MEETING REPORT

Aperiodic crystals*

Aperiodic crystals are characterized by the discrete diffraction patterns which cannot be indexed with the conventional three indices but require additional ones. They occur in almost every type of solid including organic and inorganic compounds, minerals, metals and alloys, and even macromolecules. It is convenient to describe their structures in superspace (higher dimensional space), a conceptual environment, in which three-dimensional aperiodic crystals recover their periodicities. The inconvenience of visualization due to extra dimensions is compensated by the mathematical elegance achieved through recovering periodicity. Studies of aperiodic structures have greatly enriched our understanding of the physics and chemistry of atomic orders, and have opened up new perspectives for correlating structure with the properties of complex materials.

The Aperiodic-09 conference was attended by 110 participants from all over the world including two participants from India – N. K. Mukhopadhyay (Banaras Hindu University (BHU)) and T. P. Yadav (BHU). The details of the conference and the abstract of the papers presented in the conference can be found at http://www.aperiodic09.org/. There were 16 technical sessions consisting of 46 presentations including one tutorial session and 2 poster sessions of 45 papers. There was an interesting public lecture delivered by Sir Roger Penrose who discovered the quasiperiodic tiling long before the experimental discovery of quasicrystals (QCs) in 1984. Such a tiling is now popularly known as Penrose tiling. He elegantly demonstrated how the simple set of shapes tiles the plane without repetition, gaps and overlaps. Many explicit examples of aperiodic sets were presented in his talk, showing different types of symmetry. In addition to the public lecture, during the conference there were lively discussions on topics related to QCs, modulated (incommensurate) crystals and complex metallic alloys (CMA). Some of the issues emerging out of this conference are highlighted here.

*A report on the 'Sixth International Conference on Aperiodic Crystals (Aperiodic '09)' organized by R. McGrath and U. Grimm during 13–19 September 2009 at Liverpool under the auspices of the Commission on Aperiodic Crystals of the International Union of Crystallography (IUCr).

Quasicrystals

Several workers presented the structure, properties, and stability of QCs. E. Abe (Japan) discussed the microscopic view of QC symmetry in order to elucidate, 'where are the atoms'. Through a direct, real-space imaging of the decagonal structure at a sub-angstrom scale, the degree of ordering in the most perfect quasicrystalline compounds was shown to be close to Penrose tiling. The characteristic localized-distributions of point defects, existing in the best-ordered quasicrystalline specimen were explained as being due to a phason-degree of freedom. H. Takakura (Japan) presented a unified viewpoint of the atomic structure of P-type icosahedral QCs in CdYb and ZnMgHo system based on six-dimensional models. These QCs belonging to the family of Tsai- and Bergman-type QC are explained as structures with different atomic decorations of the same building units: (i) rhombic triacontahedron, (ii) acute rhombohedron and (iii) obtuse rhombohedron. The model of ZnMgHo P-type QC was extended to F-type QC in reference to the recently analysed ZnMgHf 1/1 approximant crystal[1] that is considered to be an approximant crystal to the corresponding F-type QC. N. Fujita (Japan) discussed the various possibilities of orders and disorders in ternary decagonal tilings. It was shown that phason fluctuations could be introduced into the perfect structures by exciting phason flips in a canonical Monte Carlo simulation. A. Yamamoto (Japan) advocated the theory of short-range order magnetic diffuse scattering in QCs. The analytical formula giving the short-range order diffuse scattering (SRODS) intensity of QCs for X-ray was discussed. For the first time, the analytical formula for neutron magnetic scattering giving the short-range order diffuse scattering analysis was provided. H. Abe (Japan) discussed atomic short-range and medium-range order in Al–Ni–Co decagonal QCs, while analysing diffuse scattering by Monte Carlo simulations. The diffuse scattering was correlated to an order–disorder phase transition on $Al_{72}Ni_{20}Co_8$.

S. Deloudi (Switzerland) studied Al–Co–Ni decagonal QC structures. A fundamental cluster with 20 Å diameter was presented to model all decagonal phases in Al–Co–Ni system including the approximants, with small changes in the atomic structure. Y. Yokoyama (Japan) investigated the preferred occupation at the transition metal (TM) sites in the decagonal unit cluster of two-dimensional Al–Co–Ni and Al–Co–Cu QCs. Analysis on the bonding character and bond energy for local clusters around the TM sites showed that Al–Co–Cu favours the Cu and Co occupations at the first and second inner TM sites respectively. A. Strutz (Japan) presented an average structure solution of the decagonal basic $Al_{72.5}Co_{18.5}Ni_9$ QC based on the refinement of single-crystal five-dimensional data using a higher dimensional structure model. The determined higher dimensional space group is noncentrosymmetric P10*m*2. The best-fit model structure with 229 parameters resulted in $wR = 0.109$ and $R = 0.1263$ for 957 reflections.

