“Physico-chemical nanomaterials science”

Crystal structure peculiarities of mixed ferrites $La_{1-x}Sm_xFeO_3$

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The interest in the rare earth ferrites is stimulated by their unique properties, such as high electrical conductivity, specific magnetic properties including spin reorientation phenomena, as well as significant electrochemical and catalytic activity. $R FeO_3$ compounds are used in thermoelectric devices, solid oxide fuel cells, as membranes for partial oxidation of methane and oxygen cleaning and as sensory materials.

Samples with nominal compositions $La_{1-x}Sm_xFeO_3$ (x = 0.2, 0.4, 0.6, 0.8) were obtained by solid state reactions technique. Precursor oxides La_2O_3, Sm_2O_3 and Fe_2O_3 were ball-milled in ethanol for 5 h, dried, pressed into pellets and annealed in air at 1473 K for 40 h with one intermediate redrinding. X-ray phase and structural characterization was performed by using Huber imaging plate Guinier camera G670 (Cu K_1 radiation, = 1.54056 Å). Spot-check examination of the cationic composition was performed by energy dispersive X-ray fluorescence (EDXRF) analysis by using XRF Analyzer Expert 3L. It was established that all samples synthesized adopt orthorhombic perovskite structure isotypic with $GdFeO_3$. Structural parameters of the mixed ferrites obtained derived by full profile Rietveld refinement agree well with the data of the "pure" $LaFeO_3$ and $SmFeO_3$ compounds, thus proving formation of continuous solid solution $La_{1-x}Sm_xFeO_3$ in the $LaFeO_3$–$SmFeO_3$ system. Peculiarity of this solid solution is the lattice parameters crossover and formation of dimensionally tetragonal structure at x = 0.04 (Fig.). The unit cell volume of $La_{1-x}Sm_xFeO_3$ series decreases almost linearly with decreasing R-cation radii according to the Vegard’s rule.

	Fig. Concentration dependencies of unit cell dimensions of $La_{1-x}Sm_xFeO_3$ at room temperature. Lattice parameters and cell volume of the orthorhombic cell are normalized to the perovskite ones as follows: $a_p = a_o/\sqrt{2}$, $b_p = b_o/\sqrt{2}$, $c_p = c_o/2$, $V_p = V_o/4$.