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Crystal structure of bismuth ferrite based compounds prepared by sol-gel method

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In the last decade, materials belonging to the class of multiferroics have attracted the increased interest of researchers. One of the most famous multiferoics is bismuth ferrite, which has high transition temperatures to the magnetically ordered and ferroelectric state. Doping in the A- position of perovskite lattice allows to modify the ferroelectric subsystem, even though such doping schemes are usually associated with the difficulties in determination of the crystal structure, especially in the vicinity of the phase boundary regions. The system doped $Bi_{1-x}La_xFeO_3$ exhibits a number of structural transitions driven by changes in ion dopend concentration.

Experimental. Samples of $Bi_{1-x}La_xFeO_3$ system with concentrations of the dopant ions up to x = 0.50, were prepared by the sol-gel method. Structural measurements have been performed using neutron powder diffraction (NPD) measurements were performed using high-resolution neutron powder diffractometer FIREPOD (λ=1.7977Å, E9 instrument, HZB).

Results and discussion. The neutron powder diffraction patterns obtained for the compositions $Bi_{1-x}La_xFeO_3$ (x<=0.15) at room temperature were successfully refined using the antiferromagnetic rhombohedral model (space group R3c). It should be noted that the structural distortions of the indicated compositions suggest an antiphase tilt of the *B*O6 oxygen octahedra ($a^-a^-a^-$ in the Glazer notation) and polar displacements of ions along the $[111]_C$ direction of the base cubic cell. It is assumed that the ordering of the magnetic moments of Fe^{3+} ions in the rhombohedral phase is characterized by spatial modulation with a period of ~ 50-100 nm; a more accurate determination of the modulation period is limited by the resolution of the diffractometer used in the experiment (FirePod, HZB). The magnetic contribution to the neutron diffraction spectrum is described under the assumption of antiferromagnetic ordering of the Fe^{3+} G-type magnetic moments (the calculated magnetic moment is ~ 3.6 μB), the magnetic moments are oriented along the ***a*** - parameter of the hexagonal axis. The diffractogram of the $Bi_{0.82}La_{0.18}FeO_3$ composition was refined in the model assuming an orthorhombic structure (space group Pnam), combining the inclination of oxygen octahedra $(a^-a^-c^+)/(a^-a^-c^-)$, similar to the $PbZrO_3$ composition with antipolar displacements A cations along the $[110/\bar{1}\bar{1}0]_C$ directions of the original perovskite cell. The magnetic moments of iron ions are oriented along the ***c*** - axis of the orthorhombic cell and form an antiferromagnetic

G-type structure. For compounds $Bi_{1-x}La_xFeO_3$ ($0.2 < x < 0.5$), neutron powder diffraction patterns showed a pattern that consists of basic reflections of perovskite, completely consistent with an orthorhombic unit cell with the metric $\sqrt{2}a_c \times 2a_c \times \sqrt{2}a_c$, and small superstructural reflections incompatible with any commensurate superstructure.

Conclusion. The neutron diffraction data obtained for the compositions $Bi_{1-x}La_xFeO_3$ ($x <= 0.15$) at room temperature are characterized by a single-phase antiferromagnetic rhombohedral structure (space group R3c) for the compositions $Bi_{1-x}La_xFeO_3$. The neutron powder diffraction patterns obtained for the compositions$Bi_{1-x}La_xFeO_3$ ($0.2 <x <0.5$) at room temperature were successfully refined using the orthorhombic model.

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