Applied Physics Letters

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Cite as: Appl. Phys. Lett. **117**, 052903 (2020); https://doi.org/10.1063/5.0017781
Submitted: 09 June 2020 . Accepted: 25 July 2020 . Published Online: 07 August 2020

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Applied Physics Letters ARTICLE scitation.org/journal/apl

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AFFILIATIONS

[1]G I ι , C f G , ι 430074, C
[2]I ι f M , A I f , 47, K 04001,
[3] f E M , ι M , f L , L E1 4N , K I
[4]N K L f D I ι f F ι , C A I f E , M 621900, C
[5]N L , H I , 11 0L , K I
[6]E L , F I , ι G 9 9 , K I
[7] f , L ι , L ι 730000, C

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ABSTRACT

M . H , - - . , - A , D . H , A B 5.25L 0.75F C 3O18 P . - A , *in situ* . - F 3+ O F 3+, C 3+ O C 3+, F 3+ O C 3+ - . - . A , C /F - , - .

M (FE) A B 5F 3O15 (= 4) B 6F 2 3O18 (FM) (= 5), B 4 3O12 , , B F O3, FE FM .[12,13] B - , .[1 4] H , - C F B- , B 5F 0.5C 0.5 3O15 - (= 4) B 6F C 3O18 (= 5) .[5] , - A - (B 2O2)2+(A -1B O3 +1)2− (A -, .[14,15] H , -, 12- - , B - - , D -)[6] .[16] , - B- - A B F O3 - .[7 11] .

I , A B 5.25L 0.75F C 3O18 (BLFC) P (P). P L , C , - F , .[14,17] D 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 (:// . .).

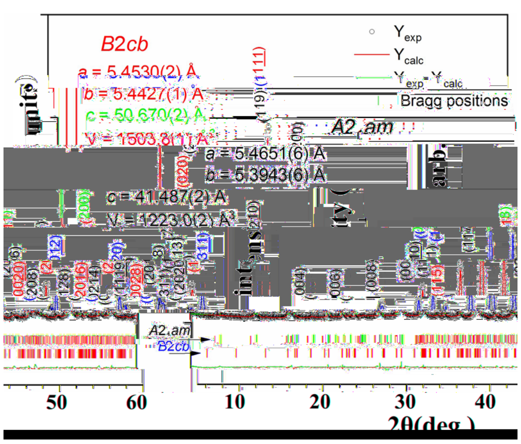

FIG. 1. -a a a B .

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 2F O4 - . - A B 5F 0.5C 0.5 3O15.[16] F 2( ) BLFC P (50, 70 100, 300, 500 H). 1060 K FE T BLFC . H , BLFC B 6 3F 2O18 (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

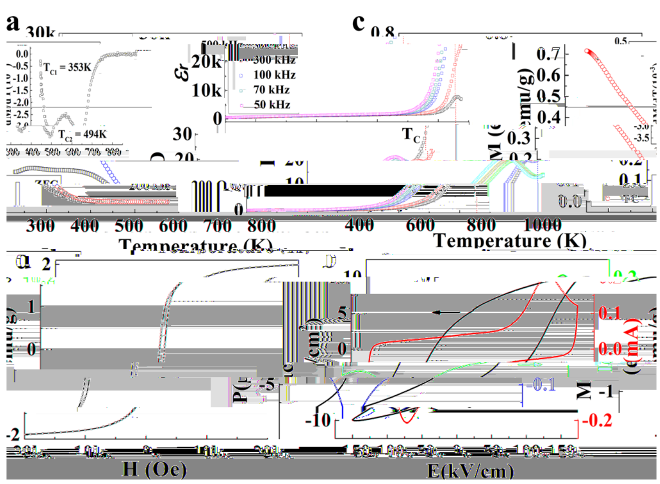

FIG. 2. (a) a a (a) a ( ) B a a a ⊥ . ( ) a B a a a . a a a a a . ( ) a a a B a ⊥ / a = 200 . a a - a / a a a . ( ) a a- a 300 B a .

