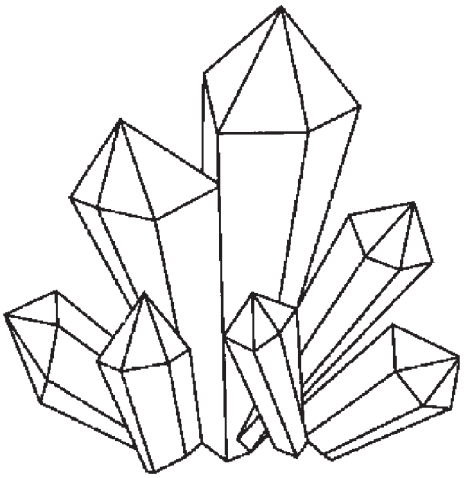
www.iucr.org

INTERNATIONAL UNION OF Crystallography

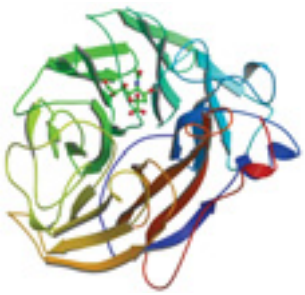
NEWSLETTER

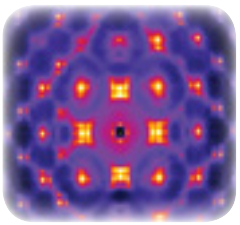
Volume 14, Number 1 ♦ 2006

CRYSTALLOGRAPHY IN

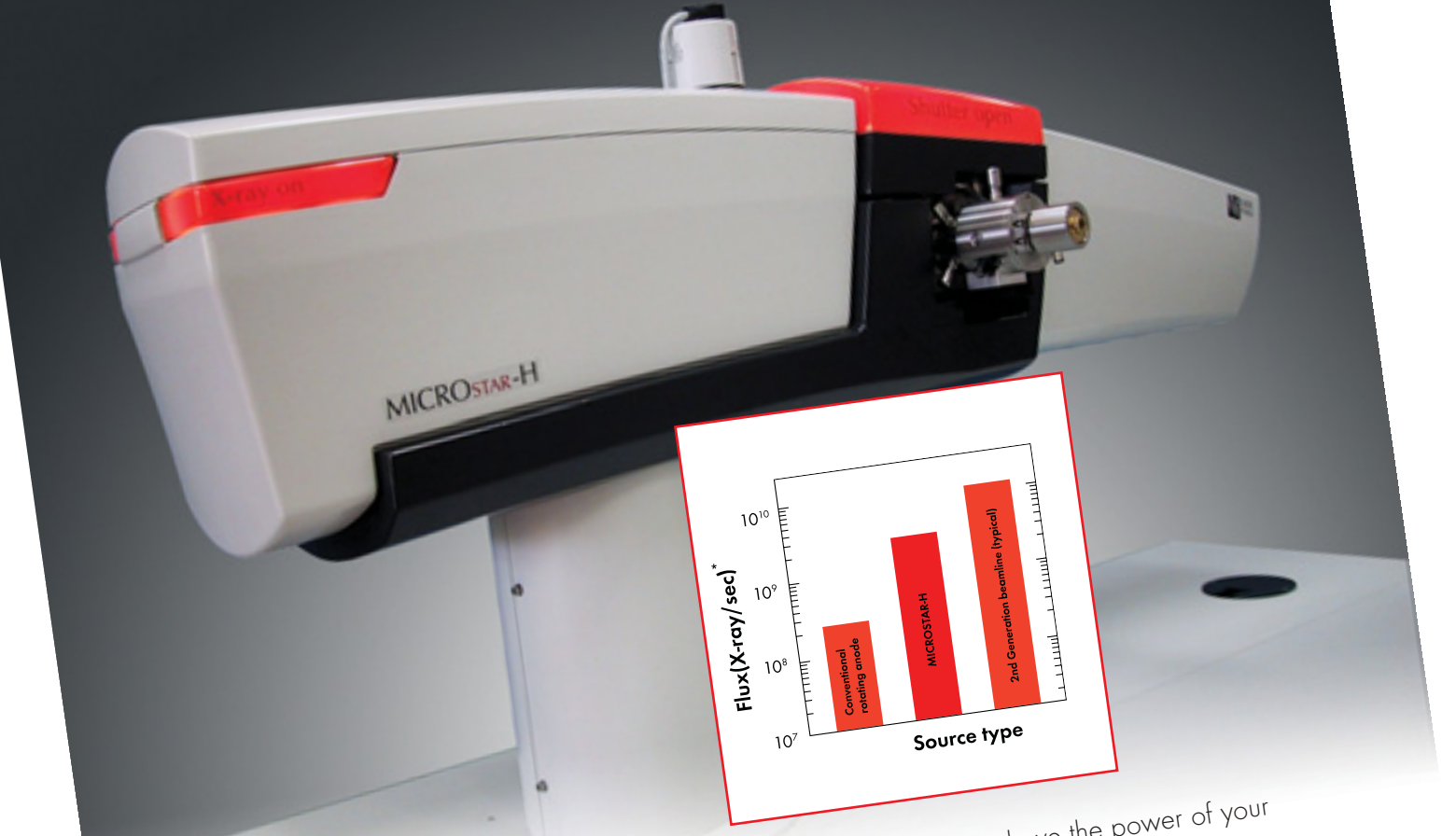


SCANZ





AUSTRALIA AND NEW ZEALAND



New MICROSTAR-H

Take your home data collection to a whole new level.

How would you like to have the power of your own Personal Beamline in your homelab, available to you 24 hours a day, 7 days a week? With more than 10 times the flux of a conventional rotating anode (up to $3x10^9$ X-rays/sec*) the new MICROSTAR-H micro-focus rotating anode gives your home laboratory X-ray intensities that approach typical second generation beamlines. And yet, it is simpler and less expensive to operate and maintain than most conventional rotating anodes.

