

*Structural phase transition in  $(Y_{0.95}Bi_{0.05})Fe_3(BO_3)_4$  iron borate*

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Some of rare earth iron borates  $RFe_3(BO_3)_4$  are assigned to multiferroic family due to coexisting of spontaneous electric polarization, magnetoelectric and magnetoelastic properties. The diverse iron borates properties are attributed to the presence of two magnetic subsystems formed by iron and rare earth ions. The presence of non-magnetic Y ion allows tracing the mutual influence of the Fe and R sublattices to the magnetic and crystal structure.

The  $YFe_3(BO_3)_4$  single crystals under studying were grown using flux method with a presence of  $Bi_2Mo_3O_{12}$ . Bi atoms from the flux were detected in the structure by X-ray spectroscopy method using a FEI Quanta 200 3D Dual Beam scanning electron microscope equipped with an EDAX EDS system. The complete XRD data were collected in 90–500 K temperature range using CCD Xcalibur S (Rigaku Oxford Diffraction) diffractometer equipped with Cobra Plus (Oxford Cryosystems) cryosystem and using PILATUS@SNBL diffractometer with Oxford Cryostream700+ heater. The Mossbauer spectroscopy on  $^{57}Fe$  nuclei were performed in temperature range 40–500 K on standard spectrometer MS-1104Em equipped with closed cycle liquid free helium cryostat CryoFree-104 (RTI Cryomagnetic Systems) and high temperature resistive air furnace.

The refined composition of the structure based on the XRD data is  $(Y_{0.95}Bi_{0.05})Fe_3(BO_3)_4$ . It was found that the crystal is a merohedral twin. Unit cell parameters temperature dependence has not let to confirm the temperature of phase transition. However, after sp.gr. R32 systematic absences analysis it was shown that crystal undergo a phase transition in the 350–370 K range at about 370 K. The structures were solved in P3121 sp.gr. at 90–370 K and in R32 sp.gr. at 375–500 K. The crystal structure is made of Y(Bi)O<sub>6</sub> prisms, edge-sharing FeO<sub>6</sub> octahedra chains and two types of BO<sub>3</sub> triangles in R32 sp.gr. For the structure relating to P3121 sp.gr. there are two types of FeO<sub>6</sub>-chains and three types of BO<sub>3</sub> triangles. The distortions of Y(Bi)O<sub>6</sub>, FeO<sub>6</sub>, B(2)O<sub>3</sub> and B(3)O<sub>3</sub> coordination polyhedra were observed upon lowering the temperature. The Fe<sub>1</sub>–Fe<sub>1</sub> distances in the helical chains along c axis decrease, the Fe<sub>2</sub>–Fe<sub>2</sub> distances increase, the angles Fe–O–Fe change nonuniformly. The shortest distances between 3 chains in ab plane become reduced, the most long distances increase. The existence of two Fe crystallographic positions lead to emergence of two magnetic Fe positions below the Neel temperature. The effect of the distortion of the crystal structure was analyzed on the magnetoelectric properties. Dynamic of temperature dependence of the quadrupole splitting (structural sensitive Mossbauer hyperfine parameter) in high temperature range 300–500 K correlates with our XRD results in general, but has some specific features.

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