Crystal and magnetic structures of novel Heusler alloys inducing martensitic transformation

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First-principles band calculations of the ternary *X*-*Y*-*Z* Heusler alloy in this study predicted half-metallic behavior with a spontaneous magnetization $M_s = 3\ \mu_B$/f.u. at stoichiometric composition. However, the synthesized Heusler alloy exhibited composition-dependent ferromagnetism, with a measured M_s of approximately 1 μ_B /f.u. Powder X-ray diffraction measurements revealed that, for compositions exhibiting paramagnetism, the (220) reflection of the austenitic (A)-phase at 300 K splits into the (002), (400) and (221) reflections of the martensitic (M)-phase below 160 K. This experimental result provides clear evidence of the discovery of a novel Heusler alloy exhibiting a martensitic transformation. Furthermore, a sharp ferromagnetic-paramagnetic phase transition was observed in compositions with low *Z*-element content, suggesting the existence of a quantum critical point. These findings indicate that the ternary *X*-*Y*-*Z* Heusler alloy is a promising multifunctional material that combines a martensitic transformation with a quantum critical point. In this study, we performed powder neutron diffraction experiments to determine the crystal structure and chemical ordering of the M-phase in the paramagnetic state of the ternary *X*-*Y*-*Z* Heusler alloy.

Powder neutron diffraction experiments were performed using the HERMES powder diffractometer installed at the T1-3 beamline of the Japanese Research Reactor-3 (JRR-3) at JAEA. Approximately 7 g of powdered sample was loaded into a 6 mm diameter vanadium cell and mounted in a cryostat equipped with a 4 K Gifford-McMahon (GM) refrigerator. Diffraction patterns were collected over the temperature range from 3 K to 300 K.

Figure 1 presents the neutron diffraction pattern of the ternary *X*-*Y*-*Z* Heusler alloy with the specified composition in the paramagnetic A-phase at 300 K. As shown in Fig. 1, the ternary *X*-*Y*-*Z* Heusler alloy crystallizes in the ordered $L2_1$ structure with a minor impurity phase at 300 K. Temperature-dependent neutron diffraction measurements of the ternary *X*-*Y*-*Z* Heusler alloy reveal that the (220) reflection of the cubic $L2_1$ structure splits into the (002), (400) and (221) reflections of the martensitic structure below 160 K upon cooling. This splitting indicates that the M-phase adopts an orthorhombic $B19$ structure. The neutron diffraction results are in good agreement with the X-ray diffraction results. Systematic investigations of the prepared samples revealed that martensitic transformation occurs preferentially in *X*-rich and *Z*-poor compositions, where the ternary *X*-*Y*-*Z* Heusler alloys remain in the paramagnetic state. In addition, the martensitic transformation temperature increases as the composition shifts toward the *X*-rich and *Z*-poor regions.

We are continuing to perform Rietveld refinements to investigate the crystal structure associated with the martensitic transformation and chemical ordering of the ternary *X*-*Y*-*Z* Heusler alloys. Preliminary results suggest that the crystal distortion is very small.

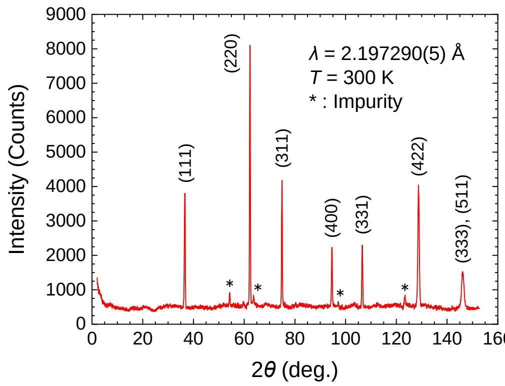

Fig. 1. Powder neutron diffraction pattern measured at 300 K.