MS12.24.4
Acta Cryst. (2005). A**61**, C22
Diffuse Scattering Study of 2D Superstructure in a T' Electron-Doped Cuprate Superconductor
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It is well-known that electron-doped superconductor $Nd_{0.85}Ce_{0.15}CuO_4$ can be reversibly rendered a superconductor or non-superconductor by appropriate high-temperature treatments in reducing or oxidizing environments, respectively. We find that superconducting samples exhibit diffuse (0, 0, L) rods of scattering at superlattice positions in the (H, K, 0) plane corresponding to a larger $2\sqrt{2} \times 2\sqrt{2}$ unit cell. We present a synchrotron x-ray diffuse scattering analysis of this rod scattering in related compound $Pr_{0.88}LaCe_{0.12}CuO_4$ (PLCCO) and demonstrate that it arises from a two-dimensional superstructural distortion of the CuO_2 sheets rather than from cubic Nd_2O_3 (bixbyite) impurities.
Keywords: diffuse scattering, superconducting oxides, superstructures

MS12.24.5
Acta Cryst. (2005). A**61**, C22
Cooperative Evolution - a New Algorithm for Refining Disordered Structures
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The combination of evolutionary algorithms and Monte Carlo simulation is a powerful tool for the investigation of disordered crystals [1]. In analogy to natural evolution, Monte Carlo parameters are optimized by selection, mutation and recombination of previous, suboptimal solutions ("individuals"). In contrast to the technique used in [1] the method proposed in this contribution is not based on competition, but takes advantage of cooperation between individuals. Each of the individuals is allowed to live as long as it is capable of improving the structure. It is shown that this technique leads to a better performance than the algorithm described in [1]. The principle of Cooperative Evolution and its application to disordered structures will be presented.

[1] Weber T., Bürgi H. B., *Acta Cryst.*, 2002, A**58**, 526.
Keywords: diffuse scattering, optimization algorithms, disorder

MS13 Advances in Computational Methods for Powder Diffraction

Chairpersons: Brian H. Toby, Lachlan M. D. Cranswick

MS13.24.1
Acta Cryst. (2005). A**61**, C22
Application of Symmetry to Magnetism and its Consequences for Crystallography
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The microscopic picture of magnetism developed by Néel required extensions to be made to the description of symmetry in crystalline solids. Historically, the first of these was the application of the so-called "coloured" groups or Shubnikov groups, created by the addition to the conventional symmetry elements of crystallography of an operation that reverses magnetic moments. Whilst these are conventionally tabulated for simple commensurate periodicities defined by the Lifshits condition they can be used to describe both commensurate and incommensurate symmetries. There are, however, fundamental restrictions to the types of symmetry that can be effectively characterized using the coloured groups which limits greatly their usefulness. The most general description of symmetry in crystalline solids is that developed by Wigner and is based on the use of irreducible corepresentations.

This presentation will explain the fundamentals behind Shubnikov's space groups and Wigner's theory, and will detail how unspecialized researchers can use corepresentation theory to determine magnetic structures from neutron diffraction data using the computer program SARA*h* (ftp://ftp.ill.fr/pub/dif/sarah/) in combination with the refinement programs GSAS or Fullprof [1,2].

[1] Wills A.S., *Physica B*, 2000, **276**, 680. [2] Wills A.S., Lappas A., *J. Phys. Chem. Solids*, 2004, **65**, 65.
Keywords: magnetic structures, symmetry theory, neutron scattering

MS13.24.2
Acta Cryst. (2005). A**61**, C22
CrysFML: a Library to Develop Crystallographic Programs in Fortran 95. Powder diffraction examples
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CrysFML is a set of Fortran 95 modules to be *used* in crystallographic and diffraction computing programs [1]. Modern array syntax and new features of Fortran 95 are used through the modules. We take advantage of all object oriented programming techniques already available in Fortran (user-defined types, encapsulation, overload of procedures and functions). The lacking features (e.g. inheritance and class methods) will be easily implemented as soon as compilers of the new standard become available. We aim to preserve the efficiency, the simplicity and the adequacy of modern Fortran for numerical calculations. All aspects of symmetry and handling of reflections and structure factor calculations are treated in dedicated modules. Main programs using the adequate modules may perform more or less complicated calculations with only few lines of code. The documentation is written in the source code. A document, in HTML format can be generated using a program.

We shall present an overview of the present status of the library and a series of examples useful for powder diffraction: simple crystallographic calculations, bond-valence sums, aids to space group determination, profile fitting, powder diffraction simulations, kernel of the Rietveld method, etc.

[1] Rodríguez-Carvajal J., González-Platas J., *Compcomm Newsletter* 2003, **1**, 50.
Keywords: computational crystallography, algorithms, modelling

MS13.24.3
Acta Cryst. (2005). A**61**, C22-C23
Peter Piper Picked a Problem Trickier than most. Can Computer Science Solve the Problem Peter Piper Picked?
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Modern materials of scientific and technological interest are notoriously complex. This is exemplified by efforts to control the atomic organization of materials on the nanoscale to give them directed functionality. Clearly it is necessary to be able to characterize the structure of these materials. This is a difficult problem. In a crystal there is a good match between the information required to solve the problem (atomic positions, symmetry and unit cell metrics) and the information in the data (Bragg peak positions and intensities). We are all aware of the power of crystallography. In a nanostructured material the peaks broaden and become overlapped resulting in diffuse scattering which contains much less information. On the other hand the number of degrees of freedom needed to specify the model increases (in principle of order the number of atoms in the