The outstanding intensity and stability of the MICROSTAR-H make it ideal for the most demanding SAD experiments or for high throughput screening of the smallest crystals.

The new MICROSTAR-H.

BETTER DATA...FASTER.

find out what's inside

*Flux through 0.2 mm aperture with mutilayer optics.

BRUKER AXS

BRUKER ADVANCED X-RAY SOLUTIONS

North America: BRUKER AXS INC. ■ Tel. (+1) (608) 276-3000 ■ Fax (+1) (608) 276-3006 ■ www.bruker-axs.com ■ info@bruker-axs.com
The Netherlands: BRUKER AXS B.V. ■ Tel. (+31) (15) 2152 400 ■ Fax (+31) (15) 2152 500 ■ www.bruker-axs.nl ■ info@bruker-axs.nl
Germany: BRUKER AXS GMBH ■ Tel. (+49) (721) 595-28 88 ■ Fax (+49) (721) 595 45 87 ■ www.bruker-axs.de ■ info@bruker-axs.de

TABLE OF CONTENTS

Editors
Judith L. Flippen-Anderson
flippen@rcsb.rutgers.edu

William L. Duax
duax@hwi.buffalo.edu

Newsletter Design & Production
Patricia Coley

Assistant Editor
Jane Griffin

Send Contributions to: P. Coley, c/o Hauptman-Woodward Med. Research Inst. 700 Ellicott St., Buffalo, NY 14203, USA
Tel.: 716 898-8691 · FAX: 716 898-8695
e-mail: patti@hwi.buffalo.edu
www.hwi.buffalo.edu/iucr/IUCr-News/Home.html

Matters pertaining to Advertisements should be addressed to P. Coley at the above address.

On the Cover: Images taken from the article on Crystallography in Australia and New Zealand. Article begins on page 26.

Contributors: See Page 34

IUCr Executive Secretary
Michael Dacombe (execsec@iucr.org)
International Union of Crystallography
2 Abbey Square, Chester, CH1 2HU, England

The IUCr Newsletter (ISSN 1067-0696; coden IUC-NEB) Volume 14, Number 1. Published quarterly (4x) by the International Union of Crystallography. Members receive the IUCr Newsletter by virtue of country membership in the IUCr. Periodical postage rates paid at Buffalo, NY and additional mailing offices. POSTMASTER: Please send changes of address to IUCr Newsletter Editorial Office, c/o Hauptman-Woodward Medical Research Inst., 700 Ellicott St., Buffalo, NY 14203 USA.


Yuji Ohashi

In May 7 to 12, I attended the 3rd Moroccan Crystallographic School held in Agadir. There were more than 70 crystallographers including the students. The meeting of the Moroccan Crystallographic Association was also held in one evening. I am very sorry to say that the Moroccan Crystallographic Association is a member of European Crystallographic Association, ECA, but is not a member of IUCr. I considered what IUCr should do for the crystallographers in such developing countries.

As written in Statues, one of the objects of IUCr is to adhere to the International Council of Science, ICSU. The most important mission of ICSU is to strengthen international science for the benefit of society since its establishment in 1931. The principle of the universality of science has been embedded in the statutes of ICSU from its very early days. All members agree to adhere to this principle and it provides a model of equity and non-discrimination across the international science community.

The membership of ICSU is consisting of three categories. The first one is composed of national members. The number of the national members is 104 in 2006. The second one is scientific union members, in which are included not only the IUCr but also IUPAB (International Union of Pure and Applied Biology), IUPAC (International Union of Pure and Applied Chemistry), IUPAP (International Union of Pure and Applied Physics), IUGS (International Union of Geological Sciences), IUBMB (International Union of Biochemistry and Molecular Biology), IUMRS (International Union of Materials Research Societies) and so on. The number of the union members is 29. The third one is composed of scientific associates, whose number is 23. In the General Assembly 76 of 104 national members and 29 scientific unions have full voting rights. The past president of IUCr, Dr. W. Duax, attended the General Assembly as a representative of IUCr. In order to achieve the objects of ICSU, the close contact and cooperation between science council and scientific unions in each country are indispensable.

The number of membership countries of IUCr is only 40 national crystallographic associations and adhering body. This is too small compared with 104 or 76 national members of ICSU. Morocco is, of course, one of national members of ICSU. However, the Moroccan Crystallographic Association is not a member of IUCr. When I saw the list of national members of ICSU, there are many countries in the same circumstance as Morocco.

It must be emphasized that the member of IUCr should pay the membership fee. There are five categories for the membership fee from I to V. For the category I the fee is CHF 1,000 per each year, which is about USD 830. This payment is not so easy for the national crystallographic associations with small members. I know several Asian countries, in which there are only a few crystallographers. It seems difficult for such crystallographic associations to pay the membership fee.

In order to welcome their opinions and activities to IUCr, we must invite them to IUCr as members. To find out the ways how to reduce their financial duty and how to get the benefit from IUCr is the most important for the future of IUCr. I already sent one proposal to Executive Committee. In the Leuven meeting of EC the proposal will be discussed. The result will be informed to the regional and national crystallographic associations as soon as possible.

Yuji Ohashi, yohashi@spring8.or.jp

The IUCr Newsletter is distributed to 587 libraries and 15,000 crystallographers and other interested individuals in 39 countries. The IUCr also runs Crystallography Online, available at www.iucr.org, as a complement to the IUCr print newsletter. Feature articles, meeting announcements and reports, information on research or other items of potential interest to crystallographers should be submitted to the editor at any time. Submission of text by electronic mail and graphics, slides or photographs by express mail is requested. Items will be selected for publication on the basis of suitability, content, style, timeliness and appeal. The editor reserves the right to edit. Cost of distribution in Algeria, Australia, Colombia, Croatia, Cuba, Czech Republic, France, India, Italy, Japan, Malaysia, New Zealand, Poland, Portugal, South Africa, Switzerland, Taiwan, The Netherlands, Thailand, and Venezuela is borne by crystallographic associations or institutions or by individual crystallographers in these countries. Address changes or corrections and requests to be added to the mailing list should be addressed to the editorial office.

