

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

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AFFILIATIONS

¹G...
²I...
³E...
⁴N...
⁵N...
⁶E...
⁷

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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)
 (FM)
 H...
 A...
 (B₂O₂)²⁺(A₋₁B O₃ +1)²⁻
 12-
 B...
)⁶
 B-...
 B F O₃
 7 11

~ 494 K (M/),
 $B_6FC_{3O_{18}}$ (526 K).²³
 BLFC
 $F^{3+} O F^{3+}, C^{3+} O C^{3+}, F^{3+} O C^{3+}$ (.
 ED
 FC ~ 353 K
 $C_2F_4O_4$ (460 K) ^{16,25}
 (M) $C_2F_4O_4$ 1.4 %
 $16.235 / .25$, 0.22 0.32 / ,
 $C_{2-} F O_4$ BLFC
 $M = 1.85 / , F . 2() . I$
 M H
 $2 (F . 3)$ 1
 425 K 1.58 / . 0.27 / ,
 ED
 BLFC
 A
 $F 3$
 $F^{3+} O C^{3+}$
 (DF) *ab initio*
 (A P)
 $F = 2$ $C = 3$ F C ,
 (GGA) I
 BLFC
 $F . 3(a)$, F^{3+} C^{3+} (3.1 $2.1 \mu_B/a$),
 $0.1 \mu_B/a$.
 $F O_6$ $C O_6$
 F/C
 $F . 3()$
 F^{3+} C^{3+}
 $E_{FM} - E_{AFM} = -144.1$
 (FM)
 43.5 (., 504.6 K), FM
 FC/FC $F . 2()$
 a b
 010
 $F 4$
 BLFC I
 399 O .
 PFM BLFC , a $F .$
 5(). A a a a F -

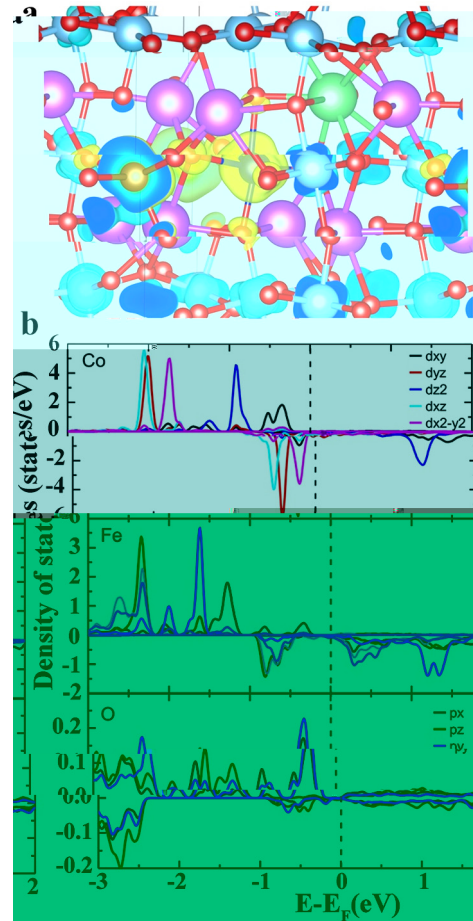


FIG. 3. (a) Crystal structure of BLFC (space group $R\bar{3}m$, $a = b = c = 0.38$ nm, $\alpha = \beta = \gamma = 90^\circ$). (b) Density of states (DOS) for Co, Fe, and O atoms. The DOS is calculated using the Perdew-Burke-Ernzerhof (PBE) functional and the projector augmented wave (PAW) method. The Fermi level (E_F) is set to 0 eV.

BLFC is a layered structure with Fe and Co ions in octahedral sites and O ions in tetrahedral sites. The structure is shown in Fig. 3(a). The DOS for Co, Fe, and O atoms is shown in Fig. 3(b). The DOS for Co shows a sharp peak at $E - E_F = 0$ eV, which is the Fermi level. The DOS for Fe and O shows a gap at $E - E_F = 0$ eV. The DOS for Fe and O is calculated using the Perdew-Burke-Ernzerhof (PBE) functional and the projector augmented wave (PAW) method. The Fermi level (E_F) is set to 0 eV.

