

P21.01.03*Acta Cryst.* (2008). **A64**, C618**Point groups in crystallography**Massimo Nespolo¹, Bernd Souvignier²¹Nancy Université, LCM3B UMR-CNRS 7036, BP 239, Vandoeuvre-lès-Nancy, Meurthe-et-Moselle, 54506, France, ²Radboud University Nijmegen, The Netherlands, E-mail: massimo.nespolo@lcm3b.uhp-nancy.fr

Two dual spaces are extensively used in crystallography: the point space E^n , hosting the crystal pattern; and the vector space V^n , where face normals and reciprocal-lattice vectors are defined. The term "point group" is used in crystallography to indicate four different types of groups in these two spaces. 1) Morphological point groups in V^n : They can be obtained from maximal holohedries (holohedries not properly contained in another holohedry) by iteratively descending to proper subgroups: this gives 21 point groups in V^2 and 136 point groups in V^3 , which are then classified into 10 and 32 point-group types, respectively (on the basis of which geometrical crystal classes are defined), and into 9 and 18 abstract isomorphism classes. 2) Symmetry groups of atomic groups and coordination polyhedra in E^n : They coincide with molecular point groups and fall into infinitely many different isomorphism classes, since due to the absence of periodicity these groups are not subject to the crystallographic restriction. 3) Site-symmetry groups in E^n : They are the finite subgroups of space groups. For each site-symmetry group, conjugation by the translation subgroup yields infinitely many different groups, but transforming the fixed point to the origin of E^n allows to classify them into geometric crystal classes exactly like point groups in V^n . A finer classification of site-symmetry groups into *species* is however introduced that takes into account their orientation in space: species of site-symmetry groups in E^n uniquely correspond to point groups in V^n . 4) Groups of matrices representing the linear parts of space group operations in E^n : They are isomorphic both to the point groups in V^n and to the factor groups G/T , where T is the translation subgroup of a space group G .

Keywords: point groups, Site-symmetry groups, symmetry

P21.02.04*Acta Cryst.* (2008). **A64**, C618**Hierarchical structural analysis of supramolecular isomers of organic crystalline host compounds**

Kazuaki Sakaguchi, Norimitsu Tohnai, Tsuyoshi Watabe, Ichiro Hisaki, Mikiji Miyata

Graduate School of Engineering, Osaka University, Department of Material and Life Science, 2-1 Yamadaoka, Suita, Osaka, 565-0871, Japan, E-mail: sakaguchi@molrec.mls.eng.osaka-u.ac.jp

Supramolecular isomerism has attracted considerable attention currently in the field of supramolecular chemistry from the viewpoints of the development of new materials. However, the appearance of unexpected supramolecular isomers has been seen as a problem from the supramolecular architectural design. To better understand the isomerism, we have prepared the supramolecular isomeric crystals of host-guest complexes, and elucidated their crystal structures starting from the chiral host molecules hierarchically. Taking inclusion crystals of alkaloid for instance, here we describe the hierarchical interpretation of the supramolecular isomerism and chirality. Recrystallization from various organic solvents afforded the guest-induced supramolecular isomeric inclusion crystals composed of common 21 helical columnar assemblies. Thus, the inclusion crystallization can be interpreted

hierarchically as follows; (i) fixing a conformation of host molecule with three-directional chirality for making the subsequent molecular architecture, (ii) forming a bimolecular aggregate, and piling up the bimolecular aggregates to form a helical columnar assembly with supramolecular tilt chirality, (iii) stacking the columns in a parallel or anti-parallel fashion to produce supramolecular isomeric bundles, (iv) accommodating guest molecules in the cavities of the bundles to yield host-guest complexes characterized by molecular recognition. Such an interpretation leads to a reasonable elucidation of supramolecular isomerism starting from molecules focused on intermolecular interactions, and will serve as models to better understand complicated self-assembled phenomena.

