MagStREXS: a crystallographic software for magnetic structure determination through resonant X-ray magnetic diffraction data

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Resonant elastic X-ray scattering (REXS) is a unique element, site, and valence specific probe to study the charge, spin and orbital degrees of freedom and multipole orders in solids and thin films [1, 2]. This technique, which combines elements of diffraction and spectroscopy, has been successful in unraveling different order parameters and solving magnetic structures.

Concerning magnetic structure determination, REXS is complementary to neutron techniques. Several situations make it essential: when the involved magnetic species present a neutron absorption cross-section that is too large, like Eu, Dy, Gd… [3], when the magnetic moments cannot be determined unambiguously with neutron experiments [4], or when more than one magnetic species are involved.

Different types of data can be collected during a REXS experiments: intensities of a set of magnetic reflections, full linear polarization analysis of a specific magnetic reflection, or its azimuthal dependence. The analysis of these experimental data is highly complex and no crystallographic software has been developed yet to enable users to perform this analysis.

MagStREXS is a crystallographic software dedicated to the determination of **Mag**netic **St**ructures through **R**esonant **E**lastic **X**-ray **S**cattering. It is under development since mid-2017 at beamline P09 [5] at PETRA III (DESY) and is based on CrysFML, a library developed to facilitate the creation of crystallographic software that includes also some functionalities especially oriented to deal with magnetic structures. The aim of this program is to facilitate this type of analysis to the non-specialist in this technique and also to provide tools for the preparation of these magnetic diffraction experiments.

Hereby, we will present an overview of MagStREXS, its current status and some of the magnetic structures which have already been determined with it in the field of highly correlated systems.

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