

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

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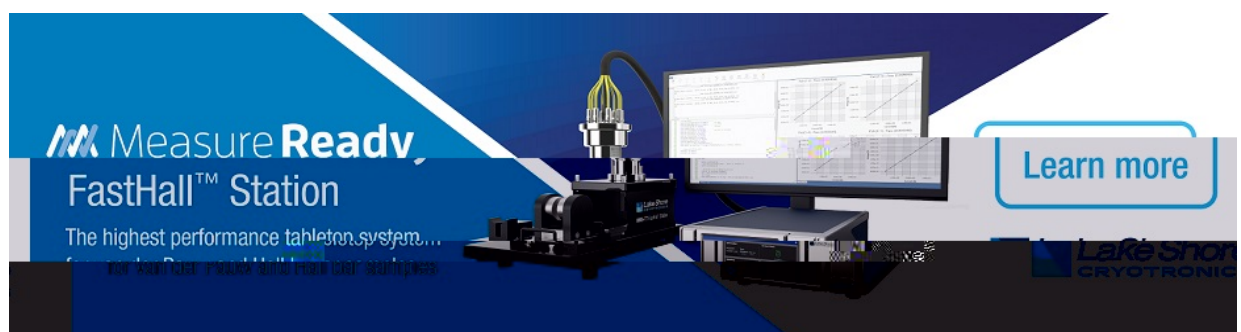
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AFFILIATIONS

¹G... 430074, C
²I... 47, K 04001, ...
³E... E14N, ... K f E
⁴N... 621900, C
⁵N... 110L, ... K
⁶E... G 99, ... K
⁷f... 730000, C

a)Email: ...@... .

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

ABSTRACT

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

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M... (FM) (FE) ... B₅F₃O₁₅ (= 4) ... B₆F₂O₁₈ ... B₄F₃O₁₂ ... B₅F_{0.5}C_{0.5}O₁₅ ... (B₂O₂)²⁺(A₋₁B₁O₃)²⁻ ... A ... H ... B- ... B₆F₃O₁₈ (= 5) ... B- ... A ... B- ... B F O₃ ... 7 11 ... A ... 16 ... D ...

I A B $_{5.25}L_{0.75}F_{1-x}C_{x-3}O_{18}$ BLFC \rightarrow A N
 (BLFC) L () =4 =5 .N \rightarrow D
 F, A C, D \rightarrow F 1 EM (a-b) M
 BLFC a b A a b F . 1 1.4 % (F . 2
 A A A \rightarrow D. ED
 N F , AL, D , O , K. 1) F, C, O, C₂F₂O₄ BLFC B₅F_{0.5}C_{0.5}F₃O₁₅¹⁶ (50, 70 100, 300, 500 H) . FE T BLFC . H , B₆F₃F₂O₁₈ 1060 K BLFC 2() P-E I-E BLFC I-E BLFC BLFC 10 μ C/ F 2() (FC) BLFC BLFC A B2cb A A21 BLFC A B2cb A^{19,20} A a = 5.4530(2) Å, b = 5.4427(1) Å, c = 50.670(2) Å A2₁am a = 5.4651(6) Å, b = 5.3943(6) Å, c = 41.487(2) Å V = 1223.0(2) Å³ (://) .

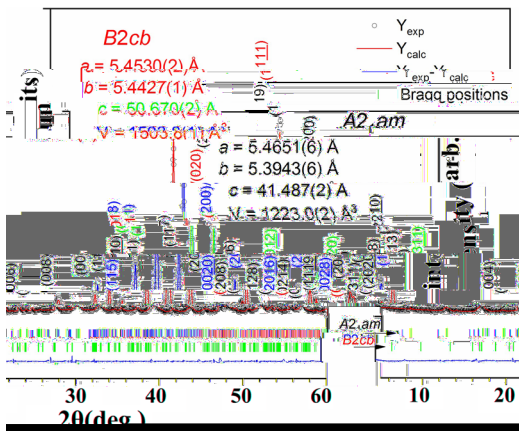


FIG. 1. XRD patterns of B2cb and A21am phases.