If you would like to see a copy of the IUCr Newsletter in your college or university library, send the address to the Newsletter office so that we can add it to our mailing list.

Letters to the Editor

Dear Editors,

Thank you very much for publishing in Newsletter 4/2005 the reports concerning the activity of the Commission on Inorganic and Mineral Structures (CIMS) at IUCr- XX in Florence. Unfortunately, in part due to myself (non clear submission of the reports) and in part due to editing of the reports, the following mistakes need a correction.

Page 12 - The photo marked L. Cario is that of T.R. Welberry.

Pages 12-13 - The report Modularity and Modulation in Inorganic and Mineral Structures must be signed by Emil Makovicky and Stefano Merlino.

Page 13 - The report Polytypism and Twinning must be signed by Giovanni Ferraris and Elena Belokoneva.

Page 14 - The photo marked E. Makovicky is that of L. Cario. On line 10 of the report Open Commission Meeting on Inorganic and Mineral Structures (CIMS) there is mistake which looks like a joke: OD is the acronym of Order Disorder not of Object Discovery!

Giovanni Ferraris

Statement of Ownership, Management, and Circulation

1. Publication Title: International Union of Crystallography Newsletter
2. Publication Number: 1067-0696
3. Filing Date: November 10, 2005
4. Issue Frequency: Quarterly
5. Number of Issues Published Annually: 4
6. Annual Subscription Price: $0.00
7. Complete Mailing Address of Known Office of Publication: IUCr Newsletter, c/o Hauptman-Woodward Medical Research Inst., 700 Ellicott Street, Buffalo, NY, 14203-1102, Erie County
8. Complete Mailing Address of Headquarters or General Business Office of Publisher: Same as above
9. Full Names and Complete Mailing Addresses of Publisher and Editor: Publisher: International Union of Crystallography, 2 Abbey Square, Chester CH1 2HU, UK; Editor: Judith Flippen-Anderson, 3521 Lancelot Way, Annandale, VA 22003
10. Owner: International Union of Crystallography, 2 Abbey Square, Chester CH1 2HU, UK
11. Known Bondholders, Mortgagees, and Other Security Holders Owning or Holding 1 Percent or More of Total Other Securities: None
12. Tax Status: Not Changed During Preceding 12 Months
13. Publication Title: International Union of Crystallography Newsletter
14. Issue Date for Circulation Data Below: September 2005

15. Extent and Nature of Circulation			Average No. Copies Each Issue During Preceding 12 Months	No. Copies of Single Issue Published Nearest to Filing Date
a. Total Number of Copies (Net press run)			17,250	17,500
b. Paid and/or Requested Circulation	(1)	Paid/Requested Outside-County Mail Subscriptions Stated on Form 3541	6,009	5,931
	(2)	Paid In-County Subscriptions Stated on Form 3541	0	0
	(3)	Sales Through Dealers and Carriers, Street Vendors, Counter Sales, and Other Non-USPS Paid Distribution	10,331	10,799
	(4)	Other Classes Mailed Through the USPS	0	0
c. Total Paid and/or Requested Circulation [Sumof15b.(1),(2),(3),and(4)]			16,340	16,730
d. Free Distribution by Mail	(1)	Outside-County as Stated on Form 3541	226	225
	(2)	In-County as Stated on Form 3541	0	0
	(3)	Other Classes Mailed Through the USPS	0	0
e. Free Distribution Outside the Mail			342	341
f. Total Free Distribution (Sum of 15d. and 15e.)			568	566
g. Total Distribution (Sum of 15c. and 15f.)			16,908	17,296
h. Copies not Distributed			342	204
i. Total (Sumof15g.andh.)			17,250	17,500
j. Percent Paid and/or Requested Circulation			97%	97%

I certify that all information furnished on this form is true and complete.
(signed) Patricia Coley, Production Manager

FINDING A NEEDLE IN THE HAYSTACK HAS NEVER BEEN EASIER.

(And we didn't stop there.)

Emerald BioSystems offers a wide variety of sophisticated laboratory automation, software tools, and consumable products for gene to protein crystal structure research.

VISIT US ON THE WEB OR REQUEST A CATALOG TODAY!

Start your search with the right tools and see how close you are to finding something special.

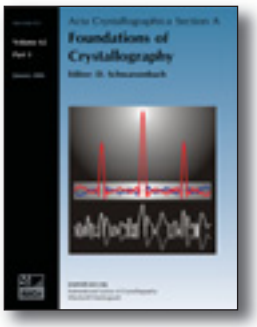
Emerald BioSystems

Integrated solutions for biotechnology

www.emeraldbiosystems.com

7869 NE Day Road West | Bainbridge Island, WA | 98110 | (888) 780-8535 | (206) 780-8535 | emerald@emeraldbiosystems.com

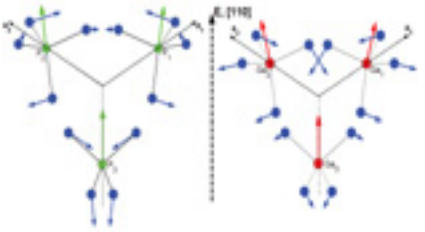
Acta Cryst. (2006). A**62**, 1–10 (doi: 10.1107/S0108767305036111)



X-ray diffraction by a crystal in a permanent external electric field: electric-field-induced structural response in α-$GaPO_4$

Semen Gorfman, Vladimir Tsirelson, Andreas Pucher, Wolfgang Morgenroth and Ullrich Pietsch

A permanent external electric field induces the displacements of atoms within a unit cell and variation of crystal lattice parameters. These microscopic changes causing dielectric polarization and converse piezoelectric effect can be observed experimentally by means of X-ray diffraction. The theory of X-ray diffraction in an *E*-field is developed and used for planning a synchrotron X-ray diffraction experiment. Based on 54 measured Bragg reflections, the electric-field-induced distortion of PO_4 and GaO_4 tetrahedra in α-$GaPO_4$ crystals was evaluated. It shows that the *E*-field-induced changes are larger at the PO_4 tetrahedra compared with those of GaO_4, which can be explained by the higher pseudoatomic charge of the P ion compared with Ga.