Keywords: alkaloid structures, helical structure, hydrogen bonds

P21.02.05*Acta Cryst.* (2008). **A64**, C618**The (3+1)-dimensional scheelite structure type**

Alla Arakcheeva, Gervais Chapuis

Laboratoire de Crystallographie, Ecole Polytechnique Fédérale de Lausanne, Dorigny BSP-Cubotron, Lausanne, Lausanne, CH-1015, Switzerland, E-mail: Alla.Arakcheeva@epfl.ch

The concept of structure type (ST) is a well-known crystallographic term, which is widely used in physics, chemistry, and material science. This term refers to a family of periodic crystal structures sharing similar features [1]. In classical crystallography, the relations between structures belonging to the same ST are rather intuitive than quantitative. We propose to improve and extend the notion of ST by applying the concept of superspace symmetry. We show [2] that an incommensurately modulated structure (IMS) described in superspace can be used as a model, capable of generating and describing a family of compounds belonging to a unique higher dimensional structure type (HD-ST). This superspace model and the corresponding HD-ST are characterized by a superspace group (SSG), a number of building units in some basic unit cell occupying certain Wyckoff sites. The occupation and displacive atomic modulations along with variable coefficients of the vector \mathbf{q} are able to uniquely specify any structure belonging to the HD-ST. An INS taken as a superspace model indicates the primary variable(s), which is (are) responsible for the structure manifold in the HD-ST family. The symmetry of the 3D structures and topological manifold in the structure type family are restricted by the SSG. The new concept of ST has been illustrated with the example of the scheelite-like incommensurately modulated structure (3+1)D $\text{KNd}[\text{MoO}_4]_2$. The concept has been applied for the description and derivation of scheelite-like compounds differing widely in chemical composition and topology [2].

[1] Lima-de-Faria, J., Hellner, E., Makovicky, E. & Parthé, E. (1990). *Acta Cryst.* **A46**, 1-11.[2] Arakcheeva, A. & Chapuis, G. (2008). *Acta Cryst.* **B64**, 12-25.

Keywords: incommensurately phase crystallography, structure type, Incommensurately modulated structure

P21.04.06*Acta Cryst.* (2008). **A64**, C618-619**A model of decagonal Al-Cu-Co**

Zorka D. Papadopolos

Universitaet Tuebingen, Institut fuer Theoretische Physik, Auf der

Morgenstelle 14/D8, Tuebingen, Baden Wuerttemberg, 72076, Germany,
E-mail: ptipz01@tphys.physik.uni-tuebingen.de

Decagonal Al-Cu-Co had been modelled by Burkov [1], based on the electron microscopy [2] and x-ray diffraction data [3]. A variant of the model was latter founded over the decagonal tiling of the two golden triangles, $T^*(A4)$ [4], projected from the 4-dimensional root lattice A_4 . The recent STEM data of the same material [5] show that the previous models must be updated. We try to interpret the new data also as a decoration of the decagonal tiling $T^*(A4)$.

[1] S.E. Burkov, Phys. Rev. B, 47 (1993) 12325.

[2] K. Hiraga, W. Sun, and F. J. Lincoln, Jpn. J. Mod. Phys. 30 (1991) L302.

[3] W. Steurer and K. H. Kuo, Acta Crystallogr. Sect. B 46 (1990) 703; J. Phys. C3 (1991) 3397.

[4] P. Kramer, A. Quandt, M. Schlottmann, and T. Schneider, Phys. Rev. B 51 (1995) 8815.

[5] S. Taniguchi and E. Abe, Highly-perfect decagonal quasicrystal $Al_{64}Cu_{22}Co_{14}$ with non-centrosymmetry, to appear in Phyllos. Mag. 2008.

Keywords: decagonal quasicrystal, modelling, tiling

P21.03.07

Acta Cryst. (2008). A64, C619

The pseudosymmetry of atomic structures in crystals of organic and organoelemental compounds

Nikolay V. Somov, Evgeni V. Chuprunov

Nizhniy Novgorod Sate University, Physical department, Russian Federation, Nizhniy Novgorod city, Gagarin av. 23 building 3, Physical department, Nizhniy Novgorod, Nizhniy Novgorod region, 603950, Russia, E-mail: somov@phys.umn.ru

A study of translational and inversion pseudosymmetry of crystal structures retrieved from the Cambridge Structural Database is presented. In this work, the results of translational and inversion pseudosymmetry investigation of 211162 crystal structures are given. The value of the pseudosymmetry determined as degree of invariance of crystal electron density function. The analysis method for pseudosymmetric structure was offered. The percentage of crystals with pseudo inversion (~18%) is higher than the percentage of crystals with translational pseudosymmetry (~5%). The increase in symmetry with respect to the inversion center has two mechanisms. The first one is special superposition of orbits which are invariant with respect to the inversion. The second one is the occupancy of special orbits by heavy atoms. Besides, there are some space groups where every orbit is invariant with respect to inversion. The crystal described by a locally centrosymmetric group will be pseudo-invariant with respect to the center of inversion if it has a heavy atom. In the case of translational pseudosymmetry, there are no groups where every orbit is invariant with respect to superlattice translation. In all the crystals, the increase in the symmetry depends on a special distribution of atoms in the unit cell. Heavy atoms occupy special positions whose location is pseudo-invariant with respect to pesudotranslations.

