

Magnetic Structure of the Antiferromagnetic $\text{Au}_{68}\text{Ga}_{18}\text{Dy}_{14}$ 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 variety of exotic magnetic phases, including *whirling* ferromagnetic (FM) and antiferromagnetic (AFM) states, that have been discovered in Tb-contained 1/1 ACs. However, thus far, there has been no report on magnetic structures of Dy-contained FM or AFM Tsai-type compound. Slight difference in electron configurations between Tb^{3+} ($4f^8$) and Dy^{3+} ($4f^9$) could affect the crystalline electric field (CEF) potential and might lead to novel magnetic phases in Dy-contained systems. In fact, recent theoretical studies have predicted a wide spectrum of nontrivial magnetic textures in these compounds, including hedgehog, whirling, and anti-whirling structures. Given these facts, in this present proposal, we focused on the $\text{Au}_{68}\text{Ga}_{18}\text{Dy}_{14}$ 1/1 AC to investigate its magnetic structure through neutron diffraction. This compound stands out among Dy-contained compounds because it exhibits AFM order, making it critical to test whether any of the theoretically predicted magnetic phases appear in practice. Also, it is interesting to check similarity/dissimilarity of the magnetic structure of the present Dy-contained AFM phase and formerly observed non-coplanar whirling structures in Tb-contained AFM phases. To explore this, we performed neutron powder diffraction (PND) measurements on the $\text{Au}_{68}\text{Ga}_{18}\text{Dy}_{14}$ 1/1 AC using the HERMES diffractometer, which is optimal for such magnetic structure analysis.

At $T = 2$ K, as shown in Fig. 1, the PND data revealed the presence of magnetic Bragg reflections at hkl : $h + k + l = 2n + 1$, as a hallmark

of AFM order. The strongest reflection was observed at $2\theta = 11^\circ$, corresponding to the 021 peak. Through Rietveld refinement, an AFM structure with spins whirling around the $[111]$ axis, aligning nearly perpendicular to the pseudo-fivefold axis, with a canting angle of 77 degrees was identified. The refinement was based on a combination of two basis vectors, yielding coefficients of $C_1^2 = 6.160$ and $C_2^2 = -1.816$. This is slightly lower than the 86-degree canting seen in the whirling AFM structures of Tb-contained ACs, such as $\text{Au}_{65}\text{Ga}_{21}\text{Tb}_{14}$ and $\text{Au}_{73}\text{Al}_{13}\text{Tb}_{14}$.

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.

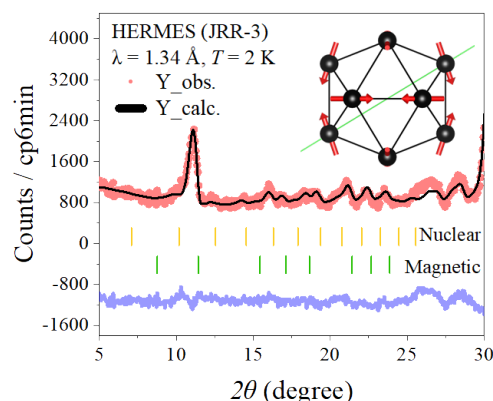


FIG. 1. Rietveld refinement of $\text{Au}_{68}\text{Ga}_{18}\text{Dy}_{14}$ 1/1 AC at $T = 2$ K. The inset shows the refined magnetic structure on a single icosahedron with the magnetic moments being canted away from the pseudo 5f-axis by approximately 77 degrees.