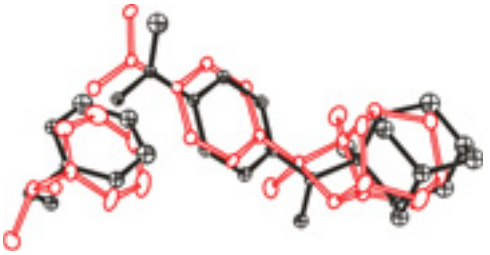
The displacement of pseudoatoms in PO_4 (left) and GaO_4 (right) sublattices induced by the external electric field parallel to the [110] lattice direction.

Acta Cryst. (2006). B**62**, 128–134 (doi: 10.1107/S0108768105034014)

Monitoring structural transformations in crystals. 8. Monitoring molecules and a reaction center during a solid-state Yang photocyclization

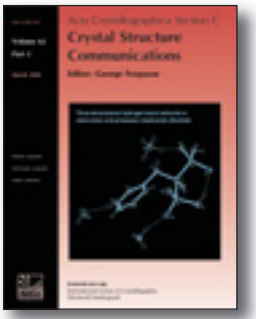
I. Turowska-Tyrk, E. Trzop, J. R. Scheffer and S. Chen

Structural changes in a single crystal, brought about by an intramolecular photochemical reaction, were monitored step-by-step using X-ray diffraction analysis. Special attention was paid to monitoring variations in the relative orientation of reactant and product molecules, changes in geometrical parameters describing the reaction center, and variations in the cell constants. Although rarely met in the scientific literature, such studies are important because they provide detailed information about the course of reactions in crystals. The results of the present study are compared with analogous data published for other single-crystal to single-crystal photochemical reactions.



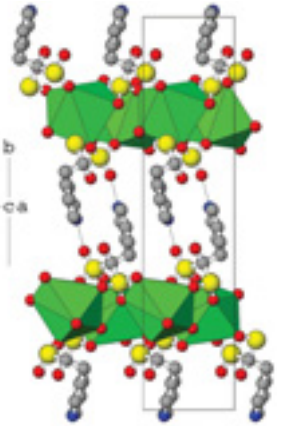
The product molecule (in red) superimposed on the reactant molecule (in black) for one of the stages of the photoreaction.

Acta Cryst. (2006). C**62**, m112–m115 (doi: 10.1107/S0108270106002782)



Ammonium 1-hydroxy-2-(2-pyridinio)ethane-1,1-diyldiphosphonate dihydrate and potassium 1-hydroxy-2-(2-pyridinio)ethane-1,1-diyldiphosphonate dihydrate

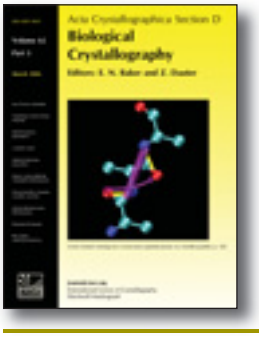
K. Stahl, J. Oddershede, H. Preikschat, E. Fischer and J. S. Bennekou



The crystal packing of potassium risedronate viewed along the *c* axis, showing the layers of seven-coordinated potassium ions connected by hydrogen bonding.

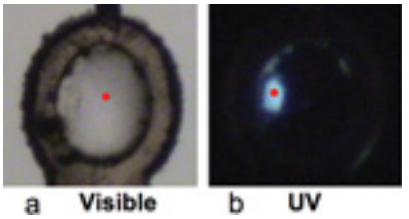
Risedronic acid is nowadays one of the preferred active substances used for the treatment of osteoporosis. However, the currently used sodium salt of risedronic acid displays different degrees of hydration giving rise to formulation problems. The potassium as well as the ammonium salt, on the other hand, reproducibly forms dihydrates, which are both well defined and very stable. In potassium risedronate, the potassium ions are 7-coordinated in layers connected by hydrogen bonding, while ammonium risedronate molecules form a three-dimensional hydrogen-bonding network.

Acta Cryst. (2006). D**62**, 253–261 (doi: 10.1107/S0907444905041429)



UV laser-excited fluorescence as a tool to visualize protein crystals mounted in loops

X. Vernede, B. Lavault, J. Ohana, D. Nurizzo, J. Joly, L. Jacquamet, F. Felisaz, F. Cipriani and D. Bourgeois



Fluorescence images of a protein crystal (~20 μm long) under visible light (a) or UV light (b). Red points show the crystal centre as detected by automation software. The crystal is hardly detectable under visible light but easily identified under UV-laser illumination.

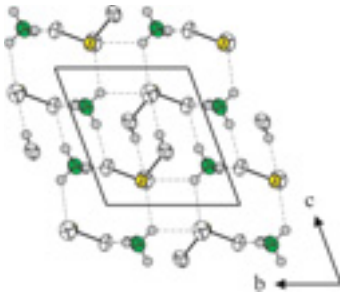
The automation of protein structure determination by crystallography encounters a serious bottleneck. Automated sample alignment along the synchrotron X-ray beam is often hampered by the difficult visualization of protein crystals. We have used the fluorescence from aromatic amino acids to identify reliably even tiny

crystals. The use of a 266 nm UV laser in combination with an optimised illumination geometry and non-fluorescent sample holders provides an efficient solution to collect fluorescence images in milliseconds with standard camera optics. The low UV exposures do not generate detectable structural damage.

