Magnetic structure of rare-earth palladium bronze NdPd3S4

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The rare-earth (R) palladium bronzes RPd3S4 crystallizes into a cubic NaPt3O4-type crystal structure. The R atoms form a body-centered cube and are subjected to a cubic crystalline electric field (CEF) represented by the cubic point group Th [1]. Systematic studies along the R series have revealed that the CEF ground states of 4f electrons in RPd3S4 have orbital degeneracy [1].

NdPd3S4 shows an antiferromagnetic (AFM) transition at TN = 2 K [1]. TN shows an anomalous magnetic-field dependence. By applying a magnetic field below 1 T, TN decreases with increasing magnetic field, while it increases with increasing magnetic field above 1 T. The increase in TN above 1 T implies that the field-induced antiferroquadrupolar (AFQ) ordering occurs above 1 T. To examine the magnetic structure of AFM phase and the possibility of the existence of field-induced AFQ phase, we have planned to perform a neutron powder diffraction experiment of NdPd3S4 in magnetic fields. However, we could not perform a diffraction experiment in magnetic fields because of a technical trouble of dilution refrigerator. The experiment without applying magnetic field has been performed using HERMES installed at the JRR-3M reactor in JAEA. Neutrons with a wavelength of 1.84772(9) A were obtained by the 3 3 1 reflection of the Ge monochromator.

Fig. 1(a) and (b) show the diffraction patterns of NdPd3S4 measured at 3 K (> TN) and 1.57 K (< TN), respectively. At 3 K, all of the Bragg peaks can be indexed as a NaPt3O4-type structure. The diffraction pattern at 1.57 K shows some additional Bragg peaks and the increase in intensity of some nuclear Bragg peaks as shown in Fig. 1(b). For example, the new peak which can be indexed as 1 0 0 appears at 15.69 as well as the increase in the intensity of nuclear 2 1 0 peak at 35.95 . Fig. 1(c) shows the temperature dependence of the integrated intensity of the 1 0 0 peak. The integrated intensity increases steeply below TN = 2.0 K, implying that the appearance of additional Bragg peaks is due to AFM ordering. The gradual increase in the integrated intensity below 3 K can be ascribable to the development of a short-range ordering. The diffraction pattern at 1.57 K is qualitatively the same to that at 1.3 K for TbPd3S4, which shows an AFM order at 2.9 K with the wave vector of k = [100] [2]. We therefore conclude that the magnetic structure of the AFM phase in NdPd3S4 is a type-I AFM structure, i.e., the direction of magnetic moments of Nd ions on the corner sites in the unit cell is opposite to those on the body-centered sites.

[1] K. Abe et al., Phys. Rev. Lett. 83 (1999) 5366.
[2] E. Matsuoka et al., J. Magn. Magn. Mater. 231 (2001) L23.

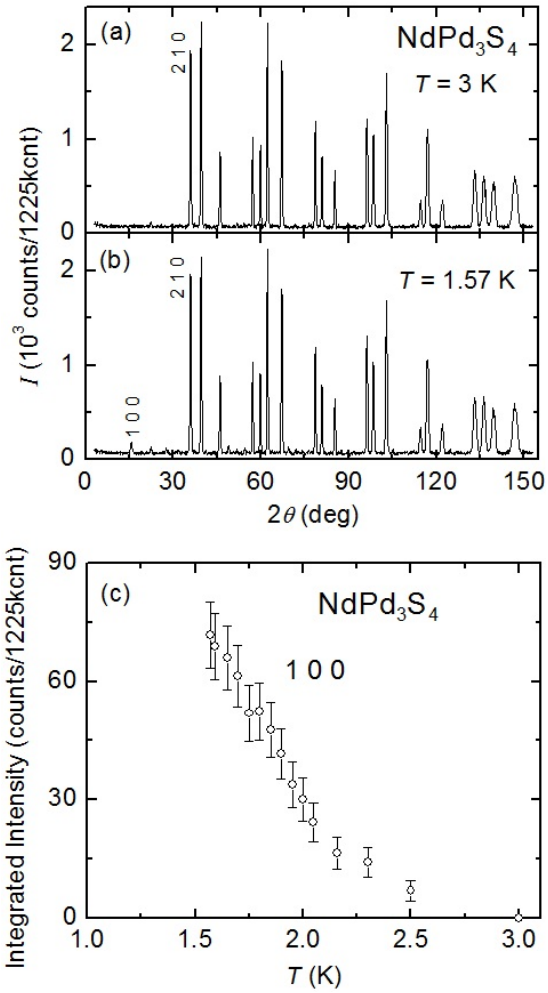

Fig. 1. Neutron powder diffraction patterns of NdPd3S4 measured at (a) 3.0 and (b)1.57 K. Temperature dependence of the integrated intensity of magnetic 1 0 0 peak is shown in (c).