Study of the magnetic structure for a novel Ce-based layered material

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Ce-based intermetallic compounds have been actively studied as a fertile ground for the strongly correlated phenomena, such as complex magnetism, Kondo effect and unconventional superconductivity. One of the most typical crystal structures is the $ThCr_2Si_2$-type tetragonal layered structure (so-called '122' phase). A similar layered structure called the $ZrCuSi_2$-type structure ('112' phase) also forms an important group of materials, as exemplified by the layered material CeTX_2 (T: transition metal, X: group 14-16 element). The structure of the 112 phase consists of an alternative stacking of the X square net and the Ce-T-X layer. The latter forms a part of the $ThCr_2Si_2$-type structure, whose magnetic order can be coupled to the high-mobility Dirac fermions on the X square net. Therefore, this class of materials is a candidate for topological magnets[1].

We have been exploring Ce-based compounds with various layered structures and have recently succeeded in synthesizing a new material with different numbers of Ce-T-X layer sandwiched by the X square nets. The conventional 112 material $CeAuBi_2$ has two Ce layers sandwiched by Bi square nets [2], while the new material $Ce_3Au_4Ge_2Bi_4$ has three Ce layers. Interestingly, the magnetic order varies significantly depending on the number of Ce layers. $CeAuBi_2$ shows an antiferromagnetic transition at T_N = 18 K, whereas $Ce_3Au_4Ge_2Bi_4$ shows a ferromagnetic-like transition at T_C = 6 K. Below T_C, the magnetization steeply increases with decreasing temperature, followed by another magnetic transition at T^*=3.5 K. This temperature dependence of the magnetization suggests that the zero-field ground state for the new material is not a simple ferromagnetic order but a ferrimagnetic or canted-antiferromagnetic order.

To elucidate the magnetic structure, we conducted neutron diffraction experiments using the 5G PONTA triple-axis spectrometer at JRR-3. Figure 1 shows the temperature dependence of (2 0 l) line scans. Clear magnetic contribution is superimposed on nuclear Bragg peaks, which evolves with decreasing temperature. This result reveals magnetic reflections with a Q-vector of (0 0 0) below T_C.

To determine the ordering pattern of the Ce moments, we performed magnetic structure analysis based on diffraction data collected at 3.8 K. The best fit between the observed and calculated intensities was obtained by assuming ferromagnetic alignment within the *ab*-plane and ferrimagnetic stacking along the *c*-axis. Specifically, an up–down–up moment ordering is stabilized within the Ce trilayer.

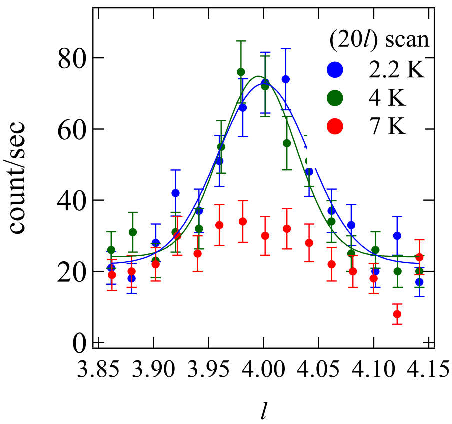

Fig. 1. Neutron diffraction intensity versus l in (2 0 l) at selected temperatures. 2.2 K < T^* < 4 K < T_C <7 K.

[1] S. I. Hyun *et al*, Phys. Rev. B **98** 165108 (2018).
[2] M. M. Piva *et al*, Phys. Rev. B **101** 214431 (2020).