Y. Ishii (Japan) dealt with the electronic structures and stability of Ag–In–Ca QC surfaces. Such characteristic electronic structures were shown to affect chemical properties of QC surfaces. Charge density distributions simulating STM (scanning tunnelling microscope) images were calculated for relaxed surface and it was found that Ag and In sites were distinguishable by changing a bias voltage. A role of the sp-d hybridization on surface electronic structures was discussed. M. Krajč (Slovakia) proposed a structural model of the quasiperiodic Pb monolayer grown on the fivefold i–Al–Pd–Mn surface at the coverage close to saturation. The proposed model reproduced the quasiperiodic ordering of the monolayer described. The calculated electronic structure revealed that the density of states of the quasiperiodic monolayer exhibited a pseudogap at the Fermi level. S. Olsson (Sweden) suggested that QC thin film should be produced keeping the substrate temperature around 500°C. When annealing the Al–Cu–Fe thin films grown on Al_2O_3 substrates, the individual layers first mixed into several binary AlCu phases (Al_2Cu, AlCu and Al_4Cu_9)

and thereafter ternary Al–Cu–Fe phases (e.g. Al_7Cu_2Fe) before the $Al_{62.5}Cu_{25}Fe_{12.5}$ icosahedral quasicrystalline phase was formed. The formation temperature of the quasicrystalline phase was between 400°C and 490°C. H. R. Sharma (UK) determined the surface structure of Ag–In–Yb QCs by STM and low energy electron diffraction (LEED). The surfaces are found to be consistent with bulk terminations at the centre of the rhombic triacontahedral clusters, the building blocks of these materials. M. K. Mukhopadhyay (India) studied the evolution and structural transition of quasicrystalline phases in Al–Fe–Cu–Cr and Al–Fe–Cu–Mn alloys during high-energy ball milling. The evolution of nanoicosahedral and nanodecagonal phases were found to occur. The formation of nanospinel phase was reported from these systems. M. Loquias (Philippines) discussed the recent developments in the mathematics of grain boundaries. The examination of coincidence site lattices (CSLs) from a more mathematical point of view was readily extended to aperiodic situations, which was possible through their underlying translation modules with 5-, 8-, 10- and 12-fold symmetry. The notion of a colour symmetry, originally defined for symmetries of a lattice was extended to coincidence isometries of the lattice. J. Roth (Germany) explored the QCs of higher irrationality. Up to now only n-fold symmetric QCs with quadratic irrationalities, i.e. 5-, 8-, 10-, 12-fold, and icosahedral symmetry have been observed in nature. QCs with cubic (7- and 9-fold) or higher irrationalities have been studied only in static artificial nanostructures. A. P. Tsai (Japan) reviewed the basis for synthesis of QCs. He emphasized that by following the Hume–Rothery's rule (i.e. e/a criteria) for phase stability, several new QCs had been found out earlier. R. Lifshitz (Israel) studied the stability of QCs (soft QC) composed of soft isotropic particles. A model using a coarse-grained description for a system of soft isotropic particles was proposed to explain the experimental observation of Zeng *et al.*[2]. It was shown that entropy plays an important role in introducing effective three-body interactions in these systems.

