category and the present paper reports the results of single crystal structural analysis for theses approximants. The present study reveals the fundamental atomic arrangement of the pentagonal columnar structure with 0.8nm periodicity and clarifies its linkage so as to form crystalline structures. Such structural information allows us to discuss the atomic structure of decagonal quasicrystals by reproducing the images of HREM and HAADF-STEM.

Keywords: alloy structurte, single-crystal diffraction, quasicrystals

MS.84.3

Acta Cryst. (2008). A**64**, C142

New phenomena in epitaxial growth: Solid films on quasicrystalline substrates

Vincent Fournee
LSG2M, UMR 8584 CNRS-INPL, Ecole des Mines, Parc de Saurupt, Nancy, Nancy, 54042, France, E-mail：fournee@lsg2m.org

A quasiperiodic arrangement of atoms has only been realized in binary or ternary alloys, known as quasicrystals. These are complex intermetallics with long-range aperiodic order and non-crystallographic rotational symmetry (usually five-fold or ten-fold symmetry). The physical properties arising from the quasiperiodic arrangement of the metal atoms significantly depart from that of periodic alloys and have attracted a broad interest. A long standing issue has been to understand the relative influence of the quasiperiodic order on the physical properties of quasicrystals, independently from the complex chemistry associated with such alloys. This has been the starting point of recent attempts to grow new quasiperiodic systems by using quasicrystalline surfaces as templates to force a quasiperiodic structure in metal thin films deposited on such substrates. Here I will give an overview of the research conducted in the field of solid film growth on quasiperiodic surfaces. An atomistic description of quasicrystalline surfaces will be presented and discussed in relation to bulk structural models. Then the various phenomena occurring during thin film growth on quasiperiodic surfaces will be outlined. Emphasis will be placed on the nucleation mechanisms of the solid films, on their growth modes in relation to the nature of the deposited metals, on the possibility of alloying at the interface, and on the epitaxial relationships at the crystal-quasicrystal interfaces. We will also describe situations where the deposited elements adopt a quasiperiodic structure, which opens up the possibility of extending our understanding of the relation between quasiperiodicity and the physical properties of such structurally and chemically complex solids.

Keywords: surface science, quasicrystals, thin films

MS.84.4

Acta Cryst. (2008). A**64**, C142

Mesoscopic quasicrystalline and Archimedean tilings in polymer alloys

Tomonari Dotera[1], Kazunari Ueda[1], Tohru Gemma[2], Kenichi Hayashida[3], Atsushi Takano[3], Yushu Matsushita[3]
[1]Kyoto University, Department of Polymer Chemistry, Kyoto University, Katsura, Nishikyo-ku, Kyoto, Kyoto, 615-8510, Japan, [2]Graduate School of Arts and Sciences, University of Tokyo, Tokyo 153-8902, Japan, [3]Department of Applied Chemistry, Nagoya University, Nagoya 464-8603, Japan, E-mail：dotera@phys.polym.kyoto-u.ac.jp

Tilings and patterns are known not only to mathematicians and crystallographers, but also to designers and visual artists as the basis of decorative art appearing on furniture, curtains, wall papers, kilts, ceramics, ties, etc. In this talk, we show that star-polymers can produce elegant self-assembled periodic and quasiperiodic patterns without fabrication technique. We have been creating several complex but periodic patterns known as antique Archimedean tiling patterns, and finally, we have found evidence of a “polymeric quasicrystal” tiling for the first time [1]. Quasicrystals are the avant-garde structures that have noncrystallographic symmetry, and initiated a revolution of crystallography and solid-state physics in 1980’s. Remarkably, our polymeric dodecagonal quasicrystal has a hundred times length-scale compared to metallic systems, and thus it approaches the scale of visible light, where a promising photonic application has been considered [2]. The present result indicates the universality of quasicrystalline order from atoms to polymers.
Reference:
[1] Kenichi Hayashida, Tomonari Dotera, Atsushi Takano, and Yushu Matsushita, Phys. Rev. Lett. 98, (2007) 195502.
[2] Kazunari Ueda, Tomonari Dotera, and Tohru Gemma, Phys. Rev. B 75 (2007) 195122.

