

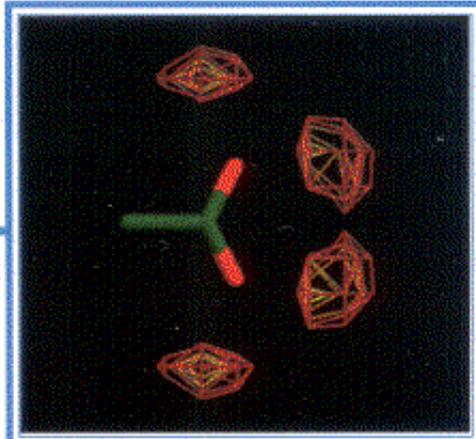
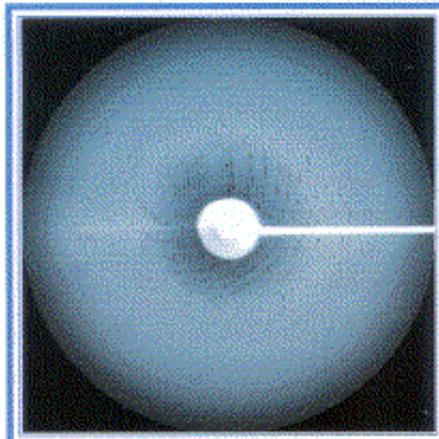


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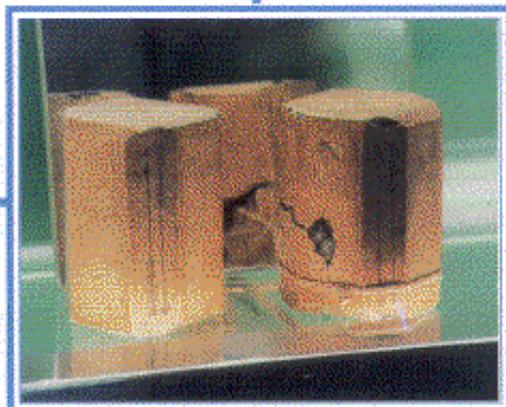
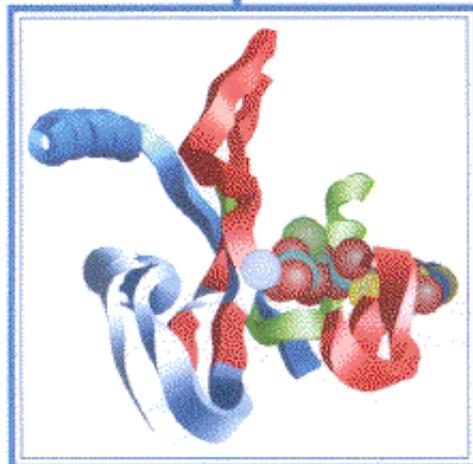
NEWSLETTER

Volume 7, Number 4 ♦ 1999



CRYSTALLOGRAPHY

**ACROSS THE
SCIENCES**





Henk Schenk

The last issue of the Newsletter already paid much attention to the very successful Congress in Glasgow, so I will be very brief. Scientifically and socially it was a great Congress, every day a feast! There were also a number of innovations, like the Closing Ceremony being part of the Farewell Party, the poster prize presentation, and the dance to very lively music! My congratulations go to our UK colleagues, especially to the two Chairs, Professors Judith Howard and Chris Gilmore!

The General Assembly in Glasgow had the difficult task of electing the next President from two candidates. Although the statutes of the IUCr provide for this possibility, there has never before been more than one candidate for this post, so this was an exceptional occasion. Indeed, for the candidates themselves it was also an exceptional experience as I can assure you. On Sunday evening, the day before the election, Hartmut Fues and I were having a beer together, discussing our chances and concluding that it was completely unclear which of us was going to win. I will never forget how surprised I was when Ted Baker told the General Assembly that in a close finish I had been elected President. I am glad that Hartmut

will remain a member of the Executive Committee and will be the Chair of the Sub-committee on the Union Calendar.

The few remaining days of the Congress went through my fingers as in a dream. To be President of the IUCr I feel is a great honour, not just for myself, but also for my very supportive colleagues in Amsterdam and for the Dutch crystallographic community. On my return from Glasgow my group had decorated my room and the lab, my family and friends had filled the house with a sea of flowers, and the congratulations were numerous and heart warming. So the dream was going on.

In the last three months the work has started. I have had my first meetings and many email conversations with the numerous people who work so hard to make our Union the strong organisation that it is. As a matter of course, I have seen in the last six years as an Executive Committee member how the IUCr retains its vitality through the enormous input of so many volunteers and through the enthusiastic competent professional staff in Chester. But as President the view on all that is going on is more intense and I am very much impressed by what I see. This is something we must treasure and maintain in the next century!

All that Ted Baker wrote in his last letter about the challenges for the IUCr and the 'I' in its name I endorse fully. I told the General Assembly that I also think that our so-

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Journals on-line

<http://journals.iucr.org>

ciety should make it clear to the rest of the world why we are so dedicated to and so enthusiastic about our profession. Through the Internet we have a real chance to reach the people easily. It is my intention to initiate an educational website about crystallography in many languages meant for primary school children, kids of 10 years old. They will be the University students of 2010 and enthusiastic young scientists, perhaps the crystallographers of 2020! You will hear more about this in future columns.

*Hendrick Schenk
hs@cryst.chem.uva.nl*

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On the Cover: Illustrations taken from the cover of the 50th anniversary publication of the International Union "Crystallography Across the Sciences" reflect the remarkable variety of areas to which crystallography makes a vital contribution.

Contributors: D. Balzar, P. Barnes, M. Bellotto, P.T. Beursken, U. Bismayer, R. Caram, K. Crennell, R. Delhez, M.T. Dove, P.F. Fewster, F. Frey, W. Fuller, E. Garman, J.M. Guss, A. Hewat, R. Hock, H. Klapper, A. Le Bail, B. LeBeck, P. Mallinson, P. McArdle, K.A.R. Mitchel, S. Popovic, R.J. Read, C. Ruiz-Pérez, H. Saibil, C. Sansom, A.L. Spek, A. Tonejc, M. Vijayan, D. Watkin, and R. Withers.

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Crystallography Across the Sciences

This issue of the Newsletter contains reports from the scientific sessions at the XVIII IUCr Congress in Glasgow, summaries of selected articles from recent issues of journals published by the IUCr, reports from national and international symposia and workshops sponsored by the IUCr in all parts of the world, information on resources for crystallography and news about and awards received by crystallographers.

The remarkable scope of applications of crystallography is reflected throughout the Newsletter and in the superb anthology "Crystallography Across the Sciences" the publication with which the IUCr celebrated its 50th anniversary. The cover illustrations of this issue of the Newsletter are taken from the book.

"Crystallography across the Sciences" is a rich collection of state of the art reports on advances and applications of crystallography in its myriad forms. The volume includes chapters by the ten plenary lecturers at the IUCr 50th anniversary sessions held in the US, Europe, and Asia in 1998 and a dozen other chapters by authorities in special areas of crystallography, ranging from small angle scattering and powder diffraction, to drug design and macromolecular structure. The book provides a crash course in where crystallography stands near the end of its first century. Every crystallographer, materials scientist, and structural biologist should have a copy of this book in their personal library. It also makes an excellent gift if you are invited to lecture on crystallography and want to present your host with a valuable reminder of your visit. Copies are available at IUCr headquarters in Chester.

Due to space limitation, only a few of the reports from the IUCr Congress are published in this issue. More will follow in future issues. All the reports that were filed (25) can be found on the IUCr website, together with photographs of the speakers in 90% of the sessions.