Modulated crystals

M. Baake (Germany) discussed the mathematical diffraction theory of aperiodic crystals. It was shown that the understanding of systems with continuous and mixed spectra has improved considerably. Moreover, the fascinating phenomenon of homometry was found to exhibit various unexpected new facets. G. Chapuis (Switzerland) elaborated how incommensurate and composite crystals are part of a more general class of compounds currently known as aperiodic crystals. It was discussed that there are obvious advantages of using the superspace concept for understanding the structure of aperiodic crystals. J. L. Ribeiro (Portugal) demonstrated the modulated magnetic order parameter in the orthorhombic rare-earth manganites $RMnO_3$ (R = Gd, Tb, Dy), a novel class of frustrated magnets. The existence of secondary order parameters, such as strain, magnetization, electric polarization or toroidal moment, has been examined in order to elucidate the possible co-existence of different ferroic orders. R. L. Withers (Australia) presented a careful phase analysis and TEM investigation of the $(Bi_{1-x}Ca_x)Fe^{III}O_{3-x/2}V_{x/2}$(V for vacancy), $0.20 \le x \le 0.50$, and $(Bi_{1-x}Sr_x)Fe^{3+}O_{3-x/2}V_{x/2}$, $0.2 \le x \le 0.67$, perovskite related solid solution. Both solid solution fields are, in general, $(3 + 1) - d$ incommensurately modulated with an incommensurate primary modulation wave-vector magnitude. High resolution (HR) TEM imaging was used to show the presence of at least 6-fold twinning. Perez-Mato (Spain) discussed two approaches for the solution of modulated structures: (i) the use of symmetry adapted modes and (ii) the superspace method. He demonstrated that both the approaches are closely related, being equivalent in simple cases. However, if the unit cell of the distorted phase is much larger than the parent one, the superspace description is more efficient. On the other hand, for distorted phases with supercells which are only a small multiple of the parent phase and involve modulations along several directions, the mode description is much more convenient. A. Arakcheeva (Switzerland) presented the contributions of superspace to structure–property investigations. From various compounds of the $Na_xEu^{3+}_{2/3-x/3}MoO_4$ ($0 \le x \le 0.5$) series of scheelite related compounds (SRCs) it has been demonstrated that the degree of luminescence could be correlated with the various types of modulations developed due to composition change. C. Ecolivet (France) presented direct observations by neutron and X-ray scattering of structural phase transitions in the urea-alkane family which were mostly driven by an intermodulation modification, whereas the average structure of the sublattices did not vary concomitantly. It was shown that the urea-alkane family members may present a sequence of two structural phase transitions. A. Schonleber (Germany) studied phase transitions and modulated structures of Co (sepulchrate)-trinitrate $C_{12}H_{30}N_8Co^{3+} \cdot 3(NO_3)$ at low temperatures. Applying spectroscopic measurements, phase transitions have been observed at $T_1 = 133$ K and at $T_2 = 106$ K. By single-crystal neutron diffraction upon cooling the appearance of satellite reflections in the diffraction pattern at $T_1 = 133$ K was discovered.

V. F. Degtyareva (Russia) discussed the electronic origin of the incommensurate-modulation (IM) in the structure of phosphorus IV using high-pressure X-ray diffraction studies. All IM structures were observed when elements become metallic. The stability of this IM structure was attributed to the lowering of the electronic band structure energy due to Brillouin zone Fermi surface interaction. A. Ustinov (Ukraine) studied the diffraction effects due to modulation of orthorhombic crystals by aperiodically arranged twin boundaries (TB). Based on the model, the intensity curves were simulated to give a reasonable fit to the diffraction pattern of a layered Ni–Mn–Ga martensite that showed irregular positions of the extra peaks due to the presence of aperiodic TBs in the crystal.

Complex metallic alloys

CMA are alloys which belong to the family of intermetallics and are characterized by complex structures, with large unit cells containing up to thousands of atoms[3]. A. Beni (Switzerland) described how a CMA could be used for industrial applications, such as tribological, adhesion and corrosion resistance properties. Those systems exhibit several unusual properties, like very low electrical and heat conductivity, ascribed to the presence of a pseudo-gap at the Fermi level. Various CMA ternary Al-alloys, belonging to the Al–Cr–Fe family, were found to be highly corrosion resistant in aqueous media. J. Ledieu (France) presented a detailed investigation of the (100) surface of the orthorhombic $Al_{13}Co_4$ crystal using experimental tools and *ab initio* electronic structure calculations. This CMA surface, approximant of the decagonal QC, was used as a template for Pb and Cu adsorption. A pseudomorphic thin film is also obtained. O. Degtyareva (Russia) investigated modulated super-

structure of γ-brass CuZn compressed to 90 GPa. The structural distortion of the γ-brass of CuZn in the pressure range up to 90 GPa, using synchrotron X-ray diffraction was detected. In the diffraction patterns above 40 GPa, the splitting of the bcc reflections, as well as appearance of weak superstructure reflections were observed. Splitting of the main reflections is explained by a trigonal distortion of bcc, while the additional reflections are due to a positional modulation along the trigonal axis.

