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 type of half-metallic Heusler alloy that is 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, is sensitive to crystalline disorder. Our success of synthesizing polycrystalline $Ru_{2-x}Fe_xCrSi$ samples by arc-melting has led us to investigation of their physical properties [2]. With regards to Ru_2CrSi, a clear peak was observed at $\sim$ 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 may conclude that an AFM transition occurs at $T_N \sim 14$ K in Ru_2CrSi.

In this study, we performed the 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, WAND, installed in HB-2C at the HFIR in the ORNL. A powdered sample (about 11 grams) was loaded in the vanadium cell with the diameter of 9 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 the low temperatures 1.5 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 $T_N \sim 14$ K, as shown in Fig. 1(a). Figure 1(b) shows the difference between the patterns observed at 1.5 K and at 50 K, exhibiting that the AFM peaks appeared at low temperature 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, if the fcc type-2 order was assumed in the AFM structure, we found that the positions of the AFM Bragg peaks in Fig. 1(b) were slightly shifted to low angle, as compare with the positions of the nuclear Bragg peaks in Fig. 1(a). Magnetic as well as crystallographic structure analysis is now in progress using the Rietveld analysis. At the same time, Ru_2CrSi sample quality is also improved by the post-annealing treatment to promote homogeneity and chemical ordering.

[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).

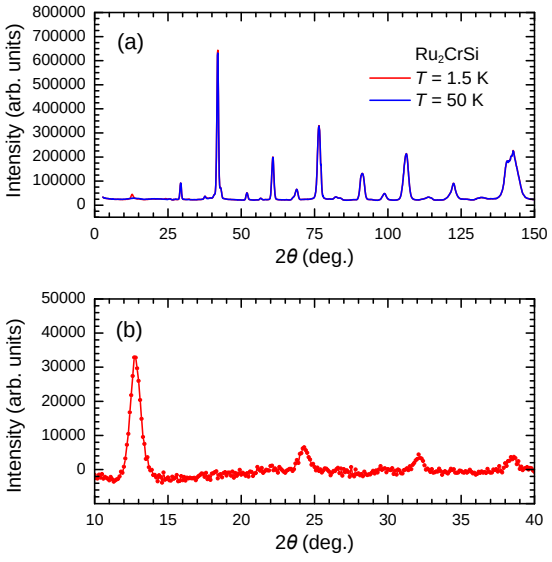

Fig. 1. (a) Neutron powder diffraction patterns at 1.5 K (red line) and at 50 K (blue line). (b) Difference between the patterns at 1.5 K and at 50 K showing appearance of AFM peaks at low temperature.