XAFS STUDY OF ZrO_2–BASED SOFC MATERIALS

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A XAFS study of yttrium stabilized manganese doped zirconia solid solutions is presented. The materials are promising candidates for intermediate layers between electrolyte and cathode in solid oxide fuel cells. Presence of manganese in the zirconia solid solution is expected to bring about electronic conductivity owing to the formation of electron defects at manganese ions. In consequence, the resistance for charge transfer between electrolyte and cathode would be reduced.

Powder samples of $Mn_x(Y_{0.08}Zr_{0.92})_{1-x}O_{2-\delta}$ ($0 < x < 0.25$) used for XAFS study were prepared by co-precipitation-calcination method and then sintered for 2 h at 1500°C. The dependence of the lattice parameters on x follows the Vegard rule from zero to about 18 mol.% of manganese where the cubic zirconia structure of the solid solution is preserved.

The measurements have been carried out in Hasylab/DESY, Hamburg, in the XANES (X-ray Absorption Near Edge Structure) and EXAFS (Extended X-ray Absorption Fine Structure) ranges at the manganese and yttrium K edges at room temperature and at 10 K. The XANES spectra at the Mn K edge are presented in Fig. 1.

The absorption edge energies of the samples studied derived from the spectra were compared to those of the reference samples. Assuming a linear dependence between the valence and the edge energy, the valences of Mn in the samples studied were obtained. They are collected in the table below and show that the Mn average oxidation degree is between +2 and +3. It increases with increasing manganese content.

Sample	Edge energy [eV]	Average oxidation
5% Mn	6547.0	2.44± 0.02
10% Mn	6547.2	2.47± 0,02
15% Mn	6547.7	2.60± 0.02

Fourier transforms of EXAFS spectra obtained at the Y K edge are presented in Fig. 2. They show significant changes with Mn content in the second coordination shell (3.6 Å) corresponding to metal ions, whereas only slight modifications in the first coordination shell (2.1 Å) corresponding to oxygen neighbours is found.

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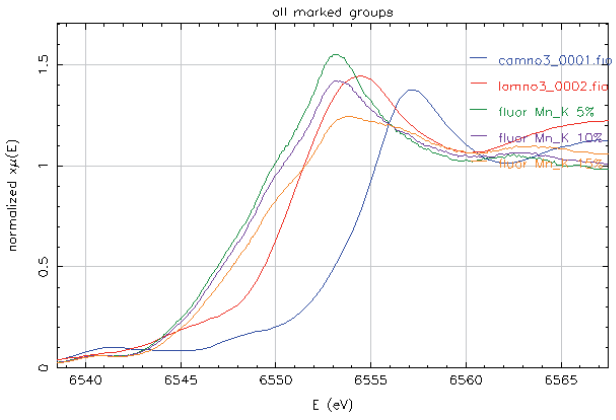

Figure 1. XANES spectra of Mn:K edge of yttrium stabilised zirconia oxide doped with 5, 10 and 15% of manganese.

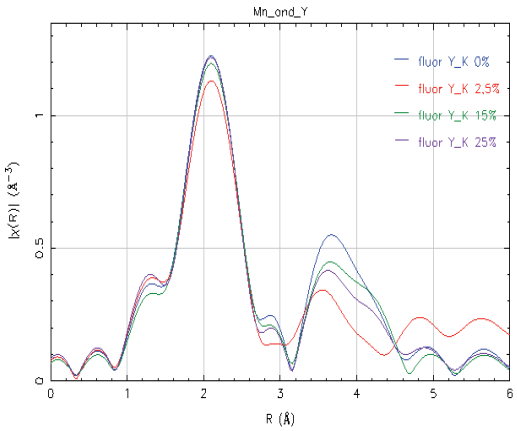

Figure 2. Fourier transforms of the EXAFS spectra obtained at the Y K edge at room temperature for the zirconia oxide doped with 2.5%, 15% and 25% Mn.