Antiferromagnetic state of Heusler alloy $Ru_{2-x}Fe_xCrSi$

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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 noteworthy because the spin polarization of well-known half-metallic Heusler alloys, such as Co_2MnSi and NiMnSb, is sensitive to crystal 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 regard to the end material Ru_2CrSi, a clear peak indicating an antiferromagnetic (AFM) transition was observed at a specific heat $C_p(T)$ of ~14 K. Partial element substitution of Ru by Fe in Ru_2CrSi seems to cause the sudden elimination of 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 the specific heat measurements are concerned, we can conclude that an AFM transition occurs at T_N~14 K only 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 and $Ru_{1.9}Fe_{0.1}CrSi$. 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 (approximately 7 grams) was loaded into a 6 mm diameter vanadium cell, and then mounted in a cryostat equipped with a GM refrigerator. Powder diffraction patterns were recorded in the range of 4 K to 300 K.

New peaks attributed to the AFM state were observed in diffraction patterns of Ru_2CrSi below T_N~14 K. Figure 1(a) shows the difference between the diffraction patterns observed at 4 K and 50 K for Ru_2CrSi, indicating that the AFM peak appeared at low temperatures below T_N~14 K. Figure 1(b) represents the difference between the diffraction patterns at 4 K and 50 K for $Ru_{1.9}Fe_{0.1}CrSi$. 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) only for Ru_2CrSi in Fig. 1(a), 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).

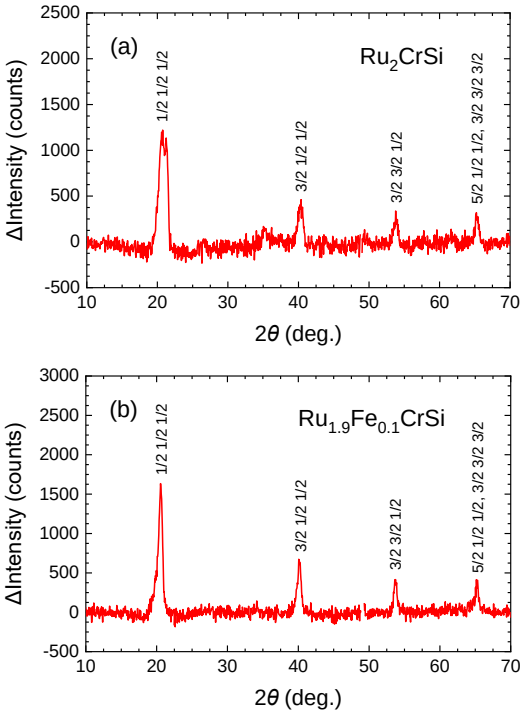

Fig. 1. Difference between the neutron powder diffraction patterns at 4 K and 50 K for (a) Ru_2CrSi and (b) $Ru_{1.9}Fe_{0.1}CrSi$, showing the appearance of AFM peaks at low temperatures.