Enhancement of $L2_1$ ordering and spin-polarization of Co$_2$FeSi thin film by substitution of Fe with Ti

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Introduction

According to theoretical calculation reported by Miura et al.$^1$, Co$_2$TiSi Heusler alloy has high spin polarizations in the ordered $L2_1$ structure and high tolerance for the Co-related atomic disorder. On the other hand, Co$_2$FeSi Heusler alloy is known to have $L2_1$-ordering even in as-deposited state and has large exchange stiffness.$^2$ By combining these two alloys, Co$_2$Fe$_{1-x}$Ti$_x$Si could be a promising Heusler alloy which has both high spin polarization and high $L2_1$-ordering properties.

Experiment

Samples with layer structure of MgO(001)-subs./Co$_2$Fe$_{1-x}$Ti$_x$Si(50nm), $x = 0, 0.1, 0.2, 0.3$ were fabricated using an ultrahigh vacuum magnetron co-sputtering machine. The films were annealed at temperatures ranging from 400 to 650 $^\circ$C after the deposition. The crystal structure of the films was examined by 4-axis X-ray diffraction (XRD) using Cu-Kα radiation. The AMR property was measured by Physical Property Measurement System (PPMS).

Result

Figure 1 shows the calculated density of states (DOS) for Co$_2$FeSi and Co$_2$Fe$_{0.75}$Ti$_{0.25}$Si Heusler alloy with different Ti composition $x$ by using Generalized Gradient Approximation (GGA) +U method. From the calculation results shown in Figure 1, we found that position of Fermi level shifted from the edge of conduction band in Co$_2$FeSi toward the inside of half-metallic gap in Co$_2$Fe$_{0.75}$Ti$_{0.25}$Si alloy. Therefore, it was suggested from calculation that half-metallic property at finite temperature can be improved by partly substitution of Fe with Ti due to the shift of $E_F$ toward the center of half-metallic gap.

The XRD patterns for 50 nm-thick CFTS epitaxial films on MgO (001) single crystal substrate annealed at 650$^\circ$C with different $x$ are shown in Figure 2. The strong (002) super-lattice peak, indicating a highly B2-orderd structure, was observed in all CFTS films. The position of (004) fundamental peak gradually shifted toward higher $2\theta$ angel with increasing $x$, suggesting a reduction of out-of-plane lattice constant with higher Ti content.

In order to check the degree of $L2_1$ ordering of CFTS thin films, the ratio of $L2_1$-superlattice (111) peak intensity to fundamental (004) peak intensity $I_{L2_1}^{obs}$ as a function of Ti composition is plotted in Figure 3. In the case of Co$_2$FeSi thin film, a high annealing temperature of 650$^\circ$C was needed to achieve the $L2_1$ ordering crystal structure. When substituting 10% of Fe with Ti, we found that the $L2_1$ ordering started to appear at 500$^\circ$C. The $L2_1$ ordering temperature was further reduced to 400$^\circ$C when the Ti composition rises up to 20%. These results clarify that the driving force for $L2_1$ ordering can be significantly improved by small amount of substitution (10-30%) of Fe in Co$_2$FeSi with Ti, which can be explained by higher tolerance for Co-related atomic disorder in Co$_2$Ti-based Heusler alloy compared with Co$_2$Fe-based Heusler alloy as suggested from the calculation of the formation energy.$^3$

Reference