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AFFILIATIONS

[1] G I ι , C f G , ι 430074, C
[2] I ι f M , A f , 47, K 04001,
[3] f E M , ι M , f L , L E1 4N , K
[4] N K L f D I ι f F ι , C A f E , M 621900, C
[5] N L , H , 11 0L , K
[6] E L , F , ι G 99 , K
[7] f , L ι , L ι 730000, C

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ABSTRACT

M . H , - - . , - A , D . H , A $B_{5.25}L_{0.75}F$ C $_3O_{18}$ P . - A , *in situ* . - F^{3+} O F^{3+}, C^{3+} O C^{3+}, F^{3+} O C^{3+} - . - . A , C /F - , - .

M (FE) (FM) , , . [1-4] H , - - . [5] , (B $_2O_2)^{2+}$(A $_{-1}$B O$_3$ $_{+1})^{2-}$ (A -, 12- - , B - - ,)[6] B- - B F O$_3$ - .[7-11] . A B $_5$F $_3O_{15}$ (= 4) B $_6$F $_2$ $_3O_{18}$ (= 5), B $_4$ $_3O_{12}$ B F O$_3$, FE FM .[12,13] B - C F B- , B $_5$F $_{0.5}$C $_{0.5}$ $_3O_{15}$ (= 4) B $_6$F C $_3O_{18}$ (= 5) - -, .[14,15] H , D - - .[16] , A .

I , A $B_{5.25}L_{0.75}F$ C $_3O_{18}$ (BLFC) P (P). P L , C , [14,17] D F , A a b , P BLFC a b . A - - , , [18] . - - A , in situ I H I I N , AL, D , O , K. F - ( ). , A BLFC P . BLFC P . , - , . F 1 - (D) BLFC . A B2cb - A , $A2_1$, - A [19,20]. - B2cb $a = 5.4530(2)$ A, $b = 5.4427(1)$ A, $c = 50.670(2)$ A - $A2_1am$ $a = 5.4651(6)$ A, $b = 5.3943(6)$ A, $c = 41.487(2)$ A F P (:// . .).

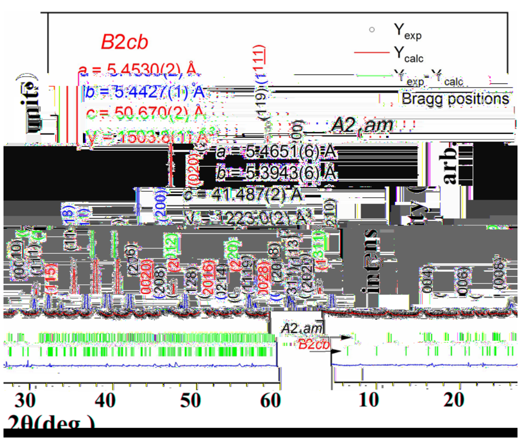

FIG. 1. -a a a e e B e .

BLFC - A = 4 = 5 . N D' . F 1 EM - BLFC . - (a–b) P . M , F . 1 . - 1.4 . %, D. ED (F . 2 1) F , C , O, . , C $_2$F O_4 - . - A $B_5F_{0.5}C_{0.5}$ $_3O_{15}$.[16] F 2( ) BLFC P (50, 70 100, 300, 500 H). 1060 K FE T BLFC . H , BLFC B_6 $_3F_2O_{18}$ (973 K).[13] F 2( ) P–E I–E BLFC P . I–E [21,22] . BLFC 10 μC/ ^{2}. F 2( ) - (FC) - (FC) 200 O BLFC . BLFC

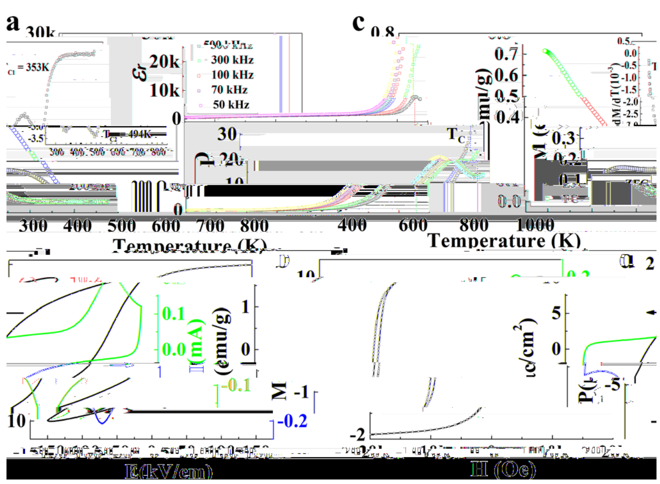

FIG. 2. (a) e e ea ue e e e e e ea e ee e (a e) a a e ( ) B e a ea ue e e ua ⊥ e P e ue e . ( ) e P a e e e e ue B e a ea ue e e ua e P e ue e . e u e e a e e a a a e a e ee . ( ) e e ea ue e e e e e a e a B e a ⊥ e / e ea ue = 200 e . e e e e a e a e- / a a u e e a ue . ( ) e e e e e e a e a- a 300 e B a e .

