Antiferromagnetic state of Heusler alloy Ru_2CrSi

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The first-principles band calculations predicted that $Ru_{2-x}Fe_xCrSi$ is a new half-metallic Heusler alloy insensitive to crystalline disorder [1]. This insensitivity is worth noting because the spin polarization of well-known half-metallic Heusler alloys, such as Co_2MnSi and NiMnSb, is sensitive to crystalline disorder. Our success in synthesizing polycrystalline $Ru_{2-x}Fe_xCrSi$ samples by arc-melting has led us to investigate their physical properties [2]. With regards to Ru_2CrSi, a clear peak was observed at ~14 K in the specific heat $C_p(T)$, indicating the antiferromagnetic (AFM) transition. Partial element substitution of Ru by Fe in Ru_2CrSi seems to suddenly eliminate the AFM order. For $Ru_{1.9}Fe_{0.1}CrSi$, for example, no anomaly in $C_p(T)$ was observed at any temperatures. As far as based on the specific heat measurement, we can conclude that an AFM transition occurs at T_N~14 K in Ru_2CrSi.

In this study, we performed powder neutron diffraction experiments to determine the AFM structure as well as the chemical ordering of the crystal structure at low temperatures in Ru_2CrSi. The experiments have been performed using a powder diffractometer, HERMES, installed in T1-3 at Japanese Research Reactor 3 (JRR-3) in JAEA. A powdered sample (about 7 grams) was loaded in the vanadium cell with a diameter of 6 mm, and then attached to a top-loading liquid helium cryostat. The powder diffraction patterns were recorded in the range from 1.5 K to 290 K.

Figure 1(a) shows the resulting powder diffraction patterns at low temperatures of 3.2 K (red line) and 50 K (blue line). No significant changes in the diffraction patterns were observed on cooling to 50 K, but new peaks appeared below T_N~14 K, as shown in Fig. 1(a). Figure 1(b) shows the difference between the diffraction patterns observed at 3.2 K and at 50 K, exhibiting that the AFM peaks appeared at low temperatures below T_N. Based on the results of Figs. 1(a) and 1(b), we expected that the structure had fcc type-2 AFM order; the magnetic moments were ferromagnetically aligned within 111 planes with adjacent planes coupled antiferromagnetically. However, we found the AFM peak splitting at (1/2 1/2 1/2) in Fig. 1(b), due to the reduction of symmetry of the magnetic or crystallographic structure. Magnetic and crystallographic structure analysis is now in progress using the Rietveld refinement technique.

[1] S. Mizutani *et al.*, Mater. Trans. **47** (2006) 25.

[2] K. Matsuda *et al.*, J. Phys. Condens. Matter **17** (2005) 588; 18 (2006) 1837(E).

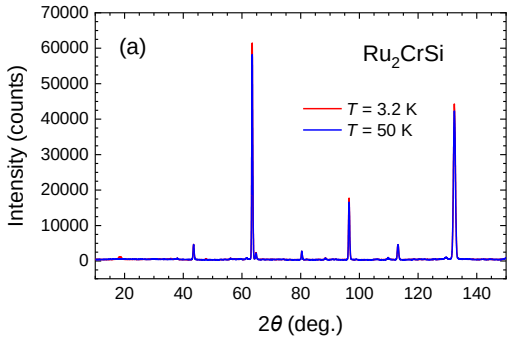
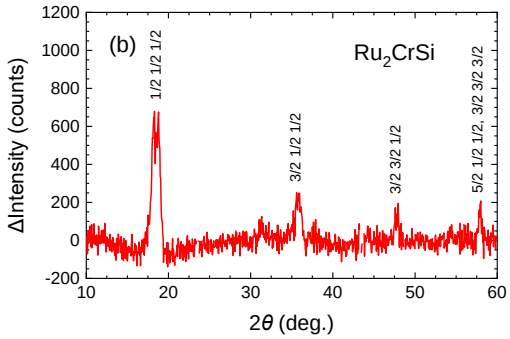


Fig. 1. (a) Neutron powder diffraction patterns at



3.2 K (red line) and at 50 K (blue line). (b) Difference between the diffraction patterns at 3.2 K and at 50 K showing the appearance of AFM peaks at low temperatures.