“Physico-chemical nanomaterials science”

Structural behavior of solid solutions in the $NdAlO_3$-$SrTiO_3$ system

N.A. Ohon`[1], L.O. Vasylechko[1], R.V. Stepchuk[1], I.I. Syvorotka[2]

[1] *Lviv Polytechnic National University, 12 Bandera St, Lviv-79013, Ukraine.*
E-mail: nat.ogonj@gmail.com

[2] *Scientific Research Company “Carat”, Lviv, Ukraine*

Materials with perovskite structure based on rare earth aluminates $RAlO_3$ and their solid solutions with strontium titanate $SrTiO_3$ are considered and already used as prospective functional materials, such as electrode materials in solid oxide fuel cells, radio-frequency ceramics, phosphors and refractory materials due to their excellent dielectric properties.

Mixed aluminates-titanates $Nd_{1-x}Sr_xAl_{1-x}Ti_xO_3$ (x = 0.3÷0.9) were prepared from stoichiometric amounts of constituent oxides Nd_2O_3, Al_2O_3, TiO_2 and Sr carbonate $SrCO_3$ by solid-state reaction technique in air at 1773 K for 9 h. X-ray powder diffraction examination revealed pure perovskite structure for all samples synthesized. The $Nd_{1-x}Sr_xAl_{1-x}Ti_xO_3$ samples with x=0.7, 0.8 and 0.9 show ideal cubic perovskite structure, whereas the samples with x=0.3 and 0.5 addopt rhombohedral structure isotypic with $NdAlO_3$. Full-profile Rietveld refinement, performed in corresponding space groups *Pmm* and *Rc* show good fits between experimental and calculated profiles for all compositions, thus confirm their phase purity and crystal structures. Comparison of the obtained structural parameters of the mixed aluminates-titanates with the literature data for the end members of the system $NdAlO_3$ and $SrTiO_3$ prove a formation of two kinds of solid solution $Nd_{1-x}Sr_xAl_{1-x}Ti_xO_3$ with rhombohedral (x < 0.7) and cubic (x 0.7) perovskite structure (Fig. 1).

	Fig. 1. Concentration dependencies of the unit cell dimensions illustrating concentration-induced continuous phase transition *Rc-Pmm* in $Nd_{1-x}Sr_xAl_{1-x}Ti_xO_3$ series. Lattice parameters and cell volume of the rhombohedral (*Rh*) cell are normalized to the perovskite ones as follows: $a_p = a_r/\sqrt{2}$, $c_p = c_r/\sqrt{12}$, $V_p = V_r/6$.