

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

Cite as: Appl. Phys. Lett. **117**, 052903 (2020); <https://doi.org/10.1063/5.0017781>

Submitted: 09 June 2020 . Accepted: 25 July 2020 . Published Online: 07 August 2020

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Published Online: 7 August 2020 · Corrected: 11 August 2020



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AFFILIATIONS

¹G - f l u , C - f G f , u 430074, C
²l u 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 - D l u f u , C A - f E ,
M 621900, C
⁵N L , H - , 110L , K -
⁶E L , F - , u G 99 , K -
⁷f l u , L u - , L u 730000, C

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b)Author to whom correspondence should be addressed: . . @ -

ABSTRACT

M . H , - A -
. H , A B_{5.25}L_{0.75}F₃O₁₈
P . D
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) B₆F₂₃O₁₈
(= 5), B₄₃O₁₂
, .^{1,4} H , , B F O₃, FE FM .^{12,13} B -
C F B- , B₅F_{0.5}C_{0.5}₃O₁₅
(= 4) B₆F₃C₃O₁₈ (= 5)
⁵ , - A
(B₂O₂)²⁺(A₋₁B O₃ +1)²⁻ (A - , .^{14,15} H ,
- , B
)⁶ , .¹⁶ ,
B- .^{7,11} A

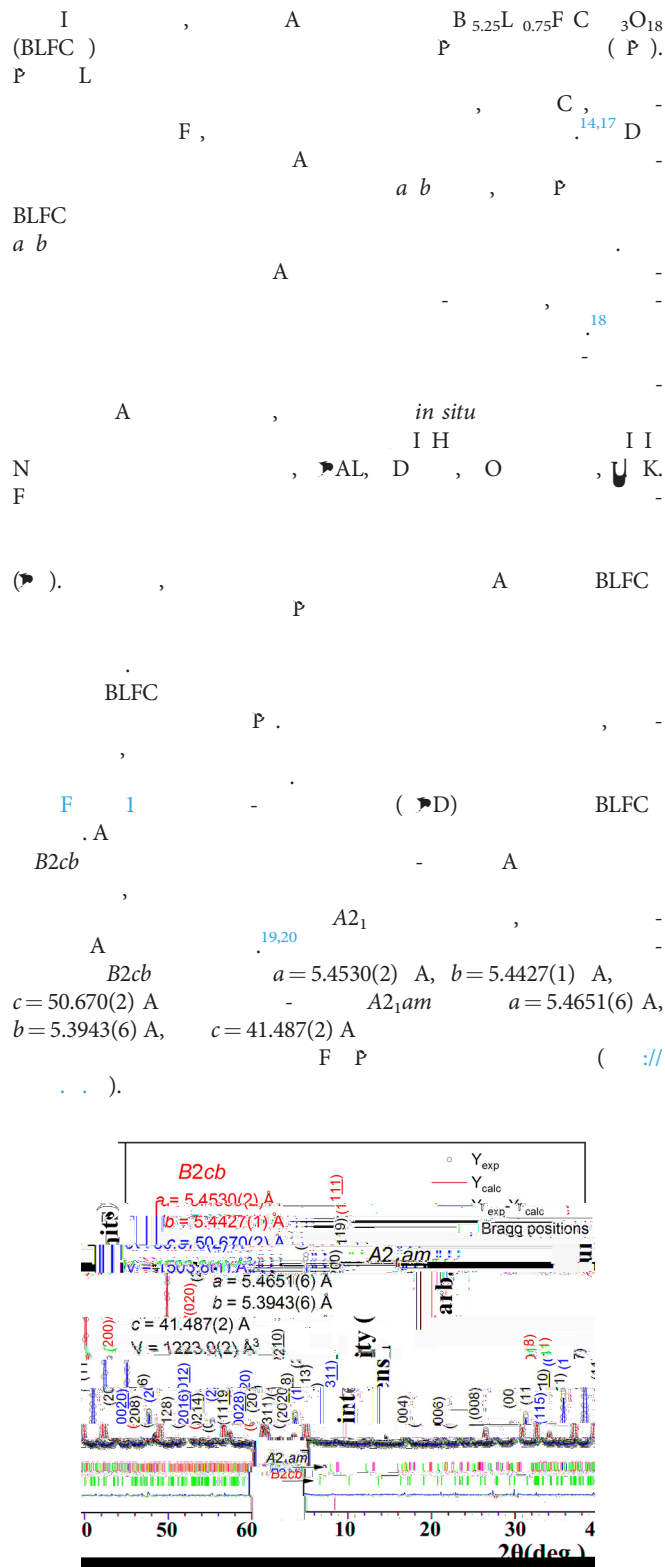


FIG. 1. $a a a B$

BLFC = 4 = 5 A N

BLFC F 1 EM (a-b) M

F 1 1.4 %, (F 2

D. ED

1) F, C, O, C $2F O_4$

A $B_{5F_{0.5}C_{0.5}O_{15}}$ ¹⁶

BLFC (50, 70 100, 300, 500 H). 1060 K FE T BLFC H, BLFC (973 K).¹³ F 2() P-E I-E BLFC I-E

BLFC $10 \mu C / 2(\dots)$ (FC) BLFC BLFC

200 O BLFC BLFC

^{21,22}

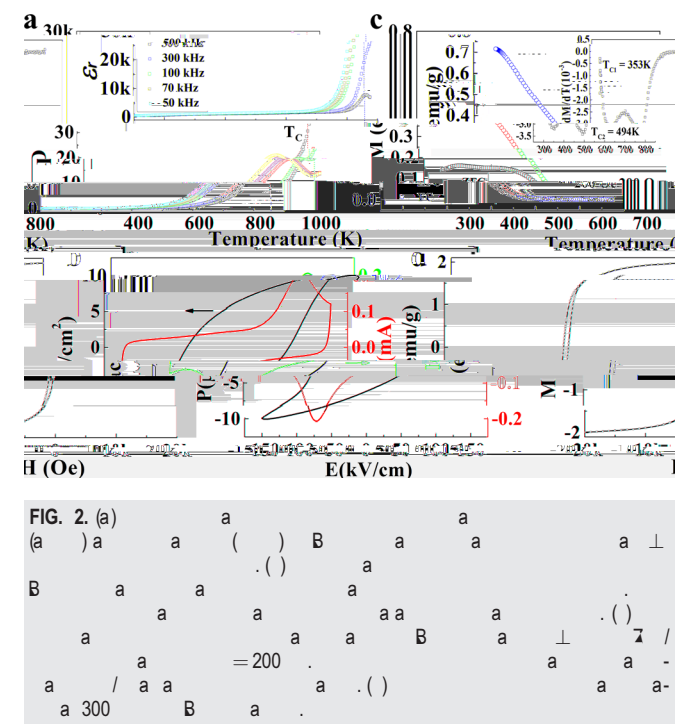


FIG. 2. (a) $a a () B a a a \perp$
 $() a a a a a a a \perp$
 $B a a a a a a a \perp$
 $a a a a a a a \perp$
 $a / a a = 200 a a$
 $a 300 B a () a a$

~ 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
 $C_2F O_4$.
 $C_2F O_4$ (460 K) 2 .^{16,25}
 (M) $C_2F O_4$.
 $16 \ 23.5$ / .²⁵ , 1.4 . %
 $C_{2-} F O_4$ $0.22 \ 0.32$ / , BLFC
 $M = 1.85$ / , $F . 2() . I$, $M H$
 $2 (F . 3)$.
 425 K 1.58 / . 0.27 / , ED
 $BLFC$, A
 $F 3$.
 (DF) $F^{3+} O C^{3+}$ *ab initio*
 $(A P)$. H
 $U_F = 2$ $U_C = 3$ $F C$,
 (GGA) . 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
 $BLFC$, $399 O$.
 $F .$
 PFM $BLFC$, $F -$
 $5() . A$

