Magnetic Structure of the $Au_{65}Ga_{21}Dy_{14}$ 1/1 Approximant Crystal

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Magnetic properties of quasicrystals (iQCs) and their periodic approximant crystals (ACs) have been the subject of increasing interest due to the discovery of exotic magnetic phases such as whirling ferromagnetic (FM) and antiferromagnetic (AFM) [1]. While Tb-contained Tsai-type 1/1 ACs have been well-studied, the magnetic structures of Dy-contained QCs and ACs remain largely unexplored. The slight difference in electron configurations between Tb^{3+} ($4f^8$) and Dy^{3+} ($4f^9$) could significantly affect the crystalline electric field (CEF), potentially leading to novel magnetic phases in Dy-contained ACs. In fact, recent theoretical studies have predicted a wide range of potential nontrivial magnetic textures, including hedgehog, whirling, and anti-whirling structures in these compounds [2].

In this study, we focused on the $Au_{65}Ga_{21}Dy_{14}$ 1/1 AC to investigate its magnetic structure through neutron diffraction. This compound is an intriguing candidate as it exhibits FM order, making it a prime candidate for examining the appearance of novel magnetic structure anticipated in theoretical works. Moreover, comparing the magnetic structure of the present Dy-contained FM phase with the well-known noncoplanar whirling FM structures found in Tb-contained samples [1,3] is of great interest. For that purpose, we performed neutron powder diffraction (PND) measurements on the $Au_{68}Ga_{18}Dy_{14}$ 1/1 AC using the HERMES diffractometer.

At $T = 2$ K, as shown in Fig. 1, the PND data revealed the presence of magnetic Bragg reflections at hkl with $h + k + l = 2n$ (n being an integer), which is consistent with the symmetry of underlying crystal structure. The strongest reflection was observed at $2\theta = 16.2^\circ$, corresponding to the 031 peak. Through Rietveld refinement, a whirling FM structure is identified. The canting angle of the spin from the mirror plane equals 42.03˚, which is much larger than nearly 7˚ observed in $Au_{70}Si_{17}Tb_{13}$ 1/1 AC [3] but comparable to the 50(5)˚ observed in the $Au_{60}Ga_{26}Tb_{14}$ 1/1 AC [1]. Additionally, the magnetic moments are oriented approximately 70(1) degrees away from the pseudo 5f-axis.

Our results demonstrate that Dy^{3+} ions in Tsai-type 1/1 ACs behave as Ising spins, driven by strong local anisotropy from the CEF effect. These findings are currently under submission to one of the prestigious international journals and will be published soon.

[1] F. Labib *et al.*, Mater. Today Phys. 40 (2024) 101321. [2] S. Watanabe*et al.*, Phys. Rev. B. 108 (2023) 045110. [3] T. Hiroto, *et al.*, J. Phys. Condens. Matter. 32 (2020) 415802.

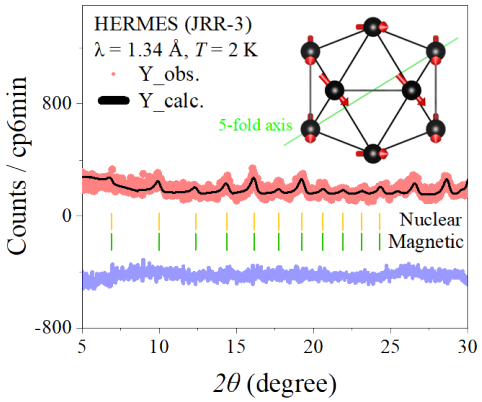

FIG. 1. Rietveld refinement of $Au_{65}Ga_{21}Dy_{14}$ 1/1 AC at $T = 2$ K. The inset shows the refined magnetic structure on a single icosahedron with the magnetic moments being canted away from the pseudo 5f-axis by approximately 70˚.