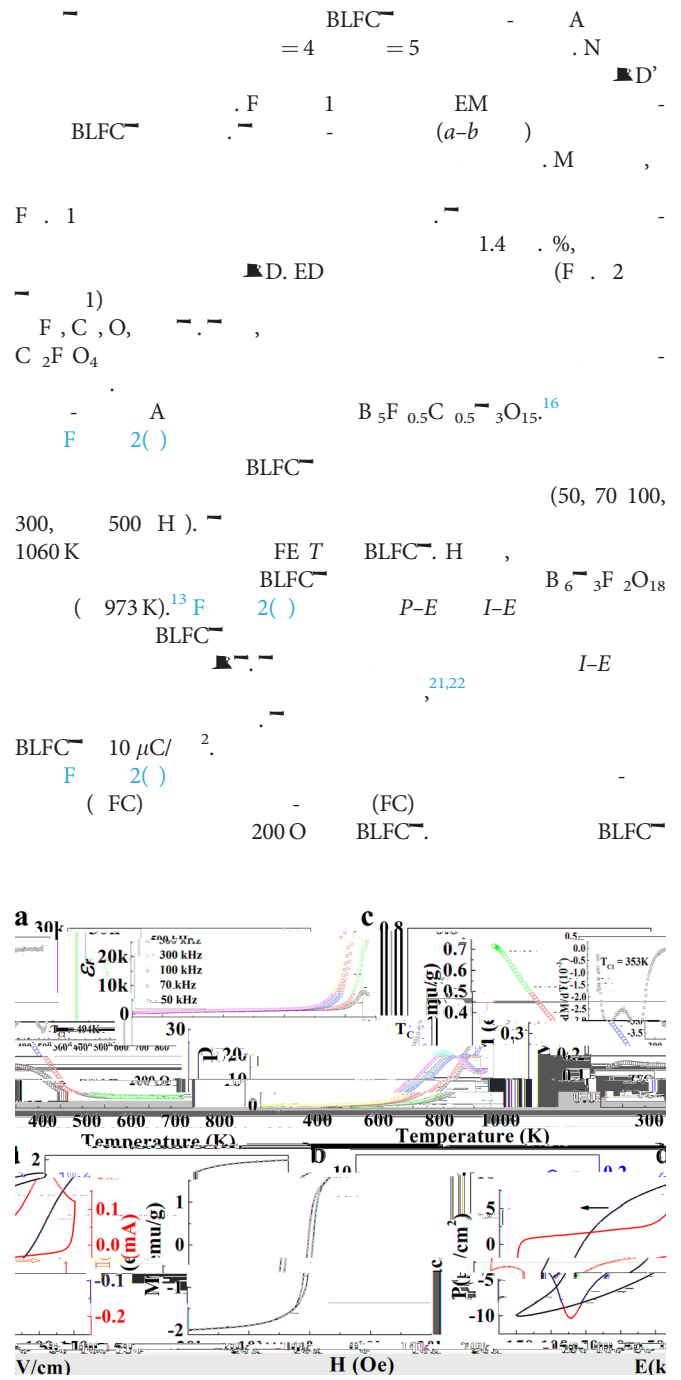


FIG. 2. (a) EPR spectra of BLFC at various frequencies. (b) Temperature dependence of magnetic field H and polarization P. (c) Temperature dependence of the derivative of the second derivative of absorption. (d) Temperature dependence of polarization P. (e) Temperature dependence of the derivative of the second derivative of absorption.

~ 494 K
 M/μ_B ,
 $B_6F_2C_{18}O_{18}$ (526 K).²³
 BLFC
 $F^{3+} O F^{3+}, C^{3+} O C^{3+}, F^{3+} O C^{3+}$ ().²⁴
 ED
 FC
 ~ 353 K
 $C_2F_4O_4$ (460 K)
 $(M) C_2F_4O_4$ 16 23.5 / .²⁵ 1.4 .%
 $C_2F_4O_4$ 0.22 0.32 / ,
 $M = 1.85$ / , $F = 2(1.1)$ BLFC
 $M H$
 ~ 425 K 1.58 / .
 0.27 / , ED
 BLFC
 A
 $F^{3+} O C^{3+}$
 (DF) *ab initio*
 (A) $F H$
 $\mu_F = 2$ $\mu_C = 3$ $F C$,
 (GGA)+ μ . I
 BLFC
 $F = 3(1)$, $F^{3+} C^{3+}$ (3.1 2.1 μ_B / ,) ,
 $(0.1 \mu_B /)$.
 $F O_6 C O_6$ F/C
 $F O$ / $F = 3(1)$.
 $F^{3+} C^{3+}$,
 (\dots) ,
 (\dots) ,
 $E_{FM} - E_{AFM}$
 $= -144.1$.
 H , (FM)
 43.5 (, 504.6 K),
 ~ 1 FC/FC . $F = 2(1)$.
 $a b$
 010 .
 BLFC
 $F = 4$. I
 , ,

