


Experiment title:

Structural control of the magnetic and electrical properties in a new multiferroic rare earth ferrobates crystal family at low temperatures

Experiment number:

MA-2970

Beamline: BM-01	Date of experiment: from: 01.07.2016 to: 04.07.2016	Date of report: 26/07/2016
Shifts: 9	Local contact(s): Dmitry Chernyshov	<i>Received at ESRF:</i>

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Report:

The aim of the project was to study the correlations between the crystal structure, magnetic and electrical properties of the new multiferroic crystal family $LnFe_3(BO_3)_4$ ($Ln = Gd, Nd, Y, Ho, Sm$) at low temperatures.

We have successfully collected sets of diffraction data as a function of temperature between 11 K and 500 K. All the data were processed preliminary with SNBL Tool Box[1] and CrysAlis[2] software and crystal structures were examined with JANA2006[3] software. Examples of reciprocal space layer reconstruction for crystals belonging to different space groups are shown in Fig.1. Experimental statistics for some samples is presented as an example at Table 1. The Fig. 2 demonstrates general view of $YFe_3(BO_3)_4$ crystals in space group $P3_121$.

Table 1. Crystallographic parameters, X-ray data collection and preliminary refinement statistics for the $GdFe_3(BO_3)_4$, $YFe_3(BO_3)_4$ and $SmFe_3(BO_3)_4$

Composition	$GdFe_3(BO_3)_4$	$YFe_3(BO_3)_4$	$SmFe_3(BO_3)_4$
Space group	Trigonal, $P3_121$	Trigonal, $P3_121$	Trigonal, $R32$
$a, b, \text{\AA}$	9.5437(1)	9.5145(1)	9.4784(8)
$c, \text{\AA}$	7.563(1)	7.5433(1)	7.5282(5)
$V, \text{\AA}^3$	596.57(1)	591.38(1)	585.72(8)
$D_x, \text{g/cm}^3$	4.6764	4.1418	4.7044
Wavelength, \AA	0.6742		
μ, mm^{-1}	11.729	11.007	13.517
T, K	9	5	11
Sample diameter, mm	0.2	0.2	0.2
Scanning mode	ϕ -scans		
$\theta_{\text{max}}, \text{deg}$	31.86	31.96	32.15
h, k, l ranges	$-13 \leq h \leq 13;$ $-13 \leq k \leq 13;$ $-11 \leq l \leq 11$	$-13 \leq h \leq 13;$ $-14 \leq k \leq 14;$ $-11 \leq l \leq 11$	$-14 \leq h \leq 14;$ $-14 \leq k \leq 14;$ $-10 \leq l \leq 10$
Number of reflections: measured/unique /with $I > 3\sigma(I)$	5086/1312/1015	4922/1171/945	1912/1280/1280

Flack parameter	0.58(4)	0.514(9)	1
$R1/wR2$	0.0386/0.0502	0.0214/ 0.0232	0.0410/ 0.0515
S	1.08	1.18	1.27
$\Delta r_{\min}/\Delta r_{\max}$, e/ \AA^3	-2.86/2.07	-2.90/ 2.45	-1.28/ 1.35
Programs	SNBL Tool Box [1], CrysAlis [2], Jana2006 [3]		

