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IUCr 2014

Satellite Workshop:

Introduction to Aperiodic Crystals

Commission on Aperiodic Crystals

Chair: **Ron Lifshitz** (lifshitz@caltech.edu)

WORKSHOP PROGRAM — Tuesday, 5 August 2014

07:45 – 08:30	**Registration and Gathering**	
Session 1	**Fundamentals**	***Uwe Grimm*** *Open University, UK*
08:30 – 09:15	**Aperiodic Crystals: How is that even possible?**	**Ron Lifshitz** *Tel Aviv University, Israel and Caltech, USA*
09:15 – 10:00	**Tiling Models for Aperiodic Crystals**	***Marjorie Senechal*** *Smith College, USA*
10:00 – 10:30	**Coffee Break** (provided)	
Session 2	**Crystallography**	***Václav Petříček*** *ASCR, Czech Republic*
10:30 – 11:15	**Structure Solution of Modulated and Composite Crystals**	***Sander van Smaalen*** *University of Bayreuth, Germany*
11:15 – 12:00	**Structure Solution of Quasicrystals**	***Walter Steurer*** *ETH Zurich, Switzerland*
12:00 – 13:30	**Lunch** (on your own)	
Session 3	**Systems**	***Ted Janssen*** *University of Nijmegen, Netherlands*
13:30 – 14:15	**Incommensurate Modulated and Composite Crystals: A survey**	***Artem Abakumov*** *University of Antwerp, Belgium*
14:15 – 15:00	**Quasicrystals: A survey**	***An-Pang Tsai*** *Tohoku University, Japan*
15:00 – 15:30	**Coffee Break** (provided)	
Session 4	**Advanced Topics**	***Marc de Boissieu*** *Grenoble-INP, France*
15:30 – 16:00	**Phonons and Phasons in Quasicrystals**	***Yasushi Ishii*** *Chuo University, Japan*
16:00 – 16:30	**Discovery, Growth, and Physical Characterization of Quasicrystalline Systems**	***Paul Canfield*** *Iowa State University, USA*
16:30 – 17:00	**Soft Matter Quasicrystals**	***Tomonari Dotera*** *Kinki University, Japan*
17:30	**Congress Opening & 10th Ewald Prize**	***Ted Janssen & Aloysio Janner*** *University of Nijmegen*

Abstracts

Speaker: ***Ron Lifshitz****, Tel Aviv University, Israel; and Caltech, USA*

Title: **Aperiodic Crystals: How is that even possible?**

Abstract:

For over a century it was understood that crystals were a form of matter in which the atomic constituents were ordered periodically. Already 50 years ago it started to become evident that long-range order survives, even when the periodicity is removed via incommensurate modulations, or the inter-growth of two or more crystals with incommensurate periodicities. Yet, it was only about 30 years ago, with the announcement of the discovery of quasicrystals, that the periodicity paradigm had to be fully abandoned and the notion of crystallinity had to be redefined. In this lecture, which will serve as an introduction for the whole day, I will explain some of the basic notions of aperiodic crystals—What does it mean to have long-range order without periodicity? What does an aperiodic crystal look like? How can we model such crystals? What do we really mean when we say that a crystal has a certain rotational symmetry? Can we still talk about point groups, space groups, and systematic extinctions?—and possibly more if time permits.

Further reading:

1. R. Lifshitz, "What is a crystal?" *Z. Kristallogr*. **222** (2007) 313.
2. R. Lifshitz, "Quasicrystals: A matter of definition." *Foundations of Physics* **33** (2003) 1703.
3. R. Lifshitz, "Symmetry breaking and order in the age of quasicrystals." *Isr. J. Chem*. **51** (2011) 1156.
4. R. Lifshitz, "Theory of color symmetry for periodic and quasiperiodic crystals." *Rev. Mod. Phys*. **69** (1997) 1181.

Speaker: ***Marjorie Senechal****, Smith College, USA*

Title: **Tiling Models for Aperiodic Crystals**

Abstract:

"All models are wrong but some are useful."* I will show, through a case study, that tiling models for aperiodic crystals are surprisingly useful. They explain why "aperiodic crystal" is not an oxymoron. More generally, they show us what aperiodic order can look like, the properties it can have, and ways that order can be measured. More generally still, aperiodic tilings sharpen and deepen our thinking, expand our vision, and pose new problems for crystallographers and mathematicians.

