Acta Cryst. (2002). A58 (Supplement), C180

CONSTRUCTING A DODECAGONAL STRUCTURE BY PROJECTION IN TWO STAGES

S.I. Ben-Abraham[1] Y. Lerer Y. Snapir
Department of Physics, Ben-Gurion University of the Negev, POB 653, IL-84105 Beer-Sheba, Israel

The covering cluster approach offers a plausible mechanism for the formation of aperiodic (as well as periodic) crystals. Thus, decagonal and octagonal tilings can be constructed by covering with a single cluster (or patch). The approach fails in the dodecagonal case where two clusters are needed to guarantee a quasiperiodic structure. Considering the cut-and-project method one may guess that this is due to the extra freedom when projecting from 6D to 2D. To explore this line of thought, we projected a 6D simple cubic lattice into 3D so that a further projection to 2D yields a dodecagonal structure.
A 6D cube projects into a 3D triacontahedron different from the Keplerian; its symmetry is -3*m*. The final result is a dodecagonal layer structure quasiperiodic in the basal plane and periodic in the perpendicular direction. We also explore this approach in the octagonal case where it yields a structure quasiperiodic in one direction and periodic in the two perpendiculars.

Keywords: **DODECAGONAL STRUCTURE; 2-STAGE CUT-AND-PROJECT**

Acta Cryst. (2002). A58 (Supplement), C180

SIMULATION OF THE LOCALLY DISORDERED STRUCTURE IN DECAGONAL $Al_{71}Co_{13}Ni_{16}$

M. Kobas Th. Weber W. Steurer
Laboratory of Crystallography Earth Science Sonneggstr. 5 ZUERICH 8092 SWITZERLAND

The nickel rich decagonal quasicrystal in the ternary system Al-Co-Ni, the so-called Edagawa-phase, shows complex but nevertheless very structured diffuse scattering phenomena. After solution of the average structure and of the superstructure [1], it is the aim of this project to understand the disordered structure. Through gradual analysis of the diffuse scattering and simulation of disorder, it is tried to reproduce the experimental diffuse scattering and by that to understand the disordered structure. At the present stage, the calculations are restricted on disorder on the scale of single clusters, using models based on electron microscopy [2]. First results show that most of the diffuse scattering in the Bragg-layers can be explained by orientational disorder. This kind of disorder model includes clusters that are randomly oriented by 0°, 72°, 144°, 216° and 218°. The diffuse interlayers are not yet sufficiently understood, but the origin of the corresponding diffuse intensity is assumed to be due to anti-phase domain structure caused by shifts of the columnar clusters along the tenfold axis.
References
[1] Cervellino, A., Haibach, T. & Steurer W. (2002). Acta Cryst. B, 58, 8-33.
[2] Steinhardt, P.J., Jeong, H.C., Saitoh, K., Tanaka, M., Abe, E. & Tsai, A.P. (1998). Nature, 396, 55-57.

Keywords: **SIMULATION DIFFUSE SCATTERING DECAGONAL QUASICRYSTAL**

Acta Cryst. (2002). A58 (Supplement), C180

STUDY OF THE THERMOTROPIC PHASE TRANSITIONS OF THE $K_2Mo_xW_{1-x}O_4$ COMPOUNDS USING RIETVELD ANALYSIS

N. L. Speziali[1] A. A. Guarnieri[2] A. M. Moreira[1] G. Goulart Silva[1] C. B. Pinheiro[3] G. Chapuis[3]
[1]Universidade Federal De Minas Av. Antonio Carlos, 6627 BELO HORIZONTE MG 31 123 970 BRAZIL [2]Universidade Federal de Vicosa - Brazil [3]Univeriste de Lausanne - Switzerland

Alkali A_2Mo/WO_4 (A = Na, K, Rb or Cs) are highly hygroscopic compounds presenting the phase transition sequence : Monoclinic <= T_{C1} => Modulated or β-K_2SO_4 <= T_{C2} => α-K_2SO_4 According to the literature, K_2MoO_4 and K_2WO_4 are isomorphic with *C*2/*m* symmetry (Z = 4) at room and $P6_3/mmc$ symmetry (Z = 2) at high temperature; the former is incommensurate (q near 0.30 between 593 and 733 K) and the latter commensurate (q = 0.25 between 643 and 733 K). In the modulated phase the average structure is isomorphic to the β-K_2SO_4. It was recently reported that the monoclinic phase of the parent compound Rb_2WO_4 is hydrated and that the anhydrous compound has *Pcmn* symmetry.
Results from differential scanning calorimetry (DSC) and qualitative X-ray powder diffraction indicate similar characteristics for K_2MoO_4 and K_2WO_4. Polycrystalline samples of $K_2Mo_xW_{1-x}O_4$ have been synthesized and characterized by X-ray diffraction and DSC. The lattice parameters are sensitive to the Mo/W concentration. The values of T_{C2} does not depend on the Mo concentration while T_{C1} decreases with increasing x. DSC diagrams obtained with hydrated and anhydrous powder samples reveal that water molecules strongly influence the structural phase transformation. Results of X-ray powder diffraction show clear differences in the crystal structure of both compounds at room temperature before and after heating.

Keywords: **MODULATION RIETVELD ANALYSIS PHASE TRANSITIONS**

Acta Cryst. (2002). A58 (Supplement), C180

QUASICRYSTAL STRUCTURE ANALYSIS, A NEVER-ENDING STORY?

W. Steurer[1] A. Cervellino[2]
[1]Laboratory of Crystallography ETH Zurich ZURICH CH-8092 SWITZERLAND [2]CNR-IRMEC, c/o Dipartimento Geomineralogico, Universita di Bari, Via Orabona 4, I-70125 Bari, Italy

Twenty years ago, D. Shechtman discovered a novel phase with icosahedral diffraction symmetry in rapidly solidified Al-Mn alloys. It took two years until the renowned international journal Physical Review Letters accepted the manuscript reporting the discovery of this novel ordering state of matter (Shechtman et al., 1984). Nowadays, stable decagonal, dodecagonal or icosahedral quasicrystals are known in more than 40 ternary and binary intermetallic systems. More than 6000 publications on quasicrystals already appeared and almost every day one further paper on this topic is published. Nevertheless, fundamental questions are not answered yet: * What governs formation and stability of quasicrystals? * Are quasicrystals entropy stabilized high-temperature phases or are they thermodynamically stable also at zero K (are they a ground state of matter)? * Is the structure of quasicrystals quasiperiodic in the strict sense? The knowledge of the structure of quasicrystals is a prerequisite for answering all these fundamental questions. On the example of decagonal Al-Co-Ni, the status of quasicrystal structure determination is critically discussed from the first structural paper (Yamamoto et al., 1990) to the most recent one (Cervellino et al., 2002).
References
Cervellino, T. Haibach, W. Steurer, Acta Crystallogr. B58 (2002) 8-33.
Shechtman, D., Blech, I., Gratias, D., Cahn, J.W., Phys. Rev. Lett. 53 (1984) 1951-1953.
Yamamoto, A., Kato, K., Shibuya, T., Takeuchi, S., Phys. Rev. Lett. 65 (1990) 1603-1606.

Keywords: **QUASICRYSTAL, STRUCTURE ANALYSIS, DECAGONAL Al-Co-Ni**