L-10 **Session B, Tuesday, 14.06., 11^{40} - 12^{20}**

Study of oxide materials for energy applications with X-ray spectroscopies

Cz. Kapusta[1*], K. Kollbek[1,2], J. Stępień[1], M. Sikora[1,2], K. Schneider[3], K. Zakrzewska[3] and J. Szlachetko[4,5]

[1]*AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Kraków, Poland*
[2]*AGH University of Science and Technology, Academic Centre for Materials and Nanotechnology, Kraków, Poland*
[3]*AGH University of Science and Technology, Faculty of Computer Sciences, Electronics and Telecommunications, Kraków, Poland*
[4]*Paul Scherrer Institute, Swiss Light Source, Villigen-PSI, Switzerland*
[5]*Institute of Physics, Jan Kochanowski University, Kielce, Poland*

Keywords: titania nanomaterials, doped zirconia, perovskites, photoelectrolysis, fuel cells, XAS, XES, RIXS

*e-mail: kapusta@agh.edu.pl

In the lecture selected applications of X-ray spectroscopies for the study of materials for energy conversion are to be presented. Three groups of materials are discussed: titania nanofilms/ nanopowders, yttria stabilized/doped zirconia and the lanthanide – 3d element perovskites. The titania based materials attract nuch interest due to their applications in photovoltaics and catalysis. Yttria stabilized zirconia and perovskites are the materials used for fuel cells. Results obtained with the following X-ray spectroscopic methods will be presented: High Resolution XAS/XES (X-ray Absorption Spectroscopy / X-ray Emission Spectroscopy) derived from RIXS (Resonant Inelastic X-ray Scattering) measurements, as well as a conventional XAS in the XANES (Near Edge Absorption Structure) and EXAFS (Extended X-ray Absorption Structure).

For the study of doped titania nanopowders and nanofilms of various oxygen stoichiometry, crystal structure and the cation and anion sites doping, two dimensional RIXS dependences have been measured at the Ti:K edge. They delivered HR-XES and HR-XANES spectra which provided information on e.g. band gap (Fig. 1, [1]) or the location of dopants in the next neighborhood of the Ti site.

The yttria stabilized zirconia doped with manganese, of the formula $Mn_x(Y_{0,148}Zr_{0,852})_{1-x}O_{2-\delta}$, has been studied with conventional XAS spectroscopy in the XANES and EXAFS range at the Mn:K, Zr:K and Y:K edges [2]. The Mn spectra, Fig. 2, show a considerable change of the edge energy and shape corresponding to changes of Mn average valence and symmetry of its local environment with x, in contrast to Zr (Fig. 2) and Y, where slight changes in the spectra are observed only.

A combination of XANES and XES methods was applied to $LaMn_{1-x}Co_xO_3$ system [3]. It provided the information on the charge and spin evolution of manganese and cobalt on x.

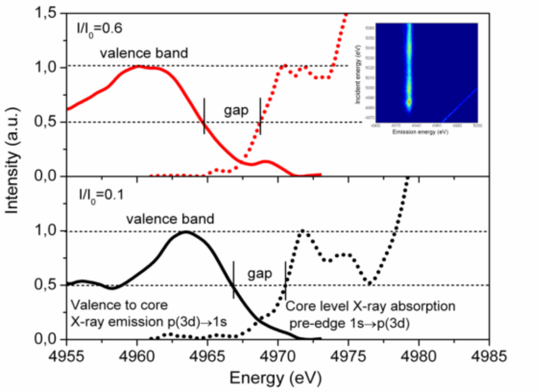

Figure 1. Pre-peak of Ti-K-edge HR-XANES (dashed) and Kβ lines of XES spectra (solid) of TiO_{2-x} for different x (I/I_0), after [1]. The extracted band gap energy is marked. Inset - the RIXS plane, from which XES and XANES spectra were derived.

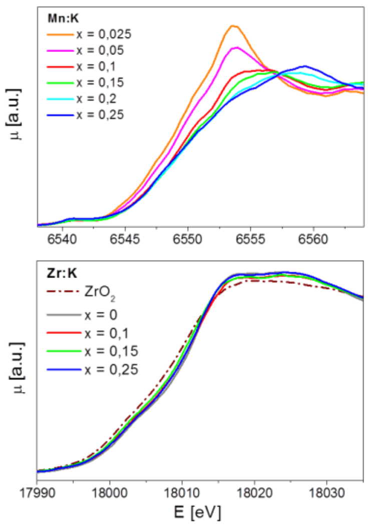

Figure 2. XANES spectra of $Mn_x(Y_{0,148}Zr_{0,852})_{1-x}O_{2-\delta}$ at the Mn:K and Zr:K edges (after [2]).

The results are analysed in terms of unique information on the individual element valencies, projected bands, site symmetries, charge and spin states provided by the synchrotron radiation exploiting X-ray spectroscopies. The relation of these data to those obtained by other methods, e.g. magnetometry, and to the crucial applied properties and parameters of the materials is discussed.

[1] K.Kollbek, M.Sikora, Cz.Kapusta, J.Szlachetko, K.Zakrzewska, K.Kowalski, M. Radecka, *Appl. Surf. Sci.* **281** (2013) 100.

[2] J. Stępień, *PhD Thesis*, AGH University of Science and Technology, Kraków, 2015.

[3] M. Sikora, K. Knizek, Cz. Kapusta, P. Glatzel, *J. Appl. Phys.* **103** (2008) 07C907.