* G.E.P. Box, and N.R. Draper, *Empirical Model Building and Response Surfaces* (John Wiley & Sons, New York, 1987), p. 424.

Further reading:

1. M. Senechal, *Quasicrystals and Geometry* (Cambridge University Press, 1996).
2. M. Senechal and J. Taylor, "Quasicrystals: the view from Les Houches," *The Mathematical Intelligencer* **12** (2) (1990) 54.
3. M. Senechal and J. Taylor, "Quasicrystals: the view from Stockholm," *The Mathematical Intelligencer* **35** (2) (2013) 1.

Speaker: ***Sander van Smaalen***, *University of Bayreuth, Germany*

Title: **Structure Solution of Modulated and Composite Crystals**

Abstract:

Crystal structures of incommensurately modulated compounds and composite crystals can most favorably be described with the aid of superspace, a special variety of four-dimensional or higher-dimensional space. The concept of superspace was originally introduced by P.M. de Wolff, A. Janner and T. Janssen, and in the early 1980s it was applied to the structural analysis of a series of modulated crystals by A. Yamamoto. Superspace is the Swiss knife of the crystallography of aperiodic crystals. It allows to describe and to understand symmetry and diffraction, including the so-called satellite reflections violating the translation symmetry. It is an indispensable tool for structure solution by charge flipping and the maximum entropy method, for visualizing electron densities and for the crystal chemical analysis of the structures of aperiodic crystals. Here, the concept of superspace will be introduced and applications in the aforementioned fields will be illustrated by selected examples.

Further reading:

1. S. van Smaalen, *Incommensurate Crystallography* (Oxford University Press, Oxford, 2007). Published in paperback (with corrections) 2012.
2. S. van Smaalen, "An elementary introduction to superspace crystallography." *Z. Kristallogr.* **219** (2004) 681.
3. S. van Smaalen, B. J. Campbell, and H. T. Stokes, "Equivalence of superspace groups." *Acta Crystallogr. A* **69** (2013) 75.
4. A. Wölfel, P. Dorscht, F. Lichtenberg, and S. van Smaalen, "Anisotropic thermal expansion of $La_n(Ti,Fe)_nO_{3n+2}$ (n = 5 and 6)" *Acta Crystallogr. B* **69** (2013) 137.
5. A. Wölfel, Liang Li, S. Shimomura, H. Onodera, and S. van Smaalen, "Commensurate charge-density wave with frustrated interchain coupling in $SmNiC_2$." *Phys. Rev. B* **82** (2010) 054120.

Speaker: ***Walter Steurer***, *ETH Zurich, Switzerland*

Title: **Structure Solution of Quasicrystals**

Abstract:

Quasicrystal (QC) structure analysis is all but a straightforward process because QCs cannot be described by just a smaller or larger deviation from a periodic basic structure [1,2]. The main problem is that one has to determine both the long-range order as well as the short-range order from scratch. In case of a tiling-based approach, one needs a basic assumption about the underlying tiling [3]. If a higher-dimensional structure analysis is performed, the basic assumption is that the structure is really quasiperiodic [4]. Once this basic decision is taken, the charge-flipping method will provide a reasonable starting model for the 3D or *n*D structure refinements. However, the resulting structure will always be an averaged structure, which can be close to the actual structure in case of rather perfect QCs [3] or just reflect some basic features in case of poor-quality QCs [4]. The most important question to be posed is "What do I want to know about the QC structure, and what do I want to do with this structural information?"

Further reading:

1. W. Steurer, S. Deloudi, *Crystallography of Quasicrystals. Concepts, Methods and Structures* (Springer Series in Materials Science, Vol. 126, 2009).
2. W. Steurer, "Quasicrystal structure analysis, a never-ending story?" *J. Non-Cryst. Solids* **334** (2004) 137.