Acta Cryst. (2006). E**62**, i38–i40 (doi:10.1107/S1600536806003850)

Ammonium hydrogenselenate(IV)

M. Weil



One of the starting materials for aqueous ammonium selenate(IV) solutions, which are frequently used for precipitation of other, more insoluble selenate(IV) compounds, is $NH_4(HSeO_3)$. This compound is accessible by dissolving SeO_2 in an ammonia solution and by subsequent recrystallization. The crystal structure comprises NH_4^+ cations and trigonal-pyramidal $HSeO_3^-$ anions, the latter containing two short Se–O bonds and one long Se–OH bond. The structure packing is accomplished by an intricate network of weak hydrogen bonds, with donor–acceptor distances (N···O and O···O) between 2.80 and 3.07 Å.

Acta Cryst. (2006). F**62**, 180–185 (doi:10.1107/S1744309106005847)

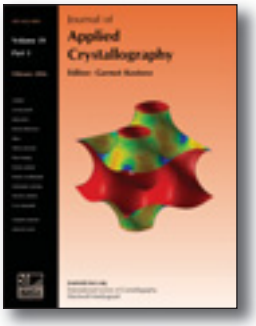
Structure of the conserved hypothetical protein MAL13P1.257 from *Plasmodium falciparum*

M. A. Holmes, F. S. Buckner, W. C. Van Voorhis, C. Mehlin, E. Boni, T. N. Earnest, G. DeTitta, J. Luft, A. Lauricella, L. Anderson, O. Kalyuzhniy, F. Zucker, L. W. Schoenfeld, W. G. J. Hol and E. A. Merritt

This structure establishes a mapping of sequence family PF05907 onto a novel fold containing 15 β-strands in 4 sheets.

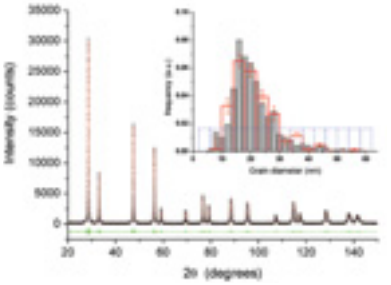
The structure of *P. falciparum* MAL13P1.257 is the first structure determined for a member of Pfam sequence family PF05907. The biological function of these proteins is unknown. The structure is almost entirely β-sheet and represents a new protein fold. There are two regions of high sequence conservation with other family members. One forms a hydrophobic core; the second contains both core and surface residues. Curiously, several distinctive sequence motifs that are highly conserved across other family members are not present in the *P. falciparum* protein.

J. Appl. Cryst. (2006). **39**, 24–31 (doi: 10.1107/S0021889805032978)



Line profile analysis: pattern modelling *versus* profile fitting

P. Scardi and M. Leoni



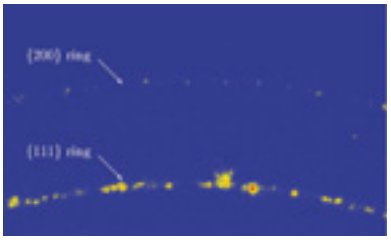
WPPM results for a nanocrystalline ceria sample. In the inset, TEM grain diameter distribution (full column) with WPPM final results (open column) and starting (prior) distribution (dashed column).

Grain size determination is a primary issue in the study of nanocrystalline materials. The recently developed Whole Powder Pattern Modelling (WPPM) was applied to data collected on a nanocrystalline ceria sample. Unlike traditional profile fitting, WPPM makes no use of arbitrary analytical profile functions: diffraction profiles are directly modelled in terms of microstructural parameters, like, e.g., grain shape and size distribution, dislocation density, effective outer cut-off radius, faulting and anti-phase domain boundary probabilities. The results are in close agreement with those of transmission electron microscopy.

