





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

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$B_{5.25}La_{0.75}FeC_{3O_{18}}$  (BLFC) is a perovskite structure with  $P6_3/mc2$  space group. The lattice parameters are  $a = 5.4530(2)$  Å,  $b = 5.4427(1)$  Å, and  $c = 50.670(2)$  Å. The structure is distorted along the  $c$ -axis. The  $B2cb$  phase is characterized by  $a = 5.4651(6)$  Å,  $b = 5.3943(6)$  Å, and  $c = 41.487(2)$  Å. The structure is distorted along the  $c$ -axis. The  $A2_1am$  phase is characterized by  $a = 5.4651(6)$  Å,  $b = 5.3943(6)$  Å, and  $c = 41.487(2)$  Å. The structure is distorted along the  $c$ -axis.

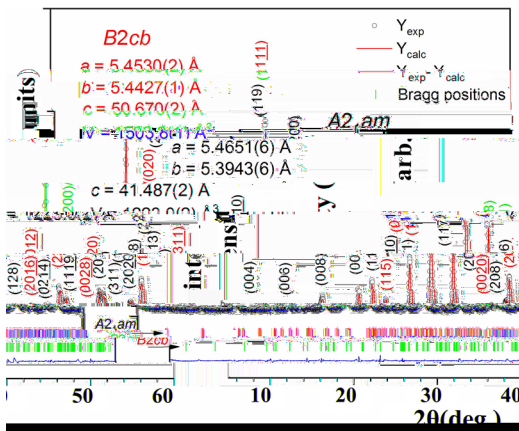


FIG. 1.

BLFC is a perovskite structure with  $P6_3/mc2$  space group. The lattice parameters are  $a = 5.4530(2)$  Å,  $b = 5.4427(1)$  Å, and  $c = 50.670(2)$  Å. The structure is distorted along the  $c$ -axis. The  $B2cb$  phase is characterized by  $a = 5.4651(6)$  Å,  $b = 5.3943(6)$  Å, and  $c = 41.487(2)$  Å. The structure is distorted along the  $c$ -axis. The  $A2_1am$  phase is characterized by  $a = 5.4651(6)$  Å,  $b = 5.3943(6)$  Å, and  $c = 41.487(2)$  Å. The structure is distorted along the  $c$ -axis.

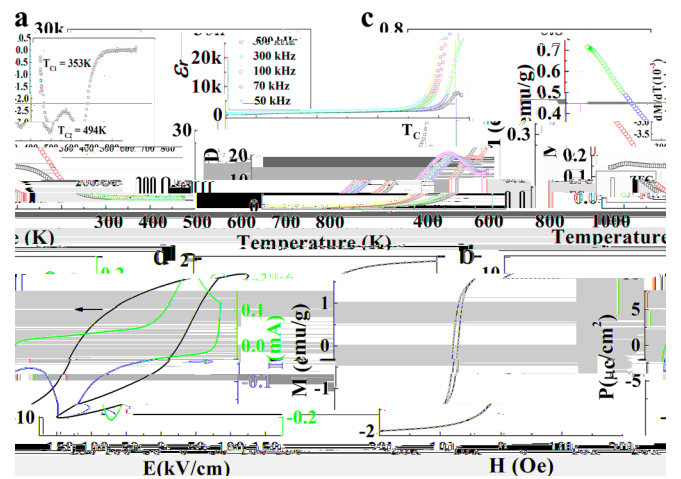


FIG. 2. (a) Temperature dependence of dielectric loss ( $\tan \delta$ ) for BLFC at various frequencies (500 Hz to 50 kHz). (b) Temperature dependence of dielectric constant ( $\epsilon'$ ) for BLFC at various frequencies. (c) Temperature dependence of magnetic susceptibility ( $\chi$ ) for BLFC at various frequencies. (d) Temperature dependence of magnetization ( $M$ ) for BLFC at various frequencies. (e) Temperature dependence of piezoelectric coefficient ( $P$ ) for BLFC at various frequencies.

$\sim 494$  K (M/),  
 $B_6FC_{3O_{18}}$  (526 K).<sup>23</sup>  
 BLFC  
 $F^{3+} O F^{3+}, C^{3+} O C^{3+}, F^{3+} O C^{3+}$  (.  
 ED  
 $FC$   $\sim 353$  K  
 $C_2FO_4$  (460 K)  $^{16,25}$   
 $(M) C_2FO_4$   
 $16.235 / .^{25}$ ,  $0.22 0.32 /$ ,  $1.4 .\%$   
 $C_{2-} F O_4$  BLFC  
 $M = 1.85 / , F . 2( ) . I$   
 $M H$   
 $2 (F . 3)$   
 $425$  K  $1.58 /$ ,  $0.27 /$ , ED  
 BLFC  
 $F 3$   
 $F^{3+} O C^{3+}$   
 $(DF)$   $ab initio$   
 $(A P)$   
 $F = 2$   $C = 3$   $F$   $C$ ,  
 $(GGA)$   $I$   
 BLFC  
 $F . 3(a)$ ,  $F^{3+}$   $C^{3+}$  ( $3.1$   $2.1 \mu_B/a$ ),  
 $O$   $0.1 \mu_B/a$ ).  
 $F O_6$   $C O_6$   
 $F / C$   $F . 3( )$   
 $F$   $O$   $F^{3+}$   $C^{3+}$   
 $(. , )$   $(. , )$   
 $E_{FM} - E_{AFM}$   
 $= -144.1$   
 $H$  (FM)  
 $43.5$  ( $\dots, 504.6$  K), FM  
 $FC/FC$   $F . 2( )$   
 $a b$   
 $010$   
 $F 4$   
 BLFC  $I$   
 $399$  O  $F$   
 $5( ) . A$   $P F M$  BLFC  $F$

