

Room-temperature multiferroic behavior in layer-structured Aurivillius phase ceramics

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AFFILIATIONS

¹G... 430074, C
²I... 47, K 04001, ...
³E... M... L... E14N, ... K...
⁴N... D... L... A...
⁵N... 110L, ... K...
⁶E... G 99, ... K...
⁷L... 730000, C

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ABSTRACT

M... H... A...
 ... D... H... A... B_{5.25}L_{0.75}F₃O₁₈
 P... A... *in situ*
 F³⁺ O F³⁺, C³⁺ O C³⁺, F³⁺ O C³⁺
 ... A... C / F

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M... (FE) A... B₅F₃O₁₅ (= 4) B₆F₂O₁₈
 (FM) (= 5), B₄F₃O₁₂
 ...^{1,4}H... FE FM^{12,13}B...
 ... (= 4) B₆F₃O₁₈ (= 5) B₅F_{0.5}C_{0.5}O₁₅
⁵... A...
 (B₂O₂)²⁺(A₋₁B O₃ +1)²⁻(A ...^{14,15}H...
 ...⁶...¹⁶...
 B-... A
 B F O₃ ...^{7,11}...

BLFC (BLFC) $P L$

$B_{5.25}L_{0.75}F C_{3O_{18}}$ (P).

F, A, C, D ^{14,17}

$a b, P$

BLFC $a b$

A

in situ

$I H, D, O, U, K$

N F

(P).

BLFC

BLFC

$F, A, B2cb$

A_{21}

A_{21am}

$a = 5.4530(2) \text{ \AA}, b = 5.4427(1) \text{ \AA}$

$c = 50.670(2) \text{ \AA}$

$b = 5.3943(6) \text{ \AA}, c = 41.487(2) \text{ \AA}$

$a = 5.4651(6) \text{ \AA}$

$V = 1223.0(2) \text{ \AA}^3$

$(//)$

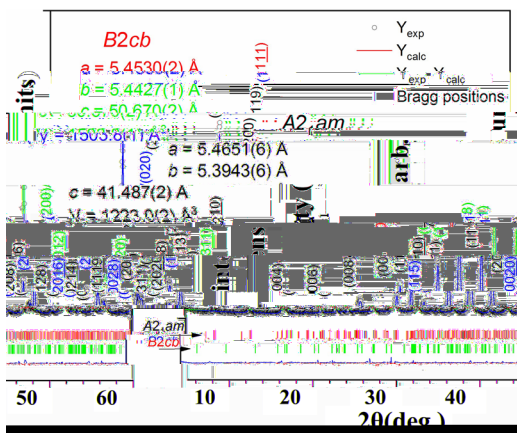


FIG. 1. $a a a B$

BLFC = 4 = 5

A, N

D'

BLFC $F, 1, EM (a-b), M$

$F, 1$

$1.4 \% (F, 2)$

D, ED

$1) F, C, O, C_2F O_4$

$A B_{5F 0.5C 0.5} O_{15}$ ¹⁶

BLFC $(50, 70 100, 300, 500 \text{ H}), 1060 \text{ K}$

FE T BLFC H

BLFC (973 K) ¹³ $F 2()$ $P-E I-E$ $B_6 F_2 O_{18}$

BLFC P

$I-E$ ^{21,22}

BLFC $10 \mu C/ F 2()$

(FC)

$200 O$ BLFC BLFC

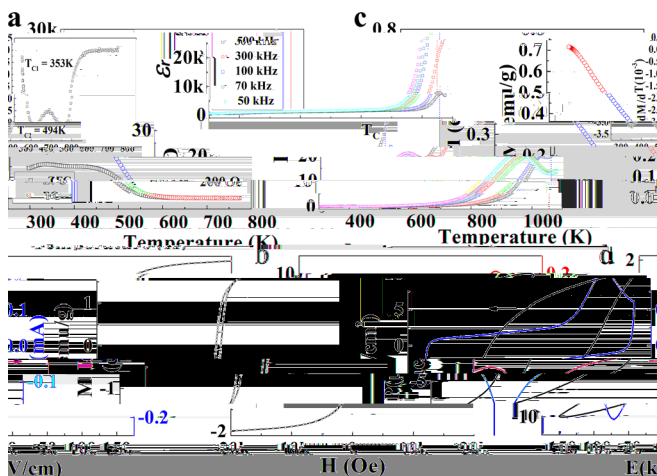


FIG. 2. (a) $a a () B a a a \perp$
 $(.) a a a$
 $B a a a a a a a \perp (.)$
 $a a a a a a a a$
 $a a a = 200 a a -$
 $a 300 B a . () a a$

