Magnetic structure determination in R5Ru3Al2 (R = Ce and Pr)

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Crystalline materials without inversion symmetry are of growing interest recently, because of the possibility for non-trivial spiral or helical spin structures. R5Ru3Al2 (R = Ce and Pr) is one of such new materials without inversion symmetry[1]. We found a second-order-like anomaly at T = 0.8 K in the specific heat measurement for Ce5Ru3Al2, whereas an antiferromagnetic ordering was observed at T = 3.8 K in the magnetic susceptibility for Pr5Ru3Al2. Details of the microscopic magnetic structures of the ordered phases in R5Ru3Al2 cannot be known from the macroscopic measurements, but such information is definitely necessary to understand the effect of the loss of inversion symmetry on their magnetic behavior.

To study the microscopic magnetic structure in R5Ru3Al2 at the low temperatures, we performed neutron powder diffraction measurements using the high-resolution powder diffractometer ECHIDNA of ANSTO. In this report, we describe the neutron powder diffraction result of Pr5Ru3Al2.

The resulting diffraction patterns are shown in Fig. 1(a). For the patterns observed at the paramagnetic temperatures 300 K and 10 K, we performed the Rietveld refinements using the existing structural model with the space group I213[1]. The result is also shown in Fig. 1(a). Reasonable agreements were seen between the observed and calculated patterns, as evidenced by the difference shown in the panels, indicating the correctness of the existing structure model.

At further lower temperatures, magnetic reflections start to develop, and become clearly visible at 1.5 K. Fig. 1(b) shows the magnified view of the diffraction patterns in the lower two-theta range measured at 10 K and 1.5 K. Clearly, the 1.5 K data show extra reflections which were not observed at 10 K. Magnetic satellite reflections were observed in the vicinity of nuclear reflections. This clearly indicates that magnetic ordering is neither simple ferromagnetic nor antiferromagnetic, but incommensurately modulated with a long modulation period. Under the cubic symmetry, the eight satellite reflections along the (1, 1, 1) direction around the 110 nuclear peak appear as three reflections at in the powder diffraction pattern. Indeed, this is the case for the magnetic satellite reflections visible in the present powder pattern. Thus, the magnetic propagation vector q is most likely along the (1, 1, 1) direction, i. e., q = (delta, delta, delta). From the peak position, we estimate delta = 0.066 (r.l.u.).

To find a possible microscopic model for the magnetic structure, the magnetic representation analysis was performed using the paramagnetic space group I213 and determined magnetic wave vector. As a result, we proposed a ”block-helical” structure, where the sum of the magnetic moments on each orbit rotates helically[2]. This is a rare example of long period modulated structures in the cubic rare-earth compounds.

[1] E. V. Murashova et al., Mater. Res. Bull. 45 993-999 (2010).

[2] K. Makino et al., J. Phy. Soc. Jpn (accepted to publication)

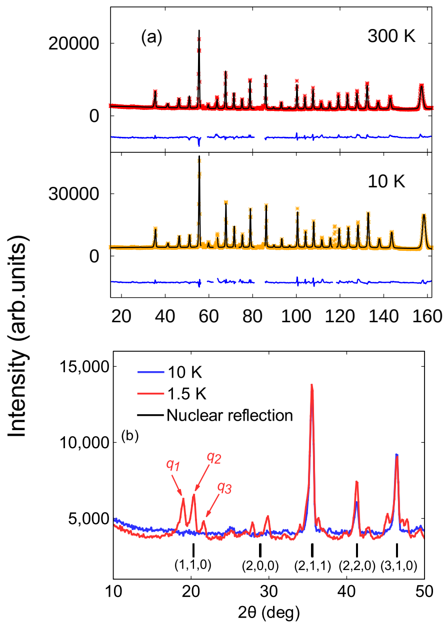

Fig. 1. (a) Powder neutron diffraction patterns of Pr5Ru3Al2 together with Rietveld analysis results at 300 K and 10 K. (b) Powder neutron diffraction patterns of Pr5Ru3Al2 at 10 K and 1.5 K together with the positions of nuclear reflections.