The format for presentation of highlights of recent IUCr publications has been revised in this issue of the Newsletter in order to identify their source clearly and provide full reference of the articles selected by the Editors for discussion.

This issue contains no Letters to the Editor. Either we are making fewer errors or our gentle readers have decided it's hopeless to try to correct us. This Newsletter is a forum for open communication among all crystallographers. Please let us hear from you. In particular, we would like to hear the opinion of the readers concerning the inclusion of highlights from Acta Cryst journals, reports of IUCr Commissions and essays on the current focus and future trends in crystallography.



Current and past issues of the *IUCr Newsletter* can be viewed on the web at

<http://www.hwi.buffalo.edu/iucr/>



BCA Spring Meeting

The BCA Spring meeting will be held April 3-5, 2000. As at previous meetings, there will be a Plenary session on Monday with speakers from each of the BCA interest groups. This year the Plenary session will be on Refinement. Session themes will include cellular assemblies, structural genomics, hot structures, software for chemical crystallography, crystal growth, pharmaceutical, specimen preparation, controlled environment x-ray diffraction, disordered materials. More information can be found on the BCA website at <http://gordon.cryst.bbk.ac.uk/BCA/meets/BCA00.html>.

Imaging of the Helical Arrangement of Cellulose Fibrils in Wood by Microfocus X-ray Diffraction

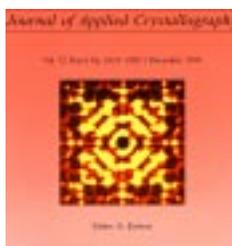
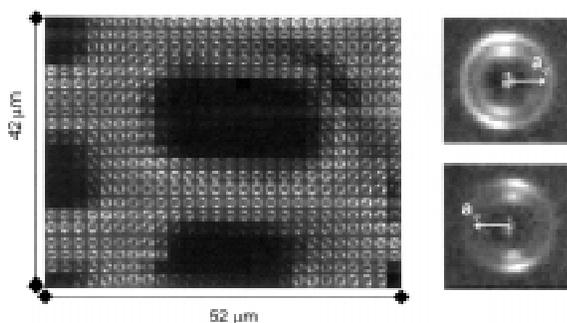
J. Appl. Cryst. **32** (1999), 1127-1133

Third-generation X-ray synchrotron sources with microfocusing optics can provide information about structural variation in partially ordered materials with a resolution of ~ 1 micron. Early examples of the exploitation of this capability using the microfocus beamline ID13 at the European Synchrotron Radiation Facility, Grenoble, France allowed variation in polymer orientation and crystallinity across a spherulite of Biopol [Mahendrasingam et al., *J. Synchrotron Rad.* **2** (1995), 308] and across the wall of a "Coke" bottle [Martin et al., *J. Synchrotron Rad.* **4** (1997), 223] to be determined. Lichtenegger et al. [*J. Appl. Cryst.* **32** (1999), 1127-1133] have recently reported an extremely interesting development of this approach in which a nonstandard fibre diffraction geometry has been used to characterize the local orientation of cellulose fibrils in wood.

X-ray diffraction patterns were recorded with a wavelength of 0.78 \AA from cross-sections ~ 10 microns thick oriented perpendicular to the X-ray beam. The figure shows a two-dimensional array of 21×26 diffraction patterns recorded as the specimen was systematically stepped across the X-ray beam with a step size in each direction of 2 microns. The relative position of cell walls containing ordered cellulose fibrils gives rise to the well-defined X-ray fibre diffraction patterns illustrated in the figure. The dark regions in the matrix correspond to the region of intervening lumina. The two typical diffraction patterns displayed at higher magnification show a striking asymmetry which contrasts with the symmetry about the meridional axis typical of fibre diffraction patterns. This asymmetry was used to determine local fibril orientation and hence to trace the path of cellulose spirals through the specimen.

As the authors state, the technique is most interesting and powerful because it provides information about two length scales simultaneously, i.e., on the micrometric scale through the positional resolution of the scan of ~ 2 microns and on the nanometre scale through the diffraction patterns recorded at each point. The approach developed in these studies, and in particular the extensive mathematical description of the diffraction geometry for this type of sample, can be expected to have wide applications in the investigation of texture in industrial polymer materials and in the characterization of structural hierarchies in biological materials where the dimensions of ordered domains are comparable to the diameter of the X-ray beam.

Watson Fuller, Keele U., Staffordshire, UK



Combined Experimental Techniques and Glass Ceramics

J. Appl. Cryst. **32** (1999), 1090-1099

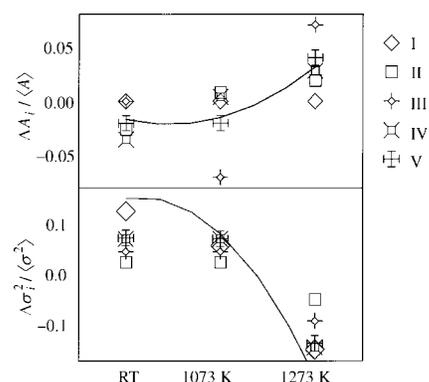
Mass produced glass and glass ceramics are found everywhere in our daily lives. The glass-making industry has accumulated a wealth of knowledge – often empirically – about glass recipes and manufacturing processes. Despite the technological importance and widespread use of these materials in everyday use as well as high-technology applications, the detailed atomic structure of many-component glasses is often not well known and the processes governing their formation are not understood on a microscopic scale.

To gain insight into the atomic structure of crystalline matter, diffraction techniques and absorption spectroscopy are routinely combined. A problem arises in composite materials where the pair correlation function $g(r)$ is the sum of convolution products between the individual partial pair correlation functions of the atomic constituents. Thus the information obtained from single measurements is difficult – if not impossible – to interpret without ambiguity.

Element contrast variation by resonant scattering of X-rays, scattering length differences related to isotope variation for neutrons and contrast enhancement with polarized neutrons can help to solve the problem. Using anomalous small-angle X-ray scattering and differential anomalous wide-angle scattering experiments at an absorption edge of elements in the glass, the individual partial pair correlation functions of these elements become accessible.

Recently, such a "multitechnique approach" was successfully adopted for the study of the devitrification and recrystallization phenomena in the systems $\text{MgO-Al}_2\text{O}_3\text{-SiO}_2$ doped with the nucleants TiO_2 and ZrO_2 ["Phase Formation Kinetics in a Glass Ceramic Studied by Small-Angle Scattering of X-rays and Neutrons and by Visible-Light Scattering", U. Lembke, R. Brückner, R. Kranold & Th. Höche, *J. Appl. Cryst.* **30** (1997), 1056-1064] and in the as-quenched $\text{CaO-SiO}_2\text{-ZrO}_2$ glass ceramic ["Differential anomalous wide-angle X-ray scattering and X-ray absorption experiments to investigate the formation of glass ceramics in the $\text{CaO-SiO}_2\text{-ZrO}_2$ system", C. Meneghini, A.F. Gualtieri & C. Siligardi, *J. Appl. Cryst.* **32** (1999), 1090-1099].

Combinations of resonant and nonresonant small-angle scattering experiments (SAX, ASAX, SANS), transmission electron microscopy, electron microprobe analysis (EDX) and visible-light scattering, X-ray absorption spectroscopy (EXAFS)

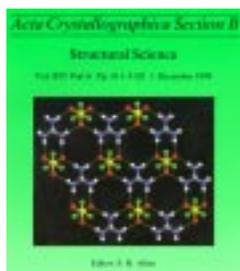


Structural modifications in a $\text{CaO-SiO}_2\text{-ZrO}_2$ glass ceramic as a function of annealing temperature. The devitrification of the system is accompanied by a decrease of the Debye-Waller factors with increasing temperature, indicating that a progressive re-ordering occurs in the bulk glass matrix. The Zr-Si and Zr-Zr coordination numbers increase, indicating a progressive ordering of the Zr environment with temperature.

and differential anomalous X-ray scattering experiments led to a detailed picture of the crystallization routes for the two oxide systems. Special attention was paid to the role of ZrO_2 and TiO_2 additives in the nucleation of crystalline phases. The articles by Meneghini *et al.* and Lembke *et al.* show impressively the high level of detailed structural information about the formation of glass ceramics that can be achieved through a combination of experimental techniques where element contrast variation plays a key role.