~ 494 K
 $M/$),
 $B_6F C_3O_{18}$ (526 K).²³
 BLFC
 $F^{3+} O F^{3+}, C^{3+} O C^{3+}, F^{3+} O C^{3+}$ (.
 ED).²⁴
 A FC $2 \sim 353$ K
 $C_2F O_4$ 2 $16,25$
 $C_2F O_4$ (460 K) (M) $C_2F O_4$ 1.4 . %
 $16 \ 23.5$ / .²⁵ , 0.22 0.32 / , BLFC
 $C_{2-} F O_4$ M = 1.85 / , F . 2() . I
 $M H$
 $2 (F . 3)$ 1
 425 K 1.58 / . 0.27 / , ED
 $BLFC$
 A
 $F 3$
 $F^{3+} O C^{3+}$ *ab initio*
 (DF)
 $(A P)$. F H
 $U_F = 2$ $U_C = 3$ F C ,
 $(GGA)U$. I
 $BLFC$
 $F . 3()$, $F^{3+} C^{3+}$ (3.1 2.1 $\mu_B/$,)
 O
 $(0.1 \mu_B/)$.
 $F O_6 C O_6$ F / C -
 $()$ O - / . F . 3() .
 F $F^{3+} C^{3+}$ -
 $(. ,)$ (. ,)
 $E_{FM} - E_{AFM}$
 $= -144.1$.
 H , (FM)
 43.5 (. , 504.6 K), FM
 1 FC/FC . F . 2() .
 $a b$
 010 .
 $BLFC$ F 4 . I
 $5() . A$ PFM BLFC , 399 O .
 $F -$

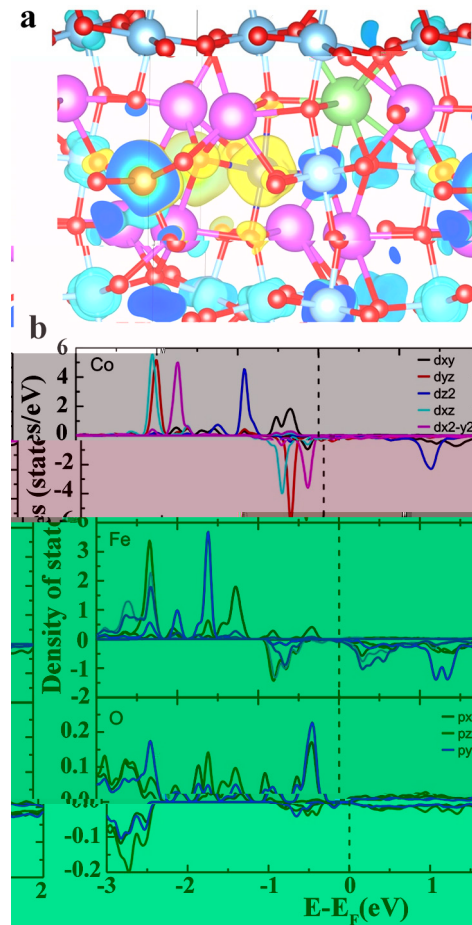


FIG. 3. (a) Crystal structure of BLFC (Ba₂FeCoO₆) with lattice parameters $a = b = 0.38$ nm, $c = 0.38$ nm, and $\beta = 90^\circ$. (b) Density of states (DOS) plot for Co, Fe, and O atoms, showing the contribution of different orbitals (dxy, dyz, dz², dxz, dx²-y², px, py, pz) to the total DOS. The x-axis is energy relative to the Fermi level ($E - E_F$ in eV) and the y-axis is the density of states in states/eV.

