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Supporting information for article:

Crystal structure, phase transition and structural deformations in iron borate (Y0.95Bi0.05)Fe3(BO3)4 in the temperature range 90–500 K

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Acta Crystallographica Section B supporting information

Crystal structure, phase transition and structural deformations in iron borate (Y0.95Bi0.05)Fe3(BO3)4 in the temperature range 90–500 K

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S1. Supporting information

Fe K-, Y K-, and Bi L_3-edge XANES and EXAFS spectra were measured at room temperature at the Structural Materials Science beamline of the Kurchatov Synchrotron Radiation Source (National Research Center "Kurchatov Institute", Moscow, Russia) (Chernyshov *et. al.*, 2009). For the measurements, single-crystalline specimens were finely ground in a mortar. The fine powder was carefully spread over the Kapton adhesive tape. The tape was folded into a few layers to achieve an adsorption edge jump $\Delta\mu$=0.5-10. Fe and Y K-edge spectra were measured in the transmission mode using ionization chambers filled with N_2/argon mixtures providing 20% and 80% transmission for I_0 and I_t, respectively. Due to the low Bi concentration in the material, the transmission mode was not suitable for the data acquisituion. And thus Bi L_3-edge spectra were measured in the X-ray fluorescence yield mode using an FMB Oxford (UK) Si avalanche diode.

The experimental spectra were processed using Athena and Artemis procedures from the IFEFFIT package (Ravel B. & Newville, 2005). Non-linear curve-fitting was performed based on *ab initio* theoretical photoelectron back-scattering phase and amplitude functions calculated using the FEFF8 code (Newville, 2001). Normalized EXAFS curves for fitting were weighted with k^3-functions. The extrinsic loss amplitude reduction factor S_0^2 was fixed at 0.75. Only interatomic distances and Debye-Waller factors were allowed to vary. The coordination numbers were kept fixed at nominal values derived from crystallographic data.

Experimental XANES spectra are shown in Fig. S1. EXAFS Fourier transforms both experimental and best-fit theoretical are given in Figs. S2-S4, whereas local-structure parameters obtained from EXAFS fits and some other relevant refinement parameters are listed in Table S1.

Table S1 Local structure parameters around Bi, Fe, and Y atoms in $(Y_{0.95}Bi_{0.05})Fe_3(BO_3)_4$ according to non-linear curve-fitting of EXAFS spectra: coordination numbers (N), interatomic distances (R), and Debye-Waller factors (σ^2)

Edge	Δk range, Å^{-1}	ΔR range, Å	Path	N	R, Å	σ^2, Å^2	ΔE, eV	R_f
Bi	2.0-12.3	1.6-3.7	Bi-O1	6	2.46	0.00344	8.3	0.067
L3			Bi-O2	2	2.62	0.00344		
			Bi…B	6	3.21	0.01251		
			Bi…Fe	6	3.83	0.00752		
Fe K	2.0-14.0	1.15-3.3	Fe-O	6	2.01	0.00488	1.8	0.005
			Fe…B	6	3.07	0.00267		
			Fe…Fe	2	3.19	0.00379		
Y K	2.0-14.3	1.6-3.7	Y-O1	6	2.34	0.00579	2.7	0.011
			Y-O2	2	2.90	0.00579		
			Y…B	6	3.08	0.01478		
			Y…Fe	6	3.79	0.01040		

