Study of the magnetic order for a new square-net magnet

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Square-net compounds with the $HfCuSi_2$-type framework have been a promising platform for realizing topological electronic states and their interplay with quantum many-body phenomena. In these materials, the transition-metal tetrahedral layer sandwiched between square-net layers plays a crucial role in determining the correlated physical properties, yet their structural variety has been limited to the single-layer type. Recently, we have discovered $Ce_3Au_4Ge_2Bi_4$, a new square-net compound that is the bilayer member of a homologous series bridging the $HfCuSi_2$-type $CeAuBi_2$ (112 phase) and $ThCr_2Si_2$-type $CeAu_2Ge_2$ (122 phase). The bilayer structure of $Ce_3Au_4Ge_2Bi_4$ is formed by combining two tetrahedral layers of the 112 phase through the insertion of a 122-like block, resulting in two mixed-anion antifluorite-type layers. [1]

To elucidate the magnetic structure for this new square-net magnet, we conducted neutron diffraction experiments using the polarized neutron triple-axis spectrometer (PONTA) at 5G beamline of Japan Research Reactor 3 (JRR-3) in Japan. The spectrometer was operated in the unpolarized two-axis mode with the horizontal beam collimation of open-80'-80'. An unpolarized monochromatic neutron beam with the energy of 34.05 meV was obtained using a pyrolytic graphite (PG) monochromator. The single crystal sample (with a dimension of ~ 3 × 3 × 0.2 mm^3) was loaded into a ^{4}He cryostat with the (h 0 l) scattering plane.

For the magnetic structure analysis, we measured integrated intensities of Bragg reflections (h 0 l), where h and l were integers. The magnetic intensities were extracted by subtracting the nuclear contribution measured at 10 K (> T_C). Assuming the ferrimagnetic order shown in Fig. 1a, we obtained good agreement between the observed and calculated magnetic structure factors with a reliability factor of R = 10.0% and ordered moment m_{Ce} = 1.01μ_B at 3.8 K (Fig. 1b). [1] We have also determined the direction of the ordered Ce moments using polarized neutron diffraction.

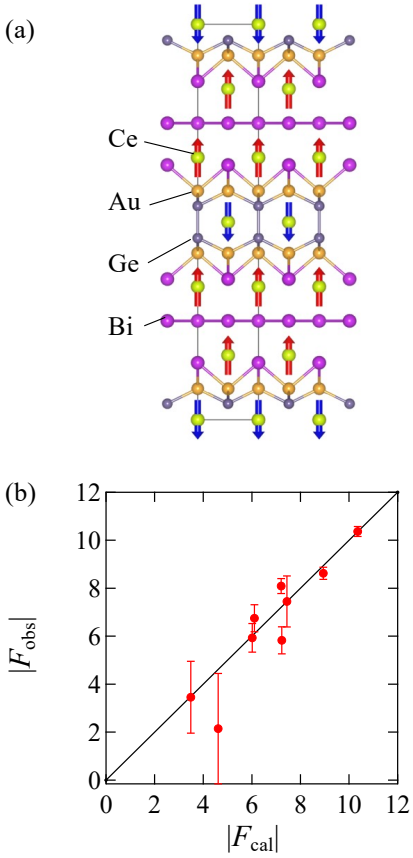

Fig. 1. (a) Crystal and magnetic structure for $Ce_3Au_4Ge_2Bi_4$. (b) Comparison of the calculated (F_{cal}) and observed (F_{obs}) magnetic structure factors at 3.8 K, assuming the ferrimagnetic order shown in (a).

[1] A. Yamashita, H. Sakai *et al.*, J. Am. Chem. Soc. 148, 28302–28309 (2026).