J. Synchrotron Rad. (2006). **13**, 1–7 (doi: 10.1107/S0909049505038811)

Radiation driven collapse of protein crystals

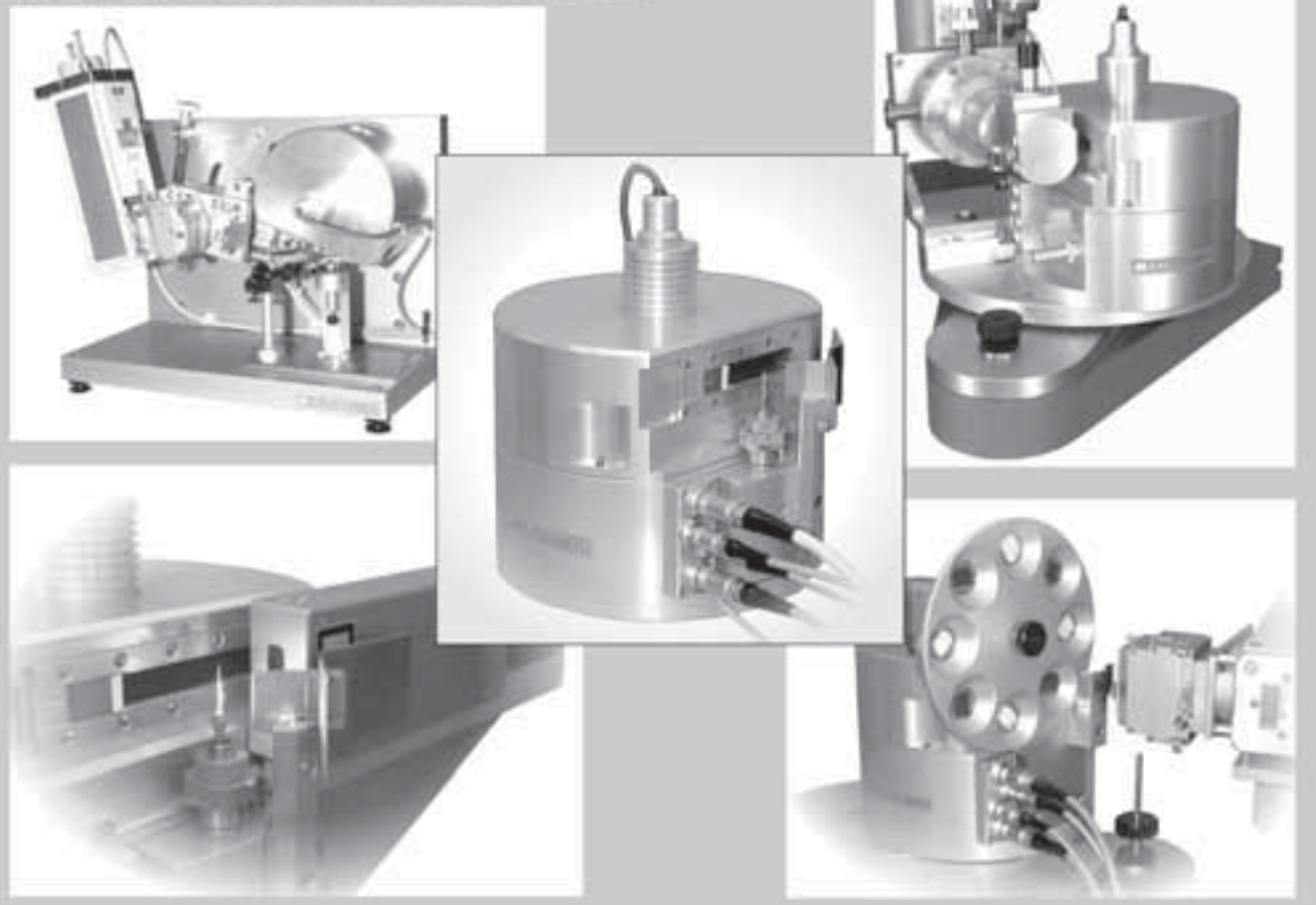
S. Boutet and I. K. Robinson



This paper describes the effects of intense synchrotron radiation beams from the Advanced Photon Source on small ferritin crystals suspended in solution. Typical powder diffraction, shown in the figure, identifies a number of individual crystals within the X-ray beam. After exposures in the range 2×10^7 Grays, the crystals were found to disintegrate suddenly in a spectacular way, as captured on the JSR cover image. The peak evolution to larger momentum transfer implies that the crystals *collapse*, possibly due to loss of hydration.

SPEED...

in X-ray Powder Diffractometry



HUBER Imaging Plate Guinier Camera 670

- ☑ A factor of more than100 faster compared to conventional step scan
- ☑ X-ray powder diffraction in 45° (asymmetric) transmission, 0° to 100° 2-theta
- ☑ Bulk samples in 17°(fixed grazing incidence) reflection, 50° to 150° 2-theta
- ☑ Plane foil or capillary samples. 8-fold sample changer for plane foil samples
- ☑ Vertical mount for liquids, 0° to 20°(adjustable grazing incidence) reflection
- ☑ Focussing monochromatic radiation, Kα, stripping not required
- ☑ Range of Bragg angles 100° 2-theta, 20001 steps @ 0.005°
- ☑ Laser scans signals @ 16 Bit A/D resolution. Linear dynamic range up to 200,000 counts
- ☑ Creates all common ASCII file types ready for data evaluation like Rietveld-Refinement
- ☑ Low-temperature attachment: Closed cycle He-refrigerator, 10 to 320 K
- ☑ Hi-temperature attachment: Diode laser heater, 300 to 1800 K
- ☑ Hi-pressure attachment: Diamond anvil cell, upto 70 GPa

HUBER

X-RAY DIFFRACTION EQUIPMENT

HUBER Diffraktionstechnik GmbH & Co. KG
Sommerstrasse 4
D-83253 Rimsting / Chiemsee
Germany

Tel: +49 (0)8051 68780
Fax: +49 (0)8051 687810
info@xhuber.com
www.xhuber.com

A Crystallographic Information File for Specular Reflectivity Data

Since the early nineties X-ray and neutron specular reflectivity have been the scattering techniques of choice for materials scientists who want to study the vertical density profile of thin films, whether crystalline, amorphous or liquid. Important structural parameters, such as the electronic or nuclear density, the thickness, and the interfacial roughness of thin layers, can be deduced from specular reflectivity data using more or less straightforward modelling techniques (1). Although initially developed by physicists, the technique is now used by chemists and biologists, each however tends to speak their own reflectivity language. This has led to a large variety of ways in which results from specular reflectivity experiments are presented, making reflectivity papers sometimes rather difficult to read, even for specialists in the field.

Some of us working in the field have thought it worthwhile to standardize the terminology by defining a Crystallographic Information Framework (CIF) Dictionary for specular reflectivity data. The benefits provided by CIF for single-crystal diffractometry are well known (2), and the CIF developed for powder diffraction (pdCIF, 3) has become more popular with the development of CIF-exporting modules in programs such as GSAS (4). In view of these developments it is expected that a CIF for specular reflectivity data (rfCIF) could make it easier to exchange specular reflectivity measurements between researchers working in different or multidisciplinary fields. It would also simplify archiving and interpreting this information.

