NEUTRON DIFFRACTION STUDIES OF AL-SUBSTITUTED HEXAFERRITES WITH GIANT COERCIVITY

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High-coercivity magnetic materials are indispensable for applications spanning permanent magnets to high-frequency electromagnetic filters; however, the scarcity and high cost of rare-earth and noble-metal-based benchmarks necessitate the development of cost-effective alternatives. While M-type hexaferrites (MFe12O19) offer a sustainable platform, their coercivity (Hc) is typically constrained by high saturation magnetization (Ms) compared to the traditional hard magnetic materials. Recent studies have demonstrated that Fe^{3+} substitution, in particular Al^{3+}, Cr^{3+}, Mn^{3+}, will significantly enhance magnetic property of strontium hexaferrite. Recently we report a systematic study on SrFe*12-xAlxO*19 (x = 0∽8) synthesized via a modified citrate-nitrate auto-combustion method, which produces highly porous precursors that effectively suppress grain growth below the single-domain limit (≈100 nm). In this work, the coercivity (Hc) and natural ferromagnetic resonance (NFMR) frequencies of strontium hexaferrite ($SrFe_{12}O_{19}$) have been significantly enhanced after Al-substitution in Fe^{3+} sites, a fundamental understanding of the site-specific substitution mechanism is critical for property optimization.

In this study, neutron powder diffraction (NPD) was employed to resolve the cation distribution across the five distinct crystallographic sublattices (2a, 2b, $4f_1$, $4f_2$, 12k). In contrast to transition metal dopants (Mn, Cr), NPD reveals that Al^{3+} ions exclusively occupy the octahedral 2a and 12k sites, while rigorously avoiding the trigonal bipyramidal 2b site—the primary locus of magnetocrystalline anisotropy. This selective occupancy of uncompensated spin-up sublattices triggers a rapid reduction in saturation magnetization (Ms) relative to the anisotropy constant (K1), thereby significantly elevating the effective anisotropy field (Ha).

Magnetic characterization correlates these structural findings with record-breaking performance: at x = 5.5, the compounds exhibit a giant room-temperature coercivity of 40 kOe and an NFMR frequency of 280 GHz. Temperature-dependent analysis further identifies a characteristic coercivity maximum at T ≈Tc/2. These results underscore the efficacy of neutron diffraction in elucidating the microscopic origins of macroscopic magnetic hardening, providing a robust framework for the development of rare-earth-free permanent magnets and high-stability components for next-generation terahertz communications.