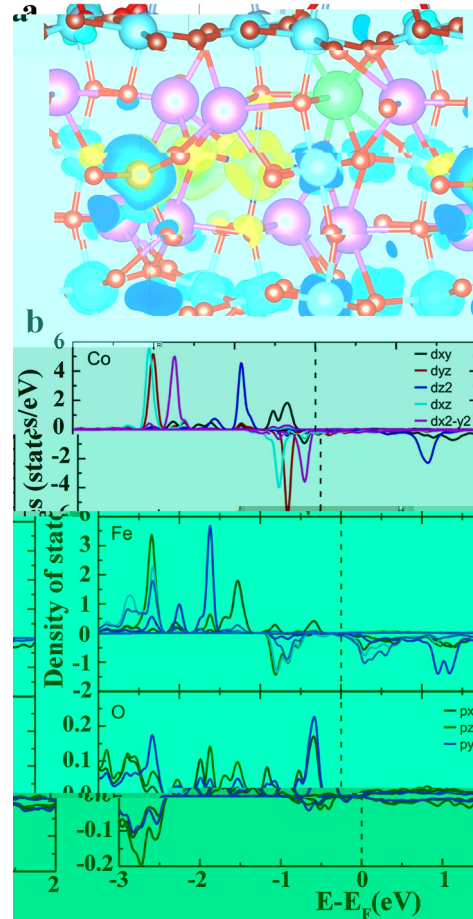


FIG. 3. (a) Crystal structure of BLFC. (b) Density of states (DOS) for Co, Fe, and O atoms. The DOS is plotted in states/eV versus energy  $E - E_F$  (eV). The legend indicates the contributions of different orbitals: dxy (red), dyz (green), dz2 (blue), dxz (cyan), dx2-y2 (magenta), px (black), py (grey), and pz (white).

$N$   
 $I$   $F . 4$   
 $(0 1 20)$   
 $2 < H < 5$ ,  
 $M H$   $F . 2( )$   $3. F$   
 $F 5$   
 BLFC  $P$   $F M$   
 $399$  O  $F$   
 $5( ) . A$   $P F M$  BLFC  $F$

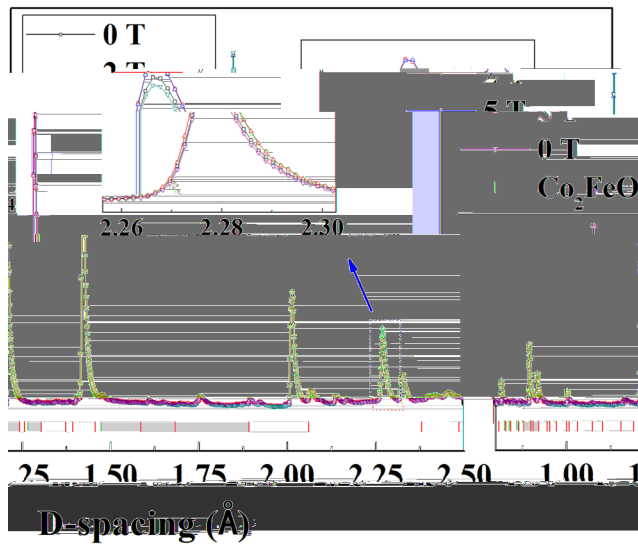


FIG. 4. XRD patterns of BLFC at 0 T and 2 T. The inset shows a magnified view of the peak at 2.28 Å.

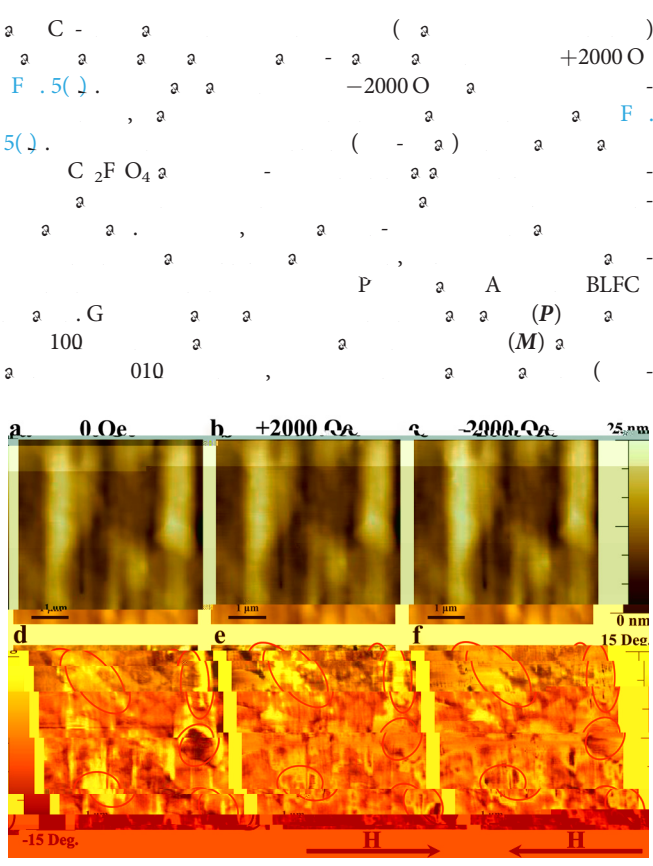


FIG. 5. TEM images of BLFC at different magnetic fields: (a) 0 Oe, (b) +2000 Oe, (c) -2000 Oe. Scale bars are 1 μm and 25 nm.

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

DATA AVAILABILITY

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