Keywords: pseudosymmetry, pesudotranslation, pseudoinversion

P22.01.01

Acta Cryst. (2008). A64, C619

Local structure study in decagonal quasicrystals

Hiroshi Abe

National Defense Academy, Materials Science and Engineering, 1-10-20 Hashirimizu, Yokosuka, Kanagawa, 239-8686, Japan, E-mail: ab@nda.ac.jp

Atomic short-range order (SRO) and size effect (SE) were investigated in $Al-Ni-Co^1$ and $Al-Ni-Fe^2$ decagonal quasicrystals. $Al_{72}Ni_{20}Co_8$ is described by an ideal Penrose tiling without a phason. $Al_{72}Ni_{20}Co_8$ possesses an order-disorder phase transition at high temperature. SRO diffuse scattering appeared around the ideal positions of superstructure reflections. Correlation length is estimated to be 2 nm. The SRO diffuse scattering disappeared completely above T_c . By anomalous X-ray scattering and quantitative analysis, total diffuse scattering is decomposed into three kinds of partial diffuse intensities, which are derived from SRO on a quasiperiodic lattice. Also, two significant points are found; i) SE is quite remarkable only between Al and transition metal (TM), not between TMs. ii) The partial diffuse intensity in TM pairs (Ni-Co or Ni-Fe) is largest. These suggest that decagonal quasicrystals suppress the additional strains, which are generated by SE. The effect is connected with the phase stability of an Al-based decagonal quasicrystal in addition to phason contributions. On the other hand, reverse Monte Carlo refinements can determine the Warren-Cowley SRO parameters. Here, SRO parameters are the conditional average of a pair-correlation function. SRO in decagonal quasicrystals develops over the medium-range, though SRO is very weak. It is considered that the peculiar feature is similar to medium-range order (MRO) in amorphous alloys. The idea of MRO parameters³ will be applied to decagonal quasicrystals.

¹H. Abe, H. Saitoh, T. Ueno, H. Nakao, Y. Matsuo, K. Ohshima and H. Matsumoto, J. Phys.: Condens. Matter 15 (2003) 1665.

²H. Abe, K. Yamamoto, S. Matsuoka and Y. Matsuo, J. Phys.: Condens. Matter 19 (2007) 466201.

³H. Abe, J. Phys. Soc. Jpn. 76 (2007) 094601.

Keywords: short-range order, diffuse scattering, size effect

P22.02.02

Acta Cryst. (2008). A64, C619-620

Structure refinement of a decagonal $Al_{72}Ni_{20}Co_8$ quasicrystal by convergent-beam electron diffraction

Koh Saitoh, Hiroki Murakami, Nobuo Tanaka

Nagoya University, EcoTopia Science Institute, Furo-cho, Chikusa-ku, Nagoya, Aichi, 464-8603, Japan, E-mail: saito@esi.nagoya-u.ac.jp

In order to perform structure refinement of quasicrystals in a nanometer area, we have developed a structural refinement method of the quasicrystals by using convergent-beam electron diffraction (CBED). In the present study, we applied the method to an $Al_{72}Ni_{20}Co_8$ alloy, which is known as a highly ordered decagonal quasicrystal. Zero-loss CBED patterns of a water-quenched $Al_{72}Ni_{20}Co_8$ with an energy-selecting slit of 10 eV were taken at the [11110] incidence, which is one of the two-fold axes. The probe size of electron beam was 10 nm in diameter. A dynamical CBED simulation was carried out on the basis of the Bethe method with about 250 beams including strong reflections observed in experimental CBED patterns. The structural model used in the present study consists of pentagonal (P) and Star-shaped (S) clusters with about a 0.4 nm radius, which are located at vertex positions of two different hexagon-boat-star tilings whose scales are mutually different by τ times [1]. A high-dimensional description of