**Coupled charge, orbital, and spin degrees of freedom in geometrically frustrated YFe2O4**

Thomas MUELLER1, **Manuel ANGST2**

1Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Garching, Germany

2Jülich Centre for Neutron Science-2, Forschungszentrum Jülich GmbH, Jülich, Germany

Rhombohedral rare earth ferrites *R*Fe2O4 have a strong tendency for coupled charge (Fe2+/3+) and spin order, despite strong geometrical frustration of the interactions [1]. For *R*=Lu or Yb corresponding superstructure reflections or diffuse scattering appear at . However, the size of Y3+ is considerably larger, with calculations [2] suggesting smaller in-plane propagation, .

Here, we focus on single-crystal x-ray diffraction performed on highly stoichiometric single crystals [3] of YFe2O4. Magnetization vs *T* indicates two subsequent highly hysteretic magnetic transitions, separating a low-temperature (LT), an intermediate (IT), and a high-temperature (paramagnetic, HT) phase. XRD shows that these transitions are structural as well. In the HT phase, diffuse scattering at is similar to other rare earth ferrites. However, cooling into the magnetic phases, sharp superstructure reflections at different positions appear, with propagation in IT and in LT. We refined the superstructure in both phases and applied bond-valence-sum (BVS) analysis to probe the charge order [4].

In the LT phase, the structure is refined in , with the inversion center between the two Fe layers. The BVS indicates a full charge order, with two of the Fe sites having valence close to 2+ and the other two close to 3+. Although of -type, the arrangement of the valences differs from the prediction in [2]. Structural distortions also suggest (ferro) orbital order of the Fe2+ sites.

The IT phase is also refined in . A clear splitting of one Y indicates the presence of disorder, which is likely connected to a fragile nature of this phase, which was not theoretically predicted. Of the 7 Fe sites, BVS shows 3 to have valences very close to 2+, indicating a strong localization of 3 electrons on these sites. However, the BVS of one of the sites is about 2.5, and for the remaining sites also further away from the ideal 3 (BVS~2.8). Thus the localization of electrons in the IT phase is incomplete, and it must be a dynamic situation with electron hopping occurring.

[1] M. Angst, Physica Status Solidi RRL, **7**, 383 (2013).

[2] M. Naka, A. Nagano, and S. Ishihara, Phys. Rev. B, **77**, 224441 (2008).

[3] Th. Mueller, J. de Groot, J. Strempfer, and M. Angst, J. Crystal Growth, **428**, 40 (2015).

[4] Th. Mueller and M. Angst, submitted to PRB.

E-mail of the corresponding author: m.angst@fz-juelich.de