An informal working group of specialists worldwide has recently been formed to produce a reflectivity CIF dictionary (rfCIF). A draft version of the dictionary is being prepared in collaboration with COMCIFS, the committee that oversees the CIF project for the International Union of Crystallography. A number of practitioners in the field have already commented on a first draft of the dictionary and any one else with an interest in this project is invited to contact one of the members of the working group listed below and can be found on the website (www.iemm.univ-montp2.fr/xrayweb/main_uk.html) under "Contacts":

A. van der Lee (chair) U. of Montpellier, France.
E. Bontempi, Un. of Brescia, Italy
D. Chateigner, CRISMAT-ENSICAEN, France
P.F. Fewster, PANalytical Research Centre, England
B. Harzallah, U. of Monastir, Tunisia
P. Kienzle, NIST, USA
K. Sakurai, U. of Tsukuba, Japan
A. Ulyanenkov, Bruker AXS, Karlsruhe, Germany.

A. van der Lee and I.D. Brown

REFERENCES
(1) see e.g. J. R. Lu, E. M. Lee and R. K. Thomas, Acta Cryst. (1996). A52, 11-41
(2) International Tables for Crystallography Volume G: Definition and exchange of crystallographic data, Eds. S. Hall and B. McMahon, Springer.
(3) B. H. Toby and N. Ashcroft, Acta Cryst. (2005). A61, C483
(4) B. H. Toby, R. B. Von Dreele and A. C. Larson, J. Appl. Cryst. (2003). 36, 1290-1294

IUCr poster prizes

Three IUCr poster prizes were awarded at the International School on Biological Crystallization (Granada, Spain; 22–26 May 2006). First prize and a copy of *International Tables for Crystallography* Volume A: *Space-group symmetry* went to P-26: "*In-situ* Characterization of Defects during Protein Crystal Growth" and Erika Ono (Co-authors: Peter Dold, Masako Koizumi, Katsuo Tsukamoto and Gen Sazaki) from Tohoku U., Sendai, Japan. Second prize and Volume F: *Crystallography of biological macromolecules* went to P-29: "Macromolecular crystallization on 'nucleant' surfaces" and Giovanna Tosi (Co-authors: Giuseppe Falini, Simona Fermani and Alberto Ripamonti) of U. Bologna, Italy. Third prize and the Brief teaching edition of Volume A went to P-27: "Structural analysis of FPR and NifF, two redox proteins from *Rhodobacter capsulatus*" and Inmaculada Pérez-Dorado (Co-authors: Cristian Bittel, Néstor Cortez, Néstor Carrillo and Juan A. Hermoso) of CSIC, Madrid, Spain.

The award panel covered the range of course topics: industrial crystallization, biomineralization and protein crystallization, and consisted of four members of the editorial board of *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* (journals.iucr.org/f): Howard Einspahr (Panel Chair), JuanMa García-Ruiz (School Director), Alex McPherson (UC Irvine, CA, USA) and Terese Bergfors (Uppsala U., Sweden) along with Madeleine Ries (U. Paris, France), Kevin Roberts (U. Leeds, UK) and Yves Nys (INRA, France).

Reports continued from Volume 13, Number 4

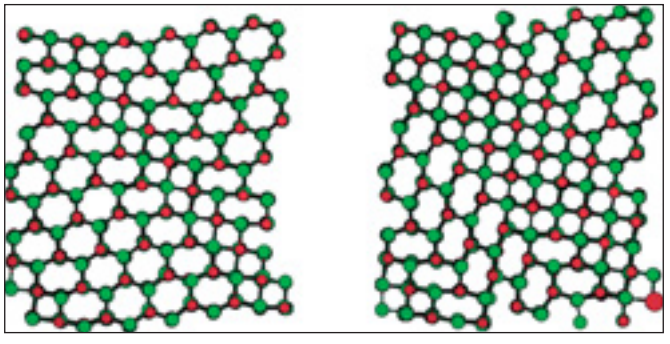
Structural Phase Transitions

The standing room only crowd attending the microsymposium on Structural Phase Transitions reflected the intense interest in this topic among crystallographers worldwide and the lively growth of activity on the subject during the last three years. In fact, many other microsymposia at the Congress included aspects of the field of structural phase transitions from different perspectives. This session focused on structural phase transitions and methodology.


C.J. Howard

The first lecture by C.J. Howard (Australia) highlighted the extreme efficiency of systematic use of group theoretical methods when analysing complex sequences of phase transitions in compound families. The use of tools such as those provided by the software package ISOTROPY (physics1.byu.edu/~stokesh//isotropy.html) by H.T. Stokes and D.M. Hatch (USA), was presented considering the particular case of some double and some cation deficient perovskites [*Acta Cryst.* B59, 463 (2003)]. Perovskites were also the subject of the second talk by D. Pandey (India), more specifically, the morphotropic tetragonal-rhombohedral boundary in the phase diagram of relaxor ferroelectrics. The existence of a difficult to characterize intermediate monoclinic phase in PZT has been the subject of intense discussion and has become a central feature for understanding the high piezolectric response of these sytems at this particular composition. M. Braden (Germany) presented a review of the properties of the system [Ca,Sr]RuO_4 as a function of composition and temperature. In spite of the isovalent character of the substitution, the system exhibits a rich variety of physical phenomena: unconventional superconductivity, a Mott-insulating phase, one of the highest Cp/T low-temperature ratios observed in a transition metal oxide and a metamagnetic transition. The smaller ionic radius drives a series of structural phase transitions which are intimately coupled with physical properties. As a function of Ca^{+2} concentration the octahedra exhibit tilts and rotations which strongly reduce the electronic hybridization thereby decreasing the electronic band widths. In this sense the increasing structural distortions enhance the role of electronic correlations. Strongly distorted Ca_2RuO_4 is even an antiferromagnetic Mott-insulator. Although centered on neutron diffraction and inelastic scattering, the talk reviewed the results of a remarkable variety of experimental methods, showing the power of combining different techniques when interpreting such complex systems.


