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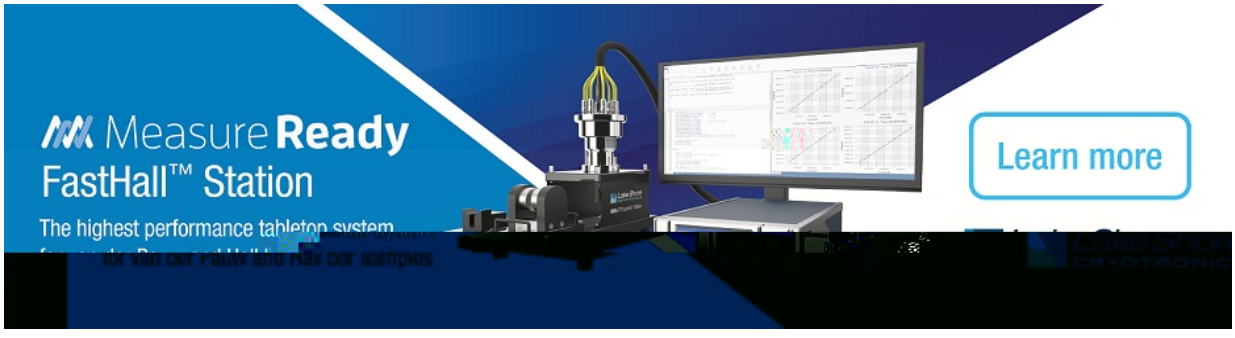

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ABSTRACT

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 O 3 +1)2− (A -, .[14,15] H , -, 12- - , B - , D -)[6] .[16] , - B- - A B F O3 - .[7 11] .

I , A $B_{5.25}L_{0.75}F$ C $_3O_{18}$ (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 - (P). , 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 (:// . .).

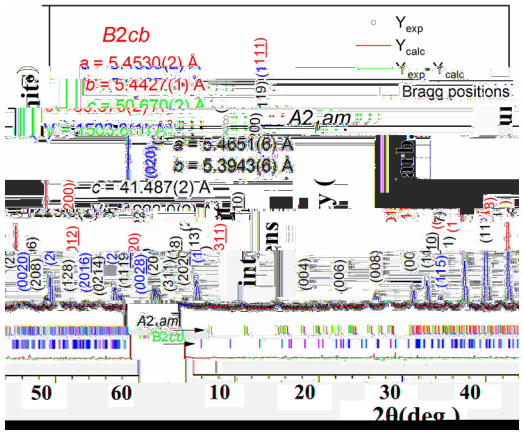

FIG. 1. - a a a B .

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 $_2F$ 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

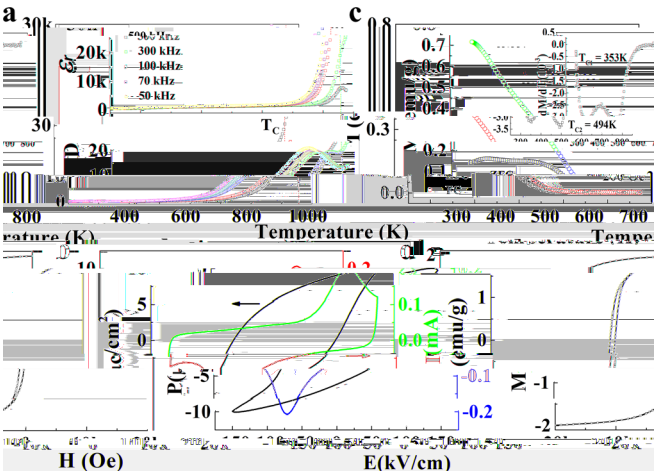

FIG. 2. (a) a a (a) a a ( ) B a a a ⊥ . ( ) a B a a a a . ( ) a a a B a ⊥ / a = 200 . a a - a / a a a . ( ) a a- a 300 B a .

