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Practical: neutron diffraction for magnetic structure determination

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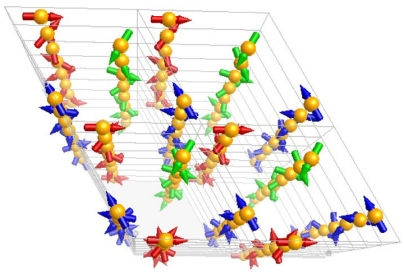
Neutron scattering has progressed over the last fifty years to become an invaluable tool to probe experimentally condensed matter. As far as magnetism is concerned, this technique has been recognized from the early days as unique. The most widespread use of this tool is the determination of magnetic structures that is the determination of the directions in which moments point in a magnetically ordered material. Since the first experiment on MnO published by Shull and Smart in 1949, which was an experimental proof of the antiferromagnetism predicted by Louis Néel, thousands of structure determinations have been reported and have revealed much more complicated magnetic arrangements than the simple ferromagnetic or antiferromagnetic cases. The comprehension of the stability of these new structures was at the origin of numerous theoretical developments, leaving the study of magnetic structures completely open.



The aim of this practical is to present some basics of the neutron scattering magnetic structure determination on powder or single-crystal materials, and some useful tools to achieve this. The theory of magnetic neutron diffraction will be briefly recalled, in particular the concept of propagation vector that allows to describe the periodicity of magnetic structures.

After a presentation of some characteristic neutron diffraction instruments, the practical will start with a description of a typical experiment:
-Powder diffraction: diffractograms recorded above and below the transition temperature in order to determine, by difference, a set of magnetic reflections, and the propagation vector.
-Single-crystal: search for some nuclear Bragg peaks, centering of the crystal in the neutron beam and determination of the orientation matrix associated to the sample, before the collect of integrated intensities of Bragg peaks knowing the propagation vector in order to determine a set of magnetic reflections.

Then some data sets collected on various materials will be analyzed with the help of symmetry analysis using group theory. In practice, we will perform some simple "hand" calculations of the magnetic structure factors at some Bragg positions, before using some dedicated software such as FULLPROF, to do Rietveld analysis of powder diffractograms or least-square refinements of integrated intensity data set for single-crystal.