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

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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

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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].

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[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

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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

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Rietveld refinement of single-crystal and/or powder Bragg diffraction intensities is a powerful method of elucidating the magnetic structure of magnetic materials; however there are inherent limitations in that Bragg intensities are sensitive only to the angle between the scattering vector and the spin orientations, rather than to the absolute orientations themselves. It is a direct consequence that a number of important problems in magnetic structure refinement (e.g. spin orientations in antiferromagnetic MnO) have remained unsolved. This talk will explore the possibility that local structure information contained in neutron total scattering data can help where average structure studies begin to fail - the idea being that local deviations from average structure allow some additional sensitivity via the magnetic diffuse scattering. The process of modelling this "local" information using atomistic reverse Monte Carlo methods will be discussed, with particular reference to its implementation in the program RMCProfile.

Keywords: reverse Monte Carlo, magnetic structures, diffuse scattering

MS.61.5

Acta Cryst. (2008). A**64**, C108

An ion sputtering epitaxial FePt ultra-thin film studied by magnetic circular dichorism

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The best material for the future high density hard disk is the FePt alloy in a L10 ordered structure due to its high magnetocrystalline anisotropy constant and perpendicular magnetic anisotropy (PMA) property. Low energy ion assisted sputtering deposition of Fe/Pt multilayer was grown eptiaxially on the MgO(001) substrate. After annealing at 973 K, the order parameter reached above 0.95, the L10 ordered FePt film with growing along (001) orientation epitaxially was obtained. The out-of-plane MCD signals increases with increasing annealing temperatures. The out-of-plane orbital-to-spin ratio is found to be proportional to the order parameter. The strong interfacial hybridization between Fe and Pt layers produces enhanced perpendicular orbital moment in the L10 structure with strong PMA effect.

Keywords: magnetic film, magnetic behavior, ordering

MS.62.1

Acta Cryst. (2008). A**64**, C108

Keeping a promise of the XFEL: Crystallography without crystals

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A primary scientific justification for construction of X-ray free electron lasers (XFEL's) has been the determination of the structure of non-crystallized macromolecules, such as proteins, from a set of diffraction patterns (DPs) obtained from randomly oriented single molecules exposed to ultra-short X-ray pulses [1]. It has been suggested that techniques akin to the method of "common-lines", developed for 3D electron microscopy, may be used to determine the relative orientations of the diffraction patterns. After orientation, the data from the DPs may be averaged to boost signal, and the electron density and hence molecular structure recovered by iterative phasing algorithms. We have recently demonstrated [2] that such methods can be used to recover the molecular structure in the absence of noise (i.e., at infinite signal.) However, the method breaks down for scattered photon intensities of less than about 10 per diffraction-pattern pixel. This is a far cry from the signal of ~ $4x10^{-2}$ photons per pixel expected from a typical 500 kDa protein. We describe progress in developing two algorithms for recovering protein structure from such extraordinarily weak signals: one based on the method of generative topographic mapping (GTM) [3, 4]; and one on the exploitation of the symmetry of the random orientations of the copies of the molecule.

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[2] V. L. Shneerson, A. Ourmazd, and D. K. Saldin, Acta Cryst. 64, 303 (2008).
[3] C. M. Bishop, M. Svensen, and C. K. I. Williams, Neural Computation, 10, 215 (1998).
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Keywords: XFEL, orientation and averaging, real space direct method

MS.62.2

Acta Cryst. (2008). A**64**, C108

Hybrid thresholding-projection algorithms for the crystallographic phase problem

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With the ideal algorithm, success in phase retrieval would depend solely on the prior knowledge of the object to be reconstructed and the quality of the data collected. For ab-initio phasing, which does not rely on prior information other than the fact that an object is made of a finite number of atoms, or it has a finite extent, two forms of algorithms have been developed in parallel. By doubling the Bragg sampling, increasingly sophisticated iterative projection algorithms [1] have demonstrated practical solutions to giga-element nonlinear phase retrieval problems, escaping local minima and producing images at resolutions beyond the capabilities of lens-based optical methods without the need for atomic resolution data. These methods have enabled the birth of diffraction microscopy, a.k.a. lensless imaging, a technique whereby the image of an object is obtained by computational phase retrieval of a diffraction pattern instead of using a lens to transform the pattern into an image The adaptation of these algorithms to crystallography have lagged -so far- due to sub-Nyquist sampling imposed by the crystal periodicity. Contrary to conventional wisdom, these algorithms can be adapted to allow for accurate and robust reconstruction from a number of measurements dictated by the signal's structure rather than its (finite) extent.

[1] S. Marchesini, "A unified evaluation of iterative projection algorithms for phase retrieval", Rev. Sci, Inst. 78, 011301 (2007), [arXiv:physics/0603201].

Keywords: projection algorithms, phase retrieval, *ab initio*