Rainer Hock, U. of Erlangen, Germany

The Powder Diffraction Handicap



Acta Cryst. **B55** (1999), 1068-1074

Acta Cryst. **B55** (1999), 1075-1089

With almost 400 *ab initio* structure determinations reported, powder diffraction is healthier than ever. In the last 10 years, a proliferation of new methods has extended our capability to extract detailed structural information from powder patterns. Two recent papers in *Acta*

Cryst. B illustrate the strength of current methods.

The classical approach, Patterson and direct methods applied to the extracted “ $|F_{\text{obs}}|$ ”, accounts for three-quarters of powder diffraction studies, but the most active area of research involves locating molecular fragments in known crystalline cells. Methods that use either a systematic grid search or a Monte Carlo calculation, simulated annealing and genetic algorithms have been applied successfully to nearly 50 powder patterns. A good example of such an application is described by Tremayne *et al.* [“2,4,6-Triisopropylbenzenesulfonamide: Monte Carlo structure solution from X-ray powder diffraction data for a molecular system containing four independent asymmetric rotors”, *Acta Cryst.* **B55** (1999), 1068-1074], who used the OCTOPUS program. The difficulty of application depends upon the number of degrees of freedom that a structure has, and increases with each independent torsion angle. Analogous single-crystal methods use Patterson and/or direct methods to position rigid models (e.g., PATSEE or DIRDIF programs). Because of reflection overlap – the powder diffraction handicap – the use of direct-space data is required to determine the position and conformation of a model.

The solution of a structure with unknown cell parameters using *ab initio* packing calculations is much more difficult. There are few successful applications of this approach, which requires previous knowledge of a quasi-complete molecule. In their paper, Karfunkel *et al.* [“Local similarity in organic crystals and the non-uniqueness of X-ray powder patterns”, *Acta Cryst.* **B55** (1999), 1075-1089] elucidate the crystal structure of some diketopyrrolopyrrole derivatives with surprisingly similar powder patterns, and introduce two new concepts for molecular solids, “local similarity” and “boundary-preserving isometry”. The degree of difficulty of indexing powder patterns is related to the complexity/resolution ratio. Crystallinity may strongly affect resolution. Poorly resolved powder patterns increase the ambiguity and decrease the accuracy of a structural model. The ability of distinctly different models to fit a powder pattern equally

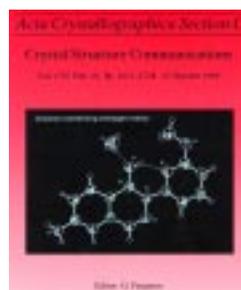
well is a recurring problem.

Owing to its one-dimensional nature, powder diffraction is less reliable than single-crystal analysis. Both of these articles address this problem. The high R factor in the Monte Carlo study ($R_F = 0.10$ for 517 reflections, 143 refined parameters, 120 geometrical restraints) suggests a problem with the model (a “local similarity” problem?) or the data. How wrong can structures determined from powder data be? The same question may be addressed to all underdetermined structural problems, including proteins, some of which are also being examined by powder diffraction!

The one-dimensional nature of powder diffraction will never be overcome. Consequently, a single-crystal study is always preferable to a powder study, when possible. The failure to obtain single crystals of many materials is the driving force behind the powder diffractionists’ quest for innovation. New methods such as those described in these articles (or at least those that are affordable, see <http://sdpd.univ-lemans.fr/iniref/progmeth.html>) may well stimulate crystallography as a whole.

Armelle Le Bail, U. du Maine, Le Mans, France

Twinning in Chemical Crystallography: New Solution to an Old Problem



Acta Cryst. **C55** (1999), 1774-1775

The cover of the November issue of *Acta Cryst. C* features a relatively simple germanium complex. Although interesting from a chemical point of view [for details see K. Hensen, A. Faber and M. Bolte, *Acta Cryst.* **C55** (1999), 1774-1775], the structure determination is of particular interest because it illustrates a solution to an old crystallographic riddle. The challenge being to sort out the twinning problem that hampered structure determination and refinement.

Twinning is an old subject with known solutions. A number of software packages provide (partial) solutions for the refinement of twinned structures (e.g., CRYSTALS, D. Watkin *et al.* and RAELS, A.D. Rae). Recently relatively easy-to-use tools for the refinement of structures based on overlapping reflection data due to twinning have become available e.g., in the widely distributed SHELXL97 program (G.M. Sheldrick) and its commercial incarnation SHELXTL.

Twinning comes in many disguises. The structure highlighted here is of the non-merohedral twin index 5 variety. Formerly, crystals like this one would usually have been discarded. Nowadays, with CCD detector systems, indexing and data collection are only slightly more troublesome for twin crystals than for routine applications. The availability of both will mean that fewer potentially interesting structural investigations on otherwise well reflecting samples will be abandoned prematurely because of twinning problems.

The current study provides an excellent example of what a professional crystallographer can do with state-of-the-art hardware and software.

A.L. Spek, Bijvoet, Utrecht U., The Netherlands



The Ewald Prize

At the opening ceremony of the XVII IUCr Congress in Glasgow, the Ewald Prize was awarded to Professor G.N. Ramachandran for fundamental contributions in the area of anomalous scattering, and the phase problem, the analysis of the structure of fibres, and the conformational analysis of macromolecular structures.

G.N. Ramachandran was born in 1922 in Kerala, a southern Indian state. He obtained his first degree in Madras and went on to pursue a Masters degree in electrical engineering at the Indian Inst. of Science in Bangalore. In Bangalore, the Nobel Laureate, C.V. Raman, urged Ramachandran to pursue a career in physics. (Raman told the Professor of Electrical Engineering that Ramachandran was simply too bright to be an electrical engineer). Ramachandran earned his M.Sc. and D.Sc. degrees with Raman working on the X-ray topography of diamond. In 1947, he went to Cambridge where he measured elastic constants using diffuse X-ray scattering.

Ramachandran returned to India and over the next 30 to 40 years, he established leading research centres of crystallography and structural biology at Madras and Bangalore. In 1952, at the suggestion of J.D. Bernal, he took up the fibre diffraction analysis of collagen and produced important early models of the structure. This modelling exercise led to a thoughtful analysis of the relationship between peptide and amino acid conformations in protein secondary structure. This analysis led to his most widely applied contribution, the Ramachandran Plot used universally to characterize protein conformations and evaluate the accuracy of protein structure determinations.

In 1956, with S. Raman, Ramachandran derived formula for calculating phase angles using Bijvoet differences that were successfully used to solve several crystal structures. Ramachandran made significant contributions to the use of Fourier transforms in structure determination. He wrote "Fourier Methods in Crystallography" with Srinivasan. Ramachandran established a remarkable scientific tradition, that thrives in the world, in India and in the two research schools he founded.

