orientation matrix and re-indexing of the corresponding reflection lists (Smart, XDS). The complete range of programs is freely available as Linux- or Windows-version upon contacting the authors.

Keywords: reciprocal space mapping; software; diffuse X-ray scattering

FA4-MS01-P08

Modeling of Decagonal Quasicrystals. Sofia Deloudi[a], Walter Steurer[a]. [a]*Laboratory of Crystallography, ETH Zurich, Switzerland.*
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Quasiperiodic phases seem to naturally withstand the quantitative description we use for most periodic structures (for an overview of the field, see [1]). Providing good models is therefore crucial in order to understand quasiperiodic structures. They have to bring down the geometric principles of quasiperiodic structures to a few simple concepts, while closely resembling the real structures. Furthermore, they are useful tools for physicists in order to provide a good starting point for simulations. These demands can be fulfilled by the well-established technique of cluster-based modeling.
Among the axial quasicrystal structures, the system Al-Co-Ni is the best studied, but the discussion about the structures within this system is still ongoing. Its suitability as a model system is excellent because of several reasons. The phase diagram is well investigated and shows a wide range of modifications of the decagonal phase as a function of composition and temperature. Large single crystals can be easily grown, and electron-microscopic and surface-imaging methods can be used due to the short translation period along the tenfold axis.
In a previous work [2] we have presented a fundamental cluster with 20 Å diameter which makes it possible to model all decagonal phases in the system Al-Co-Ni (including the approximants) systematically, with small changes in the atomic structure.
We have now extended the modeling to the systems Al-Co-Cu and Al-Fe-Ni, showing that it is possible to derive all these complex phases from only one building principle. Furthermore, it was even possible with this approach to predict and explain atomic flip positions within the structures of all phases.
Here, we will concentrate on the discussion of geometrical aspects of the models for Al-based decagonal QCs with a four-layer periodicity, such as the generation of flip positions and superstructures, and we will discuss the agreement of our models with experiment.

[1] Steurer W., Deloudi S., *Acta Crystallogr. Sect. A: Found. Crystallogr.*, **2008**, 64, 1. [2] Deloudi S., Steurer W., *Philos. Mag.*, **2007**, 87(18-21), 2727.

Keywords: quasicrystal; decagonal; modeling

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For Some Commensurately Modulated Structure, Different Index Conditions Can See Different Average Structures. A. David Rae. *The Research School of Chemistry, the Australian National University, Canberra, ACT 0200, Australia.*
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Layer stacking may allow alternative origins or orientations for adjacent layers. A different sequence may give a different origin or orientation of a structure, but different unit cells and space groups are also possible. When different sequences coexist we need to upgrade the refinement model, especially when the prototype layer adjusts for different layer sequences.
Crystals of $Bi(SPh)_3$ are a case in point. Reflections for k even, $h+k = 4N$ define a 1:1 disordered parent structure in space group $C2/c$, $\mathbf{a}_p = ½\ \mathbf{a}$, $\mathbf{b}_p = ½\ \mathbf{b}$, $\mathbf{c}_p = \mathbf{c}$ in which only the S are resolved. Disordered layers perpendicular to **a*** of $P2/c$ symmetry can only be ordered by doubling b to create a $Z = 4$ layer of $P2_1/c$ symmetry. The Bi is near a screw axis. Ordered stacking chooses between layer origins ½ **b** apart, implying 4 parameters, but 8 possible layer sequences after fixing the origin of the first layer. Four of these have $P2_1/n$ symmetry modulo **a**,**b**,**c**, but different origins. The other 4 can be formed as linear combinations of the previous 4 and have $P2_1/n$ symmetry modulo ½ **a**,**b**,**c** (two origins) and P-1 modulo ¼(**a**±**b**),**b**,**c** (two orientations). Observed intensity for reflections with k even, $h + k \neq 4N$ means the layers relax after ordering. The loss of 2/m diffraction symmetry for h odd, k odd reflections implies there is an unequally twinned triclinic component. Observation of reflections excluded by the ordered P-1 options means other component structures are present. Refinement of a twin of a prototype structure of $P2_1/n$ symmetry modulo **a**,**b**,**c** disordered over different origins is unsatisfactory. This refinement scales symmetrized components of the prototype structure and these scales vary with index condition. Excluding certain index conditions from refinement allows the remaining reflections to improve but then omitted reflections fit worse. The coexistence of different prototype structures is a necessary model extension.
I wish to thank Professor P.A.W. Dean of the University of Western Ontario for the diffraction data for this structure.

Keywords: problem structure; refinement; modulated structure

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Structures of Some 4,5-Dichlorophthalimide Derivatives. Orhan Büyükgüngör[a], Mustafa Odabaşoğlu[b]. [a]*Ondokuz Mayis University, Department of Physics, Samsun-Turkey.* [b]*Pamukkale University, Chemistry Programme, Denizli-Turkey.*
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Phthalimide derivatives have been gaining considerable interest since 1979, after recognized the hypolipidemic activity of N-substituted phthalimide derivatives [1]. Later on, researchers reported the antihyperlipidemic [2], hypolipidemic [3], anticonvulsant [4] activity and other interesting aspects [5] of phthalimide derivatives. In view