there is no significant temperature dependent change in the EXAFS signal in these spectra. On the other hand, noticeable changes can be observed in the pure compound (Figure 1 (c)). Comparison of the experimental spectra with theoretical calculations using the FEFF code not shown here shows that the monoclinic model matches the experiment much better than the trigonal model.

Conclusions: This shows that the local structure of Al doped V_2O_3 is monoclinic not only in the AFI phase, but also in the high temperature PI phase which shows a trigonal average crystal structure. Together with soft x-ray absorption results of our group published earlier³ and EXAFS analysis on pure V_2O_3 done by Frenkel⁴ these results indicate that there is a close relation between the local electronic structure and the local lattice distortion observed in V_2O_3 .

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