Structural insight using anomalous XRD into Mn_2CoAl inverse Heusler alloy films fabricated by magnetron sputtering, IBAS and MBE techniques

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Recently, spin gapless semiconductor (SGS) [1] attracts much attention due to its unique half-metallic and zero-gap semiconductor behaviors, which could be applicable to novel spintronics devices. In SGS, an almost zero band gap in the up-spin state and a usual band gap in the down-spin state are expected at the Fermi level [2]. Several recent papers on Heusler alloys reported the SGS properties that can be expected from such a band structure; however, their magnetic and transport properties such as positive linear MR ratio and semiconducting temperature dependence of resistivity are still in debate. It is known that atomic arrangements, i.e. *XA*-type and $L2_1$-type structures, and its disorder strongly influence their SGS properties. In this respect, laboratory XRD is not sufficient to distinguish structural differences in Heusler alloys due to the nearly identical atomic scattering factors of constituent elements, e.g. those of Co and Mn at Cu $K\alpha$. Therefore, careful structural evaluation of SGS materials are a key to solve the above discrepancies of magnetic behavior.

In this report, using synchrotron anomalous XRD, we evaluated atomic arrangements and their disorder in Mn_2CoAl (MCA) thin films fabricated by magnetron sputtering, ion-beam assisted sputtering (IBAS), and MBE [3]. Here, we briefly explain only on the results by MBE. The lab. XRD shown in Fig. 1(a) apparently indicates well-defined epitaxial MCA films. However, STEM-EDS (Fig1.(b)) shows there exist two phases of different elemental compositions (Mn-rich and Co-rich phases). Based on the above results, we constructed structural candidates for these two phases. AXRD results of 111, 002, and 004 reflections at Mn and Co *K* absorption edges are shown in Fig. 1(c) and (d), where calculations for the final structural models of the two phases, i.e. the $L2_1B$ and disordered $L2_1$ structures respectively shown in Fig. 1(e) and (f), well reproduced the experimental results. The synchrotron XRD were performed on BL13XU at SPring-8. This work is partly supported by JSPS KAKENHI (17H06152, 18KK0111).

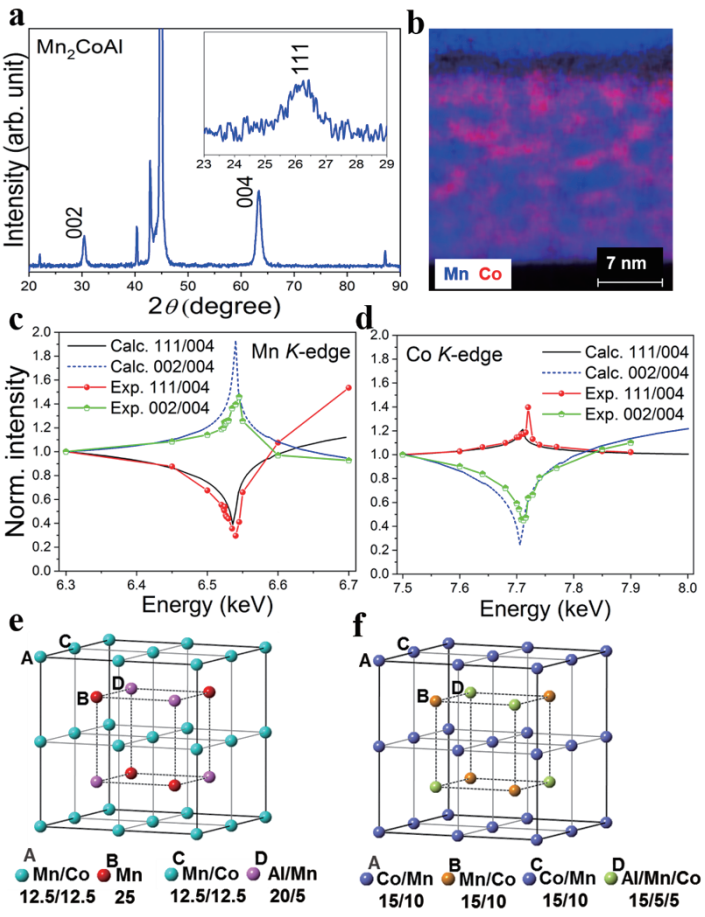

Fig.1 (a) Lab. XRD patterns of Mn_2CoAl films fabricated by MBE. Inset: 111 reflection profile. (b) STEM-EDS mapping of Mn and Co in Mn_2CoAl film. Calculated and experimental anomalous XRD I_{111}/I_{004} and I_{002}/I_{004} profiles at (c) Mn *K*-edge and (d) Co *K*-edge. Crystal structures of (e) Mn –rich phase ($L2_1B$ structure) and (f) Co-rich phase (disordered $L2_1$ structure).

Reference

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