Paul Barnes and M. Vijayan

Cryo Preservation and Decay

Opening the session on cryo-preservation methods, D. Thiel (Cornell) explained that even at cryo temperatures all crystals are mortal, that fully focused undulator radiation is lethal, that determination of cryo conditions can be problematic, particularly for membrane protein and virus crystals, and that damage mechanisms are not completely understood. G. Bunick (Oak Ridge) described the technique of crystal annealing. If cryo cooling has reduced room temperature mosaicity, crystals may be warmed to room temperature in their crystallization media for 3 minutes and flash cooled with partial recovery of the original mosaicity. S. McSweeney (EMBL-Grenoble) presented a systematic study of the structural changes induced in acetylcholinesterase by radiation damage. Successive data sets were collected from the same crystal and the structures from each were refined. The unit cell gradually increased and the molecules in the cell rotated and translated as damage increased. Disulphide bonds broke first. The study raised important questions concerning dose rate effects and the use of free-radical scavengers.

The physical processes involved when an x-ray loses energy in a crystal were reviewed by C. Nave (Daresbury), who presented his model calculations on beam heating of frozen crystals. Initially, the temperature rises a few degrees but quickly levels off. T. Tsukihara

continued on page 9

An extensive summary of G.N. Ramachandran's scientific career and accomplishments was presented by M. Vijayan at the award ceremony in Glasgow. The complete text appears on the IUCr Newsletter website

<http://www.hwi.buffalo.edu/iucr/>

(Osaka) reported the cryo-conditions and structure determination of the membrane protein cytochrome c oxidase. A combination of 5% PEG 4000 and 35% glycerol and a slow cooling protocol in a sealed capillary tube resulted in lower mosaic spread and higher quality diffraction than fast cooling in a loop. L. Liljas (Uppsala) described the structure of cricket paralysis virus from a frozen crystal despite significant problems in scaling the data due to a sudden decrease in the unit cell size during data collection.

Elsbeth Garman (Oxford), Co-Chair 05.0B

30 Years Of Rietveld Refinement

100 people queuing outside the lecture theatre were unable to get in to hear Hugo Rietveld, inventor of Rietveld Refinement that revolutionised powder diffraction. Hugo outlined development of the method from his early days at the U. of Western Australia to work on neutron structures of uranium compounds and heavy metal ceramics at the Netherlands Energy Research Foundation ECN in Petten .

A. Hewat took up the neutron story showing how primitive the original diffractometers were, even at the new European High Flux Reactor (ILL). Today's instruments have large position sensitive detectors capable of collecting all available neutrons. Powder diffraction, has had more impact than most other neutron techniques, from the study of charge reservoirs in oxide superconductors, to the structures of giant magneto-resistive ceramics.

F. Izumi showed how incommensurable structures could be refined, and described a new computer program, REMEDY combining Rietveld and Maximum Entropy techniques to increase real space resolution. He gave examples of complex spin-ladder oxide superconductors, and other inorganic materials.

D. Louer described the contribution of automatic indexing and structure solution from powders to the transformation of the study of solid state chemistry.

Finally, A. Fitch showed how increased resolution from high intensity synchrotron radiation reveals the precise line positions needed for automatic indexing, and crystal symmetry and superstructure identification. Synchrotron radiation has become a very powerful tool for the almost automatic solution of unknown structures from very small quantities of powder, and an ideal complement to neutron Rietveld refinement.

Alan Hewat



30 Years of Rietveld session speakers (left to right) are: Fujio Izumi, Hugo Rietveld, Alan Hewat, Daniel Louer, Andy Fitch.

Micro Structure and Texture of Real Materials

The microsposium included talks on size and grain distributions in crystallites, local defect structures, short-range order, stripe structures, local textures, residual strains in metal/matrix composites, strain gradients in multilayer systems, cone-like carbon or boron nitride structures forming nanotubes, and microstructures due to plastic deformation. Different systems and compounds and the relationship of structures to material properties were presented, experimental and analytical methods were explained and prospects for the future were offered. V. Massarotti described tuning ceramic oxides properties with synthesis conditions. S. Billinge showed how to exploit the total scattering pattern to study cuprates with stripe-like microstructures and mixed valence manganites where localized and delocalized phases coexist. The use of synchrotron radiation to investigate phase, purity, texture, and grain alignment in thin Bi-Sr-Ca-Cu-O tapes was outlined by H. Poulsen. The use of synchrotron microbeam lines for structural analysis of plastically deformed materials was demonstrated by M. Drakopoulos. L. Bourgeois described nano-cones, tubes, helices and hats formed by sheets of BN or carbon revealing the close relation between ring-like defects and superconductivity.

E.Frey

Macromolecular Electron Microscopy

This session included talks on isolated macromolecular complexes in solution and in two-dimensional crystals. The single particle field has been developing rapidly and is a remarkable topic for the IUCr, since it does not involve crystallography, except in the sense that 3D alignment of randomly oriented complexes is crystallization in the computer. B. V. V. Prasad presented a structural analysis of rotavirus, a double-shelled virus caught in the process of transcribing and releasing its RNA through the 5-fold vertices of its icosahedral shell. With a series of low resolution reconstructions of different states of the chaperonin GroEL, H. Saibil mapped out the domain rotations in the ATPase cycle and interpreted them by docking domain structures into the EM maps. At 10 Å resolution, a new inter-ring contact, involved in negative cooperativity, was seen in GroEL-ATP. B. Bottcher described elucidating the first complete secondary structure for a protein in a single particle complex. The 7.4 Å resolution map of Hepatitis B virus core particles revealed the fold of the α -helical capsid protein, recently confirmed by an X-ray crystallographic structure.

Moving to electron crystallography, V. Unger presented the structure of a gap junction at 7 Å resolution, with two hexameric rings forming a channel across two cell membranes. The transmembrane regions were clearly identified as 4-helix segments, and a plausible model was built with a large β -barrel forming the extracellular seal of the channel. High quality image phase maps allowed a complete secondary structure determination of the tubulin dimer described by E. Nogales at 3.7 Å resolution with the localization of bound GTP and taxol. The fold is close to that of the bacterial protein, whose structure was determined crystallographically.

Helen Saibil

X-ray and Neutron Complementarity

The complementary of X-ray and neutron diffraction was illustrated throughout the session, beginning with a study of magnetism in an anomalously non-supercon-

ducting member of the $(RE)Ba_2Cu_3O_{6+x}$ series. The elemental specificity of resonant X-ray magnetic scattering showed unambiguously that when $RE = Pr$ the structure is ordered. This led to the discovery of incommensurate modulation which energy resolved neutron magnetic scattering revealed to be static. A talk on spherical neutron polarimetry described measurement of sixteen quantities related to the sixteen independent correlation functions involved in the most general mixed nuclear/magnetic neutron scattering process.

An enlightening study by small angle neutron and X-ray scattering (SANS and SAX) of block copolymer micelles emphasized isotope effects. Optimal information on structure is obtained by SANS from neutron contrast variation measurements. Using pure deuterated or hydrogenated solvent, the core and the corona can be measured separately, while mixtures provide information on the interference term.

A highly efficient neutron imaging plate with a dynamic range of $1:10^5$ and spatial resolution of less than 0.2 mm was described.

Bente LeBeck

Industrial Analysis On-Line

This microsymposium dealt with a wide range of industrial applications of X-ray analysis including on-line production control and process optimization. C. Small (Rolls Royce) described the development of an inspection technique of single-crystal turbine blade orientation based on back-reflection Laue geometry. M. Halliwell, (Philips Analytical) talked about routine measurements of hetero-epitaxial layers, and the most recent advances in automatic fitting procedures. B. Rebours (Inst. Français du Pétrole) introduced the use of XRD for process optimization in the petro-chemical industry and heterogeneous catalysis. Applications of on-line XRD for process control in the cement and mining industries were described by M. Bellotto (CTG Italcementi Group). Finally, the importance of high-resolution XRD to



Macromolecular Structure by Electron Microscopy speakers. (left to right) Eva Nogales, Helen Saibil, B.V.V. Prasad, Bettina Bottcher, Vinzenz Unger, Richard Henderson

improved device performance, process control and product yield of InP-based fiber-optic communication lasers was discussed by J. Vandenberg (Lucent Technologies), who brilliantly showed the interplay between the analytical techniques and the priorities dictated by production.

