Electronic Supplementary Information

Bulk crystal growth and characterization of bismuth ferrite-based material $Bi_3FeO_4(MoO_4)_2$

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Table S1. Crystal data and structure refinement for BFM.

Crystal	BFM
Empirical formula	$Bi_3FeO_4(MoO_4)_2$
M_r	1066.67
Crystal system	Monoclinic
Space group	*C*2/c (No. 15)
Temperature (K)	296
a, *b*, *c* (Å)	16.927(12), 11.672(12), 5.263(4)
β (°)	107.160(10)
V (Å^3)	993.6(15)
Z	4
Dcalcd, g/cm^3	7.131
μ (mm^{-1})	56.88
F (000)	1820
Crystal size (mm)	0.10× 0.08× 0.07
R_{int}	0.092
R indices [I>2σ(I)][a]	R_1=0.0482, wR_2=0.1203
R indices (all data)	R_1=0.0584, wR_2=0.1254
Extinction coeff	0.0067(4)
GOF on F^2	1.018
CCDC	1879545

[a] $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$, $wR_2 = \{\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$

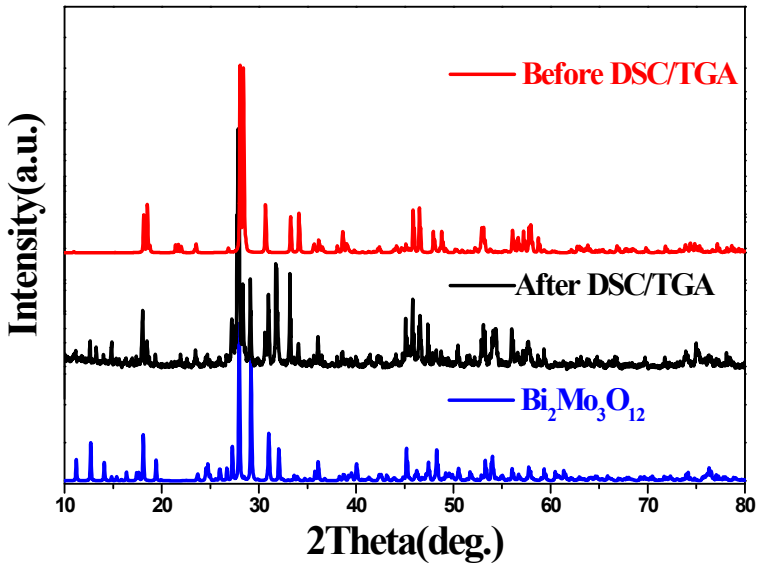

Figure S1. The experimental patterns of powder XRD of the residue in the platinum pan after DSC/TGA.

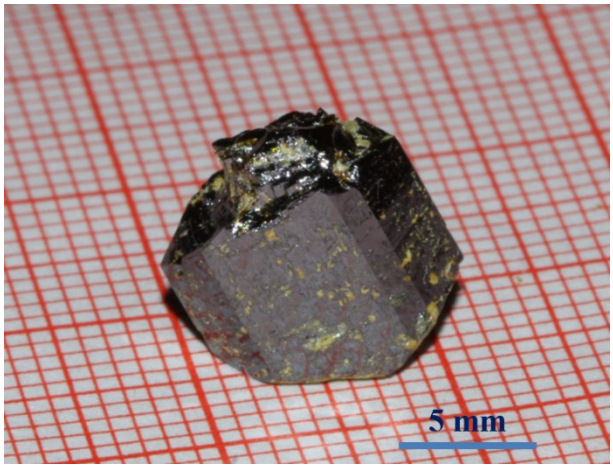

Figure S2. Photographs of the as-grown $Bi_3FeO_4(MoO_4)_2$ crystals through spontaneous crystallization with MoO_3 flux.

Table S2. Bond Distances (Å) and Angles (deg.) for $Bi_3FeO_4(MoO_4)_2$ crystal.