3. P. Kuczera, J. Wolny, W. Steurer, "Comparative study of decagonal quasicrystals in the systems Al-Cu-Me (Me = Co, Rh, Ir)." *Acta Crystallogr. B* **68** (2012) 578.
4. T. Ors, H. Takakura, E. Abe, W. Steurer, "The quasiperiodic average structure of highly disordered decagonal Zn-Mg-Dy and its temperature dependence." *Acta Crystallogr. B* **70** (2014) 315.
5. W. Steurer, S. Deloudi, "Decagonal quasicrystals - what has been achieved?" *C. R. Physique* **15** (2014) 40.

Speaker: ***Artem M. Abakumov****, University of Antwerp, Belgium*

Title: **Incommensurate Modulated and Composite Crystals: A survey**

Abstract:

Although it might not be obvious at first glance, incommensurately modulated and composite structures are abundant among advanced materials. As incommensurability often plays a key role in the material's functionality, knowing its nature is vitally important for understanding, predicting and improving the material's performance. The main goal of this lecture is providing a brief overview of the incommensurately modulated and composite crystals with particular emphasis on the compounds relevant for material science. Using several examples such as superconductors, Li-ion conductors, mixed ionic and electronic conductors, multiferroics, luminescent materials etc., I will try to demonstrate relationships between the functional properties and individual features of incommensurability in every case.

Further Reading:

1. S. van Smaalen, *Incommensurate Crystallography* (Oxford University Press, Oxford, 2007). Published in paperback (with corrections) 2012.
2. T. Janssen, G. Chapuis and M. de Boissieu, *Aperiodic Crystals: From modulated phases to quasicrystals* (Oxford Univ. Press, Oxford, 2007).
3. A.M. Abakumov, A.A. Tsirlin, E.V. Antipov, "Transition-Metal Perovskites". In *Comprehensive Inorganic Chemistry II, Vol. 2* (Elsevier, Amsterdam, 2013) pp.1-40.

Speaker: ***An Pang Tsai****, Tohoku University, Japan*

Title: **Quasicrystals: A survey**

Abstract:

Quasicrystals are no longer considered unique structures of matter since they have been confirmed as equilibrium phases in over one hundred alloys. The stability of stable quasicrystals can be understood within the framework of Hume-Rothery rules. Even more interesting, it is found that the known stable quasicrystals are strict electron compounds, which form only for alloys with precise valence electron concentration e/a (valence electrons per atom ratio). Actually, most stable quasicrystals were discovered on the basis of the e/a criterion. The discovery of these quasicrystals was extremely important as it allowed performing structural analysis and study physical properties on large single-grain samples. We recently found that icosahedral quasicrystals (IQC) and their approximant phases compete for stability, and that the phase formed depends strongly on thermal history. In the talk, I will mainly describe how stable quasicrystals were discovered, explain how first structural solutions were obtained, and discuss the stability of some stable IQCs which have been reported recently.

Further Reading:

1. A.P. Tsai, "Discovery of stable icosahedral quasicrystals: Progress in understanding structure and properties." *Chem. Soc. Rev.* **42** (2013) 5352.
2. H. Takakura, C. Pay Gómez, A. Yamamoto, M. De Boissieu, A.P. Tsai, "Atomic structure of the binary icosahedral Yb–Cd quasicrystal." *Nature Materials* **6** (2007) 58.

Speaker: ***Yasushi Ishii**, Chuo University, Japan*

Title: **Phonons and Phasons in Quasicrystals**

Abstract:

One of the most generic and interesting properties of quasiperiodic crystals is the existence of collective excitations called "phasons". As their name suggests, phasons are associated with changes in the relative phases of incommensurate density waves that make up the crystal. In an incommensurately modulated crystal, phasons arise from the freedom to set the phase of the modulation with respect to the underlying periodic crystal. In quasicrystals, which often have a high degree of rotational symmetry, the phason degrees of freedom lead to a much greater variety in structural modifications. Recently, accurate information on the atomic structure has become available for some families of quasicrystals, and hence the nature of phason excitations on the atomic scale is now understood more precisely than ever before. On the atomic scale phasons are characterized by a local rearrangement of atoms. This yields characteristic structural flexibility in quasicrystals, which seems to be universal, and plays a vital role in realizing such exotic phases of matter. Lattice-vibration (phonon) spectrum in systems with this kind of structural flexibility is of great interest—particularly in connection with the unique thermal properties of quasicrystals—and has been studied by both neutron experiments and computer simulations. In this lecture, I will illustrate the notion of phasons in quasicrystals as a basic concept for understanding the diversity of real materials, and discuss their dynamic aspect, including their characteristic influence on the phonon vibrational spectra.