Maurizio Bellotto

Interfaces, Thin Films, Multilayers

I. Kegel (Munich) described the information that can be extracted from semiconductor quantum dots, including vertical ordering in periodic structures and the composition of nanometre scale features. Composition is obtained from measurement of the strain and interference effects of the dot and the underlying substrate, using the variable penetration of grazing incidence scattering. R. Cowley (Oxford) discussed the measurement of roughness at metallic and semiconductor epitaxial interfaces. For Nb on sapphire the roughness worsened with increasing thickness, yet the measured correlation length is increased suggesting that short correlation lengths are well maintained close to the interface. For GaSb on GaAs he found a regular array of dislocations which differ in orthogonal directions indicative of orthorhombic distortion in GaSb.

M. Sanyal (Calcutta) discussed retrieving electron density profiles from specular reflectometry scans using Fourier and iterative fitting methods. Applications to semiconductors and Langmuir-Blodgett multilayers were presented including in-depth analyses of lateral correlation lengths. I. Vartanyants (Moscow) presented new developments in reconstructing surface mor-

phology using highly coherent X-ray sources. For a normal source the profile from rough surfaces will be broad and smooth, whereas for a coherent source this will become very jagged due to interference. R. Feidenhans'l (Risø) illustrated methods of analysing interfacial structures from directly bonded Si wafers where small twists create moire patterns or periodic arrays of dislocations and satellites. The satellite structure factors are fitted to a model and the detailed atomic structure can be obtained.

Paul F Fewster

Macromolecular Phasing

Macromolecular crystallographers are united by problems that plague the molecular replacement technique (multiple copies of a molecule, high crystallographic or non-crystallographic symmetry, and low homology). J. Navaza discussed combating the problem of high non-crystallographic symmetry, by exploiting the prior information available from self-rotation and Patterson functions. In complementary work, R. Read showed that likelihood functions give a much clearer indication of the correct answer than conventional scores, particularly for poor or incomplete models.

Two talks described phase information that can be gained by averaging multiple images of a structure, either through non-crystallographic symmetry or multiple crystals. K. Cowtan described combining data from a crystal at room temperature and the same crystal at cryogenic temperatures, showing how changes in cell dimensions can give useful phase information. J. Wang presented an example where 14-fold non-crystallographic symmetry was used to generate an excellent map from nearly random phases.

Finally, Q. Shen gave a lucid explanation of 3-beam X-ray diffraction and the use of a reference beam geometry to collect 3-beam data. In favourable cases, the resulting profiles give clear indications of triplet phases, which can be used in conjunction with direct methods programs to give clear electron density maps.

Randy J. Read

Phase Transitions

The microsposium opened with a de-

scription of the combination of quantum mechanical density functional theory and statistical thermodynamics to the study of the fcc-bcc Bain transformation (K. Schwartz, Austria). Other presentations concerned the crystal chemistry, displacive flexibility, and susceptibility to phase transformation of framework structures and compositionally flexible solid solutions (R. Withers, Australia), domain textures associated with ferroelastic phase transformations, the nano-structure of twin boundaries and their effect on physical properties such as ion transport along twin walls (E. Salje, UK), modulated phases of BCCD and the anharmonicity of the associated atomic modulation functions (O. Hernandez, France), and investigations of a high pressure incommensurate to normal structural phase transition in akermanite at ~ 1.7 GPa (R. Angel, Germany).

Ray Withers/Ulrich Bismayer

Applications of Line Broadening

Line-broadening analysis is a small but lively field of crystallography. There is an increasing interest in the simultaneous analysis of a number of technologically important properties of polycrystalline materials, e.g. dislocation densities and configurations, planar defects, such as stacking and twin faults, and crystallite size and shape. Simultaneous measurement of these properties is possible because of the increasing ease of modeling the full powder pattern directly. E.J. Mittemeijer (Germany) opened the session with a talk on diffraction-line broadening by lattice imperfections. The next two lectures focused on size-related and strain-related aspects of diffraction line broadening. J.I. Langford (UK) discussed the influence of a crystallite size distribution on size-broadened profiles, focusing on a log-normal distribution. T. Ungar (Hungary) gave an overview of anisotropic broadening by dislocations and emphasized the connection between the Warren-Averbach type of analysis with analysis of dislocation densities. P.W.

Stephens (New York) told of a novel approach to model the anisotropic line broadening in Rietveld programs, applicable to the general case of triclinic symmetry. D. Balzar (Colorado) described an application of diffraction line-broadening analysis to a problem of nuclear reactor containment-vessel embrittlement.

Davor Balzar and Robert Delhez

Metalloproteins, Electron Transport and EXAFS

Presentations ranged from the use of time-resolved methods in single crystal diffraction to the complementary roles played by crystallography and EXAFS in determining the structures of the metal centres in metalloproteins. I. Schlichting (Germany) described the structure of the ternary complex between P450cam/camphor/dioxygen, formed by co-crystallisation with camphor, chemical reduction, and then oxygen diffusion, and a structure of a reaction intermediate. S. Ramaswamy (Sweden) described the structure of naphthalene dioxygenase, where the initial structure surprisingly contained a reaction intermediate; an indole covalently linked to dioxygen bonded to the active site iron. Following refinement of purification protocols, an "empty" active site was achieved, and the product could be soaked into the crystals, leading to the conclusion that during the reaction indole binds before dioxygen. H. Freeman (Australia) spoke

continued on page 14



Speakers in the Phase Transitions session, back row (left to right) Karlheinz Schwarz, Ekhard K.H. Salje, Ray Withers, Olivier Hernandez. Sitting in front are: Ulrich Bismayer (left) and Ross Angel (right).

about using polarised Fe K-edge X-ray absorption spectroscopy with oriented carbonmonoxy-myoglobin crystals to obtain accurate angular geometries between the ligand and metal centre that could be used to restrain metal-ligand angles in single crystal X-ray structures. G. George (Stanford, USA) highlighted the difficulties of interpreting X-ray crystal structures with reference to spectroscopic techniques. In the case of formaldehyde ferredoxin oxidoreductase, a tungsten containing enzyme, EXAFS suggested the presence of two W-oxo ligand interactions, whereas the crystal structure only had one in the model. Re-examination of the electron density suggested the presence of the second interaction. S. S. Hasnain (Daresbury, UK) demonstrated the complementarity of EXAFS and single crystal X-ray crystallographic studies of nitrite reductase, Cu,Zn superoxide dismutase (SOD) and rusticyanin. EXAFS and single crystal structures showed that nitrite reductase was incapable of binding substrate or inhibitors, subsequent to an electron transfer between the two copper ion sites in the enzyme. Therefore, substrate nitrite must bind to the enzyme prior to electron transfer.

J. Mitchell Guss



Prizes for the best poster at the IUCr Congress in Glasgow sponsored by the Cambridge Crystallographic Data Center were awarded to: **Peter Muller**, Germany (*Holes in Crystals?*); **Alicia Beatty** and Christer Aakeroy, USA (*Beyond the first dimension: hybrid materials assembled via H-bonds*); **C. Baehtz** and H. Fuess (*Tetrathiafulvalene and tetracyano-p-quinodimethane in faujasite*) and **S. Leoni** & R. Nesper, Switzerland (*Tilings on hyperbolic surfaces*). Judith Howard and Steve Maginn (front row) presented the prizes to Muller, Leoni, Beatty and Fuess (accepting for Baehtz) (back row).

