

# Structural and magnetic phase transitions in $\text{BiFe}_{1-x}\text{Mn}_x\text{O}_3$ solid solution driven by temperature

Dmitry.V. Karpinsky <sup>1,2,\*</sup>, Maxim V. Silibin <sup>2</sup>, Siarhei I. Latushka <sup>1,2</sup>, Dmitry V. Zhaludkevich <sup>1,2</sup>, Vadim V. Sikolenko <sup>2,3,4</sup>, Hanan Al-Ghamdi <sup>5</sup>, Aljawhara H. Almuqrin <sup>5</sup>, M. I. Sayyed <sup>6,7</sup> and Alexei A. Belik <sup>8</sup>

<sup>1</sup> Scientific-Practical Materials Research Centre of NAS of Belarus, 220072 Minsk, Belarus; la-tushkasi@gmail.com (S.I.L.); geludkevichdima@mail.ru (D.V.Z.)

<sup>2</sup> Institute of Advanced Materials and Technologies, National Research University of Electronic Technology “MIET”, 124498 Zelenograd, Moscow, Russia; sil\_m@mail.ru (M.V.S.); sikolen@jinr.ru (V.V.S.)

<sup>3</sup> Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research Joint Institute for Nuclear Research, 141980 Dubna, Russia

<sup>4</sup> Division Technical Petrophysics, Institute of Applied Geosciences, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

<sup>5</sup> Department of Physics, College of Science, princess Nourah bint Abdulrahman University, 84428, Riyadh 11671, Saudi Arabia; hmalghmdid@pnu.edu.sa (H.A.-G.); ahalmoqren@pnu.edu.sa (A.H.-A.)

<sup>6</sup> Department of Physics, Faculty of Science, Isra University, Amman, Jordan; dr.mabualssayed@gmail.com

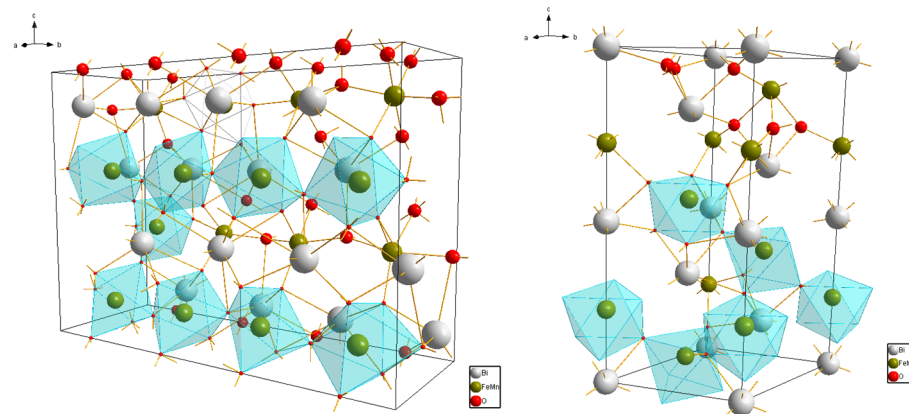
<sup>7</sup> Department of Nuclear Medicine Research, Institute for Research and Medical Consultations (IRMC), Imam Abdulrahman Bin Faisal University (IAU), Dammam, 31441, Saudi Arabia

<sup>8</sup> International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), Namiki 1-1, Tsukuba, Ibaraki, 305-0044, Japan; alexei.belik@nims.go.jp

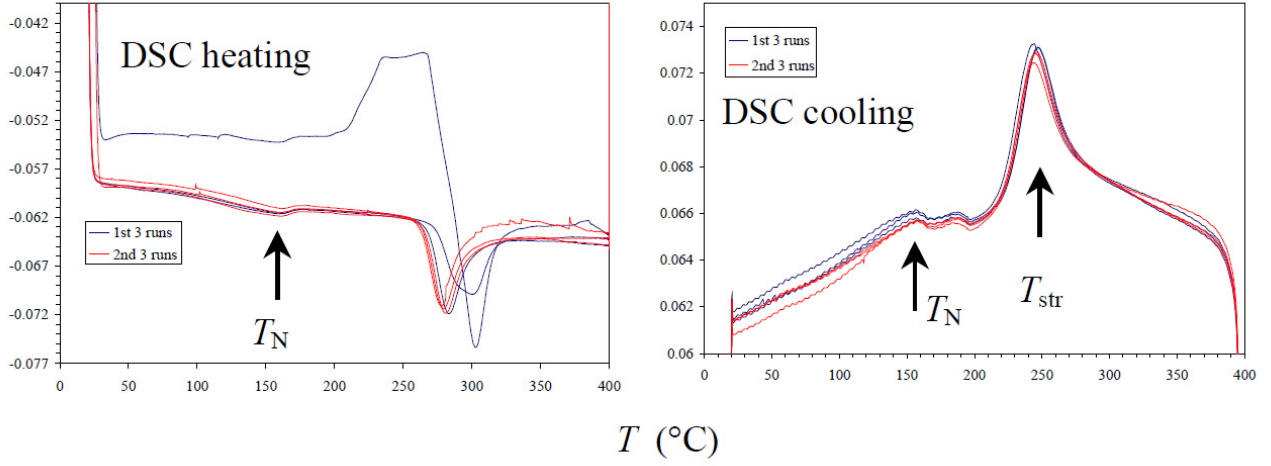
\* Correspondence: dmitry.karpinsky@gmail.com