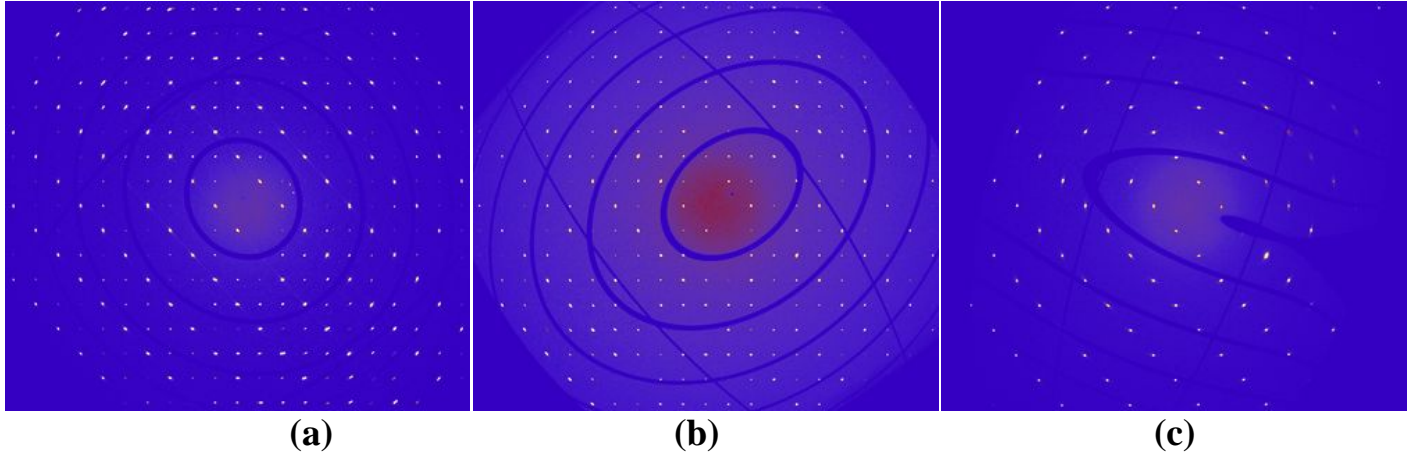


Fig. 1. Examples of a reconstructed layer $(-1, k, l)$ at 23K for (a) $\text{GdFe}_3(\text{BO}_3)_4$, pr.gr. $P3_121$, (b) $\text{YFe}_3(\text{BO}_3)_4$, pr.gr. $P3_121$ and (c) $\text{SmFe}_3(\text{BO}_3)_4$, pr.gr. $R32$

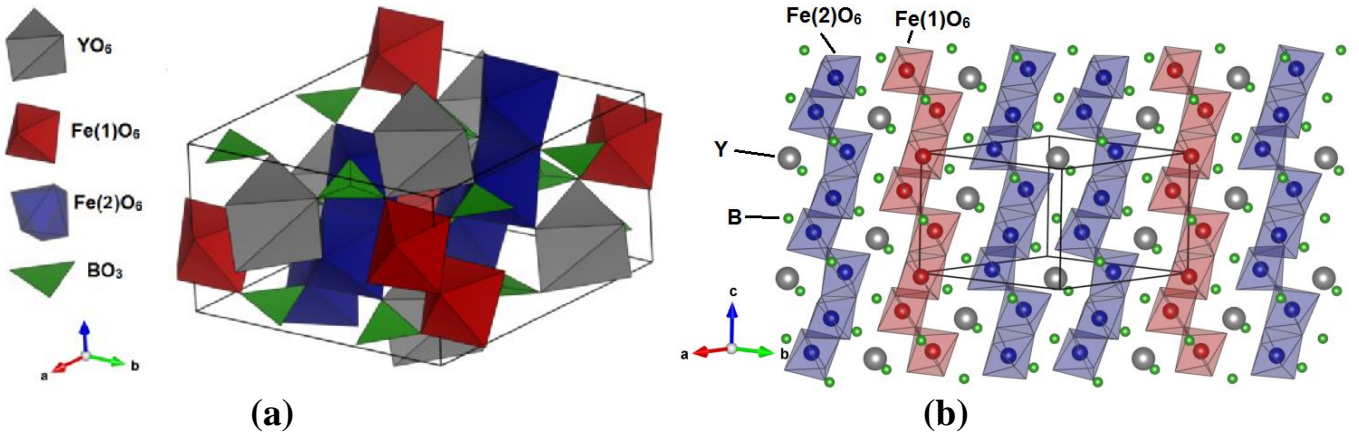


Fig. 2. (a) General view of $\text{YFe}_3(\text{BO}_3)_4$ unit cell at 5 K and (b) Fe-chains in the structure

A complete data analysis is in progress. The quality and volume of the collected data seems to be sufficient to reach the scientific goals of proposal, namely to establish correlations between the crystal structure, magnetic and electrical order in $\text{LnFe}_3(\text{BO}_3)_4$ multiferroic family in the low temperatures region.

1. Dyadkin, V., Pattison, P., Dmitriev, V. & Chernyshov, D. (2016). J. Synchrotron Rad. 23, 825–829
2. Petricek, V., Dusek, M. & Palatinus, L. (2014). Z. Kristallogr. 229(5), 345-352
3. CrysAlisPro 1.171.38.43 (Rigaku OD, 2015)