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B-site ordering state in double-perovskite La_2CrFeO_6 films

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Introduction

Double-perovskite La_2CrFeO_6 has been intensively studied because there is a possibility to have a ferri-magnetic ground state with a net spin moment $2\mu_B$/f.u. through the $3d^3$(Cr)-$3d^5$(Fe) superexchange interaction [1]. In contrast, the (111)-oriented $LaCrO_3/LaFeO_3$ super-lattice shows ferromagnetism, though the measured saturation magnetic moment is much less than the expected value [2]. To clarify this inconsistency, we fabricated La_2CrFeO_6 films on (111)-oriented $SrTiO_3$ substrates using pulsed-laser deposition method under the various conditions and examined the degree of order of Cr and Fe by using synchrotron x-ray diffraction.

Experimental results and Discussions

Fig. 1(a) shows a schematic crystal-structure model of (111)-oriented La_2CrFeO_6 film. From the model with the antiside disorder (*AS*) fraction, which is defined as the percentage of misplaced Cr at Fe site and vice versa, and atomic displacement of La and O ions towards Fe-rich transition-metal-site plane (δ_{La} and δ_O), we calculated the structure factor at each reciprocal lattice point as follows:

$F_{(1/21/21/2)}=(1-2AS)(f_{Cr}-f_{Fe})+2f_{La}\sin(3\pi\delta_{La})+6f_O\sin(3\pi\delta_O)$
$F_{(111)}=f_{Cr}+f_{Fe}-2f_{La}\cos(6\pi\delta_{La})-6f_O\cos(6\pi\delta_O)$
$F_{(3/23/23/2)}=(1-2AS)(f_{Cr}-f_{Fe})-2f_{La}\sin(9\pi\delta_{La})-6f_O\sin(9\pi\delta_O)$
$F_{(222)}=f_{Cr}+f_{Fe}+2f_{La}\cos(12\pi\delta_{La})+6f_O\cos(12\pi\delta_O)$
$F_{(5/25/25/2)}=(1-2AS)(f_{Cr}-f_{Fe})+2f_{La}\sin(15\pi\delta_{La})+6f_O\sin(15\pi\delta_O)$
$F_{(333)}=f_{Cr}+f_{Fe}-f_{La}\cos(18\pi\delta_{La})+f_{La}\cos[9\delta(1+2\delta_{La})]$
$-3f_O\cos(18\pi\delta_O)+3f_O\cos[9\pi(1+2\delta_O)]$

Here, f_{Cr}, f_{Fe}, f_{La}, f_O, and $F_{(hhh)}$ represent atomic form factors of Cr, Fe, La, O, and structure factor of (*h h h*) reflection, respectively. The calculated intensity *I* was obtained from $I=FF^*\times L\times p\times N$. *L*, *p*, and *N* are Lorentz factor, polarization factor, and scale factor, respectively.

From the analyses of experimental data, the *AS* ratio of the condition A, B, D samples are estimated as 0.051, 0.145, 0.34, respectively (Fig. 1(b-d)). By using these samples, the magnetic field and temperature dependences of the magnetization are measured (Fig.1 (e, f)). The samples with the high degree of order (A and B) show ferromagnetic orders with $2\mu_B$/f.u. magnetic moment, which is consistent with previous theoretical prediction [1]. In contrast, the sample of the low degree of order (C) shows a ferromagnetism with a small magnetic moment. Detailed information are reported in ref. [3].

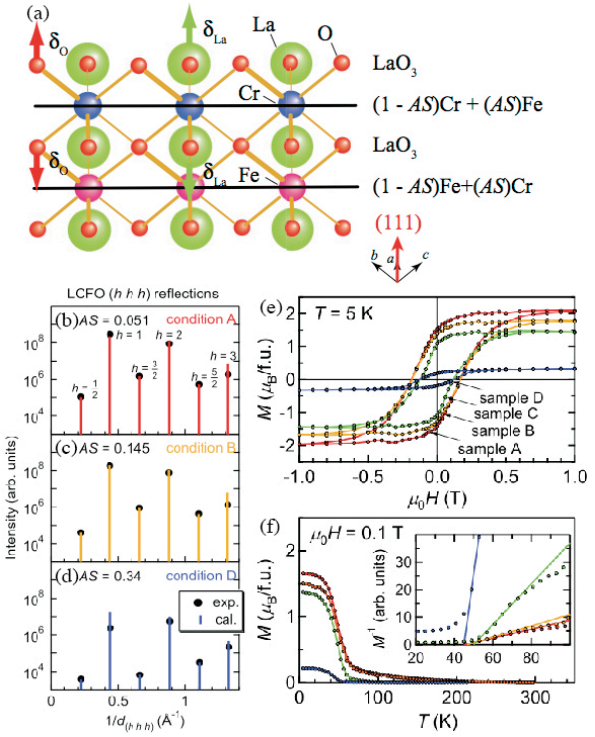

Fig. 1: (a) The schematic model of La_2CrFeO_6 thin film. (b-d) X-ray diffraction results of the samples grown under conditions A, B, and D. The observed intensity and calculated one are indicated by circles and bars, respectively. (e,f) Magnetic field and temeratpure dependences of the magnetization.

References

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