$_1 \sim 494$ 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$_4$. $_2$ - 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 - , - ,

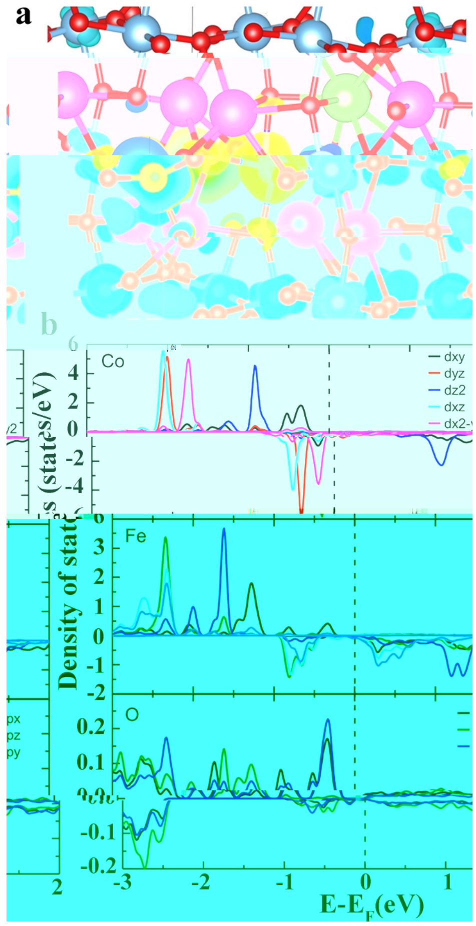

FIG. 3. (a) (a = 0.005) ( ), B ( ), a ( ), ( ), (a), a ( ) a . ( ) A a a $^{3+}$ $^{3+}$.

. . 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 -

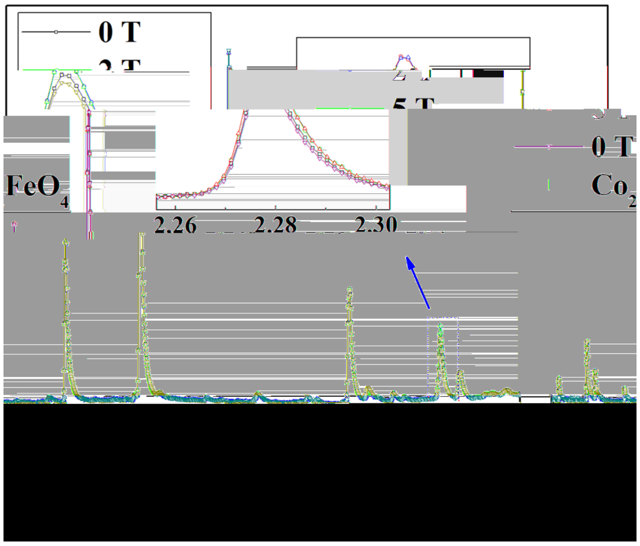

FIG. 4. - a a a a B a a a (0, 2, a 5 a a 0).

C - ( ) - +2000 O F . 5( ) . −2000 O - , F . 5( ) . (-) C $_2$F O$_4$ - - - . , - , - P A BLFC . G (*P*) 100 (*M*) 010 , (-

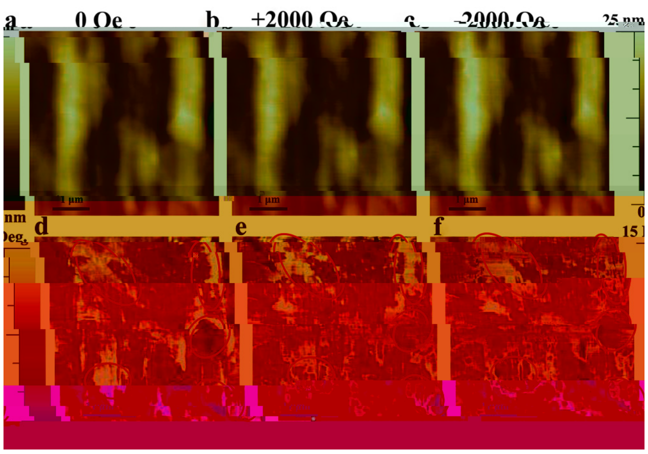

FIG. 5. a B a a (a a a). (a) a a ( ) a a a 0 ( ) a a ( ) a a a +2000 a ( ) a a ( ) a a a −2000 .

) $T = P \times M$ 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 (EMP) P IND54 N . EMP EMP AME E .

DATA AVAILABILITY

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