Bi2—Bi1^{i}	3.649 (3)	Bi1—O6^{viii}	2.722 (12)
Bi2—O2^{ii}	2.235 (12)	Bi1—O5^{ix}	2.346 (14)
Bi2—O2	2.236 (14)	Bi1—O5^{x}	2.346 (14)
Bi2—O1^{iii}	2.257 (14)	Mo1—O3	1.776 (13)
Bi2—O3^{iii}	2.652 (12)	Mo1—O6	1.758 (13)
Bi2—O3	2.546 (14)	Mo1—O4	1.775 (14)
Bi2—O4^{iv}	2.683 (13)	Mo1—O5	1.825 (14)
Bi2—O5^{v}	2.519 (14)	Fe1—O2^{xi}	1.908 (13)
Bi1—O1^{vi}	2.202 (13)	Fe1—O2	1.908 (13)
Bi1—O1	2.202 (13)	Fe1—O1	1.920 (14)
Bi1—O6^{vii}	2.722 (12)	Fe1—O1^{xi}	1.920 (14)
O2—Bi2—Bi1^{i}	106.6 (4)	O1^{vi}—Bi1—O5^{x}	77.9 (5)
O2^{ii}—Bi2—Bi1^{i}	87.5 (4)	O6^{viii}—Bi1—Bi2^{ii}	88.2 (3)

O2^{ii}—Bi2—O2	77.3 (3)	O6^{vii}—Bi1—Bi2^{ii}	136.4 (3)
O2—Bi2—O1^{iii}	80.9 (5)	O6^{vii}—Bi1—Bi2^{i}	88.2 (3)
O2^{ii}—Bi2—O1^{iii}	104.1 (5)	O6^{viii}—Bi1—Bi2^{i}	136.4 (3)
O2^{ii}—Bi2—O3^{iii}	137.9 (4)	O6^{vii}—Bi1—O6^{viii}	124.3 (6)
O2—Bi2—O3	80.9 (5)	O5^{ix}—Bi1—Bi2^{ii}	108.6 (3)
O2—Bi2—O3^{iii}	76.3 (5)	O5^{x}—Bi1—Bi2^{i}	108.6 (3)
O2^{ii}—Bi2—O3	78.6 (5)	O5^{ix}—Bi1—Bi2^{i}	43.2 (3)
O2—Bi2—O4^{iv}	126.1 (4)	O5^{x}—Bi1—Bi2^{ii}	43.2 (3)
O2^{ii}—Bi2—O4^{iv}	152.9 (5)	O5^{ix}—Bi1—O6^{vii}	94.2 (4)
O2^{ii}—Bi2—O5^{v}	77.4 (4)	O5^{x}—Bi1—O6^{viii}	94.2 (4)
O2—Bi2—O5^{v}	138.1 (4)	O5^{ix}—Bi1—O6^{viii}	100.7 (4)
O1^{iii}—Bi2—Bi1^{i}	34.6 (3)	O5^{x}—Bi1—O6^{vii}	100.7 (4)
O1^{iii}—Bi2—O3	160.5 (5)	O5^{x}—Bi1—O5^{ix}	147.9 (7)
O1^{iii}—Bi2—O3^{iii}	103.4 (4)	O3—Mo1—O5	110.5 (6)
O1^{iii}—Bi2—O4^{iv}	70.7 (4)	O6—Mo1—O3	112.6 (6)
O1^{iii}—Bi2—O5^{v}	73.7 (5)	O6—Mo1—O4	107.2 (6)
O3—Bi2—Bi1^{i}	162.4 (3)	O6—Mo1—O5	106.5 (7)
O3^{iii}—Bi2—Bi1^{i}	131.5 (3)	O4—Mo1—O3	106.4 (7)
O3—Bi2—O3^{iii}	65.2 (3)	O4—Mo1—O5	113.8 (7)
O3^{iii}—Bi2—O4^{iv}	67.5 (4)	O2^{xi}—Fe1—O2	123.3 (8)
O3—Bi2—O4^{iv}	115.4 (4)	O2^{xi}—Fe1—O1^{xi}	106.8 (6)
O4^{iv}—Bi2—Bi1^{i}	73.4 (3)	O2—Fe1—O1	106.8 (6)
O5^{v}—Bi2—Bi1^{i}	39.6 (3)	O2^{xi}—Fe1—O1	101.9 (5)
O5^{v}—Bi2—O3	125.3 (4)	O2—Fe1—O1^{xi}	101.9 (5)
O5^{v}—Bi2—O3^{iii}	141.5 (4)	O1—Fe1—O1^{xi}	117.2 (8)