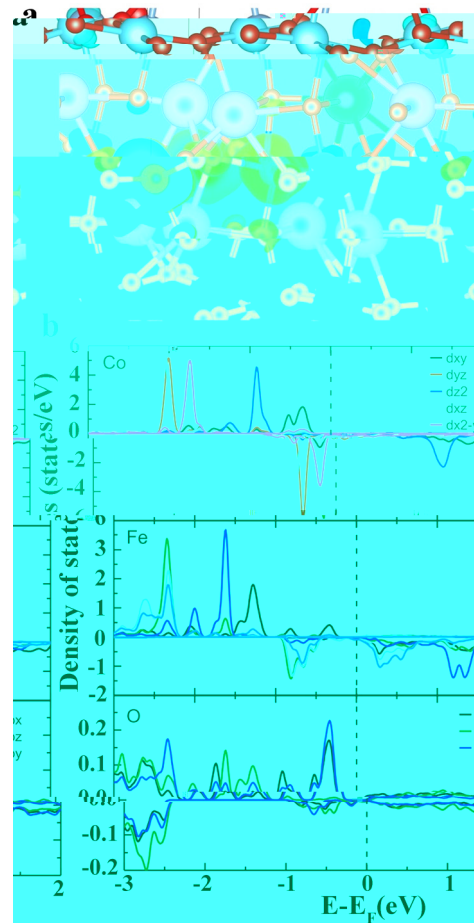


FIG. 3. (a) Crystal structure of BLFC ($B_6F_2C_{18}O_{18}$) with $a = b = 0.35$ nm, $c = 0.35$ nm, $\alpha = \beta = \gamma = 90^\circ$. (b) Density of states (DOS) for Co, Fe, and O atoms. The DOS is calculated using the Perdew-Burke-Ernzerhof (PBE) functional with a spin polarization parameter $\sigma = 0.005$. The x-axis represents the energy relative to the Fermi level ($E - E_F$) in eV, ranging from -3 to 1. The y-axis represents the density of states in states/eV. The legend indicates the contributions from different orbitals: d_{xy} (green), d_{yz} (orange), d_{z^2} (blue), d_{xz} (red), and $d_{x^2-y^2}$ (purple).

~ 399 O .
 $F = 4$,
 $(0 1 20)$.
 2 . F
 $(2^\circ < H < 5^\circ)$,
 $M H$ $F = 2()$ 3. F ,
 $F = 5$
 BLFC
 F M
 399 O .
 $F = 4$.
 $F = 4$.
 FM BLFC ,
 $5()$. A F

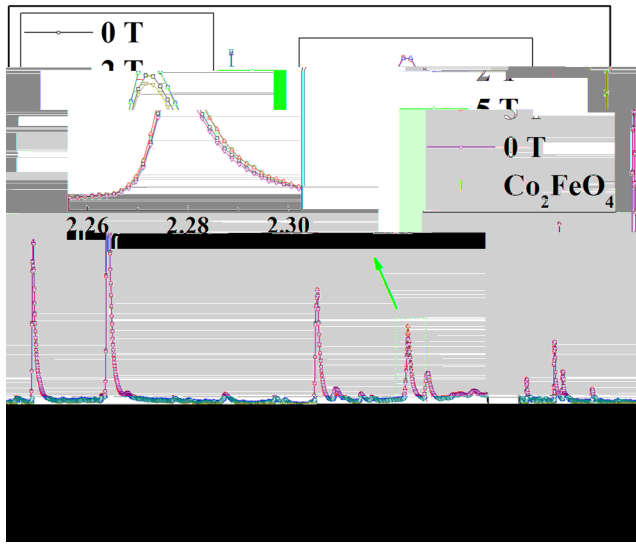


FIG. 4. XRD patterns of Co_2FeO_4 at various magnetic fields (0 T, 2 T, 5 T).

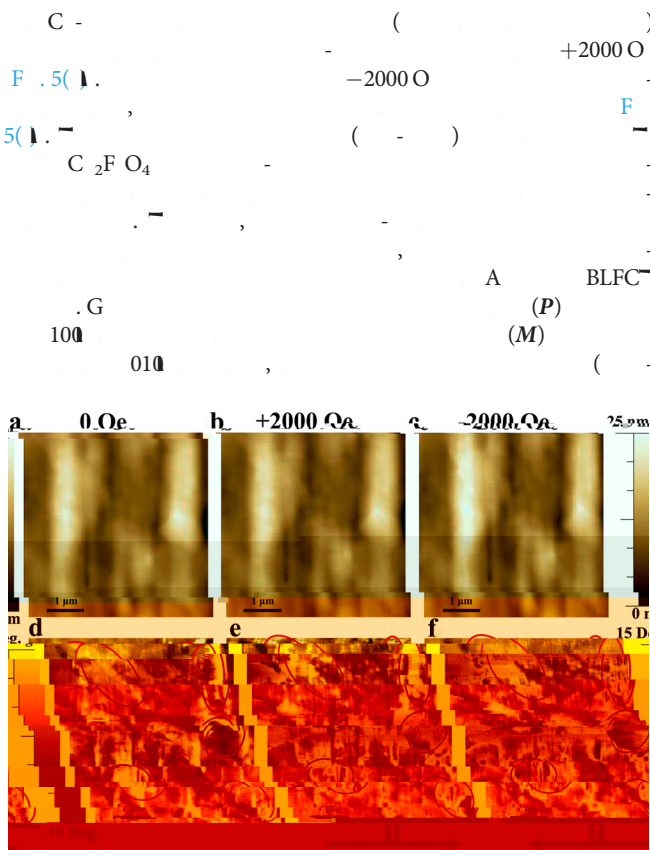


FIG. 5. HRTEM images and SAED patterns of Co_2FeO_4 at different magnetic fields (0 Oe, +2000 Oe, -2000 Oe).

$T = P \times M$
 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 E₂AME E

DATA AVAILABILITY

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 H , H , O. G , D. C. L , H. , K ,
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 E. , D. J , J. A . C . . 96, 2339
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 A . . L . 96, 222903 (2010).
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