ESRF	**Experiment title:** **The sign of the Dzyaloshinskii-Moriya vector in Fe_2O_3 hematite crystal**	**Experiment number**: HC-698
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Report

Scientific Background

The non-resonant x-ray magnetic scattering was observed in hematite Fe_2O_3 many years ago with a conventional x-ray source [1]. This crystal is antiferromagnetic owing to rather strong exchange interaction (T_N=948K) but absence of local inversion symmetry gives also rise to an antisymmetric exchange or Dzyaloshinskii-Moriya interaction [2,3] which in turn leads to a small canting of Fe spin magnetic moments. Such canting produces a net ferromagnetic moment, that's why crystals of this type are usually called weak ferromagnets. Recently it was recognized that the DM interaction could be crucial for multiferroic phenomena and many efforts are devoted to theoretical and experimental studies of its physical origins. Therefore it is important to develop and prove new quantitative methods for these studies. In hematite, owing to the crystal symmetry, the overall DM interaction can be written as $\mathbf{D}\cdot[\mathbf{S}_1\times\mathbf{S}_2]$ where $\mathbf{S}_1$ and $\mathbf{S}_2$ are the spins of neighbouring Fe atoms related by a twofold rotation axis and **D** is the DM vector directed along threefold axis. The value and sign of **D** vector are not determined by symmetry and depend on details of the spin-orbit interaction. There were very sophisticated *ab initio* calculations of **D** vectors in hematite [4] and they are still waiting for experimental proof. Recently a novel method was suggested [5] for the sign measurement in this type of crystals. It is based on the interference between charge and magnetic contributions to scattering in the single-magnetic-domain geometry obtained in the external magnetic field applied perpendicular to the threefold axis. This idea has been used recently in the experiments on crystals of FeBO3 type [6] at XMaS beamline at the ESRF. However in this case one should rely on the calculated sign of the dipole-quadrupole (E1E2) scattering amplitude and this is an obvious drawback of that method.

Experimental details

In our experiments we use the interference between non-resonant magnetic scattering and multiple wave (Renninger) diffraction. The advantage is that for both scattering channels we can perform very reliable and model-independent calculations. The amplitude of non-resonant magnetic scattering is purely imaginary whereas the amplitude of the multiple wave diffraction is almost real (anomalous absorption corrections are small far from the absorption edge). Therefore to make the interference observable we use circularly polarized X-rays and preferably at photon energies below the main absorption edge, Fe K-edge here. This technique to measure the DM vector is model independent but the signal is expected to be quite small and requires the very stable and highly sensitive set-up.

Results

Untwinned hematite single crystals (space group *R-3c*) have been fully characterized. We measured the diffracted intensities for the 111_{rh} forbidden reflection recorded with right-handed and left-handed circularly polarized X-rays. To minimize the fluorescence background from Fe, we perform measurements at photon energy of 5521 eV which corresponds to $\theta_{Bragg} = 14.67^o$ for the 111_{rh} forbidden reflection. This geometry is very well suited to a new experimental setup which is now available at the ID12 beamline.

Our preliminary estimations and available experimental data for hematite [1,7] show that the intensity of the non-resonant magnetic 111_{rh} reflection is of about 10^{-6} in comparison with the allowed 222_{rh} reflection. We performed also preliminary simulations of the 111_{rh} azimuthal Renninger plot for hematite and have found the optimal angular settings for the observation of the desirable interference (see Fig. 1). The asymmetry ratio (or circular dichroism) of this reflection $(I_{left}-I_{right})/(I_{left}+I_{right})$ depends on the azimuthal deviation from the multiple diffraction position.

An external magnetic field of 0.2 T produced by small permanent magnets were applied to saturate the weak ferromagnetism of hematite and obtain a single-domain state. Direction of the magnetic field was changed in the easy 111_{rh} plane to vary the value and sign of non-resonant magnetic scattering.

To make sure that the signal is free of any experimental artefacts we performed very careful measurements of the asymmetry ratio as a function of the azimuthal angle near the multiple diffraction positions for several orientations of magnetic field.

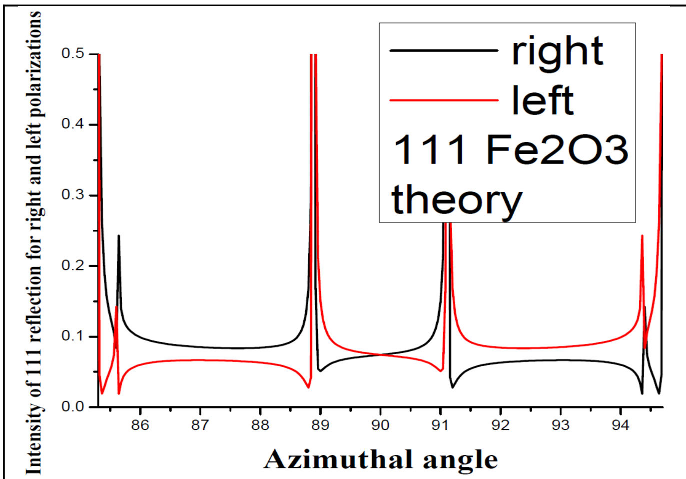

Fig. 1. The calculated azimuthal dependence for interference between magnetic and multiple-wave channels for different circular polarizations.

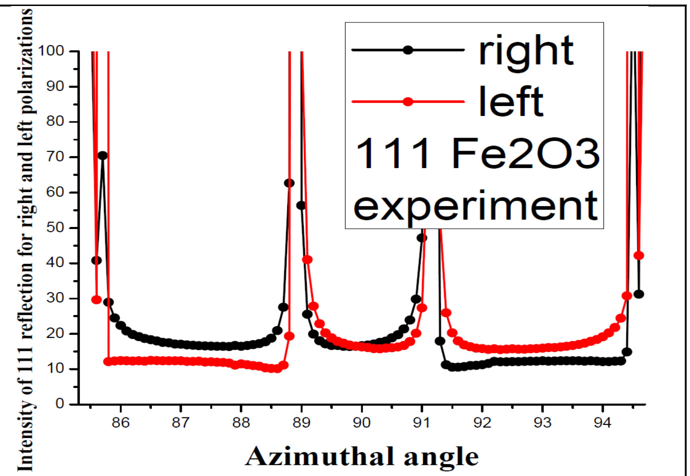

Fig. 2. The azimuthal dependence for interference between magnetic and multiple-wave channels for different circular polarizations measured at ID12.

The obtained experimental results (an example is shown in Fig. 2) demonstrate strong difference between reflection intensities for right-handed and left-handed circularly polarized X-rays and hence a rather strong interference between the magnetic and Renninger diffraction channels. Comparison with the theoretical calculations (Fig. 1) allows us to determine the sign of the Dzyaloshinskii-Moriya interaction.

References

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Report Summary

We have determined for the first time the sign of the Dzyaloshinskii-Moriya vector in hematite crystal using diffraction of circularly polarised X-rays *via* interference between non-resonant magnetic and multiple-wave contributions to forbidden hhh_{rh} (h=2n+1, rhombohedral description) reflections. This method of measurements is model independent, allows easy comparison with available *ab initio* calculations, and can be extended for other types of crystals especially when neutrons are not applicable.