O5^{v}—Bi2—O4^{iv}	75.7 (4)	Bi2^{iii}—O2—Bi2	113.0 (6)
Bi2^{ii}—Bi1—Bi2^{i}	84.42 (8)	Fe1—O2—Bi2	122.8 (6)
O1^{vi}—Bi1—Bi2^{i}	35.6 (4)	Fe1—O2—Bi2^{iii}	123.0 (7)
O1—Bi1—Bi2^{ii}	35.6 (4)	Bi1—O1—Bi2^{ii}	109.8 (6)
O1—Bi1—Bi2^{i}	72.7 (4)	Fe1—O1—Bi2^{ii}	116.1 (6)
O1^{vi}—Bi1—Bi2^{ii}	72.7 (4)	Fe1—O1—Bi1	129.9 (7)
O1—Bi1—O1^{vi}	82.8 (7)	Bi2—O3—Bi2^{ii}	91.7 (4)
O1—Bi1—O6^{vii}	159.0 (4)	Mo1—O3—Bi2^{ii}	123.8 (7)
O1^{vi}—Bi1—O6^{viii}	159.0 (4)	Mo1—O3—Bi2	138.5 (6)
O1—Bi1—O6^{viii}	76.5 (4)	Mo1—O6—Bi1^{viii}	116.8 (6)
O1^{vi}—Bi1—O6^{vii}	76.5 (4)	Mo1—O4—Bi2^{xii}	127.8 (7)
O1—Bi1—O5^{x}	78.2 (5)	Bi1^{x}—O5—Bi2^{xiii}	97.1 (5)
O1—Bi1—O5^{ix}	77.9 (5)	Mo1—O5—Bi2^{xiii}	134.3 (7)
O1^{vi}—Bi1—O5^{ix}	78.2 (5)	Mo1—O5—Bi1^{x}	127.4 (7)

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $x, -y+1, z+1/2$; (iii) $x, -y+1, z-1/2$; (iv) $-x+1/2, y-1/2, -z+1/2$; (v) $-x+1/2, y-1/2, -z+3/2$; (vi) $-x+1, y, -z+5/2$; (vii) $x+1/2, -y+3/2, z+3/2$; (viii) $-x+1/2, -y+3/2, -z+1$; (ix) $x+1/2, -y+3/2, z+1/2$; (x) $-x+1/2, -y+3/2, -z+2$; (xi) $-x+1, y, -z+3/2$; (xii) $-x+1/2, y+1/2, -z+1/2$; (xiii) $-x+1/2, y+1/2, -z+3/2$.

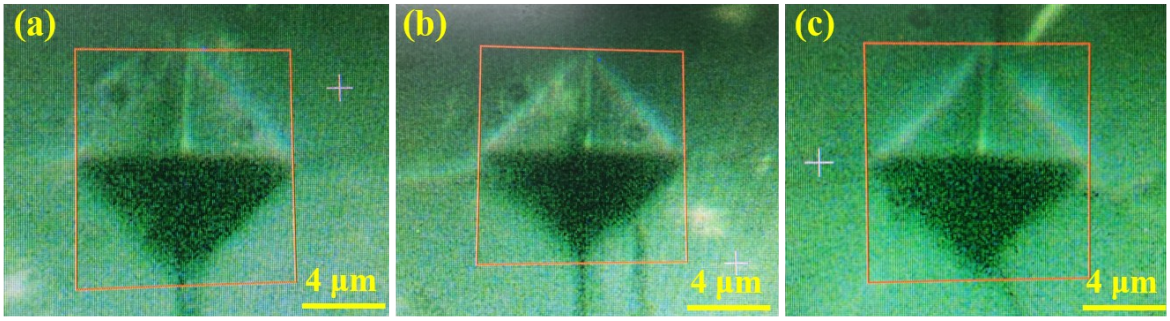

Figure S3. (a)-(c) Photographs of the indentation morphologies of the $Bi_3FeO_4(MoO_4)_2$ crystal faces (100), (010) and (001), respectively, from which they are rhombic and regular.

Table S3. Observed Raman wavenumbers (cm^{-1}) and vibrational assignments for the $Bi_3FeO_4(MoO_4)_2$ crystal.[1-3]

Raman spectra (cm^{-1})	Assignments
< 100 (vw)	O-Bi-O and O-Mo-O bond bending
124.49 (vs)	Bi-O bands and Bi and Mo translation and libration
200-600 (w)	Bi-O bonds, Mo-O bonds and translations of Fe atoms
761.12 (m)	Mo-O bonds and Mo-O-Bi bridges
868.67 (vs)	MoO_4 asymmetric stretching
870.41 (m)	MoO_4 symmetric stretching

In the table, vs: very strong; m: medium; w: weak

References

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