



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

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AFFILIATIONS

¹G... f... I... l... u... ,C... f... G... f... ,u... 430074,C
²I... l... f... M... ,... A... f... ,u... 47,K... 04001,
³f... E... f... M... ,u... M... ,... f... L... f... ,L... E14N... K... f...
⁴N... K... L... f... M... ,u... D... I... l... f... E... ,C... A... f... E...
M... 621900,C
⁵N... L... ,H... ,... 110L... K...
⁶E... f... L... ,F... ,u... G... 99... K...
⁷f... ,L... u... ,L... u... 730000,C

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^{b)}Author to whom correspondence should be addressed: ...@... .

ABSTRACT

M... ,H... ,... A...
...D... ,H... ,... A... B_{5.25}L_{0.75}F₃C₃O₁₈
...A... ,... *in situ*
F³⁺ O F³⁺, C³⁺ O C³⁺, F³⁺ O C³⁺
...A... ,... C /F...

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M... (FM) (FE) A... B₅F₃O₁₅ (= 4) B₆F₂O₁₈
(= 5), B₄F₃O₁₂
^{1,4}H... FE FM ^{12,13}B...
C... F... B... B₅F_{0.5}C_{0.5}O₁₅
(= 4) B₆F₃C₃O₁₈ (= 5)
⁵... (B₂O₂)²⁺(A₁₋₁B O₃ +1)²⁻(...
^{14,15}H...
⁶...
B-...
B F O₃...
^{7,11}...
A...

$B_{5.25}L_{0.75}F_{1-x}C_{x-3}O_{18}$
 (BLFC) (a, b, c)
 $a = 5.4530(2) \text{ \AA}$, $b = 5.4427(1) \text{ \AA}$, $c = 50.670(2) \text{ \AA}$
 $a = 5.4651(6) \text{ \AA}$, $b = 5.3943(6) \text{ \AA}$, $c = 41.487(2) \text{ \AA}$
 (FC)

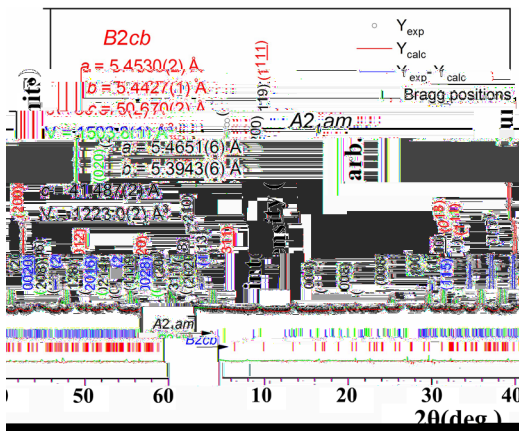


FIG. 1. XRD patterns of BLFC samples.

$B_{5.25}F_{0.75}C_{x-3}O_{18}$
 BLFC (a, b, c)
 $a = 5.4530(2) \text{ \AA}$, $b = 5.4427(1) \text{ \AA}$, $c = 50.670(2) \text{ \AA}$
 $a = 5.4651(6) \text{ \AA}$, $b = 5.3943(6) \text{ \AA}$, $c = 41.487(2) \text{ \AA}$
 (FC)

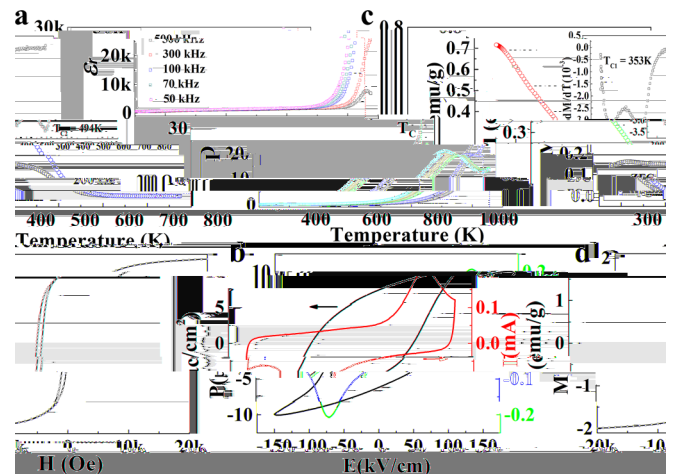


FIG. 2. EPR spectra of BLFC samples.

($\sim 1 \sim 494$ K) ~ 494 K / \sim ,
 $B_6F_2C_{13}O_{18}$ (526 K).²³ \sim
 BLFC $F^{3+} O F^{3+}, C^{3+} O C^{3+}, F^{3+} O C^{3+}$ (\sim),²⁴ \sim
 ED
 A FC $\sim 2 \sim 353$ K \sim
 $C_2F_4O_4$ ~ 2 \sim 16,25
 $C_2F_4O_4$ (460 K) (M) $C_2F_4O_4$ 1.4 %
 $16.235 / \sim$ $0.22 0.32 /$ 1.4 %
 $C_2F_4O_4$ BLFC
 $M = 1.85 /$ $F \sim 2(1.1)$ $M H$
 $\sim 2 (F \sim 3)$ ~ 1
 425 K $1.58 / \sim$ $0.27 /$ ED
 \sim $BLFC$
 $F \sim 3$ A
 $F^{3+} O C^{3+}$ *ab initio*
 (DF) (A) H
 $\uparrow_F = 2$ $\uparrow_C = 3$ F C
 $(GGA) \uparrow$ I
 BLFC $F \sim 3(1), F^{3+} C^{3+} (3.1 2.1 \mu_B/)$ \sim),
 $(0.1 \mu_B/)$ $F O_6 C O_6$
 (F) F/C $F \sim 3(1)$
 F $F^{3+} C^{3+}$
 (\sim) (\sim)
 $= -144.1$ $E_{FM} - E_{AFM}$
 H (FM) FM
 $43.5 (\sim, 504.6 K)$ FC/FC $F \sim 2(1)$ $a b$
 \sim
 010 $F \sim 4$
 BLFC I $399 O$ F F

