PS16.03.15 CRYSTAL GROWTH AND X-RAY STRUCTURE DETERMINATION OF A SERIES OF BIOLOGICALLY INTERESTING COMPOUNDS. Janet M. Moloney, J. A. K. Howard, R. Cochlin, W. J. Feast, Chemistry Department, University of Durham, South Road, Durham, DH1 3LE, UK.

Crystallogenesis has assumed increasing importance over the past decade. This is chiefly because many large molecules can be obtained as highly pure single crystals for structural studies. Therefore, the weak intermolecular interactions which govern solid-state structure can be characterised accurately.

The crystallization of peptides and organic molecules is challenging due to the harsh conditions of the vacuum environment. The pumping system allows to achieve the residual gas pressure 10⁻¹⁰ torr.

The crystal structures of three related branched cyclopentadienyl compounds, determined from low temperature (150K) on a Siemens SMART diffractometer with area detector will be provided. The similarities of these compounds will be compared and details of solid-state packing will be provided.

References:

PS16.03.16 THE RESEARCH MBE SYSTEM WITH TWO MUTUALLY SYNCHRONIZED MODULATED MOLECULAR BEAMS. AlmN. Sen'ko*, Yu. A. Gol'man, A. A. Chemov, A. F. Sen'ko, Yu. M. Dvynshits, Institute of Crystallography, Russian Academy of Science, Moscow, 117333, Russia. * Grodno State University, Grodno 230023, Belarus

The 3 chamber setup to study growth processes of the A2B6 compounds by MBE have been designed and built. There are 4 molecular beam sources based on effusion cells. Two sources are equipped with beam choppers. Chopped beams are aimed at studying adsorption, sticking coefficients, surface nucleation and another MBE growth processes. Growth chamber is equipped by RHEED setup with a system to record the RHEED oscillations and AeO2 viewport which allows one to study how in situ sample illumination by the UV and visible light (λ=250-450 nm) influences on the condensation process of thin films. The analytical chamber is equipped by RHEED, AES, QMS and duoplasmatron Ar⁺ ion gun. The pumping system allows to achieve the residual gas pressure 10⁻¹⁰ torr.

PS16.03.17 SYNTHESIS, STRUCTURE AND PROPERTIES OF Ba₂Cu₃Cl₂O₇, Zhigang Zou* and Hiroyuki Horiiuchi, Mineralogical Institute, Graduate School, Kyoto University, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan; Kunitsugu Oka and Yoshikazu Nishihara, Electron physics section, Physical science division, Electrotechnical Laboratory, 1-1-4 Umezono, Tsukuba Ibaraki 305, Japan. *Present address: Electron physics section, Physical science division, Electrotechnical Laboratory, 1-1-4 Umezono, Tsukuba Ibaraki 305, Japan.

Single crystals of a new barium copper oxochloride, Ba₂Cu₃Cl₂O₇, were grown in a Ba(OH)₂/KCl flux. Through the use of single crystal X-ray diffraction method, it was found that the compound has 4mmn Laue symmetry. The crystal structure was refined in the space group 14mm, and lattice constants a=5.19(1), b=13.83(4), c=4.72, β=101.1°. The structure is characterized by infinite layers of [CuO₃] which are perpendicular to the c-axis. The closest Cu-O distances are 2.795(2), Cu-O-Cu angles are 90, 64(2), and 187, 72(2). Ba₂⁺ is coordinated to four O₂⁻ ions of a square. The melting temperature of the Ba₂Cu₃Cl₂O₇ is 715°C. This sample is an insulator. Magnetic properties of the single crystal were also measured.

Crystal Growth IV
Controlling & Predicting Crystal Morphology

MS16.04.01 DETERMINATION OF THE CRYSTAL GROWTH UNITS BY GRAZING INCIDENCE X-RAY DIFFRACTION (GIXD) AND AFM. David Gidelevitz?, Robert Feidenhans'l and Leslie Leisersonowitz. (Dept. of Materials & Interfaces, The Weizmann Inst. of Science, Israel) The Crystal Growth of Bi-Alanine was studied by GIXD and AFM. The results show that the crystal growth units are Bi-Alanine and glycine.


The design of supramolecular motifs requires complementarity and strong interactions between the molecules to “cement” the various building blocks. Among possible motifs, interdigitated bilayers are of importance since they constitute the walls of bio- and artificial membranes. (1)

A principal way for devising new materials involves the self-assembly of molecules at interfaces. Here we propose an approach for the design of crystalline interdigitated multilayers, composed of chiral molecules A and B, where A is a water-insoluble molecule composed of a long hydrocarbon chain and a hydrophilic headgroup of acid character and B is a water-soluble base. The acid-base complementarity should ensure alternating juxtaposition between the A and B units within each layer, whereas interdigitation of the hydrocarbon chains of the A molecules would promote multilayer arrangement. Molecular chirality of both components, yielding diastereomeric arrangements, is an additional variable. The phenylethylamine mandelates(2) were chosen as suitable templates satisfying the above criteria.

The chiral amphiphile, 3-p-menthendecylmandelic acid, (R-C19-MA), when compressed over a 0.008M aqueous solution of chiral