**For full reports on sessions included in this issue and other sessions
visit our website <http://www.hwi.buffalo.edu/iucr>**

50th Anniversary of the Biomolecular Structure Lab

The Biomolecular Research Lab at Birkbeck College was opened on July 1, 1948 by Sir Lawrence Bragg. A meeting to celebrate the 50th anniversary of the event was held in **November, 1998**. Speakers, all associated with the College, reminisced about 'old times' and described their current research.

A. Mackay described Bernal's work in Cambridge. J. Finney talked about his work on the structure of water, including the newly discovered phase (VII). R. Stroud discussed structures of the recognition particle responsible for targeting membrane and secreted proteins to the endoplasmic reticulum during their synthesis. The contrast between the primitive equipment used by Bernal's group and the facilities available to modern structural biologists was emphasized by P. Lindley, director of the European Synchrotron Radiation Source (ESRF). K. Holmes, (Max Planck Inst. for Medical Research in Heidelberg) described complexes between the muscle proteins actin and myosin. A. Klug described designing a protein specifically to bind to a particular sequence of DNA bases, such as those which result from cancer-causing mutations. C. Chothia of the MRC Lab of Molecular Biology, Cambridge, and A. Sali of Rockefeller U., New York, addressed the challenge of predicting the structures of the protein products of all the genes in a microbial genome. L. Pearl described the mechanism of DNA repair. T. Blundell gave industrial and academic views of structural based drug discovery and design.

Bernal's interests were not limited to science; he was also interested in the Arts and politics. Many eminent peace campaigners were entertained in his top floor flat above the lab, including Pablo Picasso who painted a mural on the wall.

*Clare Sansom and Kate Crennell
From BCA Newsletter, March, 1999*

Tenerife School

Scientists and students from Russia, Belgium, Cuba, Czech Republic, France, Germany, Italy, Rumania, Spain, USA, and

Yugoslavia attended the fifth School on New Trends in Material Science, *Direct Methods Perspectives: From Small Molecules to Proteins* held at the U. of La Laguna (Tenerife, Spain) **March, 1999**.

Lectures covered topics ranging from basic direct-methods theory to advanced subjects such as protein substructure applications. The practical computing sessions demonstrated the use of the SIR99, SHELXD, and SnB v2.0. Lecture notes were distributed and students were encouraged to bring problems.

The school was supervised by C. Ruiz-Pérez, and the lecturers included C. Giacovazzo (Bari, Italy), G. Sheldrick (Göttingen, Germany), X. Solans (Barcelona, Spain) and C. Weeks (Buffalo, USA). The school was made possible by the financial support of the U. of La Laguna and the Cabildo Insular de Tenerife, the enthusiasm of the La Laguna LOC, and the dedication of Dr. González-Platas.

The 6th School "New Trends in Material Science: Computational Methods in Powder Diffraction" will be held July 2-8, 2000 in La Laguna. For information contact C. Ruiz-Pérez, Dpto de Física Fundamental II, U. of La Laguna, E-38204 La Laguna, Tenerife, Spain; e-mail: caruiz@ull.es.

Catalina Ruiz-Pérez

Croatian-Slovenian Crystallography

The eighth annual joint meeting of the Croatian Crystallographic Assn and the Slovenian Crystallographic Society took place in **June, 1999**, at the hotel Istra on a small island in the Mediterranean. The meeting was held under the auspices of the Croatian Academy of Sciences and Arts, and was sponsored by the Ministry of Science of the Republic of Croatia; Pliva, Pharmaceutical, Chemical, Food and Cosmetic Industry, (Croatia); Renacon, (Croatia), a representative of Philips Analytical; SCAN, (Slovenia), a representative of JEOL and Oxford Instruments MAG; Bruker AXS, (Austria); Molecular Structure Corp., (UK); and Hotel Sol Club Istra, (Croatia).

The topics of the meeting were chemical, physical, biological and applied crystallography and mineralogy. 80 participants from eleven countries, presented short oral contributions. Plenary lectures concerned: The chemistry and evolution of the catalytic struc-



Attendees and speakers at the Tenerife School

tures in serine hydrolases (G.G. Dodson, UK); Modern perspectives in XRD studies of minerals (D. Yu. Pushcharovsky, Russia); GPD-4-keto-6-deoxy-D-mannose epimerase/reductase, a key enzyme in the biosynthesis of activated L-fucose (M. Bolognesi et al., Italy); Ionic fluorides in soluble organometallics (A. Demsar, Slovenia); and Metal saccharinates and their complexes with N-donating bases (G. Jovanovski, Macedonia).

A half-day boat excursion visited an aquarium at the Centre of Marine Research, Rovinj, and a 10 km fjord, called the Limski Kanal. While on board the boat, the participants enjoyed grilled fish, Istrian wine, and a magnificent sunset.

The ninth conference will be held in June, 2000, in the Republic of Slovenia. For information contact I. Leban in Ljubljana (ivan.leban@uni-lj.si)

*A. Tonejc, Chair of the Organizing Comm.
S. Popovic, Sec. of Croatian Cryst. Assn*

Crystal Growth and Materials in Brazil

This School, held in **July, 1999** at the State U. of Campinas, SP-Brazil was organized by the Sociedade Brasileira de Crescimento des Cristais (SBCC) (R. Caram, U. of Campinas, and S. Baldochi,

U. of Sao Paulo), and the IUCr Commission on Crystal Growth and Characterisation of Materials. The SBCC was founded in 1993 and has held national schools in this field in order to establish and develop the young Brazilian crystal growth community.

The majority of the 90 young scientists participated in the School came from Brazil with smaller groups from Argentina and Uruguay. Lecture titles included: *Thermodynamic Fundamentals* (P. Rudolph, Germany), *Course of Thermal Analysis* (S. Gama, Brazil), *Cellular and Dendritic Growth* (O. Mesquita/Brazil), *Interface Kinetics* (P. Rudolph/Germany), *Growth of Compound Semiconductors from Melt* (R. Fornari/Italy), *Oxide Crystal Growth* (T. Fukuda/Japan), *Solution Growth* (H. Klapper/Germany), *Transmission Electron Microscopy* (D. Ugarte/Brazil), *Modelling of Heat and Mass Transfer* (F. Dupret/Belgium), *Kinetics of Glass Formation* (E.D. Zanotto/Brazil), *Protein Crystal Growth* (K. Balzuweit/Brazil), *Crystal Growth for New Future Functional Devices* (T. Fukuda/Japan), *Elementary Growth Process of MBE* (T. Nishinaga/Japan), *Defect Characterization and X-Ray Topography* (H. Klapper/Germany), *Vapour Phase Epitaxy of GaN for Blue LEDs and Lasers* (R. Fornari, Italy), *Atomic-Force Microscopy* (N.B. Costa/Brazil) and *Microchannel Epitaxy* (T. Nishinaga/Japan).

There were excursions to the Crystal Growth Laboratories of



Organizers and lecturers of the *International School on Crystal Growth and Advanced Materials* on the campus of the University of Campinas. From left to right: P. Rudolph, R. Fornari, K. Balzuweit, R.R. Chaves, S. Baldochi, H. Klapper, R. Caram, T. Nishinaga.

the Universities of Campinas and Sao Paulo, the National Synchrotron Light Laboratory (with a 1.37 GeV electron storage ring) and the National Laboratory of Electron Microscopy, near Campinas U. The laboratories are supported by the Brazil Ministry of Science and Technology and offer free use of their experimental facilities to users from all parts of the world.

A Proceedings was distributed and a poster session featured the work of the participants. The School was a great scientific success due to the excellent organization and the eager cooperation of the young participants.

