[1] http://www-xray.fzu.cz/jana/Jana2000/jana.html
Keywords: modulated structures, aperiodic crystals, Jana2000

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Modulation Functions of Aperiodic Crystals Determined by the Maximum Entropy Method
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The Maximum Entropy Method (MEM) can be used for the reconstruction of the electron density in the unit cell from phased structure factors [1]. The maximum entropy density map (ρ^{MEM}) may provide information about disorder and anharmonic temperature movements. If an informative prior density is employed, ρ^{MEM} may be used to derive the electron density in the chemical bond.

The MEM can also be applied to the electron density in the *n*-dimensional (*n*D) unit cell of the superspace description of aperiodic crystals [2]. We have thus shown that ρ^{MEM} in superspace may provide a model-independent, quantitatively correct determination of the shapes of the modulation functions of incommensurately modulated crystals and incommensurate composite crystals [3]. All procedures have been implemented into a computer program BayMEM, that can be used for a Maximum Entropy analysis of both periodic and aperiodic crystals. In this contribution the features and problems of the MEM will be discussed, and selected applications of BayMEM will be presented [4].

[1] Gilmore C.J., *Acta Cryst.*,1996, A**52**, 561-589. [2] Weber S., Yamamoto, A., *Phil. Mag.*, 1997, A**76**, 85-106. [3] van Smaalen S., Palatinus L., Schneider M., *Acta Cryst.*, 2003, A**59**, 459-469. [4] Palatinus L., van Smaalen S., *Z. Kristallogr.*, 2004, **219**, 719-729.
Keywords: maximum entropy method, aperiodic materials, aperiodic crystals

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***Ab Initio* Solution of Incommensurately Modulated Structures by Charge Flipping**
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"Charge flipping" is an algorithm for *ab initio* structure solution from X-ray diffraction data, which is based on alternating modifications of a trial electron density in direct and reciprocal space [1]. This algorithm makes no use of the atomicity of the chemical structure. It is instead based on the observation that the electron density of a crystal consists of a small number of high-density areas separated by large areas with very small electron density. This property is common to both electron densities of periodic structures and superspace electron densities of modulated structures. Therefore, charge flipping can be generalized towards superspace and used to reconstruct the superspace electron densities [2].

Up to now the structure solution of incommensurately modulated structures has been a two-step procedure involving solution of the basic periodic structure followed by the determination of the modulation. Charge flipping offers for the first time the possibility to solve the modulated structures directly in superspace, avoiding the often tedious task to construct and refine the basic structure.

Charge flipping was successfully applied to solve several modulated crystal structures including several organic and organometallic compounds with complex modulations [2].

[1] Oszlányi G., Sütő A., *Acta Cryst.*, 2004, **A60**, 134. [2] Palatinus L., *Acta Cryst*.,2004, **A60**, 604.
Keywords: ab initio structure determination, incommensurate structures, superspace electron density

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Pyrrhotites Revisited in Superspace with *ab-initio* Calculations Insights
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Superspace formalism has been used to describe families of compounds with flexible composition [1] with a unique structural model. A superspace model for the Pyrrhotite (Fe1-xS) family is proposed in this work.

Pyrrhotites have metal-deficient NiAs structures. S atoms form a hexagonal sublattice with Fe atoms in the octahedral interstices. Fe-deficient layers alternate regularly with full Fe layers to form superstructures with different composition, symmetry and c parameter [2].

In the common superspace construction, the atomic domains representing the Fe and S atoms are crenel functions. The only parameters which change with the composition are the size of the crenels for the Fe atoms and the modulation weave vector. The structure of a particular composition is obtained through a 3D cut of the superspace construction. For different compositions, distinct stacking sequences are obtained, in agreement with the reported 3D structures.

Ab-initio calculations have been used to study the stability of the different stacking sequences.

[1] Pérez-Mato J.M., Zakhour-Nakhl M., Weill and Darriet F., *J. Mat. Chem.* , 1999, **9**, 2795. [2] Yamamoto A., Nakazawa H., *Acta Cryst.*, 1982, **A38**, 79.
Keywords: aperiodic structures, layered systems, ab-initio calculations

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New Tool based on the Superspace Concept to discover Structure Relations
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Relations between crystal structures imply relations between their space groups, which can be expressed by group-subgroup relations. Recently, the superspace formalism has been extensively used for the unified description of sets of commensurate structures [1, 2]. The method consists of finding possible structures by identifying their space group symmetry from rational cuts in superspace. For practical purpose, the inverse problem is more useful but requires a large amount of compilation.

We constructed a complete tree linking (3+1)- and the corresponding 3-dimensional space groups derived by rational cuts. The aim is to discover possible (and impossible) space group chains for structural relations and phase transitions. The corresponding tree for (3+2)-dimensional groups will soon be completed.

A database providing the subgroup-supergroup relations is available at http://lcr.epfl.ch/page55041.html

This tool is particularly helpful in finding common superspace denominators for various series of modular ('composition-flexible') structures. We shall illustrate the use of the database with a few examples drawn from various fields of crystal chemistry.

[1] Perez-Mato J. M., Zakhour-Nakhl M., et al., *Journal of Materials Chemistry*, 1999, **9(11)**, 2795-2808. [2] Zakhour-Nakhl M., Darriet J., et al., *International Journal of Inorganic Materials*, 2000, **2(6)**, 503-512.
Keywords: superspace symmetry, composition-flexible structures, modular structures