International Union of Crystallography
Commission on Mathematical and Theoretical Crystallography

ECM26 XXVI European Crystallographic Meeting
MaThCryst Satellite Conference
Darmstadt, Germany, 27 - 29 August 2010

Program

Abstracts of Poster Presentations

http://www.crystallography.fr/mathcryst/darmstadt2010.php

27 August

Foundations of aperiodic structures made comprehensible *(in cooperation with the IUCr Commission on Aperiodic Crystals).*

1. Aperiodic crystals in the higher-dimensional description. Incommensurately modulated structures (IMS), composite structures (CS) and quasiperiodic structures (QS) - similarities and dissimilarities
2. Crystallography of Quasicrystals. Fibonacci sequence, Penrose tiling, octagonal tiling, random tilings - matching rules, symmetry, scaling. nD -embedding, symmetry, structure factor. Description of real quasicrystal structures
3. Some periodic crystal structures get simpler in higher-dimensions.

28 August

Introduction to Quaternions and Geometric Algebra and their applications in crystallography.

1. Three dimensional Euclidean space
2. Clifford's geometric algebra of R3
3. Subalgebra of quaternions
4. Reflection in terms of plane normal vector
5. Combination of reflections as geometric products
6. Representations of point groups
7. 3+1 dimensional space time
8. Time reversal as reflection at space hyperplane
9. Magnetic point groups
10. Explicit computations of symmetry transformations
11. Connection between unit quaternions and rotations. Computing the pair of unit quaternions corresponding to the (ordered) product of two rotations.
12. Coincidence site lattices (CSLs) generated by rotations of cubic lattices. Properties of the CSL that can immediately be read off the quaternions representing the rotation.
13. Twinning of cubic crystals.
14. Describing textures of polycrystals as unit quaternion distributions. Examples.

29 August

Mathematics of minimal surfaces

1. mean curvature
2. variational definition of mean curvature
3. some famous examples: helicoid, catenoid, Scherk, ...
4. triply periodic examples: P, D, G, ...
5. mathematical properties: maximum principle, stability
6. mathematical tools to construct minimal surfaces: Plateau problem, Weierstrass data, perturbation methods
7. significance of minimal versus constant mean curvature, Willmore/Helfrich etc.
8. assumed periodicity versus self organizing structures
9. minimal and cmc surfaces for given space groups: 1-parameter families, bifurcations, distinct families
10. classification problem for minimal surfaces w.r.t. a given space group
11. genus of nets via quotient graphs
12. minimal genus nets with good embeddings
13. catenated net-dual net pairs

14. minimal surfaces as bicontinuous cellular patterns whose labyrinths are defined by these net pairs
15. tricontinuous partitions and branched minima surfaces
16. off-surface properties of minimal surfaces, including domain sizes and the problem of determining a skeletal (medial) representation from a given minimal surface
17. non-cubic minimal surfaces (in particular rhombohedral and tetragonal geometry) as transition surfaces between the cubic TPMS

Schedule

- 9:00-10:30 Morning session I
- 10:30-11:00 Coffee break
- 11:00-12:30 Morning session II
- 12:30-14:00 Lunch break
- 14:00-15:30 Afternoon session I
- 15:30-16:00 Coffee break
- 16:00-18:00 Afternoon session II

Speakers

Prof. Hans Grimmer, PSI Villigen (Switzerland)
Prof. Eckhard Hitzer, Fukui, (Japan)
Prof. Walter Steurer, ETH Zürich (Switzerland)
Prof. Karsten Grosse-Brauckmann, Darmstadt (Germany)
Prof. Gerd Schroeder-Turk, Erlangen (Germany)
Prof. Stephen Hyde, Canberra (Australia)

Abstracts of contributed and poster presentations

Aperiodic structures and notions of order and disorder

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Artificial aperiodic structures have recently been the subject of extensive and intensive research, resulting in layered quasiregular heterostructures, as well as photonic and phononic metamaterials with possible applications such as optical and acoustic bandpassfilters or photonic waveguides.
Our main interests are centered on rather fundamental questions concerning determinism, or the old problem of order vs. disorder. We seek to establish possible quantifications of such concepts, to develop basic notions of complexity and entropy, and beyond. Our specific objects of study are multidimensional generalizations of the standard substitution sequences.
Here we present and discuss some two-dimensional instances of the Prouhet-Thue-Morse and paperfolding systems. We compute their rectangle complexities and find them to be at most polynomial, which means that the corresponding entropy basically vanishes. We also point out that the perfectly deterministic Champernowne sequence has entropy $\ln 2$. Thus the notion of entropy cannot serve as an unqualified measure of disorder, and there still remain many unanswered questions.