Helmut Klapper, Rubens Caram

Surface Structure

The Sixth Int'l Conference on the Structure of Surfaces (ICSOS-6), held at the U. of British Columbia in **July 1999**, covered the atomic-level structure of solid surfaces, and the role of surface and interfacial structure in influencing the properties of technologically-important materials. A special theme concerned surfaces of oxides of environmental interest, and invited speakers in this area included B. Kasemo (Chalmers U., Göteborg), G.E. Brown (Stanford U.), V.E. Henrich (Yale U.), S.A. Chambers (Pacific Northwest Nat. Lab) and M. Salmeron (Lawrence Berkeley Nat. Lab.).

Other prominent topics included metal surfaces, for which there were invited talks by B.S. Clausen (Haldor Topsøe Res. Lab., Denmark) on catalysis on nanoparticles, P.A. Thiel (U. Iowa and Ames Lab.) on quasicrystals, D. Menzel (Tech. Univ. München) on coadsorption structures, and B.A. Joyce (Imperial College, London) on surfaces of semiconductors, A.P. Hitchcock (McMaster U.) discussed passivation layers, and K. Akimoto (Nagoya U.) covered the use of surface X-ray diffraction (SXR) to quantify strains at Si(111) surfaces. Invited talks on theory were given by K. Hermann (Fritz-Haber-Institut, Berlin) on transition oxide surfaces and J. Tersoff (IBM, Yorktown Heights) on structure of the Si-SiO₂ interface; other keynote talks were those of S. Ferrer (ESRF, Grenoble) on the use of SXR to characterize ultrathin magnetic films, A. Atrai (U. Siena) on structure of semiconducting surfaces used as gas sensors, L.D. Marks (Northwestern U.) on direct methods for surface structure determination, and J. Gimzewski (IBM, Zürich) on designer molecules for fabricating nanoscaled machines. Applications of scanning tunneling microscopy (STM), low-energy electron diffraction

(LEED), photoelectron diffraction and SXR were prominent. Considerable progress is being made with the latter technique, including its use to probe structure at liquid-solid interfaces, and for giving new insight for adsorption systems with large unit mesh areas (H.L. Meyerheim, U. München).



K. Takayanagi

The Surface Structure Prize, for outstanding achievement in the field of surface and interface structure, was awarded to K. Takayanagi for his quantitative determination of the atomic geometry of Si(111)-(7x7). "This is the single most important structure determination in all of surface science. It brought together fragmentary results from a host of other techniques into single coherent structure that has withstood the test of time and revealed the amazing complexity of new two-dimensional compounds formed at semiconductor surfaces. It resolved three decades of controversy about the structure. It was a 'tour de force' of experimental sample preparation and gave new insights into the energetics of semiconductors surface reconstructions, an amazing accomplishment of truly historic proportions. The ICSOS Young Scientist Prize was awarded to Peter Broekmann (U. of Bonn). ICSOS-7 will be held in 2002 at the U. of Newcastle, Australia.

K.A.R. Mitchell (Chair ICSOS-6), U. of British Columbia

European Crystallography Prize

The European Crystallographic Association (ECA) announces the establishment of the European Crystallography Prize to recognize a significant achievement or discovery in crystallography in the past 5-10 years. Nominees should be affiliated or identified with the European crystallographic community, including South Africa, as broadly defined in the charter of the ECA.

Nominations for the prize should include a statement of the contribution for which the prize is to be awarded, reprints of relevant published papers, a short curriculum vitae of the nominee, and the signatures of at least three additional nominators, preferably with letters supporting the nomination.

The inaugural prize will be presented at the opening ceremony of 19th European Crystallography Meeting (ECM-19) to be held in Nancy, France, August 25-31, 2000.

Paul T. Beursken

Shechtman Receives 1999 Wolf Prize

Dan Shechtman (Israel Inst. of Technology in Haifa, Israel) was awarded the 1999 Wolf Prize in Physics "for the experimental discovery of quasicrystals, non-periodic solids having long-range order, which inspired the exploration of a new fundamental state of matter."

Shechtman discovered macroscopic alloys possessing fivefold symmetry. His claim was initially received with disbelief. Among the novel practical uses of quasicrystalline materials being developed are

additives for strengthening steel and aluminum composites and surface coatings for turbine engines and reduced-stick cookware.

The exact structure of these high-symmetry substances remains to be settled, but in the meantime, researchers are investigating quasicrystals' hardness, corrosion resistance, and other properties and have begun putting them to good use.

Physics Today, March, 1999

Awards and Appointments

Members of the Science Advisory Committee of ESRF include: **R. Fourme** (LURE, France), **H. Fuess** (Technische Hochschule, Germany), **R. Hilgenfeld** (Inst. Molekulare Biotechnologie, Germany), **K. Hodgson** (SSRL, Stanford, USA), **L.B. McCusker** (ETH, Zürich, Switzerland), and **D. Stuart** (U. of Oxford, UK).

Lawrence F. Dahl, R.E. Rundle Professor of Chemistry at the U. of Wisconsin, Madison, received the 88th Willard Gibbs Medal of the ACS Chicago Section for "outstanding contributions in organometallic and high-nuclearity metal-cluster chemistry synthesis and structural characterization of nanometer-sized molecules, in work that has been described as unique and superb science."

The Biophysical Society Society Fellows announced for the year 2000 include six crystallographers: **Donald L.D. Caspar**, **Carolyn Cohen**, **David Eisenberg**, **Hugh E. Huxley**, **Frederic M. Richards**, and **Michael G. Rossmann**.

Awards went to **Helen Berman**, Rutgers U. (Distinguished Service) and **Carolyn Cohen**, Brandeis U. (Elisabeth Roberts Cole).

Biophysical Society Newsletter, September 1999

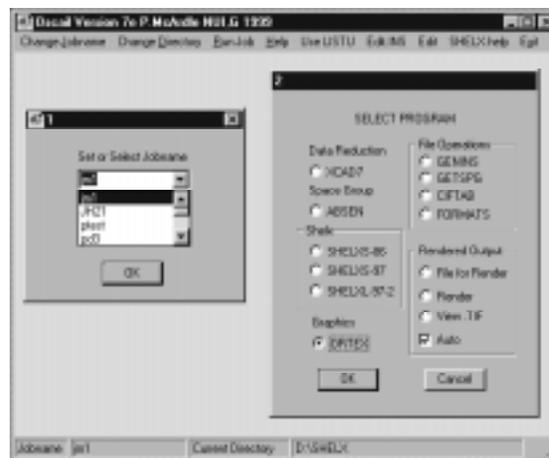
CRUSH: the Rigid Unit Mode Program

CRUSH is a program designed to probe and analyze the origin of displacive phase transitions in crystal structures that can be described as frameworks or networks of connected polyhedra. Examples are aluminosilicate minerals and zeolites. The displacive phase transitions involve low frequency phonons "Rigid Unit Modes" which, to first order, will require no distortions of the structural polyhedra moving as if they are rigid units. The RUM model can be applied to a range of problems that include understanding the nature of high-temperature phases, understanding the origin of negative thermal expansion, predicting localized distortions in zeolite structures, and identifying the flexibility of network glasses. Further information is available at <http://www.esc.cam.ac.uk/rums>.

Martin T Dove

Oscail - Single Crystal and Powder Diffraction

This Windows-based system provides the following facilities: *Space Group Determination, *Structure Solution, *Structure Refinement, *Structure Visualization and Editing, *Hardcopy in several formats including direct printing, *High quality rendered pic-



tures, *Powder pattern simulation, and *File format conversion. The software is provided free to academic users and can be downloaded from <http://www.nuiGalway.ie/cryst/software.htm>.

Patrick McArdle, National U. of Ireland

XD - A Multipole Refinement and Analysis of Charge Densities

In 1993 the IUCr Commission on Charge, Spin and Momentum Densities adopted as a project the writing of an integrated package, to be distributed, supported, documented and maintained centrally, with the objective of promoting a wide application of X-ray charge density methods to chemical problems. The outcome is the package now known as XD. Further information is available at www.chem.gla.ac.uk/~paul/xd.html.

