

“Physico-chemical nanomaterials science” (*Oral presentation*)

Coupling of electronic, magnetic and lattice degrees of freedom in $R\text{Co}_{1-x}\text{Fe}_x\text{O}_3$ cobaltites-ferrites

L. Vasylechko¹, I. Lutsyuk¹, O. Pekinchak¹, D. Sugak¹, Yu. Suhak², H. Fritze²

¹*Lviv Polytechnic National University, 12 Bandera Street, 79013 Lviv, Ukraine*
E-mail: crystal-lov@polynet.lviv.ua

²*Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Goslar, Germany*

In situ temperature-dependent powder diffraction examinations and analysis of thermal expansion is very useful tool not only for the study of structural phase transitions, but also for the investigation of diverse electronic and magnetic phase transformations occurred in complex oxide systems. Especially this is important for the Pr- and Nd-based materials, where the spin-state transition is seen much better in the thermal expansion data than in the magnetic susceptibility due to the large contribution of the $4f$ moments of rare earth ions on the magnetic properties.

Crystal structure behaviour and transport properties of the micro- and nanocrystalline powders of $R\text{Co}_{1-x}\text{Fe}_x\text{O}_3$ ($R = \text{Pr} \dots \text{Tm}$) with orthorhombic perovskite structure has been studied in detail by a combination of *in situ* X-ray synchrotron powder diffraction and temperature dependent impedance spectroscopy measurements in the temperature range of 298–1173 K. Remarkable anomalies in the lattice expansions, which are reflected in a sigmoidal dependence of the unit cell dimensions and in abnormal anisotropic increase of the thermal expansion coefficients (TEC) with broad maxima in the temperature range of 500–1000 K, are detected for all samples synthesized. Extra structural anomalies were detected in the temperature dependence of the selected bond lengths and octahedra tilt angles, as well as the atomic displacement parameters. Observed anomalies in the $R\text{Co}_{1-x}\text{Fe}_x\text{O}_3$ series become less pronounced with the decreasing cobalt content, and the temperatures of the maxima at the TEC curves shift to the higher temperatures. It is evident, that all these anomalies are associated with the transitions of Co^{3+} ions from low spin to the higher spin states and the coupled metal-insulator transitions, occurred in the rare earth cobaltites at the elevated temperatures. The temperature-dependent impedance measurements prove the change of conductivity type from dielectric to the metallic behaviour in the praseodymium cobaltite-ferrites at the elevated temperatures. The temperature of insulator-metal transition increases in $\text{PrCo}_{1-x}\text{Fe}_x\text{O}_3$ series, which is in a good agreement with the thermal expansion data.