Analysis of microstructure and transport properties in Mn_2CoAl Heusler alloy

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1. Introduction

A spin gapless semiconductor (SGS) is a new type of material in spintronics which is predicted to have a band gap in one of the spin channels and a zero band gap in the other, allowing novel spin transport functionalities such as carrier spin-polarization tunability by electric field [1]. Recently, various SGS materials have been reported in the group of Heusler compounds. Mn_2CoAl is most widely studied SGS material, which was reported to exhibit SGS-like behavior in a bulk sample [2]. However, such SGS-like properties have not been reproduced in thin films [3][4]. We have already noticed that the phase separation often happens in Mn_2CoAl thin films made by a sputtering method, therefore, we could not observe the transport properties arising from SGS such as low carrier density and positive MR ratio at low temperature. Since no one has ever investigated how the composition, atomic ordering and microstructure affect the transport properties in Mn_2CoAl, in this study we fabricated bulk Mn_2CoAl with different composition to carry out systematic investigation and find out what the critical factor to determine SGS properties is.

2. Experiment

Mn_2CoAl bulk alloy was prepared by arc melting Mn, Co, and Al high purity metals. The initial ratio of materials was Mn:Co:Al=50:25:25. The alloy buttens were annealed at 1100°C for 72h, then quenched in ice water. According to the result of ICP, the composition of the bulk was determined to be $Mn_{47.1}Co_{27}Al_{25.9}$ (at%), the Mn is less than stoichiometry. XRD is used to detect the structure. Conventional Van der Pauw method was used to measure temperature dependence of electric resistance, Hall effect and MR ratio in bulk MCA by PPMS. Microstructure of the samples was carefully investigated by SEM, TEM, 3D atom probe and EDS.

3. Results and Discussion

XRD result shows a diffraction pattern arising from single phase MCA and clear (111) super lattice peak, suggesting the presence of either $L2_1$, $D0_3$ or XA ordering. Curie temperature was 827K, which did not change by annealing. Temperature dependence of resistivity shows semiconducting behavior. The carrier density as $2.17 \times 10^{22} cm^{-3}$ at 10K, and $2.73 \times 10^{22} cm^{-3}$ at 300K, are much higher than reported for a bulk (10^{17}) and a thin film (10^{20}). The result of MR ratio has the similar trend as the reported for the bulk [4], positive at low temperature. However, the MR ratio was only 0.12% at 10K, which is much lower than the reported previously, 5% at 40K. According to the 3D atom probe map and TEM analysis, the annealed sample contained nanoscale Mn-rich second phase, while the matrix is Mn_2CoAl having inverse Heusler structure. Therefore, the observed transport property cannot be attributed to the single phase SGS.

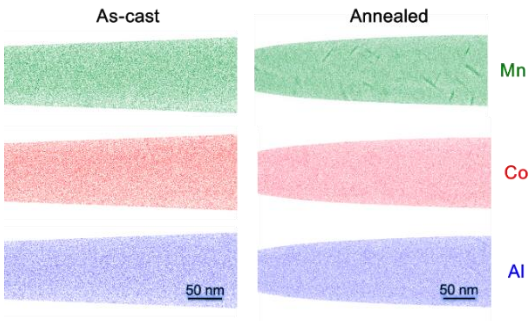

Fig.1 3D atom probe map of the samples before and after annealing.

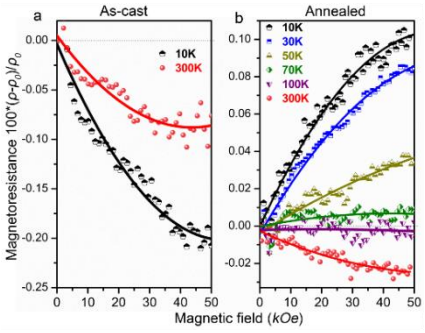

Fig.2 MR ratio measured at different temperature

Reference

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2) Michelle E. Jamer et al., Appl. Phys. Lett. 103, 142403 (2013).
3) G. Z. Xu et al., Appl. Phys. Lett. 104, 242408 (2014)
4) S. Ouardi et al., Phys. Rev. Lett. 110, 100401 (2013)