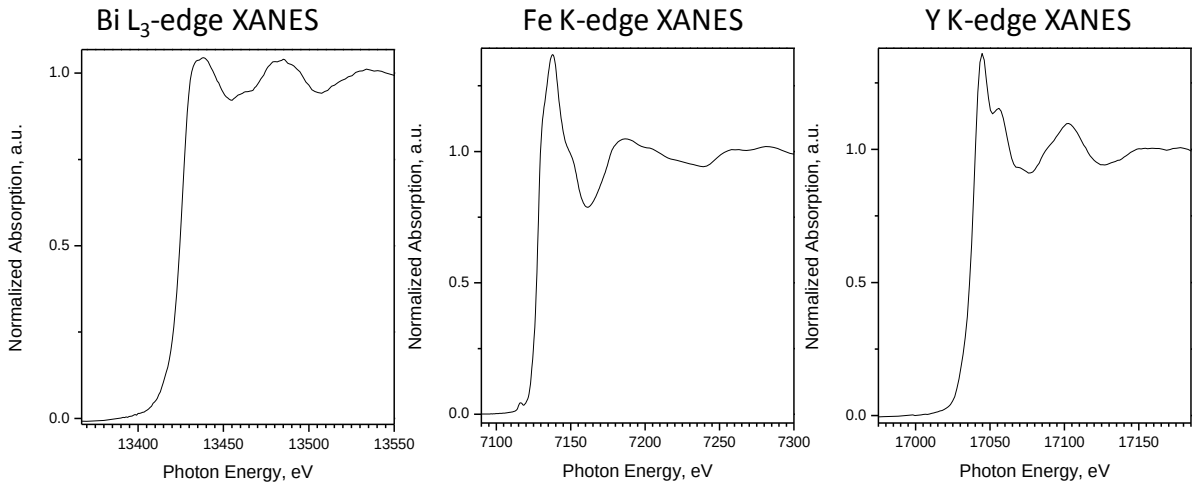

Figure S1 Experimental XANES spectra for $(Y_{0.95}Bi_{0.05})Fe_3(BO_3)_4$

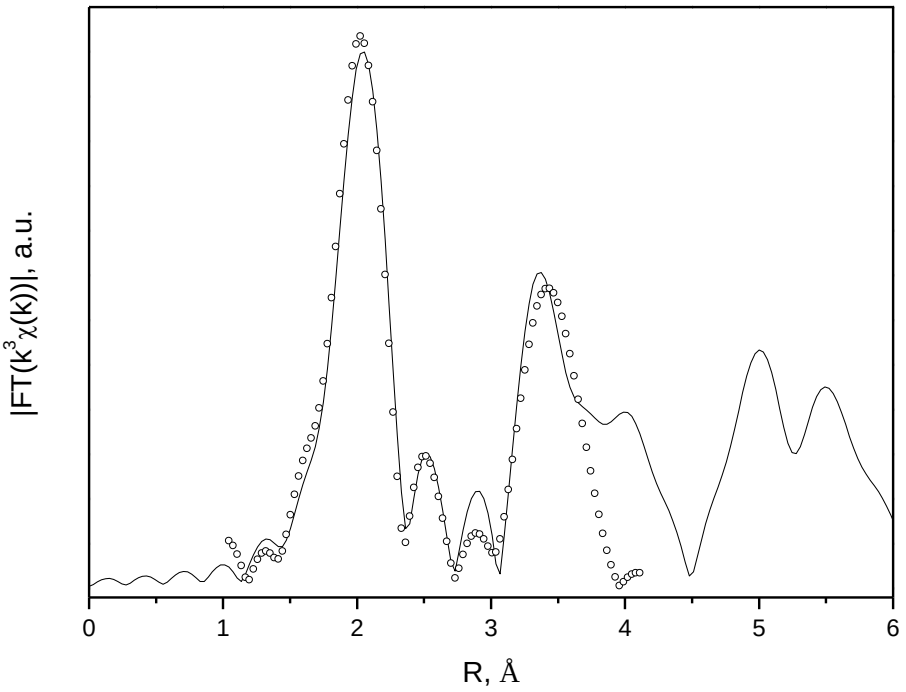

Figure S2 Fourier transforms of Bi L_3-edge EXAFS spectra: experimental (solid line) and best-fit theoretical (open circles) curves. Local-structure parameters corresponding to the structural model are given in Table S1.

