

PS10.04.09 CRYSTALS AND QUASICRYSTALS: ELECTRONIC STRUCTURE VERSUS ATOMIC STRUCTURE. Esther Belin-Ferre, LCPMR (URA CNRS 176) and GDR CINQ, 11 rue Pierre et Marie Curie, 75 231 Paris Cedex 05, France, Jean Marie Dubois, LSG2M (CNRS 159) and GDR CINQ, EMN, Parc de Saurupt, 54042 Nancy Cedex, France,

The electronic structure of all solids is closely related to their atomic structural arrangement. In this paper, we compare experimental data representative of the electronic structure of quasicrystals and of related crystalline phases showing however different medium and long range orders. Our aim is to investigate to which extent the electronic structure of quasicrystals exhibits a fingerprint that could arise from topological specificity.

Measurements have been carried out using Soft X-ray Emission and Absorption Spectroscopies and X-ray Photoemission Spectroscopy techniques. Combining these techniques allows us to obtain separately occupied and empty partial (s,p,d...) electronic distributions around each atomic site of the solid, adjusted to the binding energy scale

We present here descriptions of occupied and unoccupied bands in various binary and ternary crystalline Al intermetallic alloys as well as in Al based icosahedral and decagonal quasicrystals. We describe and discuss the electronic interactions that take place in these alloys. We emphasize that the study of the Al electronic distributions of p character gives direct evidence of the progressive appearance of non metallic character of the alloy with increasing the degree of icosahedral order. In icosahedral quasicrystals of high structural quality the Al p electronic structure is reminiscent of that of a semi-conductor. This effect is in strong relation with the increase of resistivity in the same alloys. A discussion of the results is proposed in connection with a recent model based upon hierarchically arranged clusters of atoms (the so-called McKay icosahedra).

PS10.04.10 LOCAL CONFIGURATIONS AND ALLOPHASES IN APERIODIC CRYSTALLINE STRUCTURES. Shelomo I. Ben-Abraham, Department of Physics, Ben-Gurion University, POB 653, IL-84105 Beer-Sheba, Israel

A specific instance of an aperiodic crystal is a thermodynamic phase characterized by a phase variable in the mathematical sense. It is therefore reasonable to call it an 'allopase' as an obvious generalization of 'antiphase'. Quasicrystals are routinely interpreted on the basis of tilings produced by projection of cuts through periodic structures in a hyperspace of higher dimensions. The position of the cut is determined by a phase whose variation produces an uncountable infinity of tilings of the same species, each tiling being a 'phase allele', or 'allopase', for short. A boundary between different allopases is a topological defect consisting of misplaced regular configurations as well as defective ones. More generally, a defective region constitutes a local excursion into one or more different allopases.

We (Baake et al. 1995) have recently shown that all combinatorially possible vertex configurations of the simple icosahedral tiling can be embedded in the otherwise perfect structure and, moreover, can be reached exclusively by simpleton flips. A flipped simpleton is an elementary allopase region. Its boundary is hence a topological defect.

The notion of allopase turns out to be useful also for periodic crystals with domain structures.

I formalize these notions and discuss some puzzles introducing atlases of local configurations of order p and phase shifts in hyperspace. I also try to extend the validity to deterministic aperiodic structures beyond quasiperiodic ones.

Baake, M., Ben-Abraham, S.I., Joseph, D., Kramer, P. & Schlottmann, M. (1995). *Acta Cryst.* A51, 587-588.

PS10.04.11 GROWTH OF POLYTYPIC CRYSTALS CdI_2 , PbI_2 AND STUDY OF LASER INDUCED PHASE TRANSITIONS USING X-RAY DIFFRACTION. S.K. Chaudhary, University College, U.D. University, Rohtak - 124 001 India

The single crystals of CdI_2 and PbI_2 are characterised by a marked polytypism i.e. ability of a substance to crystallize in various polytypic modifications. The crystal lattice of these polytypes is formed by structurally identical, yet translationally non-equivalent layer packets. Each layer packet forms a sandwich structure that consists of three monolayers of atoms I-Pb-I, I-Cd-I. The bonding within a sandwich is largely ionic while that between various sandwiches is predominantly Van-der Waals.

For growth of these crystals a zone-refining set up was fabricated by us. The process of purification and growth was carried out in the argon atmosphere. The purity of the crystals was checked using the atomic absorption technique. The XRD oscillation photographs were employed for structure determination. Ruby laser was used to irradiate the crystal at room temperature. The development of cracks and phase transitions in the above crystals when exposed to laser beam have been discussed on the basis of structural consideration of CdI_2 .

PS10.04.12 ATOMIC STRUCTURE, GROWTH, AND FACETING OF ICOSAHEDRAL QUASICRYSTALS.

Vladimir E. Dmitrienko and S. B. Astaf'ev A. V. Shubnikov Institute of Crystallography, 59 Leninski prospekt, 117333, Moscow, Russia

A realistic mechanism of the three-dimensional atomic growth is developed and simulated for icosahedral quasicrystals. Instead of large icosahedral clusters, previously used for such simulations, the presented mechanism exploits the atomic motives found in related crystalline structures which are called crystalline approximants. The simplest model includes atoms of two sizes, Large and Small, and the ratio of atomic radii is equal to that one in the CsCl-type structures when the S-atom in the centre of the cubic unit cell just fits the hole between L-atoms. This ratio supports the Dodecahedral Local Ordering (DLO) of atoms. The ideal DLO means that every S-atom has its closest neighbours (L-atoms) positioned at the vertices of a regular pentagon-dodecahedron, and vice versa. In crystals, the DLO is exemplified by the CsCl (B2), FeSi (B20), Hg (A10) and many other structures including also the approximants with large unit cells. To suppress the growth of crystalline DLO structures, the oscillating interatomic potentials, typical for metallic alloys, are used. More sophisticated models include atomic positions with icosahedral coordination, phasonic relaxation, etc. The grown clusters (up to 2 million atoms) have narrow Bragg peaks and rather pronounced faceting. Some preliminary results have been published elsewhere (V.E. Dmitrienko and S.B. Astaf'ev: *Phys. Rev. Lett.* v.75, 1538-1541, 1995). The report will be accompanied with computer demonstrations.