"Physico-Chemical nanomaterials science"

Structural behavior of $NdFe_xAl_{1-x}O_3$ nanopowders obtained by sol-gel method

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RAlO_3- and *R*FeO_3- based materials with perovskite structure are considered and already used as prospective functional materials, including materials for Solid oxide Fuel Cells (SOFC), materials for laser hosts, phosphors and scintillates, dielectrics, high-temperature ceramics, catalysts, sensory materials and pigments.

Series of $NdFe_xAl_{1-x}O_3$ (x = 0.1, 0.15, 0.2, 0.25, 0.3, 0.5, 0.8) nanopowders was obtained by sol-gel citrate method from $Nd(NO_3)_2 \cdot 6H_2O$, $Fe(NO_3)_2 \cdot 9H_2O$ and $Al(NO_3)_3 \cdot 9H_2O$ as initial reagents. Water solutions of the neodymium, iron and aluminium nitrates were mixed together on magnetic stirring for 30 min, after that water solution of citric acid (CA) was added to the reaction mixture under continuous stirring. The molar ratio of reagents was $n(Nd^{3+}) : n(Fe^{3+}) : n(Al^{3+}) : n(CC) = 1 : x : 1\text{-}x : 2$. Prepared solution was gelled at 343–353 K for 4 h after that head treated sequentially at 573 K and 723 K for 1 h. Obtained foamy product was calcined at 1073 K for 2 h. After X-ray diffraction (XRD) examination the part of the powders was additionally annealed at 1173 K for 2 h and then at 1473 K for 4 h. Thus three series of $NdFe_xAl_{1-x}O_3$ specimens, synthesized at different conditions, were obtained.

X-ray powder diffraction examinations of the $NdFe_xAl_{1-x}O_3$ specimens revealed morfotropic structural phase transition at x = 0.1–0.15 and formation two kind of solid solytions wiht rhombohedral and orthorhombic structures. The unit cell volume of $NdFe_xAl_{1-x}O_3$ series decreases almost linearly with decreasing *R*-cation radii according to the Vegard's rule. Also peculiarity of this solid solutions is the lattice parameters crossovers occurred at x = 0.32, 0.36 and 0.42. Evaluation of microstructural parameters of the $NdFe_xAl_{1-x}O_3$ samples from the analysis of the XRD profile broadening by full profile Rietveld technique, lead to the average grain size D_{ave} = 60–130 nm and microstrains $\langle e \rangle = \langle D_d \rangle / d =$ 0.8–0.18 %, depending on composition and heat treatment temperature.

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