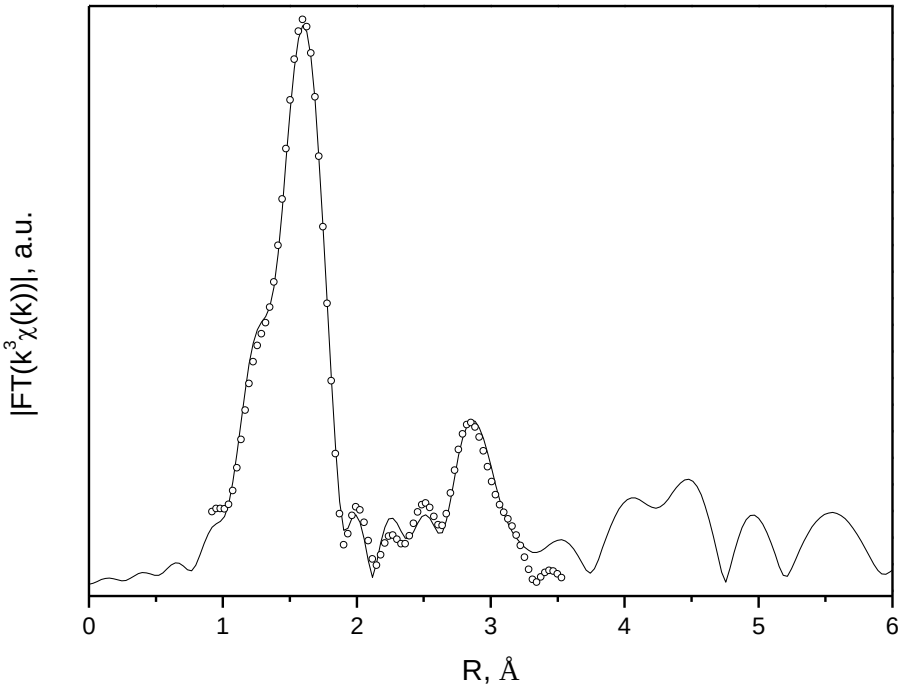

Figure S3 Fourier transforms of Fe K-edge EXAFS spectra: experimental (solid line) and best-fit theoretical (open circles) curves. Local-structure parameters corresponding to the structural model are given in Table S1.

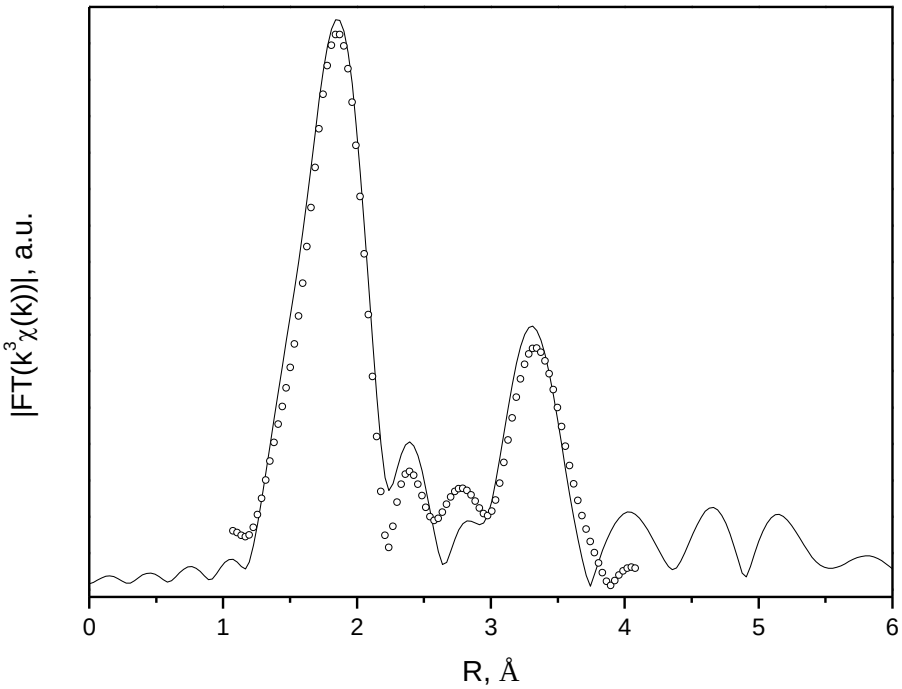

Figure S4 Fourier transforms of Y K-edge EXAFS spectra: experimental (solid line) and best-fit theoretical (open circles) curves. Local-structure parameters corresponding to the structural model are given in Table S1.

References

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