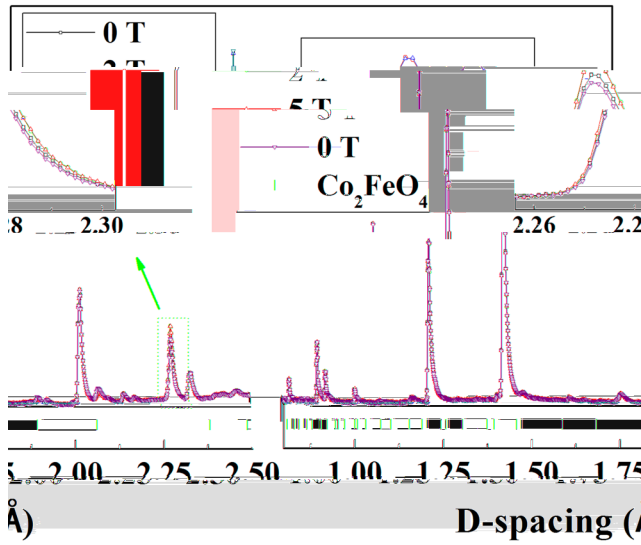


FIG. 4. XRD patterns of Co_2FeO_4 at 0 T and 5 T. The inset shows the schematic of the sample and magnetometer. The bottom panel shows the Rietveld refinement with Bragg peak positions marked at 2.00, 2.25, 2.50, 1.00, 1.25, 1.50, and 1.75 Å.

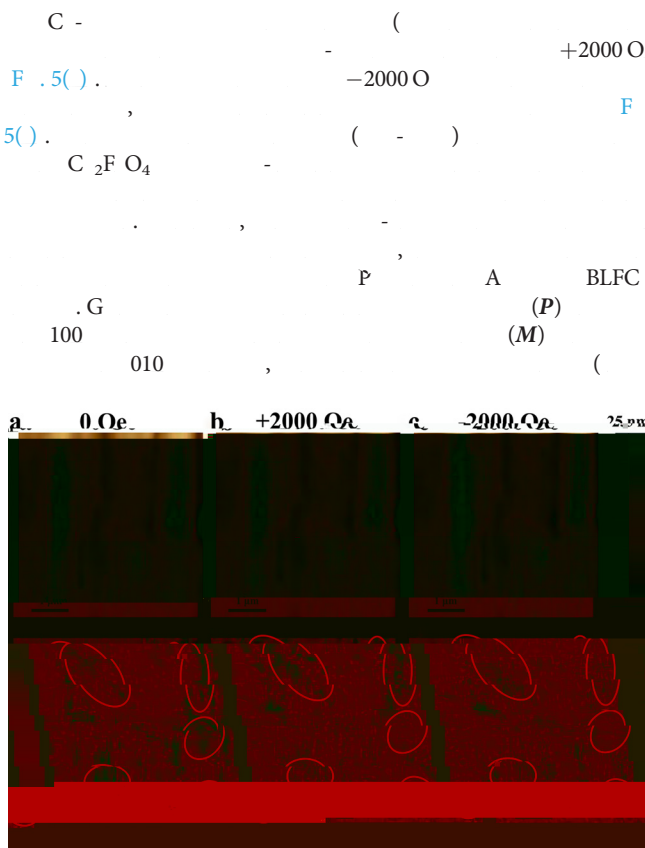


FIG. 5. TEM images of Co_2FeO_4 at 0 Oe, +2000 Oe, and -2000 Oe. The images show the morphology of the particles and the presence of magnetic domains. Scale bars are 25 nm.

$T = P \times M$
 BLFC
 I, A BLFC
 F
 $\text{C}^{3+} \text{O} \text{C}^{3+}, \text{F}^{3+} \text{O} \text{C}^{3+}$
 $\text{F}^{3+} \text{O} \text{F}^{3+}$
 A, C/F
 EM (ED)
 BLFC
 D. M, P D. K, D.
 D I H I I N, AL,
 D, O K.
 A E D F
 G A A (G N. K2015-0602006), N FC (G
 N. 11474138 11834005). A
 E M P (EM)P
 P IND54 N EM)P
 EM)P E)AME E

DATA AVAILABILITY

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