

Crystallographic and magnetic structures from neutron diffraction: the power of symmetries.

Béatrice Grenier¹, Gwenaëlle Rousse²

¹Univ. Grenoble Alpes & CEA, INAC-MEM, 17 rue des Martyrs, 38000 Grenoble, France

²Univ. Pierre et Marie Curie & Collège de France, 11 place Marcelin Berthelot, 75231 Paris, France

Abstract. The use of symmetries to understand the properties of matter is a central subject in science, in particular in crystallography and magnetism. Besides, neutron diffraction, combined with group theory, is a privileged tool to determine both a nuclear and a magnetic structure, as described in this lecture. In the first section, the basic concepts of crystallography, based on symmetries, are depicted (point groups, lattice and motif, space groups), with the final aim to be able to read and understand the international tables for crystallography. The reciprocal lattice, required for diffraction, is also introduced. The second section is devoted to the description of magnetic structures (propagation vector, the various magnetic orderings) and to their symmetries (time inversion, magnetic point groups and space groups). In the third chapter, after the description of nuclear and magnetic neutron diffraction (Bragg's law, nuclear and magnetic structure factors, extinction rules), the use of group theory to solve the nuclear and magnetic structures will be exemplified, in the case of both powder and single-crystal diffraction. All these concepts will be illustrated by various chemical compounds shown throughout the whole lecture and by the utilization of useful websites.

Suggested introductory readings (textbook, review or articles)

1. *Contribution of symmetries in condensed matter*, Edited by B. Grenier, V. Simonet, and H. Schober, EPJ Web of Conferences, Volume 22 (2012).
2. *Neutrons and magnetism*, Edited by V. Simonet, B. Canals, J. Robert, S. Petit, and H. Mutka, SNF Collection 13, EDP Science, Volume 13 (2014).