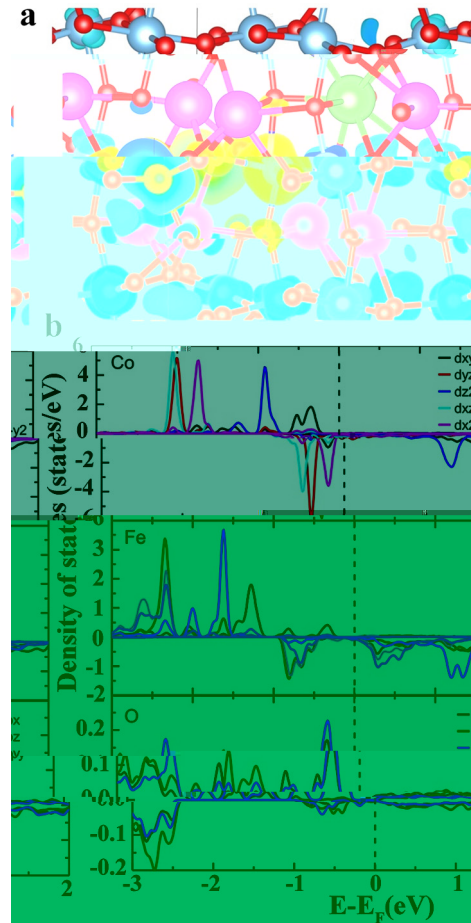


FIG. 3. (a) Crystal structure of BLFC showing layers of Co, Fe, and O atoms. (b) Density of states (DOS) plots for Co, Fe, and O atoms, showing contributions from dx^2-y^2 , dyz , dz^2 , dxz , and dx^2-y^2 orbitals.

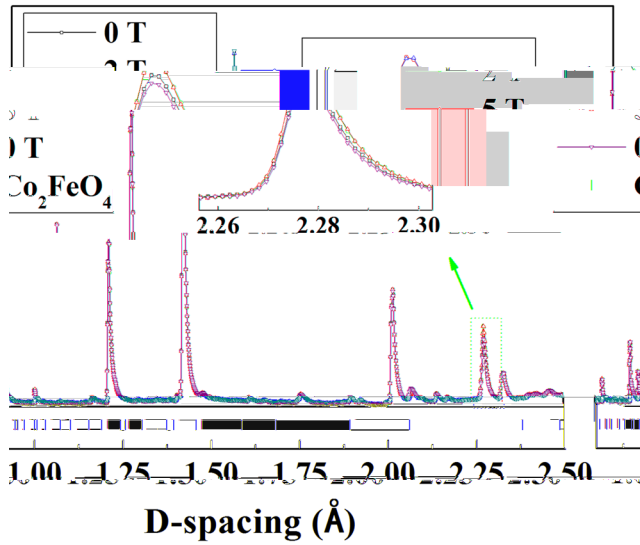


FIG. 4. XRD patterns of Co_2FeO_4 at 0 T, 2 T, and 5 T. The inset shows the crystal structure of Co_2FeO_4 with magnetic field directions.

Co₂FeO₄ (P) (M) 010

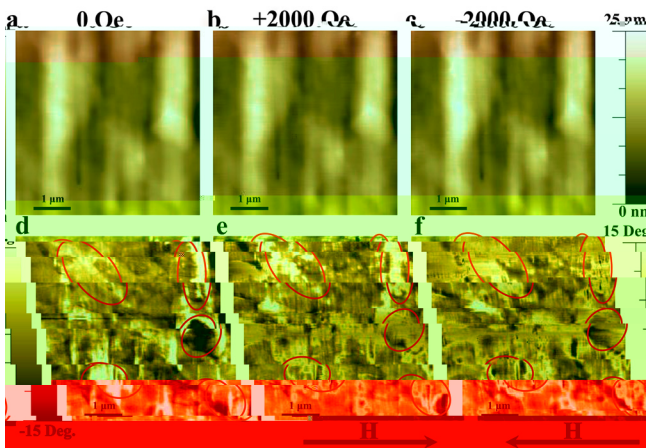


FIG. 5. MFM images of Co_2FeO_4 at 0 Oe, +2000 Oe, and -2000 Oe. (a-c) Top-view images and (d-f) cross-sectional images. Red circles in (d-f) highlight magnetic domains.

$T = P \times M$
BLFC
I, A BLFC
F
C³⁺ O C³⁺, F³⁺ O C³⁺ F³⁺ O F³⁺
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. 2/
0038/20), C (G N. K2015-0602006), N FC (G
N. 11474138 11834005). A
E M P (EMPP)
P IND54 N EMPP
EMPP E AME E

DATA AVAILABILITY

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