Quaternion based Modeling of CSL Grain Boundaries in ZnO

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The coincidence lattice site (CSL) theory [1] was developed for one-atomic-type materials like metals and works well. For materials with more than one type of atom in the unit cells several other concepts in interface crystallography have been developed, like coincidence of reciprocal lattice planes (CRLP) [2], low index lattice planes of supercells (LIPS) [3], large d-spacing perpendicular to interfaces. Among them, only at symmetrical tilt grain boundaries (STGB) new structural units can be expected which lead to new materials properties.

The application of these ideas is demonstrated on ZnO, a semiconductor with Wurzite structure. The procedure is as follows. After searching for low index planes and their corresponding perpendicular equivalent, the unit cell was orientated by quaternions and the smallest expansion searched. Then, these units were mirrored along the boundary plane and symmetrical tilt grain boundaries (STGB) were formed by considering a certain translation vector. The model showed that at the interface kites atoms next to the coincidence atoms have to be removed, before relaxing by molecular dynamics can be performed. The results are, that four different new structural units were found, and one of them is experimental confirmed. The new structural units are expected to lead to new materials properties due to Schottky barriers caused by the open structure of structural units [3].

[1] H. Grimmer, B. Bonnet, S. Lartigue, L. Priester, Acta. Cryst. A40 108 (1984).
[2] S. Stemmer, P. Pirouz, Y. Ikuhara, Phys. Rev. Letters 77 1797 (1996).
[3] W. Wunderlich, Phys. stat. sol. (a) 170, 99 (1998)

Opechowski-Guccione-like symbols of magnetic space groups

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For the magnetic space group types with black and white lattice two sets of symbols have been proposed: the BNS symbols [1] and the OG symbols [2]. Whereas generators of the group can be read off the BNS symbol, the International Tables for X-Ray Crystallography (1952) must be consulted to interpret the OG symbols in the cases where the black and white lattice is centred. We shall define OG-like symbols in the case of centred lattices in such a way that generators of the group can be deduced directly from the symbol [3]. The definition generalizes a proposal of Bertaut [4] for crystal class *mmm* to every crystal class.

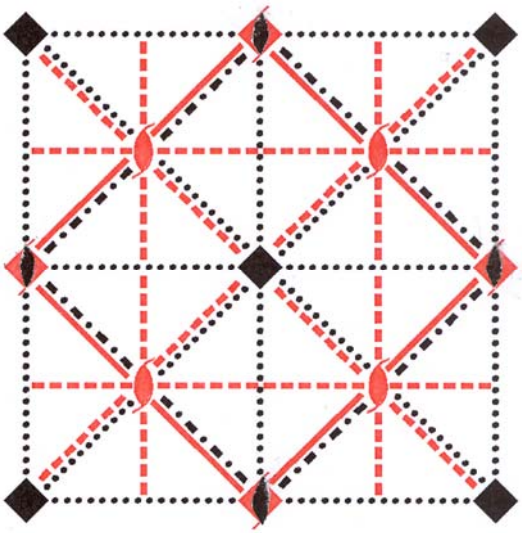

Figure 2 Symmetry diagram for the space group with
BNS symbol P_I4cc,
OG-like symbol proposed in [3] I_P4cc,
OG symbol according to [2] $I_P4c'm'$

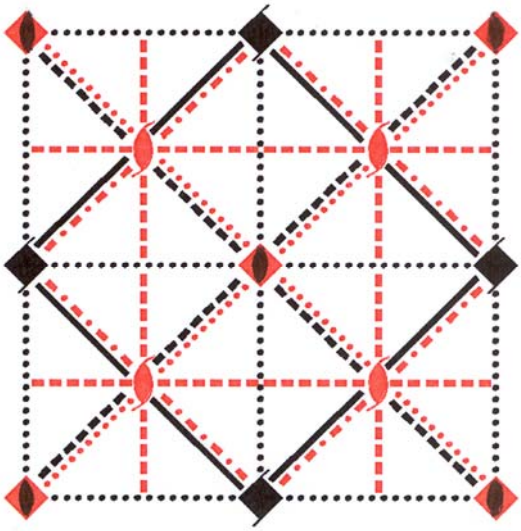

Figure 1 Symmetry diagram for the space group with
BNS symbol P_I4_2cm,
OG-like symbol proposed in [3] $I_P4'cc'$,
OG symbol according to [2] $I_P4'c'm$

[1] Belov, N.V., Neronova, N.N. & Smirnova T.S. (1957) *Sov. Phys. Crystallogr.* **2**, 311-322.
[2] Opechowski, W. & Guccione, R. (1965) *Magnetism*, edited by G.T. Rado and H. Suhl, Vol. II, Part A, 105-165. New York: Academic Press.
[3] Grimmer, H. (2010) *Acta Cryst.* A**66**, 284-291.
[4] Bertaut, E.F. (1975) *Ann. Phys.* **9**, 93-108.

