Magnetic structure at lowest temperatures of exotic valence-ordered YbPd

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YbPd, which crystallizes in the cubic CsCl-type structure at room temperature, exhibits commensurate valence order with a tetragonal symmetry below T_2=105K though it has metallic electrical resistivity at all temperatures. The valence order is intriguing since most of valence order occurs in semi-metallic or semi-conducting materials. The valence order structure is characterized by alternate stacking of Yb^{3+} and $Yb^{2.6+}$ layers (*c*-planes) along the *c*-axis. The coexistence of the integral and fractional valences is also curious. The only Yb^{3+} layers have localized magnetic moments and exhibit magnetic order below T_3=1.9K. Recently, we have clarified that the magnetic structure at T=0.59K is sinusoidal with the Yb^{3+} magnetic moments parallel to the *a*-axis, with their amplitude of 0.3μ_B, and $\boldsymbol{k}$=(0.080 0 0.32)[1]. The amplitude is smaller than that expected for the basis of the crystalline-electric-field ground state, which is suggestive of the Kondo effect of the magnetic Yb^{3+} due to sufficient conduction electrons. In addition, the incommensurate magnetic structure implies a magnetic phase transition to a commensurate one at lower temperatures. A first-order phase transition, whose mechanism remains unknown, has been reported at T_4=0.5K. Thus, the YbPd system has attracted much attention due to its complex and exotic valence and magnetic properties despite a simple cubic structure. We focus on the incommensurate-commensurate magnetic phase transition at 0.5 K since the lowest-temperature magnetic structure is certainly simple and reflected by the valence and magnetic properties. In the present study, we carried out neutron diffraction (ND) of a single crystal of YbPd using T1-1 spectrometer and a ^{3}He refrigerator. The wavelength of neutrons of 2.459Å was selected. To observe difference in propagation vector $\boldsymbol{k}$ of the magnetic structure between $T>T_4$ and $T<T_4$, we performed ω scanning (rocking curve) and ω-2θ scanning.

Figure 1 shows rocking curves of the YbPd single crystal at around (0.080 0 0.32) taken at T=0.3K, 0.7K, and 3.0K. Since there exists no peaks at T=3.0K, the peaks at T=0.3K and 0.7K are ascribed to the magnetic order. In addition, the peak position is shifted through the phase transition at T_4=0.5K, which implies change of propagation vector $\boldsymbol{k}$ of the magnetic structure. The inset of Fig. 1 depicts the peak positions in the reciprocal-lattice space with axes of a^*-c^*. Such behaviors are also found in the other satellite peaks. However, intensities of these satellite peaks are too weak to conduct magnetic structure refinements. Besides, the estimated $\boldsymbol{k}$-vector at T=0.3K is inconsistent with a commensurate magnetic structure.

[1] K. Oyama *et al.*, J. Phys. Soc. Jpn. **87**, 114705 (2018).

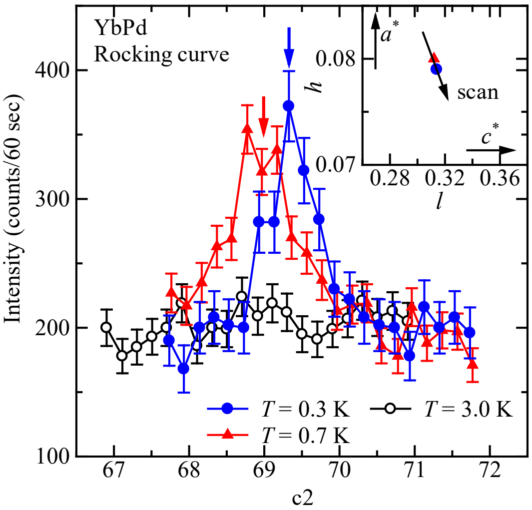

Fig. 1. Rocking curves of magnetic reflection of YbPd at T=0.3K, 0.7K, and 3.0K. There exists substantial difference in $\boldsymbol{k}$-vector between T=0.3K and 0.7 K. The inset depicts the peak positions at T=0.3K and 0.7K in the reciprocal-lattice space with axes of a^*-c^*.