**Table S1.**  $\text{BiFe}_{0.70}\text{Mn}_{0.30}\text{O}_3$  (as-prepared sample, SPD data refined at  $T = 300$  K).

O-phase (~90%): $\text{Pnma}$ space group; $a = 5.5937$ Å, $b = 15.6785$ Å, $c$ R-phase (~10%): $\text{R3c}$ space group; $a = 5.6627$ Å, $c = 13.2543$ Å, Vol. = 11.2428 Å <sup>3</sup> , Vol. = 986.00 Å <sup>3</sup> (~61.63 Å <sup>3</sup> per prim.)					= 368.08 Å <sup>3</sup> (~61.34 Å <sup>3</sup> per prim.)				
atom	site	x	y	z	atom	site	x	y	z
Bi1	8d	0.21755	0.01031	0.62373	Bi	6a	0	0	0
Bi2	4c	0.19322	1/4	0.62478	Fe Mn	6a	0	0	0.23053
Bi3	4c	0.78535	1/4	0.36228	O1	18b	0.42840	0.01486	0.95264
Fe Mn1	8d	0.22848	0.12268	0.87476					
Fe Mn2	8d	0.26247	0.62444	0.88065					
O1	8d	0.85862	0.00636	0.63359					
O2	4c	0.77883	1/4	0.59362					
O3	4c	0.18536	1/4	0.42279					
O4	8d	0.04437	0.11297	0.72374					
O5	8d	0.02537	0.63780	0.75148					
O6	8d	0.00000	0.39371	0.50000					
O7	8d	0.00000	0.37667	0.00000					



**Figure S1.** Visualization of the unit cells: the antipolar orthorhombic (O-phase, left image) and the rhombohedral one (R-phase, right image).



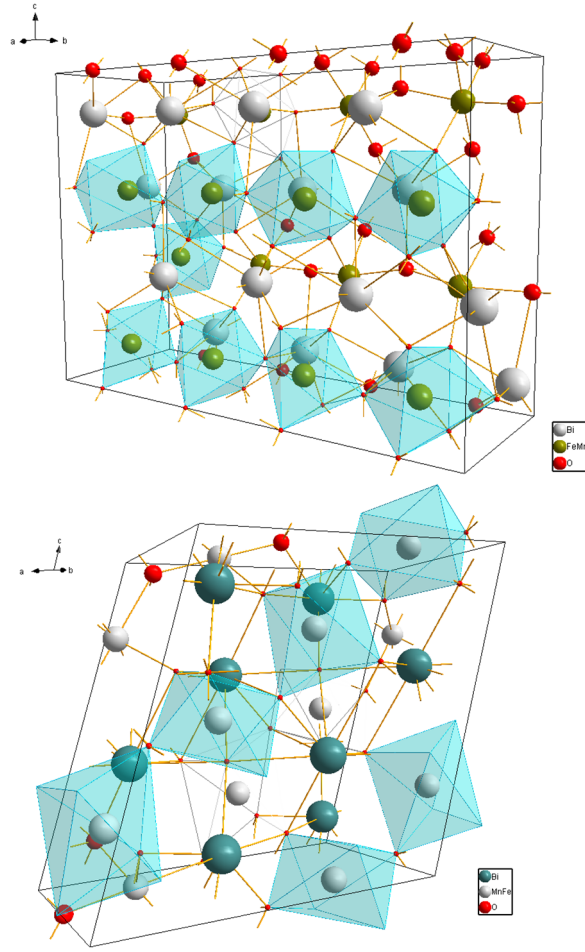
**Figure S2.** DSC data for compound  $\text{BiFe}_{0.70}\text{Mn}_{0.30}\text{O}_3$ .