Further Reading:

1. T. Fujiwara and Y. Ishii (editors), *Quasicrystals* (Elsevier, Amsterdam 2007).
2. T. Janssen, G. Chapuis and M. de Boissieu, *Aperiodic Crystals: From modulated phases to quasicrystals* (Oxford Univ. Press, Oxford, 2007).

Speaker: ***Paul Canfield**, Iowa State University, USA*

Title: **Discovery, Growth, and Physical Characterization of Quasicrystalline Systems**

Abstract:

Solution growth of single grain quasicrystals has played a vital role over the past twenty years. At a grossly qualitative level, it has produced some of the most compelling, visual evidence of the stability and symmetry of this phase of matter. At a more basic level, it has allowed for growth of single phase, single grain examples of many QC systems, thus opening them to detailed physical measurements. More recently, since solution growth is uniquely suited to growth of compounds with low peritectic decomposition temperature, it has been used as a method for discovering new quasicrystalline systems. In this presentation I will discuss how solution growth of known QC systems has been accomplished and outline a strategy for searching for new QC systems.

Further reading:

1. P.C. Canfield, I.R. Fisher, "High-temperature solution growth of intermetallic single crystals and quasicrystals." *Journal of Crystal Growth* **225** (2001) 155.
2. I.R. Fisher, K.O. Cheon, A.F. Panchula, P.C. Canfield, M. Chernikov, H.R. Ott, and K. Dennis, "Magnetic and transport properties of single-grain *R*-Mg-Zn icosahedral quasicrystals [*R* = Y, ($Y_{1-x}Gd_x$), ($Y_{1-x}Tb_x$), Tb, Dy, Ho, and Er]." *Phys. Rev. B* **59**, (1999) 308.
3. P.C. Canfield, M.L. Caudle, C.-S. Ho, A. Kreyssig, S. Nandi, M.G. Kim, X. Lin, A. Kracher, K.W. Dennis, R.W. McCallum, and A.I. Goldman, "Solution growth of a binary icosahedral quasicrystal of $Sc_{12}Zn_{88}$." *Phys. Rev. B* **81** (2010) 020201(R).
4. A.I. Goldman, T. Kong, A. Kreyssig, A. Jesche, M. Ramazanoglu, K.W. Dennis, S.L. Bud'ko & P.C. Canfield, "A family of binary magnetic icosahedral quasicrystals based on rare earths and cadmium." *Nature Materials* **12** (2013) 714.

Speaker: ***Tomonari Dotera**, Kinki University, Japan*

Title: **Soft Matter Quasicrystals**

Abstract:

Two decades after the first publication on quasicrystals in aluminum manganese alloys by Shechtman et al., a "soft matter quasicrystal of dendritic micelles" was found in 2004. Since then a number of materials successively joined the family of soft matter quasicrystals, including star and linear copolymers, nanoparticles, polymer micelles, mesoporous silica, and very recently hydrogen-bonded ferrocenecarboxylic acid. For this decade, we were convinced that there is no reason to limit quasicrystals to synthetic intermetallic systems alone. In this lecture, important experimental and theoretical advances are reviewed to introduce participants to the emerging research front of soft quasicrystalline materials. The world of quasicrystals opened by Dan Shechtman extends its reach into twenty-first century chemistry.

Further reading:

1. T. Dotera, "Quasicrystals in Soft Matter." *Isr. J. Chem.* **51** (2011) 1197.
2. T. Dotera, "Toward the discovery of new soft quasicrystals: From a numerical study viewpoint." *J. Polym. Sci. Part B: Polym. Phys.* **50** (2012) 155.
3. T. Dotera, T. Oshiro & P. Ziherl, "Mosaic two-lengthscale quasicrystals." *Nature* **506** (2014) 208.