$_1 \sim 494$ K
(M/),
B $_6$F C $_3$O$_{18}$ (526 K).[23]
BLFC
F $^{3+}$ O F $^{3+}$, C $^{3+}$ O C $^{3+}$, F $^{3+}$ O C $^{3+}$ (.
).[24] -
ED .
A FC $_2 \sim 353$ K
C $_2$F O$_4$. $_2$ -
C $_2$F O$_4$ (460 K) .[16,25]
(M) C $_2$F 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 -
$_1$
$_2$ (F . 3). -
425 K 1.58 / .
0.27 / ,
ED
. , BLFC
A .
F 3
F $^{3+}$ O C $^{3+}$ -
(DF) *ab initio*
(A P) . H
U $_F$ = 2 U $_C$ = 3 F C , ,
(GGA)-U . I -
BLFC
F . 3( ) , F $^{3+}$ C $^{3+}$ (3.1 2.1 μ_B/ ,),
O
(0.1 μ_B/).
- F O$_6$ C O$_6$
( ) F /C -
F 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 .
F 4
BLFC . I
- , - ,

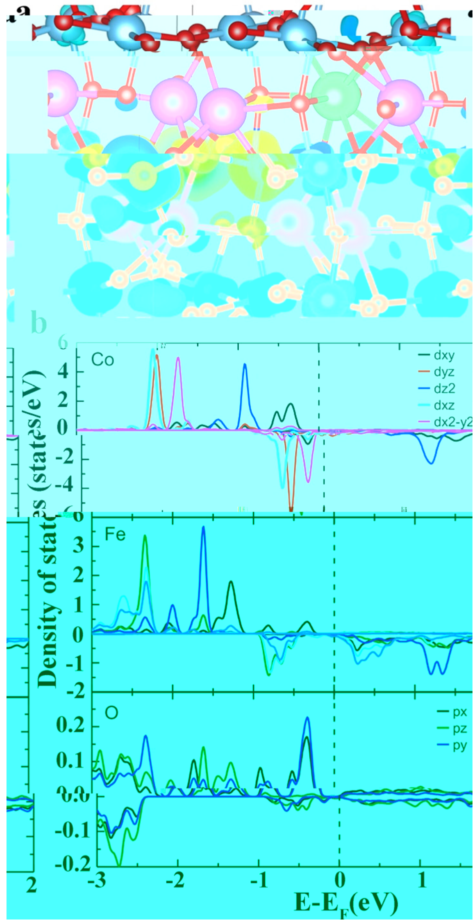

FIG. 3. (a) (u a e e e = 0.005) (e), B ( ), a (ee), (ue), (a ue), a e (e) a . ( ) A e a e e e e a e e $^{3+}$ $^{3+}$.

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

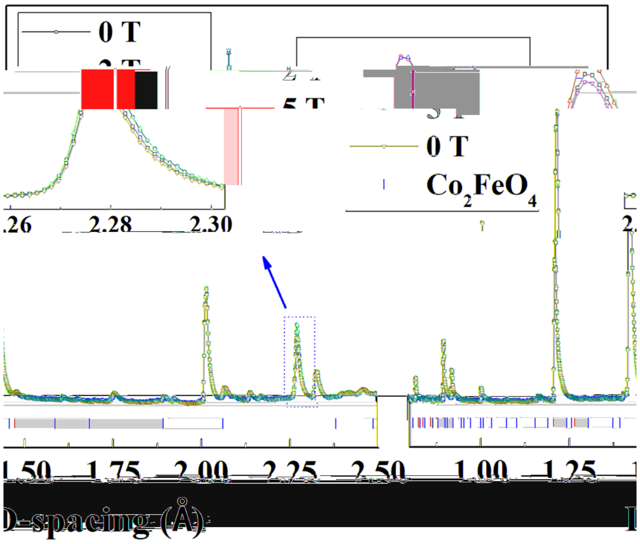

FIG. 4. e -e ea ue eu a a e a e e B e a a e e a e e (0, 2, a 5 a e a 0).

C - ( ) - +2000 O F . 5( ) . −2000 O - , F . 5( ) . (-) C_2FO_4 - - - . , - , - P A BLFC . G (*P*) 100 (*M*) 010 , (-

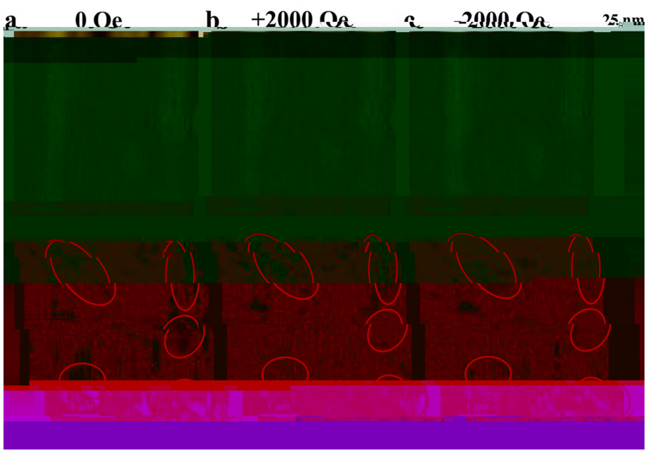

FIG. 5. e ee a B u e ea e a e e (a a e e u a e e a e). (a) a a ( ) e a P a e a 0 e ( ) a a (b) e a P a e a +2000 e a ( ) a a ( ) e a P a e a −2000 e.

) $T = P \times M$ BLFC . I , A BLFC - . F F $^{3+}$ O F $^{3+}$, C $^{3+}$ O C $^{3+}$, F $^{3+}$ O C $^{3+}$ - . - . 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 (EM P) P IND54 N . EM P EM P AME E .

DATA AVAILABILITY

.

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