BCA Spring Meeting 2012

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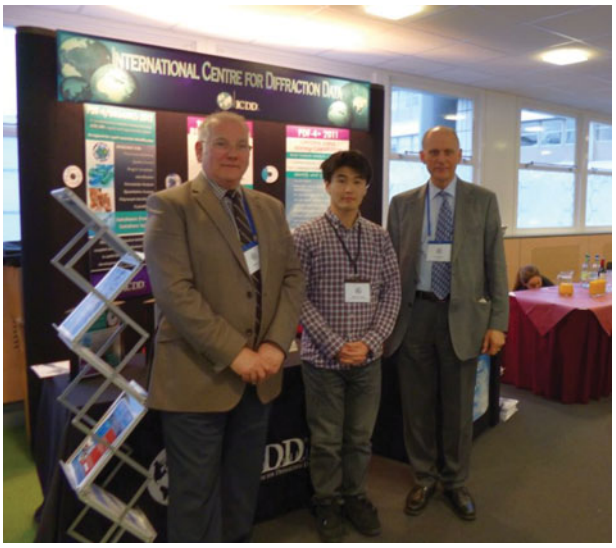
The 30th Annual Spring Meeting of the British Crystallographic Association took place at Warwick University, Coventry from 16 to 19 April 2012. The meeting comprised oral and poster sessions in traditional manner, with contributions from the Biological Structures Group, the Chemical Crystallography Group, the Industrial Group and the Physical Crystallography Group. The meeting was well attended, with 366 delegates from the four groups, supported by 20 exhibitors. The meeting also saw the retirement of the current BCA President, Elspeth Garman, who had completed her 3-year-term, and the unopposed election of David Keen from ISIS, as President for the term 2012–2015.

Monday and part of Tuesday were devoted to sessions run by the Young Crystallographers (graduate students and post-doctoral fellows within 5 years of completion of their doctoral programme), and consisted of invited plenary lectures and short (15 min) oral presentations. Kenneth Shankland of the University of Reading, UK, gave the first plenary talk entitled "Downhill all the way: an optimisation view of crystal structures from powders" in which he reviewed various global optimisation methods, and then described a novel approach that employs only a local minimisation algorithm. The second plenary by Robin Owen of the Diamond Light Source, Harwell, entitled "Seeing the full picture: combining crystallography with tomography and spectroscopy at I24", described the use of complementary experiments in structure determination from weakly diffracting or very small crystals. Of particular value in these experiments has been the high-flux microfocus and microbeam X-ray beamlines. In a Science Outreach session, Jessica Bland of the Royal Society, London, spoke on "Science in a social context". She looked into the recent history of public engagement with science in the UK, and described some of the more inventive initiatives.

Lynne Thomas of the University of Bath, UK, gave the Parkin Lecture (in honour of the late Dr Andrew Parkin's contribution to the Young Crystallographers Group) entitled "Piecing together the puzzle—multidimensional approaches". Desirable properties in molecular materials can often be accompanied by disorder in the solid state. This can take the form of static, orientational disorder or dynamic thermal motion and may be correlated over short distances, breaking the long range order. Disorder may appear within hydrogen-bonded systems, requiring quantum mechanical calculations to understand the behaviour of hydrogen atoms within these bonds. Solvent molecules contained within porous materials often show disorder because of weak interactions which hold them in place. Methods complementary to diffraction such as hot-stage microscopy, thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) have been applied to characterise such systems fully.

The Biological Structures Group plenary lecture "Structural Biology of the DNA Damage Response" was delivered by Laurence Pearl of the Genome Damage and Stability Centre, University of Sussex, UK. Understanding the structural basis of DNA damage responses is essential to understanding the process of carcinogenesis, and is also important to the development of new therapeutic approaches that take advantage of cancer-associated defects in DNA damage responses to achieve specific targeting of cancer cells. Professor Pearl discussed the attempts to understand the molecular basis for assembly, specificity and mechanism of the proteins and complexes that recognise incorrect bases, mediate repair of single-strand and double-strand DNA breaks, and trigger the DNA damage cell cycle checkpoint.

In honour of Dr Frank H. Allen (CCDC), Robin Taylor of Taylor Cheminformatics Software, Rickmansworth, UK gave the Chemical Crystallography Group's plenary talk



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"Predicting low energy conformations of small organic molecules: is crystal structure data redundant?" Reliable prediction of the low-energy conformations of organic molecules is critically important in, for example, computer-aided drug design. *Ab initio* (Hartree–Fock) and density functional methods are used for high throughput virtual screening, via docking or pharmacophore searching. The choice is between speed and accuracy, and to speed up computations, rigid bond angles are used which may result in unacceptable inter-atomic distances. Crystal structure data are used to filter out bad conformations using atom clash criteria, and to predict which intramolecular hydrogen bonds will occur in condensed phases, the latter achieved by reference to the intramolecular hydrogen bonds in the Cambridge Crystallographic Database, which even with some 600 000 entries is considered limited. The answer to the question posed in the title was—not yet!

