

**PS10.04.29 MECHANISM OF THE PHASE TRANSFORMATIONS IN DECAGONAL QUASICRYSTALS.** Walter Steurer, Matthias Honal and Torsten Haibach, Laboratory of Crystallography, ETH Zentrum, CH-8092 Zurich, Switzerland

A geometrical model for the mechanism of the transformation of decagonal quasicrystals to crystalline phases explaining the experimental diffraction phenomena has been developed.

Most decagonal phases studied experimentally so far have been found to be stable in only a small high-temperature range. Increasing the temperature transforms the decagonal quasicrystals to simple crystalline phases or leads to their peritectic decomposition. By decreasing the temperature high-order approximants are formed which can be obtained experimentally in the form of oriented nanodomain structures only. It is surprising that the coherence length of these phases, consisting of domains with  $\approx 100\text{--}400$  Å diameter, reaches up to  $\approx 10000$  Å [1].

Decagonal quasicrystals are built up from columnar clusters with fivefold orientational symmetry and  $\approx 20$  Å diameter. These clusters are packed quasiperiodically, i.e. they occupy special positions on a quasiperiodic tiling (quasilattice). In the approximant phases the same clusters decorate a translational lattice. Due to the incommensurability of a quasilattice with fivefold symmetry and a translational lattice of any kind, the geometry of a phase transformation is not simple. The particular structural properties of the clusters, however, allow a purely displacive transformation leading to a nanodomain structure.

The characteristics of these transformation mechanism in the three- and the higher-dimensional description, respectively, will be presented.

[1] Kalning, M., Kek, S., Burandt, B., Press, W. and Steurer, W. J. Phys.: Condens. Matter 6, 6177-6187 (1994).

**PS10.04.30 THE SLIDING MODE IN INCOMMENSURATE INTERGROWTH COMPOUNDS.** Sander van Smaalen, Lab. of Crystallography, University of Bayreuth, D-95440 Bayreuth, Germany, and D. Schmicker, Atomic Force Microscopes, Gneisenaustrasse 214, D-47057 Duisburg, Germany.

Phasons in incommensurately modulated structures and the sliding mode in incommensurate intergrowth compounds are zero-frequency modes of crystal vibrations, which can exist in addition to ordinary acoustic phonons. Direct experimental observation of these vibrations is possible by inelastic scattering techniques, like inelastic neutron scattering and Brillouin scattering, or by observation of the propagation of ultrasonic waves. All these techniques probe the crystal vibrations at different frequencies, and a qualitatively different behavior is expected pertaining to the sliding modes and phasons.

In the present contribution we give an overview of the experimental information about the sliding mode and phasons. A phenomenological theory is given of the long-wavelength vibrations in intergrowth crystals, within the framework of the theory of elasticity. A complete set of restrictions has been derived on the components of the extended tensor of elasticity for all (3+1)-dimensional superspace groups. The differences are discussed between the sliding mode, phasons, and acoustic phonons, and particular attention is given to pinning, damping, and the polarisation of these modes.

**PS10.04.31 APERIODIC CRYSTAL STRUCTURE IN VEGETABLE FIBRES.** Nguyen Van Tri, Pham The Vung, Le Hai Hung and Nguyen Van Thang, Institute of Technical Physics, Hanoi University of Technology, Hanoi Vietnam

The particular molecular-electronic microstructure and related properties of many different genera of vegetable fibers (such as cotton, jute, pineapple, sisal) have been studied with ESR in combination with other methods. The partner radicals  $C^\bullet$  and  $O^\bullet$ , and especially a new (2Fe-2S) exchange complex in the fibred structure were revealed. The measurement data indicate that the stable solid partner radical group  $R^\bullet(C^\bullet O^\bullet)$  is mainly by the end of two cellulose macromolecule chains. The physical local structure coupled by fivefold (2Fe-2S) rhombic combinations diagonally bonding a macromolecule chain with five neighbouring ones is based on a pentagon created by five sulfur atoms whose plane is perpendicular to the axis of the elementary fibre. A practical fiber is constituted from numerous elementary fibres spiraling about its axis by an angle  $\Theta_0 = 54,7^\circ$ . The important roles of this structure in the formation of the elementary fibres and in specific features of the material (such as the strength, the tensility, the torsional module) have been partly discovered. Some physical and biological technological treatments to improving fibre properties have been also efficiently examined.

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**PS10.04.32 FIVE DIMENSIONAL MAXIMUM ENTROPY METHOD APPLIED TO THE STRUCTURE REFINEMENT OF DECAGONAL  $Al_{70}Mn_{17}Pd_{13}$ .** S. Weber<sup>AB</sup>, A. Yamamoto<sup>B</sup>, <sup>A</sup>Institute of Applied Physics, University Tsukuba, Tsukuba, Ibaraki 305, Japan, <sup>B</sup>National Institute for Research in Inorganic Materials, Namiki 1- 1, Tsukuba, Ibaraki 305, Japan

A five dimensional structure model for the decagonal phase  $Al_{70}Mn_{17}Pd_{13}$  is proposed, whereby a combination of both the *least-squares method* and the five dimensional *maximum entropy method* was applied in the refinement. The calculations are based on a single-crystal X-ray data set using 1428 unique reflections. The superspace group is  $P10_5/mmc$  and the structure consists of ten layers (2 flat, 8 puckered), which are stacked along the tenfold screw axis with a  $\sim 12$  Å period. The model of *Hiraga and Sun (1993)* was taken as a starting model to obtain an initial 5D-model consisting of four large occupation domains (OD) in  $V_I$  (internal space). Then the size, shape and chemical occupation of the OD's was repeatedly refined to match the 5D-MEM maps. When refining the positional parameters it was found that shifts of atom positions along the tenfold screw axis play a very important role. By doing so the  $R_W$ -factor dropped by  $\sim 7\%$ . No other refined parameter shows a similar significance. In order to verify the projected structure in  $V_E$  (external space) 3D-MEM sections were used to compare the atom positions within the layers with the ones obtained by the refinement of the 5D-model. Since a good agreement was found our refinement then focused on the occupational parameters. Our 5D-model consists basically of four large and some smaller OD's, which again are subdivided in many smaller ones. The large OD's also split up due to the shifts along the tenfold screw axis so that some parts of them are situated at  $x_5$ -coordinates, which are different from the ideal positions that were formerly derived by other groups (*eg.: Steurer et al. 1993*).