$_1 \sim 494$ 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
- , - ,

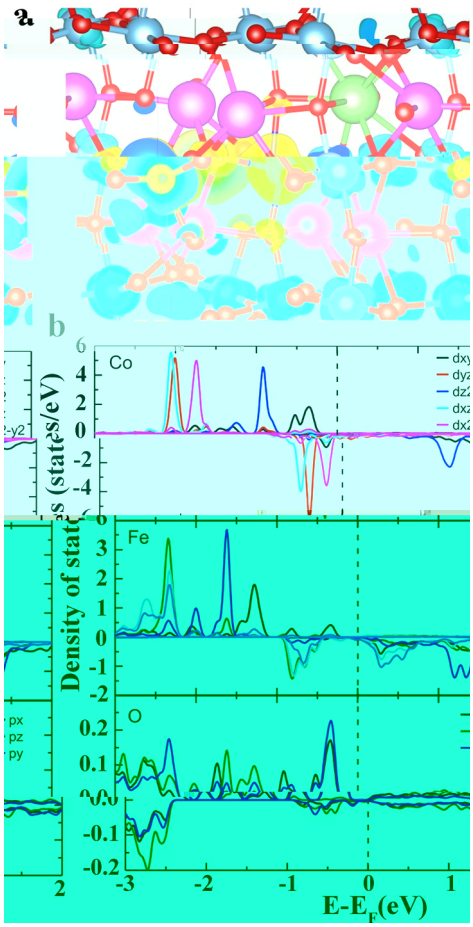

FIG. 3. (a) (a = 0.005) ( ), B ( ), a ( ), ( ), (a), a ( ) a . ( ) A a a $^{3+}$ $^{3+}$.

.
. 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 -

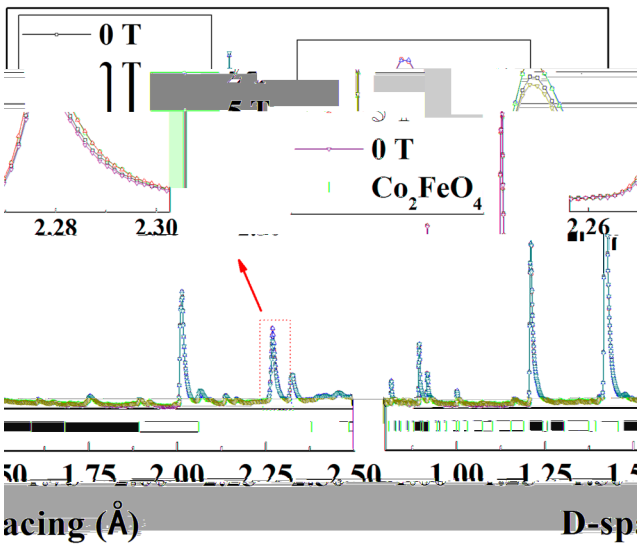

FIG. 4. - a a a a B a a a (0, 2, a 5 a a 0).

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

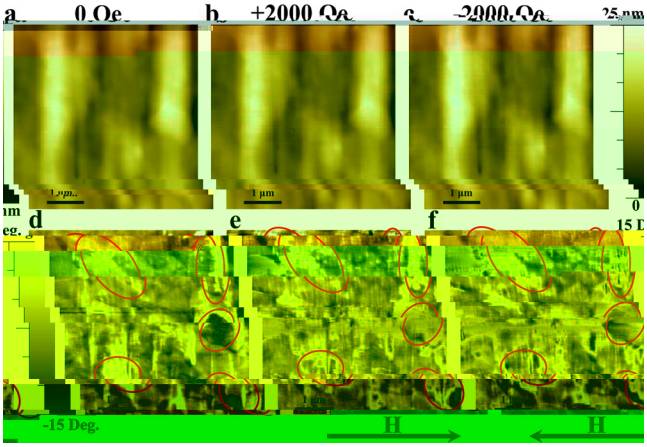

FIG. 5. a B a a (aa a a a). (a) a a ( ) a a a 0 ( ) a a ( ) a a a +2000 a ( ) a a ( ) a a a −2000 .

) $T = P \times M$ 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 E AME E .

DATA AVAILABILITY

.

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