**Table S2.**  $\text{BiFe}_{0.50}\text{Mn}_{0.50}\text{O}_3$  (as-prepared sample, SPD data refined at  $T = 300$  K).

<b>O-phase (~66%): <math>\text{Pnma}</math> space group; <math>a = 5.5677 \text{ \AA}</math>, <math>b = 15.7104 \text{ \AA}</math>, <math>c = 11.2146 \text{ \AA}</math>, Vol. = <math>980.96 \text{ \AA}^3</math> (~61.31 <math>\text{\AA}^3</math> per prim.)</b>				
atom	site	x	y	z
Bi1	8d	0.21292	0.01251	0.61724
Bi2	4c	0.23916	1/4	0.62418
Bi3	4c	0.77430	1/4	0.37469
Fe Mn1	8d	0.26408	0.11082	0.84479
Fe Mn2	8d	0.26766	0.62685	0.88304
O1	8d	0.88963	0.00375	0.69238
O2	4c	0.69420	1/4	0.60875
O3	4c	0.10489	1/4	0.46343
O4	8d	0.02852	0.17378	0.71291
O5	8d	0.05771	0.77304	0.82047
O6	8d	0.00000	0.38177	0.50000
O7	8d	0.00000	0.39019	0.00000

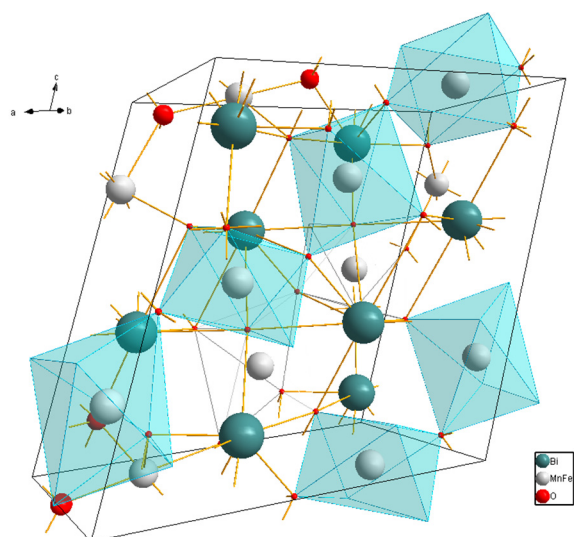
<b>M-phase (~33%): <math>\text{C2/c}</math> space group; <math>a = 9.5984 \text{ \AA}</math>, <math>b = 5.6341 \text{ \AA}</math>, <math>c = 9.6033 \text{ \AA}</math>, <math>\beta = 108.21^\circ</math>, Vol. = <math>493.34 \text{ \AA}^3</math> (~61.67 <math>\text{\AA}^3</math> per prim.)</b>				
atom	site	x	y	z
Bi	8f	0.13205	0.25310	0.13653
Mn Fe1	4e	0	0.22143	3/4
Mn Fe2	4d	1/4	1/4	1/2
O1	8f	0.05082	0.28645	0.59208
O2	8f	0.20126	0.58942	0.30602
O3	8f	0.37333	0.48382	0.10537



**Figure S3.** Visualization of the unit cells: the antipolar orthorhombic (O-phase, left image) and the monoclinic one (M-phase, right image).

**Table S3.** BiFe<sub>0.30</sub>Mn<sub>0.70</sub>O<sub>3</sub> (as-prepared sample, SPD data refined at T = 300 K).

<b>M-phase: C2/ c space group; a = 9.5172 Å, b = 5.6208 Å, c = 9.7214 Å, β = 108.2962, Vol. = 493.76 Å<sup>3</sup> (~61.72 Å<sup>3</sup> per prim.)</b>				
<b>atom</b>	<b>site</b>	<b>x</b>	<b>y</b>	<b>z</b>
Bi	8f	0.13609	0.23264	0.12793
Mn Fe1	4e	0	0.19849	3/4
Mn Fe2	4d	1/4	1/4	1/2
O1	8f	0.06125	0.20249	0.55167
O2	8f	0.16390	0.56907	0.35677
O3	8f	0.36968	0.52691	0.13010



**Figure S4.** Visualization of the monoclinic unit cell (M-phase).