Magnetic and crystal structures 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 crystalline disorder. The successful synthesis of polycrystalline $Ru_{2-x}Fe_xCrSi$ samples motivated us to investigate their physical properties [2]. With regard to Ru_2CrSi, a clear peak indicating an antiferromagnetic transition was observed at a specific heat $C_p(T)$ of ~14 K. Partial substitution of Ru with Fe in Ru_2CrSi appears to abruptly suppress the antiferromagnetic order. In the case of $Ru_{1.9}Fe_{0.1}CrSi$, no anomaly in $C_p(T)$ was detected at any temperature. Therefore, specific heat measurements indicate that an antiferromagnetic transition at T_N~14 K is present only in Ru_2CrSi

In this study, powder neutron diffraction measurements were carried out to determine both the ferromagnetic structure and the degree of chemical ordering in the crystal structures of $Ru_{0.5}Fe_{1.5}CrSi$ and $Ru_{0.2}Fe_{1.8}CrSi$ at low temperatures. The experiments were performed using the HERMES powder diffractometer installed at the T1-3 beam port of the Japanese Research Reactor-3 (JRR-3) at JAEA. A powdered sample weighing approximately 7 g was loaded into a 6 mm diameter vanadium cell and mounted in a high-temperature CTI cryostat. Powder diffraction patterns were measured between 50 and 650 K.

The Curie temperatures T_C are 500 K for $Ru_{0.5}Fe_{1.5}CrSi$ and 510 K for $Ru_{0.2}Fe_{1.8}CrSi$, respectively. As the temperature increased, the Bragg peaks systematically shifted toward lower 2θ values. However, no additional diffraction peaks beyond those expected for the Heusler crystal structure were observed in either $Ru_{0.5}Fe_{1.5}CrSi$ or $Ru_{0.2}Fe_{1.8}CrSi$ over the temperature range of 50-650 K, indicating the absence of antiferromagnetic or ferrimagnetic ordering. A comparison of the diffraction patterns at 50 and 650 K exhibits an increase in the intensities of the (111) and (200) reflections below T_C, indicating the presence of magnetic scattering. Therefore, Rietveld refinements of the neutron diffraction patterns were performed for the ferromagnetic Heusler alloys $Ru_{0.5}Fe_{1.5}CrSi$ and $Ru_{0.2}Fe_{1.8}CrSi$, which are promising half-metallic candidates. Figure 1 shows the Rietveld refinement result for $Ru_{0.5}Fe_{1.5}CrSi$, demonstrating good agreement between the experimental neutron diffraction pattern and the calculated profile based on the crystal and magnetic structures of $Ru_{0.5}Fe_{1.5}CrSi$. The refinement assumes that the Fe atoms carry magnetic moments that are ferromagnetically aligned along the (001) direction. Based on this model, the magnetic moment is determined to be 0.99 μ_B per Fe atom along the *c*-axis. The Rietveld refinements yielded similar structural results for both $Ru_{0.5}Fe_{1.5}CrSi$ and $Ru_{0.2}Fe_{1.8}CrSi$. However, they revealed that the degree of chemical disorder in $Ru_{2-x}Fe_xCrSi$ increases with increasing Fe content.

[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).

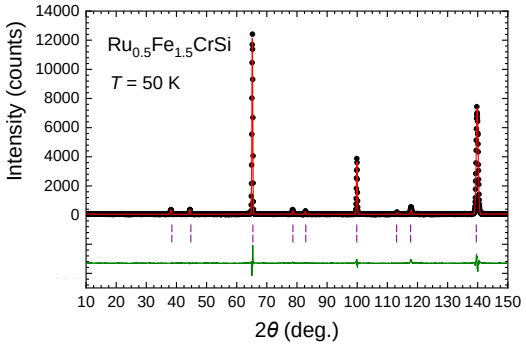

Fig. 1. Rietveld refinement of ferromagnetic Heusler alloy $Ru_{0.5}Fe_{1.5}CrSi$ at 50 K.