Keywords: quasicrystals, multicomponent polymer systems, molecular architecture self-assembly

MS.84.5

Acta Cryst. (2008). A**64**, C142–143

Atomic simulation and lattice dynamics of the ZnMgSc icosahedral quasicrystal

Marc De Boissieu[1], Marek Mihalkovic[2], Sonia Francoual[3], Kaoru Shibata[4], Hiroyuki Takakura[5], Tsutomu Ishimasa[5], An-Pang Tsai[6]
[1]SIMaP, Grenoble-INP, CNRS, UJF, Metal Physics, 1130 Rue de la piscine, BP 75, St Martin d’Heres cedex, Isere, 38402, France, [2]Institute of Physics, Slovak Academy of Sciences, 84228 Bratislava, Slovakia., [3]National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, [4]J-PARC Center, Japan Atomic Energy Agency, 2-4, Shirakatashirane, Tokai,Japan, [5]Division of applied Physics, graduate school of engineering, Hokkaido University, Sapporo, 060-8628 Japan, [6]Institute of Multidisciplinary Research for Adavanced Materials, Tohoku University, Sendai 980-8577, Japan, E-mail：Marc.de-boissieu@simap.inpg.fr

The structure of the binary CdYb icosahedral quasicrystal was recently solved using a 6D modeling approach and synchrotron radiation data. The structure of the quasicrystal is described as a quasiperiodic packing of a large triacontahedron connected along 2- and 3-fold axis [1]. Going from the atomic structure to physical properties remains a challenging problem. Indeed, an accurate derivation of the physical properties requires to, (i) have a tractable Hamiltonian and (ii) specify a realistic and unique position and chemical spicy for each atom in the quasicrystal structural model. The whole procedure is illustrated on the example of icosahedral Sc-Mg-Zn alloy, starting from the derivation of effective pair potentials from first principle database, through “energetic” refinement of uncertain structural details, and finally comparative study of lattice dynamics for 1/1 and 3/2 approximants. The simulated dynamical response function reproduces perfectly the experimental one, measured by inelastic neutron and x-ray scattering [2]. In particular the differences observed between the quasicrystal and the 1/1 approximant are well accounted for. An analysis of eigen modes and their localization on clusters will be presented. It is also found that, except for the Sc icosahedrons, all cluster shells present a significant deviation from icosahedral symmetry, related to the relative orientation of the inner

tetrahedron.
[1] Takakura H., Gomez C. P., Yamamoto A., de Boissieu M. and Tsai A. P.: Atomic structure of the binary icosahedral Yb-Cd quasicrystal, Nature Materials 6 (2007) 58-63.
[2] de Boissieu M., Francoual S., Mihalkovic M., Shibata et al.: Lattice dynamics of the ZnMgSc icosahedral quasicrystal and its ZnSc periodic 1/1 approximant, Nature Materials 6 (2007) 977-984.

Keywords: quasicrystal, lattice dynamics, simulation

MS.85.1

Acta Cryst. (2008). A**64**, C143

Structural genomic of protein families and pathways in human disease

Johan Weigelt, Pär Nordlund, Helena Berglund, Herwig Schuler, Lovisa Holmberg-Schiavone, Martin Hällberg, Susanne Gräslund, Mats Wikström
Structural Genomics Consortium and Division of Biophysics, Department of Medical Biochemistry and Biophysics, Karolinska Institutet, Stockholm, Sweden

Comprehensive molecular insights into a specific disease most often require whole pathways and processes to be considered. Structural biology together with complementing biochemical studies is the major means for achieving detailed insight into the molecular mechanisms of proteins in such pathways: how they interact, how they are regulated, and how enzymes recognize and transform substrates. This information provides a knowledge basis for current target drug design efforts and the structural information can directly assist in the rational drug design cycle. The Structural Genomics Consortium (SGC) is an Anglo-Canadian-Swedish consortium pursuing a systematic effort at generating structural insights into proteins of disease related pathways and structural families. At the SGC-Stockholm node, "the little brother" in the consortium, some 430 proteins are currently studied within areas such as; receptor signaling (Toll-, TGF-beta- and RTK-receptor based signalling), apoptosis signaling, phosphoinositol and other lipid signaling, ATPases (RNA-helicases and AAA-ATPases), poly-ADP ribose polymerase, as well as nucleotide and amino acid metabolism. Many of the proteins targeted are implied in diseases such as; cancer, inflammatory and infectious diseases. Approximately 70 novel human structures, plus follow-up structures, have been determined in the last three years at SGC-Stockholm. The specific structural genomic strategy applied on some of the pathways and families motioned above will be discussed, as well as examples of structural insights generated by this strategy.