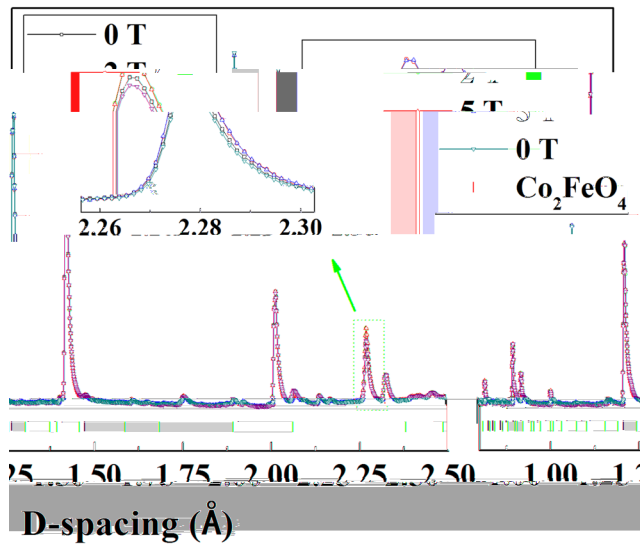


FIG. 4. XRD patterns of Co_2FeO_4 at 0 T and 5 T. The inset shows a magnified view of the 2.26–2.30 Å region.

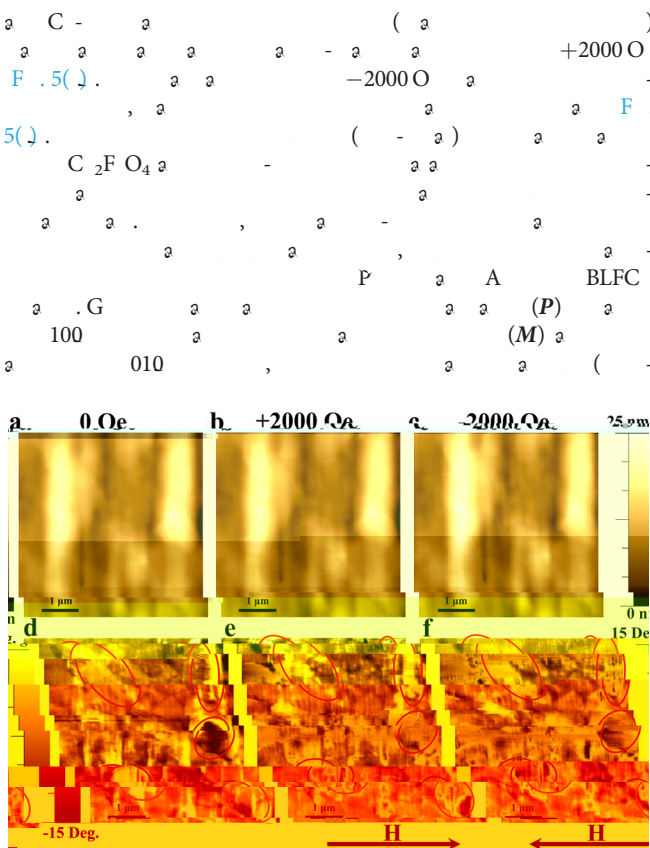


FIG. 5. MFM images of Co_2FeO_4 at 0 Oe, +2000 Oe, and -2000 Oe. The inset shows a magnified view of the 2.26–2.30 Å region.

$T = P \times M$
 BLFC
 $\text{C}^{3+} \text{O} \text{C}^{3+}, \text{F}^{3+} \text{O} \text{C}^{3+}$
 $\text{F}^{3+} \text{O} \text{F}^{3+}$
 $\text{A} \text{C} / \text{F}$
 EM (ED)
 BLFC
 D. Ma, P. Ma, D. K. Ma, D. H. Ma, I. I. N. Ma, AL, D. O. K. Ma, A. E. D. Ma, F. G. A. Ma, A. Ma (G. N. 2/0038/20), C. (G. N. K2015-0602006), N. FC (G. N. 11474138, 11834005). A. E. M. P. (EM P) IND54 Na. EM P AME E

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon request.

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