H. Euchner (France) reported on the vibrational properties of the CMA $Zn_{11}Mg_2$. This phase containing 39 atoms in the unit cell and is a cubic packing of 'mini Bergman' clusters linked by Zn octahedra. *Ab initio* simulations, conducted with the programme package VASP, PHONON, as well as recent inelastic neutron scattering experiments showed exceptional vibrational properties in the low-energy range of the generalized vibrational density of states of $Zn_{11}Mg_2$. J. Wolny (Poland) analysed the Samson phase in beta Al–Mg, being one of the most complex intermetallic structures containing 1168 atoms, distributed over 1832 atomic positions. The lattice constant of the Samson structure was shown to be a gigantic one with $a = 2.8242(1)$ nm. It was reported that at a temperature of 214°C, the structure undergoes phase transformation to the rhombohedral (space group R3m, no. 160) with $a = 1.9968(1)$ nm, $c = 4.89114(8)$ nm. T. Yamada (Japan) reported diffuse scattering in single grained Zn_6Sc (1/1 approximant) located at the position of supertlattice reflections above 157 K. The ordering transition was shown to take place at temperature around 80 K. The nature of phase transformation was interpreted to be very similar to that of Cu–Zn beta brass. A. K. Shukla (France) studied quantum size effects in the thin metallic films (Ag–Bi) grown on either the 5-fold surface of icosahedral Al–Cu–Fe QC and the (100) surface of the $Al_{13}Co_4$ periodic approximant respectively. K. Nishimoto (Japan) reported low-temperature TEM observations of Cd_6M (M = Sr, Pr, Nd and Sm) approximants. The occurrence of the phase transition at low temperature is explained by orientational ordering of the tetrahedron at the centre of Tsai type cluster. J. Ivkov (Ljubljana) studied the Hall Effect of Y–(Al–Ni–Co) and $Al_{13}Co_4$ decagonal approximants in the temperature interval from 90 to 370 K. In these intermetallics the Hall coefficient R_H exhibits well-defined anisotropy and weak temperature dependence. The anisotropy in both crystalline and quasicrystalline materials was shown to originate from the specific stacked-layer structure and the chemical decoration of the lattice. T. P. Yadav (India) studied the stability of nanocrystalline vacancy ordered phases in Al–Ni–Cu alloy by high energy ball milling. Vacancy ordered phases are a class of complex intermetallics derived from the various degrees of ordering of the vacancies along the body diagonal, causing distortion of the parent lattice. The synthesis of nanospinel was demonstrated by annealing the nano-vacancy ordered phase in air.

In the concluding session Marc de Boissieu, the chairman of the Aperiodic Commission, IUCr mentioned that there was a proposal for merging both the Aperiodic and Quasicrystal (ICQ) conference series. It was pointed out that this issue would be further discussed in the forthcoming International Conference on Quasicrystals (ICQ11) at Sappro, Japan in June 2010. In this context, Y. Ishii, the Chairman of ICQ11 extended invitations to all the delegates together with a special request to scientists from the fields of incommensurate and commensurate-modulated crystals and polytypes. It was announced that the next Aperiodic conference (Aperiodic '12) would be organized under the chairmanship of R. L. Wither in Australia in 2012. Prior to that there would be an International Congress of Crystallography (IUCr) in 2011 in Spain where a symposium on aperiodic crystals would be organized. It was also mentioned that the proceedings of Aperiodic '09, containing the selected papers after peer review will be published in the *Journal of Physics Conference Series* (http:/www.iop.org/EJ/conf).

1. Gomez, C. P. *et al.*, *Inorg. Chem.*, 2008, **47**, 8258.
2. Zeng *et al.*, *Nature*, 2004, **428**, 157.
3. Fournée, V., Banthés-Labrousse, M.-G. and Dubois, J.-M., *Solid State Phenomena*, 2008, **138**, 407.

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Infosys Prize 2009

The Infosys Science Foundation has announced winners of its Infosys Prize 2009. The foundation was established in February 2009 to 'promote world-class research in natural and social sciences in India'. Aim of the prize is to recognize Indian scientists for their 'outstanding contributions to research'. The prize is given in five categories: Engineering sciences, Life sciences, Mathematical sciences, Physical sciences and Social sciences. The winners will receive the award from the Prime Minister on 4 January 2010 in New Delhi.

According to the Infosys press release, the winners of the prize in various categories are: Life sciences: K. VijayRaghavan (National Centre for Biological sciences, Bangalore); Mathematical sciences: Ashoke Sen (Harish Chandra Research Institute, Allahabad); Physical sciences: Thanu Padmanabhan (Inter-University Centre for Astronomy and Astrophysics, Pune); Social sciences: Upinder Singh (University of Delhi, Delhi) and Abhijit Vinayak Banerjee (Massachusetts Institute of Technology, Boston). No prize was given in the Engineering sciences category this year.

The prize consisting of a citation, a medal and cash award of Rs 50 lakhs is one of the largest monetary prizes in India. The prize will be given annually to 'elevate the prestige of scientific research in India and to inspire young Indians to pursue a career in scientific research'. For further details, visit: http://www.infosys-science-foundation.com/laureates.html

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