European Community under Contract RII3-CT-2004-506008 (IA-SFS).

Keywords: X-ray absorption spectroscopy, magnetic semiconductor, occupancy

MS.61.1

Acta Cryst. (2008). A**64**, C107

Application of representation theory and SARAh to magnetic structure determination

Andrew S Wills
University College London, Chemistry, 20 Gordon Street, London, London, WC1H 0AJ, UK, E-mail：a.s.wills@ucl.ac.uk

The determination of complex magnetic orderings and the study of coupling between different types of order, such as magnetic and electric dipole in multiferroics, requires the application of advanced symmetry arguments. These provide frameworks within which symmetry rules can be developed and expressed. They also enable an understanding to be developed of exactly what a particular order is and why it occurs. SARAh was initially developed in order to allow the calculation of the different types of symmetry modes using representational theory, and refinement of neutron diffraction spectra in terms of the results. In the new release tools have been added to improve the generality of these calculations and aid the visualisation of the different types of magnetic structures. An engine has also been developed to allow the determination of commensurate and incommensurate ordering wavevectors, based on a new procedure whereby the different points, lines and planes in the Brillouin zone are explored sequentially. This procedure, termed ‘Brillouin zone indexing’, follows from the physical nature of the magnetic ordering transition and enables the translational symmetry of the magnetic order to be explored thoroughly. In SARAh its application is based on the application of reverse-Monte Carlo algorithms to the complete powder diffraction pattern, and it allows even structures with several unrelated wavevectors to be studied through automatic cycling.

Keywords: magnetic ordering, magnetic neutron scattering, symmetry theory generalization and applications

MS.61.2

Acta Cryst. (2008). A**64**, C107

The determination of magnetic structures by simulated annealing using the FullProf Suite

Juan Rodriguez-Carvajal
Institut Laue-Langevin, Diffraction Group, jrc@ill.eu, Grenoble, BP 156, 38042, France, E-mail：jrc@ill.eu

The propagation vector formalism for describing magnetic structures is the best way to treat the neutron diffraction (ND) data in order to determine experimental magnetic structures. The magnetic structure in the infinite crystal can generally be described as a finite Fourier series. The Fourier coefficients, labeled by the propagation vector and the index of the particular atom in the cell, are complex vectors to be determined experimentally. These vectors define the magnetic structure and they correspond to the unknowns of the magnetic structure. This kind of formalism is implemented within the program *FullProf* [1]. The steps for solving magnetic structures from ND are the following [2]: (a) Search for the propagation vector(s). (b) A symmetry analysis is needed to find the smallest set of free parameters. In general the Fourier coefficients are linear combinations of the basis functions of the irreducible representations of the propagation vector group. (c) Use an appropriate method for determining the coefficients of the above linear combinations. This implies an evaluation of the observed versus calculated intensity of the magnetic reflections. A trial and error method using least squares is only possible for simple magnetic structures. In general a starting model should be obtained. The simulated annealing technique is extremely efficient, for whatever kind of magnetic structure, in getting an initial model and eventually for determining hidden symmetries. In this communication we will present all the steps in solving magnetic structures by using the programs of the FullProf Suite[3].

[1] J. Rodriguez-Carvajal, Physica B 192, 55 (1993)
[2] J. Rodriguez-Carvajal, Materials Science Forum 378-381, 268 (2001)
[3] See the web site: http://www.ill.eu/sites/fullprof/

Keywords: magnetic structures, neutron diffraction, simulated annealing

MS.61.3

Acta Cryst. (2008). A**64**, C107

International-like tables for magnetic crystallography

Daniel B Litvin
The Pennsylvania State University, Eberly College of Science, Department of Physics, Penn State Berks, P.O.Box 7009, Reading, PA, 19610-6009, USA, E-mail：u3c@psu.edu

We discuss the structure, symbols, and properties of magnetic groups. While the focus is on three-dimensional magnetic space groups, analogous information on one- and two-dimensional space groups and two- and three-dimensional subperiodic magnetic groups is available. Properties of the magnetic space groups have been tabulated and are available in a format and content similar to that of the International Tables of Crystallography. For each group we have tabulated diagrams of symmetry elements, diagrams of general positions, symmetry operations, generators selected, origin, general and special positions, and symmetry of special projections. The magnetic moments allowed by magnetic symmetry are given in the diagrams of general positions and in the listing of general and special positions. The present availability of tabulations of subgroups of magnetic groups, 3D rotateable general position diagrams, and a brief review of the history of magnetic group tabulations will also be given.

Keywords: symmetry, magnetic crystal structure, magnetic ordering

MS.61.4

Acta Cryst. (2008). A**64**, C107–108

Ab initio magnetic structure refinement: Total scattering and RMCProfile

Andrew L Goodwin[1], Martin T Dove[1], David A Keen[2,3], Matthew G Tucker[2]
[1]University of Cambridge, Department of Earth Sciences, Downing Street, Cambridge, Cambridgeshire, CB2 3EQ, UK, [2]ISIS Facility, Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0QX, UK, [3]Department of Physics, Oxford University, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK, E-mail：alg44@cam.ac.uk

MS