Keywords: protein structure, structural genomics, rational drug design, cancer, inflammation, protein production

MS.85.2

Acta Cryst. (2008). A**64**, C143

Structural genomics and the expanding protein universe

Ian A. Wilson
Joint Center for Structural Genomics, TSRI, Molecular Biology, BCC206, 10550 No. Torrey Pines Road, La Jolla, CA, 92037, USA, E-mail：wilson@scripps.edu

Over the past 8 years, the JCSG has developed and integrated various methodologies and technologies into a very efficient high throughput production pipeline for all steps from target selection, cloning, expression, crystallization to structure determination. The pipeline, which was initially developed using a full proteome screen of *T. maritima* (TM), is in its 3rd year of operation as one of the 4 NIGMS, Protein Structure Initiative large-scale production centers. In order to explore the rapidly expanding sequence space from the growing genome sequencing projects, the PSI has focused on increasing coverage of the corresponding structural space at multiple levels: first, by selecting Pfam families without structural coverage; by identifying and validating new protein families; and by focusing on large families (MEGA) with inadequate structural coverage to assess evolution of structure and function. Our biomedical theme project revolves around the Central Machinery of Life, proteins that are conserved in all kingdoms of life. Other exciting new projects in our target portfolio are on metagenomes, in particular, Global Ocean Sampling and the human gut microbiome. To date, the JCSG has deposited over 555 novel structures (as of 2/19/08) in the PDB and recently completed the metabolic reconstruction of TM in collaboration with Dr. B. Palsson, UC San Diego, and Dr. A. Osterman, Burnham. The substantial contributions of the JCSG and the PSI to coverage of this expanding protein universe will be outlined. The JCSG, located at The Scripps Research Institute, Genomic Institute of the Novartis Research Foundation, U.C. San Diego, Burnham Institute, and the Stanford Synchrotron Radiation Laboratory/Stanford University, is supported through the NIGMS PSI (U54-GM074898).

Keywords: structural genomics, metagenomics, protein universe

MS.85.3

Acta Cryst. (2008). A**64**, C143-144

Using focused structural proteomics to elucidate the molecular basis of MAPK regulation in T cells

Rebecca Page, David A. Critton, Antoni Tortajada, Breann L. Brown, Katja Betz
Brown University, Box GE-4, Providence, RI, 02912, USA, E-mail：Rebecca_Page@brown.edu

Disruptions in the tight regulation of T cell activation and differentiation are correlated with numerous immunological cancers, including acute leukemias. One cause is the increased exposure of people to oxidative environmental toxins, a subset of which target and inhibit cysteine-based tyrosine phosphatases (CBTPs). Hematopoietic tyrosine phosphatase (HePTP) is a non-receptor CBTP that plays a critical role in the development of these immune disorders through its ability to regulate the activities of its only known target substrates, the MAP kinases Erk and p38. HePTP, and its only other known family members STEP and PTPRR, interacts with these targets via a unique 15 residue sequence in its N-terminus termed the kinase interaction motif (KIM). In order to investigate the regulation of MAPKs by KIM phosphatases at a molecular level, we have taken a focused structural proteomics approach. Specifically, we have produced a KIM phosphatase:MAPK specific 'toolkit', which includes KIM phosphatase substrate trapping mutants (STMs) whose activities are severely compromised, yet still able to bind target substrates, functional mutants that reflect distinct biological states of the complex and efficient methods for the robust, activation of the MAP kinases for studies of the active dephosphorylation complex, among others. Using these new biological tools, we are now investigating, using functional X-ray crystallography and NMR spectroscopy, the multiple, transient interactions of the KIM phosphatase:MAPK complexes that drive T cell differentiation at atomic detail. This work was supported through funding to RP from NIH-5P20RR016457-07 and ACS Research Scholar Grant RSG-08-