In a most entertaining Industrial Group plenary lecture, the 2011 Chemistry Nobel Laureate Dan Shechtman, from Technion, Haifa, Israel and ISU, Ames, Iowa, USA, described his discovery, in 1982, of a material exhibiting an electron diffraction pattern with apparent fivefold symmetry. Rapidly cooled 2 μm grains of the metallic solid Al_6Mn showed icosahedral symmetry, something inconsistent with conventional crystallographic teaching. It was some 2 years before Shechtman was able to publish his seminal work in 1984, having had to endure ridicule and ostracism. His critics, including Linus Pauling, maintained that what Shechtman saw was a result of twinning. Larger crystals were grown, and Laue photographs confirmed the presence of fivefold, threefold and twofold axes, consistent with icosahedral symmetry. A period of grudging acceptance followed until in 1992 the definition of a crystal was modified, by the International Union of Crystallography, to accommodate aperiodicity. Since then, many other examples of quasi-crystals have been reported, but they are all metallic in nature. Among their physical properties they exhibit extreme hardness, poor heat and electrical conductivity, and like Teflon®, low surface friction. Applications are in surgical instruments and other stainless steel appliances. Professor Shechtman concluded his talk by encouraging scientists of all disciplines to show professionalism, courage, tenacity and self-belief when advancing a new concept that flies in the face of current scientific thinking.

The Physical Crystallography Group's teaching plenary, by Branton Campbell from Brigham Young University, Provo, Utah, USA, was entitled "Symmetry modes: Nature's favoured description of structural distortions". The traditional crystal structure is defined by its atomic coordinates. A distorted structure, however, can be parameterised in terms of its deviations from a known parent structure, and in this situation the symmetry modes of a distortion provide a distinct but equivalent set of structural parameters. Phase transitions tend to break parent symmetry in specific ways, and symmetry-motivated parameters allow one to distinguish a relatively small number of structural parameters that are active in a distortion, from those which are not. Software such as ISODISTORT allows one to simultaneously employ symmetry modes involving atomic displacements, lattice strains, magnetic moments, occupancy orderings and rigid body rotations, at both commensurate and incommensurate wave vectors.

An Industrial Group session entitled "Coatings" provided some interesting talks. The first: "Evaluation of Residual stresses in coatings by X-ray Diffraction" was presented by Raja Khan from the University of Birmingham. He discussed plasma electrolytic oxidation (PEO) coatings, an advanced form of anodizing. Stresses can be induced when the applied voltage exceeds a certain critical breakdown value and short lived micro-discharges occur, also leading to high temperature phases. The deposition process influences coating properties such as hardness, adhesion and wear resistance. Thick coatings on light alloys (Al) made by anodizing, plasma spray and PEO were compared. Applications include automotive piston crowns. As a method of measuring stress, XRD is easy to use and uniquely non-destructive with macro-stress giving peak shift, and micro-stress peak broadening. CrN coatings by physical vapour deposition (PVD) were also studied by grazing incidence XRD using a PANalytical Empyrean instrument with a 1° incident angle.

Mark Farnworth from Nippon Sheet Glass (NSG) focused on the evaluation of coatings on glass. He spoke briefly about Pilkington (the inventors of the float glass process) and their acquisition by NSG. Glass from a furnace is floated on a bath of molten tin, and a chemical vapour deposition (CVD) coating applied on-line in the float bath. This produces a very hard coating with columnar growth in the (200) direction of large SnO_2 grains, each made up of smaller crystallites. The grain sizes were measured using an SEM, with crystallite size determined by XRD and the Scherrer equation. Off-line sputtering is used to produce a coating with highly textured Ag and ZnO, with pole figures used to evaluate the texture of the Ag 111 reflection. X-ray reflectometry (XRR) was used in a sequence of scans of a complex multilayer stack of: glass/TiO_2/ZnO/Ag/ZrO_2/SnO_2/TiO_2, with samples taken as the coating was built up layer by layer, illustrating the sensitivity of the technique to changes in the layers. Modelling software is used to extract layer thickness, density, surface roughness and interface roughness. Finally, he showed how XRR and time of flight secondary ionisation mass spectrometry (ToFSIMS) could be used together, with the depth profiling capability of ToFSIMS calibrated against XRR data for each coating layer type.

A novel addition to the conference was a Performing Arts production entitled "Stilled", by Fevered Sleep, staged in the Warwick Arts Centre. A performance piece for adults, it was created by collaboration between Fevered Sleep and an "advisory team of X-ray Crystallographers". According to the advertising literature, it "weaved together dance, light, music and photography, creating a meditative cross-art form event exploring perception, movement and stillness". I watched the performance for 20 min, and in terms of crystallography, I feel that even Danny Shechtman would have struggled to describe its structure. It was certainly not periodic, not even aperiodic, but amorphous.

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