

XAFS STUDY OF  $\text{BaCe}_{1-x}\text{Ti}_x\text{O}_3$  PROTONIC SOLID ELECTROLYTES

**P. Seremak-Peczki<sup>1\*</sup>, K. Schneider<sup>1</sup>, W. Zajączkowski<sup>1</sup>, Cz. Kapusta<sup>1</sup>,  
D. Zając<sup>2,3</sup>, P. Pasierb<sup>4</sup>, E. Drożdż-Cieśla<sup>4</sup>, and M. Rękas<sup>4</sup>**

<sup>1</sup> AGH University of Science & Technology, Faculty of Physics and Applied Computer Science,  
Dept. of Solid State Physics, PL-30059 Krakow, Poland

<sup>2</sup> Institute of Nuclear Physics PAS, Dept. of Magnetic Resonance Spectroscopy, PL-31342 Krakow, Poland

<sup>3</sup> Hasylab at DESY, D22607 Hamburg, Germany

<sup>4</sup> AGH University of Science & Technology, Faculty of Materials Science and Ceramics,  
PL-30059 Krakow, Poland

*Keywords: protonic electrolytes, fuel cells, barium cerate, barium titanate, synchrotron radiation, XAFS*

*\*) e-mail: kameres@interia.pl*

In this work the local structures and valence properties of Ti in  $\text{BaCe}_{1-x}\text{Ti}_x\text{O}_3$  materials were investigated. The materials belong to a new class solid electrolytes which can be used in intermediate temperature fuel cells. The series of four compounds with different titanium content  $x$  (0-0.3) was studied by means of X-ray absorption fine structure (XAFS) spectroscopy.

Powders of  $\text{BaCe}_{1-x}\text{Ti}_x\text{O}_3$  ( $x = 0.0, 0.05, 0.07, 0.10, 0.15, 0.20$  and  $0.30$ ) were prepared by solid-state reaction method. Barium carbonate  $\text{BaCO}_3$  (99.9%), cerium (IV) oxide  $\text{CeO}_2$  (99.9%) and  $\text{TiO}_2$  nanopowder (99.7%). The structural studies by X-ray diffraction have shown that undoped material crystallizes in orthorhombic phase, while the increasing concentration of Ti dopant up to  $x = 0.2$  leads to the ordering of the structure to phases with higher symmetries (tetragonal and even cubic).

The XAFS measurements have been carried out at Hasylab/DESY synchrotron facility in the XANES (X-ray Absorption Near Edge Structure) region and in the EXAFS (Extended X-ray Absorption Fine Structure) region. The Ti:K edge spectra were measured at the CEMO station with the transmission mode. The XANES results obtained at the Ti:K edge are shown in Fig. 1 and the EXAFS results are presented in Fig. 2.

The XANES spectra show a complex structure with a pre-edge peak, which is especially pronounced in the  $x=0.3$  compound. This indicates a low symmetry of the Ti environment here, in contrast to the other compounds.

The Fourier transforms of the EXAFS show the main peak corresponding to the oxygen nearest neighbours at the distance from the Ti ion closer by  $0.1 \text{ \AA}$  in the  $x=0.3$  compound than in the other. The second nearest neighbour peak, which corresponds mainly to metal ions, decreases its intensity with increasing Ti content. This is related mainly to a smaller photoelectron scattering amplitude of Ti due to its  $Z$  number smaller than that of Ce. A much smaller amplitude of the second nearest neighbour peak and its different shape in the  $x=0.3$  compound can possibly be attributed to its different structure. The results of the XAFS study are compared to those of X-ray diffraction measurements and magnetometry.

**Acknowledgements:** This paper was supported by the Polish Ministry of Science and Higher Education, Projects no. PBZ/MEiN/01/2006/57 and R15 019 02.

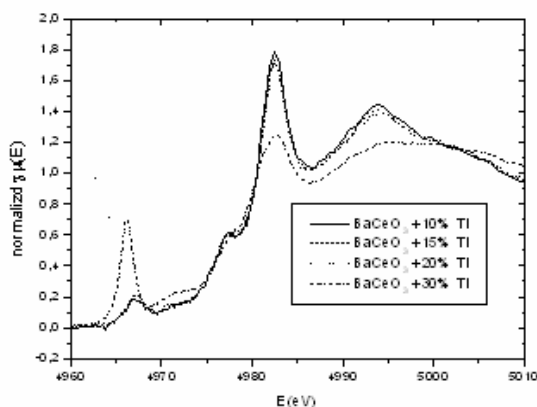


Figure 1. Normalized XANES spectra at the Ti:K edge for the  $\text{BaCe}_{1-x}\text{Ti}_x\text{O}_{3-d}$  compounds.

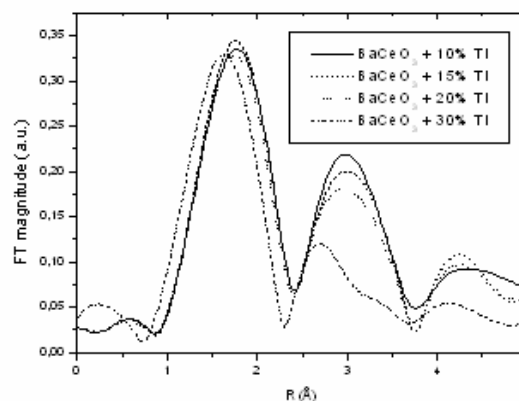


Figure 2. Fourier transforms of the Ti:K edge EXAFS function for the  $\text{BaCe}_{1-x}\text{Ti}_x\text{O}_{3-d}$  compounds.