Impact of intercalation on magnetism and charge order in rare earth ferrites

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Layered rare earth ferrites with active spin and charge degrees of freedom on the iron sites undergo complex ordering processes at relatively high temperature, despite of the geometrical frustration of the lattice. The structurally simplest compounds, with formula $R$$Fe_2O_4$ (124), contain Fe/O bilayers, which had been proposed to become polar upon charge ordering leading to an unconventional ferroelectricity, have attracted a lot of interest and were investigated intensely [1]. However, polar bilayers were identified only in one compound, with an anti-polar stacking. The seminar will focus on "intercalated" compounds $Lu_{1+n}Fe_{2+n}O_{4+3n}$, with additional Fe/O single layers inserted between the bilayers. We have grown high-quality single crystals (n=1,2) of these relatively under-investigated compounds and characterized the samples extensively [2]. Magnetization and X-ray Magnetic Circular Dichroism (XMCD) measurements indicate that the local spin arrangement in each individual bilayer is the same as in the not intercalated compound, with the Fe spins in the single layers giving rise to an additional paramagnetic-like contribution [3]. However, magnetic correlations are reduced compared to 124, as also indicated by polarized neutron diffraction [3]. XMCD suggests a similar charge ordering in the bilayers as in 124, confirmed by single-crystal x-ray diffraction: superstructure peaks are observed at positions corresponding to a propagation vector (1/3+δ,1/3+δ,0) and symmetry-equivalent, with δ=0 within error bars in some cases. Structural analysis of the data for $Lu_2Fe_3O_7$ clearly indicated that the 3-fold axis is lost, and further refinements were initially carried out in superspace groups based on *Cmcm*. The final refinements, which indicate the presence of polytypism of the charge ordered compound, will be discussed in detail. Intriguingly, the results of structural analysis suggest an out-of-plane net polarization, consistent with preliminary piezo-electric force microscopy results.

[1] For a review of early work see M. Angst, Phys. Status Solidi RRL 7, 383 (2013).

[2] S. S. Hammouda and M. Angst, J. Crystal Growth 521, 50 (2019).

[3] S. S. Hammouda, M. Angst, T. Mueller, and E. Weschke, in preparation.