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ABSTRACT

M . H , - A ' D . H , A B 5.25 L 0.75 F C 3 O 18 P A in situ F 3+ O F 3+, C 3+ O C 3+, F 3+ O C 3+ . A , C /F

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M (FM) (FE) A (= 5), B 5 F 3 O 15 (= 4) B 6 F 2 3 O 18 B 4 3 O 12 [1 4] H , B F O 3, C F B- FE FM [12,13] B (= 4) B 6 F C 3 O 18 (= 5) B 5 F 0.5 C 0.5 3 O 15 [5] (B 2 O 2)2+(A -1 B O 3 +1)2− (A A 12- , B [14,15] H [6] [16] D B- A B F O 3 [7 11]

I a , A a B$_{5.25}$L$_{0.75}$F C $_3$O$_{18}$ (BLFC) P L (P).

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$_1$am $a = 5.4651(6)$ A, $b = 5.3943(6)$ A, $c = 41.487(2)$ A F P (:// . .).

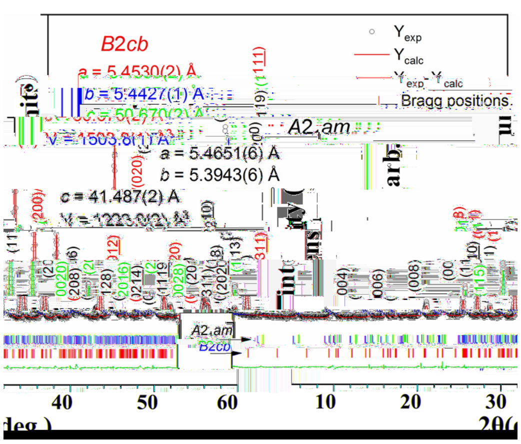

FIG. 1. -a a a B .

a BLFC a A a =4 =5 . N D' . F 1 EM (a–b) BLFC . P . M F . 1 1.4 %, D. ED (F . 2 1) F , C , O, C $_2$F O$_4$. A B$_5$F$_{0.5}$C$_{0.5}$ $_3$O$_{15}$.[16] F 2( ) BLFC P (50, 70, 100, 300, 500 H). 1060 K FE T BLFC . H BLFC B$_6$ $_3$F $_2$O$_{18}$ (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

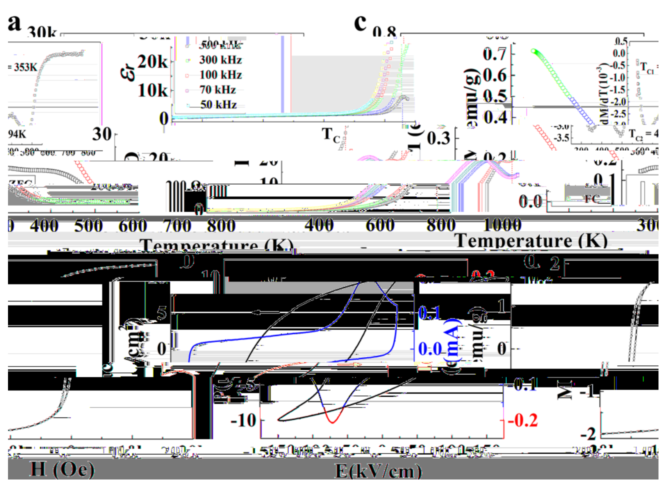

FIG. 2. (a) a (a) a ( ) B a a a ⊥ . ( ) a B a a a . a a a a . ( ) a a a B a ⊥ a =200 . a a a / a a a . ( ) a a- a 300 B a .

$_1 \sim 494$ 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$_4$.

C $_2$F O$_4$ (460 K) 2 [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

$_2$ (F . 3). 1

425 K 1.58 /

0.27 / , ED

BLFC

A

F 3

F $^{3+}$ O C $^{3+}$

(DF) *ab initio*

(A P) H

$_F$ = 2 $_C$ = 3 F C

(GGA)+ . 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 43.5 (. ., 504.6 K), (FM) FM