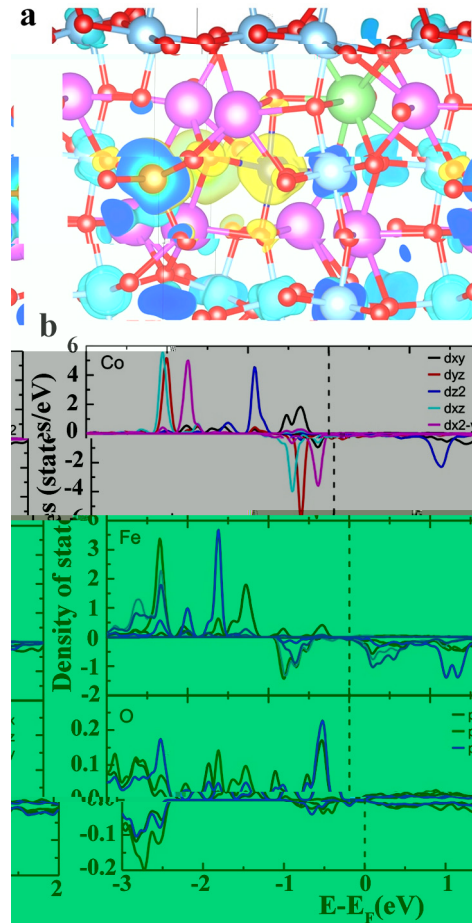


FIG. 3. (a) Crystal structure of BLFC showing layers of Co, Fe, and O atoms. (b) Density of states (DOS) plots for Co, Fe, and O atoms, showing contributions from different orbitals (dxy, dyz, dz2, dxz, dx2-y2) and spin channels (up, down).

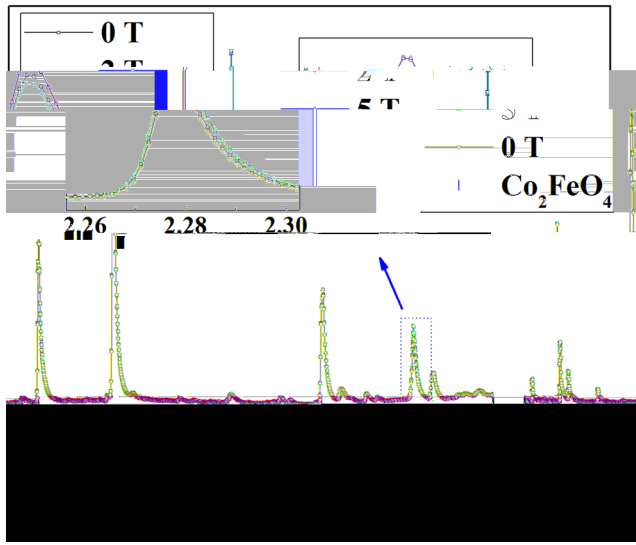


FIG. 4. XRD patterns of Co_2FeO_4 at 0 T (blue) and 2 T (red). The inset shows the schematic of the sample and measurement setup.

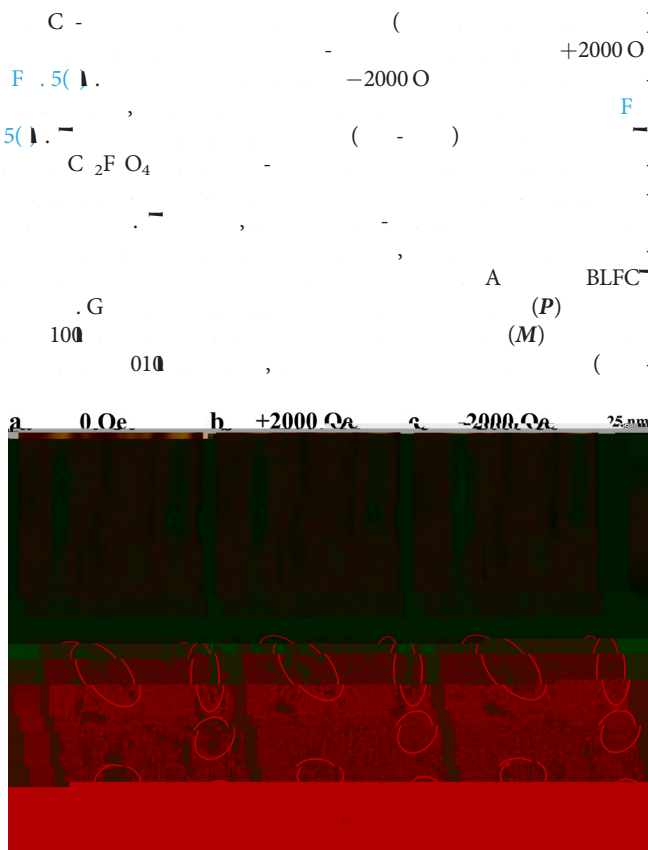


FIG. 5. TEM images of Co_2FeO_4 at different magnetic fields: (a) 0 Oe, (b) +2000 Oe, and (c) -2000 Oe. The red circles highlight the particles. Scale bar is 25 nm.

$T = P \times M$
 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 , D . K , D .
 D I H I I N , AL,
 D , O , K .
 A E D F
 G A A (G N . 2/
 0038/20), C (G N . K2015-0602006), N FC (G
 N . 11474138 11834005). A
 E M (EM)
 IND54 N EM
 EM E, NAME E

DATA AVAILABILITY

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