Application of topographs to auto-indexing of powder diffraction patterns

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Powder indexing is a special stage in ab-initio structure determination of powder crystals, not necessary for single crystals. Since three dimensional diffraction images collapse into one dimensional data in powder indexing, it is required to determine lattice parameters of a crystal using lengths of lattice vectors extracted from peak positions. While there are already a lot of indexing algorithms and software [1,2,4,6,7,8], crystallographers has pointed out there are difficult cases to solve. Particularly, powder indexing is hard to succeed when peak positions are not collected almost perfectly due to a large unit-cell, false peaks caused by some accidental reason or failure in peak search *etc*. Therefore, purpose of our investigation is to devise powder indexing algorithm robust for small errors in input data. Our new powder indexing algorithm utilizes a topograph named by J. H. Conway, which is also called the Voronoi graph in reduction theory of lattices. The main features of the algorithm are as follows:

(i) It does not require any information on crystal structure including crystal system.

(ii) It executes rapid thorough search.

(iii) By utilizing number of nodes in a topograph as a merit function, it reduces influence of small errors included in input data.

Firstly on (ii), since some pairs of different 3-dimensional lattices can have totally same set of lengths of lattice vectors, it is desirable that powder indexing algorithms can search all such candidates *i.e.* execute thorough search. On (iii), our algorithm can be regarded as improved Ito's method [7,8], one of orthodox powder indexing algorithms. From a diffraction pattern, the lengths of lattice vectors are extracted as Q-values, which is calculated from a 3-dimensional quadratic form (s_{ij}) and the Miller index *hkl* by

$$Q(hkl) = h^2 s_{11} + k^2 s_{22} + l^2 s_{33} + 2hks_{12} + 2hls_{13} + 2kls_{23}.$$

In the Ito's method, Q-values satisfying the equation $2(Q_1 + Q_2) = Q_3 + Q_4$ are searched. Then, the equation is considered to follow from the identity for Q-values of any two lattice vectors K_1, K_2:

$$2\left(Q(K_1) + Q_2(K_2)\right) = Q(K_1 + K_2) + Q_2(K_1 - K_2).$$

As a result, we can detect 2-dimensional sublattices contained in the lattice of a crystal. However, there is still possibility that the equation $2(Q_1 + Q_2) = Q_3 + Q_4$ accidentally holds and such K_1, K_2 do not exist. With regard to this problem, there seems to be no investigations to resolve it fundamentally. As a new feature of our algorithm, it utilizes a topograph as a system to confirm if K_1, K_2 really exist or not. Figure 1 shows a 2-dimensional topograph. The graph structure of a topograph is same as the Voronoi graph which is obtained from a subdivision of the space of real symmetric matrices using perfect lattices [5]. We call it a topograph because our investigation was inspired by [3]. A topograph has a nice property such that it is well connected and has infinitely long paths in spite of systematic lack of Q-values due to crystallographic extinction rule. We shall present detailed results. We'd also like to present how Q-values of extinct reflections are distributed in a 2 or 3-dimensional topograph to guarantee performance of the algorithm.

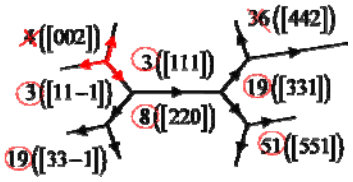

Figure 1 A topograph for a 2-dimensional sublattice of the diamond lattice. (The x-mark indicates the hkl is extinct reflection.)

[1] Le Bail A., (2002) http://www.cristal.org/McMaille/.
[2] Boultif A., Louer D., (1991) J. Appl. Cryst., **24**, p987-p993.
[3] Conway J. H., and Fung F. Y. C., (1997) "The Sensual (Quadratic) Form", The mathematical association of America.
[4] Kohlbeck F., and Horl E. M., (1978) J. Appl. Cryst., **2**, p60-p61.
[5] Martinet J., (2003) "Perfect lattices in Euclidean spaces", Springer-Verlag, Berlin.
[6] Tam K. Y., Compton R. G., (1995) J. Appl. Cryst., **28**, p640-p645.
[7] Visser J. W., (1969), J. Appl. Cryst., **2**, p89-p95.
[8] Wolff P. M., (1958), J. Appl.Cryst., **2**, p89-p95.