1 FC/FC . F . 2( ) . *a b*

010 . F 4

BLFC . I

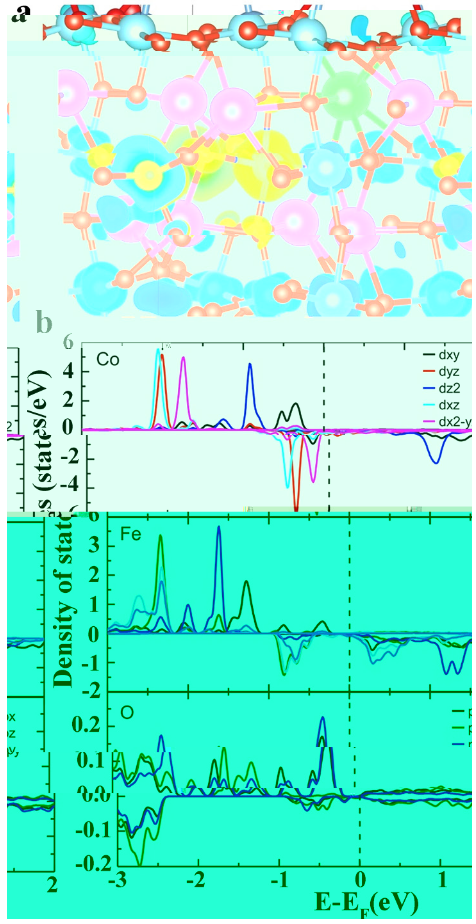

FIG. 3. (a) (a = 0.005) ( ), B ( ), a ( ), ( ), (a), a ( ) a . ( ) A a 3+ 3+.

. 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 -

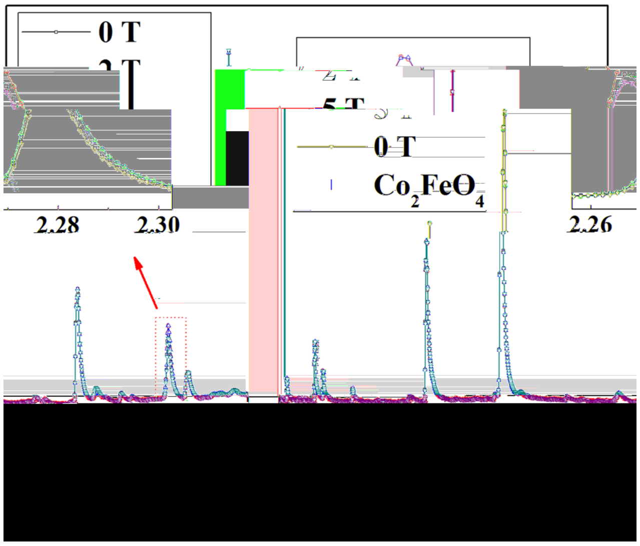

FIG. 4. - a a a a B a a a (0, 2, a 5 a a 0).

a C - a a a a a (a) a a a - a +2000 O F . 5( ) . a a −2000 O a - a a F . 5( ) . (- a) a a C 2F O4 a - a a a a . a , a - a a a - , a P a A BLFC a . G a a a (P) a 100 a (M) a 010 , (

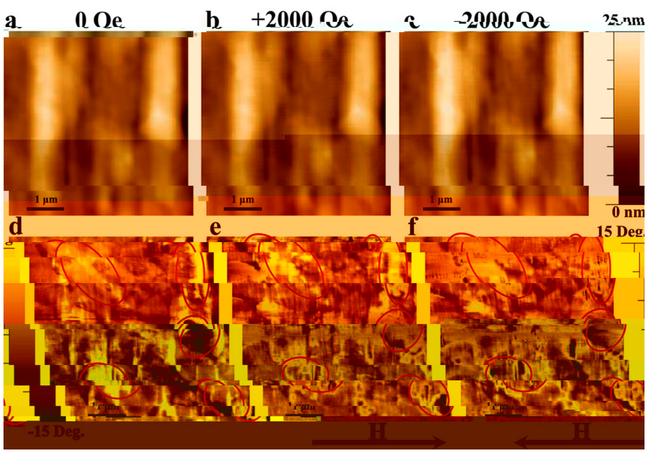

FIG. 5. a B a a (a a a). (a) a a ( ) a a a 0 ( ) a a ( ) a a a +2000 a ( ) a a ( ) a a a −2000 .

) a $T = P \times M$ a BLFC . a I , A a BLFC a a . F a F 3+ O F 3+, C 3+ O C 3+, F 3+ O C 3+ a . a A C /F a - - a a a a EM - (ED) BLFC .

a 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 E AME E .

DATA AVAILABILITY

a a a a a a a a a a a a .

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