

Magnetic structure determination of Ce₅Si₃

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The study of heavy fermion compounds with geometrically frustrated crystal structures has garnered significant interest from researchers in both the spin liquid and Fermi liquid fields. Recently, our group synthesized high-quality single crystals of two new rare-earth intermetallic compounds, Ce₅Si₃ and Ce₅Ga₂Ge, both exhibiting geometrical frustration. In these materials, one of the Ce sites features a unique structure called the Shastry-Sutherland Tetrahedron lattice, which combines aspects of both the Shastry-Sutherland and tetrahedral lattices. This unique configuration is expected to lead to the emergence of strong magnetic frustration. In Ce₅Si₃, bulk measurements have shown that while the Ce1 site exhibits antiferromagnetic ordering below 12 K, the Ce2 site lacks magnetic ordering down to 0.5 K [1]. It is currently believed that the Ce2 site in Ce₅Si₃ adopts a non-magnetic singlet ground state due to dimer formation around 4 K. Our group conducted neutron inelastic scattering experiments on Ce₅Si₃ at J-PARC/MLF using the high-resolution chopper spectrometer HRC to investigate the ground state of the Ce2 site. The results revealed a spin gap dispersion and a splitting of the triplet excitation state that cannot be explained by the conventional isolated spin dimer model [2]. To elucidate the origin of these distinctive behaviors, it is necessary to clarify not only the magnetic structure of the Ce2 site but also that of the Ce1 site. In a previous study involving neutron powder diffraction experiments on Ce₅Si₃, it was determined that the propagation vector of the antiferromagnetic order at the Ce1 site is $\mathbf{k} = (0, 0, 1)$. However, due to the weakness of the observed magnetic peaks, the magnetic structure could not be determined. In this study, we conducted single-crystal neutron diffraction experiments using the TOPAN (6G) instrument at JRR-3 to determine the magnetic structure of the Ce1 site in Ce₅Si₃.

The experiment was conducted using a ³He refrigerator, and measurements were performed at three temperature points: 0.6 K, 4.0 K, and 15 K. The temperature dependence of the 111 magnetic peak intensity was measured in the range from 0.6 K to 15 K to determine the order parameter. As a result of the experiment, it was determined that the Ce1 site in Ce₅Si₃ adopts a collinear magnetic structure with magnetic moments aligned along the *c*-axis, forming below 12 K. Furthermore, as shown in Figure 1, the critical exponent β was determined from the change in the order parameter, yielding a value of 0.56, which is close to that expected from the mean-field approximation. Currently, we are analyzing the magnitude of the ordered moment at the Ce1 site, as well as the internal magnetic field generated by this magnetic structure at the position of the Ce2 site.

- [1] T. Nishioka *et al.*, J. Phys. Soc. Jpn. **76**, pp. 45-46 (2007).
- [2] D. Ueta *et al.*, Phys. Rev. B **109**, 205127 (2024).

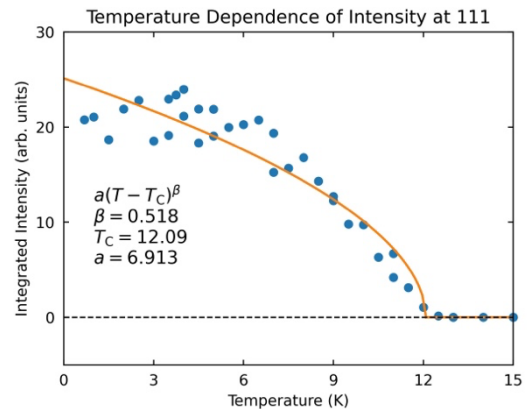


Fig. 1. The temperature dependence of the integrated intensity of the 111 magnetic peak.