Paul Mallinson, U. of Glasgow

CRYSTALS-32

CRYSTALS is a widely distributed package for single crystal structure analysis, including routines for data reduction, Fourier refinement, least-squares refinement (including absolute configuration, twinning, disorder, non-crystallographic symmetry, eigenvalue filtering and robust-resistant weighting), structure modelling and modification, analysis of structure, analysis of residuals, preparation of text and CIF tables, structure visualization and hardcopy color graphics. Because all these features are incorporated in a single package, the user can move easily from calculations to visualization to revised calculations, and as such it is a powerful environment for dealing with both routine and non-routine structures. L. Cranswick (at CCP14) set up a CRYSTALS web page to guide users through installation and initial use. <http://www.ccp14/co/uk/>. CRYSTALS-32 is being released in phases. Phase one will consist of the crystallographic code, the graphical editor and the command line script system, and as such is more-or-less a replacement for the DOS version of CRYSTALS. This release will only be available to experienced CRYSTALS users. Those interested in trying it out should contact us by E-mail at david.watkin@chem.ox.ac.uk.

David Watkin, U. of Oxford



Crystal XXI - Australia

The twenty-first meeting of the Society of Crystallographers in Australia will be held **February 1-4, 2000** in Thredbo Alpine Village, NSW. The *1987 Lecture* will be given by D.L. Dorset (Hauptman-Woodward Med. Res. Inst., Buffalo, NY USA). Other invited lecturers include I. Grey (CSIRO Div. Minerals), C. Raston (Monash U.), B. David (UK), P. Colman (BRI) and Stephen Hyde (ANU). More information is available at <http://rsc.anu.edu.au/~welberry/crystal21/>.

Crystal Chemistry - Russia

The Second National Crystal Chemical Conference, organized by the Crystal Chemical Section of the Scientific Council on Kinetics and Structure of RAS will be held on **May 22-26, 2000** near the Scientific Center in Chernogolovka. Conference Topics will include: Organic, inorganic, and organometallic crystal chemistry; Structure and properties; Chemical bonds; Reactions in crystals; Dynamics; and Applications of synchrotron radiation for X-ray research. For more information, contact Organizing Committee of the Second All-Union Crystal Chemical Conference, Inst. of Problems of Chemical Physics RAS, 142432, Chernogolovka, Moscow Region, Russia, Fax 096 576-40-09, E-mail: khn@icp.ac.ru.



ICDD Clinics

- **Fundamentals of X-ray Fluorescence Spectrometry, May 1-5, 2000.** Covering basics of X-ray spectra, instrumentation design, methods of qualitative and quantitative analysis, applications for both wavelength and energy dispersive spectrometry.
- **Advanced Methods in X-ray Fluorescence Spectrometry, May 8-12, 2000.** Quantitative methods, automated X-ray spectrometers, matrix correction procedures, and new developments in XRF.
- **Fundamentals of X-ray Powder Diffraction, June 5-9, 2000.** Covering instrumentation, specimen preparation, data acquisition, and qualitative phase analysis.
- **Advanced Methods in X-ray Powder Diffraction, June 12-16, 2000.** Computer-based methods of data collection and interpretation, for qualitative and quantitative phase analysis.

For more information, contact: J. Ginsburg, Educ. Coordinator ICDD, Tel: 610 325-9814, Fax: 610 325-9823, E-mail: clinics@icdd.com, <http://www.icdd.com/education/clinics.htm>.

Crystal Growth in China

The Chinese Crystal Growth and Materials SubSociety (CCGMS) Affiliated to Chinese Ceramics Society announces that the Twelfth Chinese Conference on Crystal Growth (CCCG-12) will be held in **May, 2000** in Shanghai. Topics to be included: Fundamental of crystal growth and exploration of new crystals; Growth from melt; Growth from solution or flux; Vapor and low dimension growth; Functional properties, structure and defects; Processing and application of crystals; and Technology and equipment. For more information contact the Secretariat at CCCG-12@sunm.shcnc.ac.cn or visit <http://www.sic.ac.cn>.

Peptides in China

The 6th Chinese Peptide Symposium 2000 will be held **July 3-6, 2000** in Huangshan City, China. The Symposium will include keynote lectures, short oral presentations and poster sessions on all aspects of peptide sciences. Exhibition spaces will be available for commercial exhibitors. More information is available at <http://www.glschina.com/cps-2000.htm>.



Twelfth American Conference on Crystal Growth and Epitaxy

ACCGE-12, **August 13-18, 2000** in Vail, Colorado, USA will provide a forum for all aspects of bulk crystal growth and epitaxial thin film growth, with sessions integrating fundamentals, experimental and industrial growth processes, characterization, and applications. Contributed oral and poster papers accepted. NASA workshop on "Applications of Experimentation in a Microgravity Environment to the Science of Electronic Materials". Abstracts due March 15, 2000.

For more information contact: T. Gentile, ACCGE-12 Sec., Tel: 805 492-7047 Fax: 805 492-4062, Email aacg@lafn.org; <http://www.aml.arizona.edu/aacg>.

Meeting Calendar

A selection of future meetings. Extensive lists appear regularly in *J. Applied Crystallography*, the *BCA Newsletter* and the *ACA Newsletter*. Corrections and new listings are invited by the Editor.

FEBRUARY 2000

1-4 ♦ **21st Meeting of the Soc. of Crystallographers in Australia (SCA)**. Thredbo, New South Wales. Contact: <http://rsc.anu.edu.au/~welberry/crystal21/>.

APRIL 2000

24-28 ♦ **Materials Research Soc. Spring Meeting**. San Francisco, CA USA. Contact: www.mrs.org/meetings/spring00/.

MAY 2000

20-23 ♦ **7th European Powder Diffraction Conf. (EPDIC-7)**. Barcelona, Spain. Contact: www.icmab.es/epdic7/.

22-26 ♦ **Second National Crystal Chemical Conf.** Moscow, Russia. Contact: See page 23.

25-4 ♦ **Methods in Macromolecular Crystallography**. Erice, Italy. Contact: www.geomin.unibo.it/orgv/erice/johnson.htm.

25-4 ♦ **Prospectives in Crystallography of Molecular Biology**. Erice, Italy. Contact: www.geomin.unibo.it/orgv/erice/johnson.htm.

JULY 2000

16-20 ♦ **18th Int'l Congress of Biochemistry and Mo-**

lecular Biology: Beyond the Genome. Birmingham, UK.

Contact: www.iubmb2000.org

22-27 ♦ **ACA 2000, American Crystallographic Assn Annual Meeting**. St. Paul MN USA. Contact: www.hwi.buffalo.edu/aca/.

AUGUST 2000

6-11 ♦ **Indaba 3, Int'l Workshop of the IUCr Structural Chemistry Commission**. Skukuza, Kruger Nat'l Park.

13-18 ♦ **Twelfth American Conf. on Crystal Growth and Epitaxy (ACCGE-12)**. Vail, Colorado, USA. Contact: see page 23.

25-31 ♦ **ECM19, European Crystallographic Meeting**. Nancy, France. Contact: www.lcm3b.unancy.fr/ecm19/.

SEPTEMBER 2000

4-7 ♦ **XVIII CAC XVIII Conf. on Applied Crystallography**. Katowice, Poland. Contact: <http://www.us.edu.pl/uniwrsytet/konferencje/2000/cac>.

AUGUST 2001

25-31 ♦ **ECM 20**. Krakow, Poland. Contact: <http://www.ch.uj.edu.pl/ECM2001.htm>.

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