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MagStREXS: a Crystallographic Software for Magnetic Structure Determination from Resonant Magnetic X-ray Diffraction Data

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Resonant X-ray elastic 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 X-ray diffraction with X-ray absorption spectroscopy, has been successful in unraveling different order parameters and solving magnetic structures.

REXS is complementary to neutron techniques for magnetic structure determination. Several situations make it essential: when the magnetic species involved present a neutron absorption cross-section 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 is 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 data is highly complex and no crystallographic software has been developed yet to enable users to solve magnetic structures from a REXS experiment.

MagStREXS is a crystallographic software dedicated to the determination of **Mag**-netic **St**-ructures through **R**-esonant **E**-lastic **X**-ray **S**-cattering and the preparation of magnetic diffraction experiments. It is under development since mid-2017 at beamline P09 [5] at PETRA III at DESY and based on CrysFML, a library developed to facilitate the creation of crystallographic software that includes some resources especially oriented to deal with magnetic structures.

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

References

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