D. Pandey


Two consecutive snapshots of the nucleation and growth mechanism for the wurtzite to rocksalt transition in CdSe, according to the molecular dynamics simulations of S. Leoni *et al.*

T. Chatterji (France) reported an isosymmetric transition in LaMnO3 with a discontinuous volume reduction, which was compared with the ice melting transition [*Phys. Rev.* **B** 69, 132417 (2004)]. The final talk by S. Leoni (Italy) covered molecular dynamics studies of reconstructive phase transitions. By means of a novel method which samples transition paths, S. Leoni *et al.* have been able to explore the most probable transition routes for this type of transformation. This work introduces the missing link between homogeneous transition paths studied theoretically and the local nucleation and growth mechanism expected in a real system. He presented the wurtzite to rocksalt transition in CdSe as an example [*Phys. Rev.* **B**72 064110 (2005)]. Inhomogeneous transient states exhibit local atomic configurations, as interfaces between the two end states, which can be identified with some of the transformation paths proposed, based on theoretical considerations. Thus for the pressure-driven transition of ClNa from the B1 (ClNa) type to the B2(ClCs) type structure, the authors could observe a local B33 (α-Tll) configuration interface between the two end structures [*Phys. Rev. Lett.* 92, 250201 (2004)], in accordance with one of the transition paths proposed for this transition.


T. Chatterji


S. Leoni

J. Manuel Perez Mato and Ulrich Bismayer

Instrumentation for Next Generation X-ray Sources

The topic of the microsymposium was the next generation of X-ray sources, in particular, X-ray free-electron lasers (FEL). Three X-ray FEL projects for hard X-ray radiation down to 0.1 nm wavelength using the self-amplified spontaneous emission (SASE) scheme are currently in construction, the Linac Coherent Light Source (LCLS) at Stanford, USA, the Spring-8 Compact SASE Source (SCSS) at Harima, Japan, and the European XFEL at Hamburg, Germany. The properties of X-ray FEL radiation are unique in that $10^{12} – 10^{14}$ photons are provided by a single pulse of typically 100 fs duration, in a bandwidth of about 0.1% of the photon energy. The radiation is furthermore transversely coherent. These properties translate into a peak brilliance about nine orders of magnitude higher than the best synchrotron radiation sources today. New and currently-impossible scientific applications have been proposed for these facilities, which will impose tough requirements on the experimental equipment. X-ray FEL experiments are expected to differ substantially from experiments at synchrotron sources. The five speakers of the session presented the state-of-the-art for different aspects of instrumentation for X-ray FEL experiments.


K. Gaffney

K. Gaffney (USA) discribed investigations of ultrafast processes on the sub-picosecond timescale using pump-probe experiments. In this type of experiment a pump pulse excites the sample and the X-ray pulse is typically used as a probe to observe the resulting rapid structural changes. The pump pulse could be either optical or X-ray, leading to different requirements for instrumentation. The use of optical lasers requires establishing a time correlation between the laser and X-ray pulses at the femtosecond level. This could be achieved either by synchronisation or by measuring the delay for each pair of pulses and appropriately tagging the data. The latter

approach has been successfully tested at the Sub-Picosecond Pulse Source at SLAC, yielding a time resolution of the order 150 fs for laser-pump/X-ray-probe experiments.


S. Marchesini

The imaging of single molecules using intense, ultrafast X-ray pulses was presented as a second X-ray FEL experiment by S. Marchesini (USA). A large number of new, difficult issues will need to be resolved: sample injection, preparation of very short X-ray pulses, absorption of X-rays in the molecules and subsequent radiation damage, and the classification of data sets and reconstruction of the 3D structures. Recent experiments using soft X-ray radiation achieved 3D reconstruction of cells and test objects at high resolution and showed that the algorithms are available.

M. Yabashi (Japan) described the role of optical elements in preserving the high degree of coherence of XFEL radiation. State-of-the-art techniques suggest that optics for coherent X-ray radiation at 0.1 nm wavelength are readily available.


C. Brönnimann

B. Lengeler (Germany) presented the latest achievements using refractive lenses and discussed the limitations for observing very small focii.

Finally, C. Brönnimann (Switzerland) presented the advances in the field of pixel detectors for synchrotron radiation applications and discussed necessary modifications and possibilities for XFEL experiments with far higher pulse intensities.

Th. Tschentscher and J. Arthur

Advances in Computational Methods for Powder Diffraction microsymposium

This microsymposium highlighted computer software advances in powder crystallography. Andrew Wills (UK) described a generalized approach to magnetic symmetry, using irreducible corepresentations that allows both commensurate and incommensurate magnetic structures to be modeled. He has implemented this complex theory with a friendly interface in a program called SARAh, which is freely distributed. Juan Rodriguez-Carvajal (France) presented his work on a huge open source subroutine library for crystallographic calculations, CrysFML, which is written in object-oriented Fortran (F95). The FullProf Rietveld program already uses parts of CrysFML and it is progressively being reimplemented to take increased advantage of the modular structure of this library. Simon Billinge (USA) discussed data analysis & modeling for total scattering and goals for a new generation of diffraction analysis envisioned as part of the DANSE project, which has been proposed to the National Science Foundation. Gavin Vaughan (France) showed how advanced computational analysis and superb microbeam diffraction capabilities allows indexing of individual crystallites in a powder diffraction sample. This allows single crystal diffraction intensities to be measured directly from powders. Finally, Samantha Chong (UK) presented her thesis work (under advisor Maryjane Tremayne) on structure solution strategies using powder diffraction.


A. Wills


J. Rodriguez-Carvajal


S. Chong

Brian H. Toby

The Big Question in Structural Genomics: Discovering Function from Structure

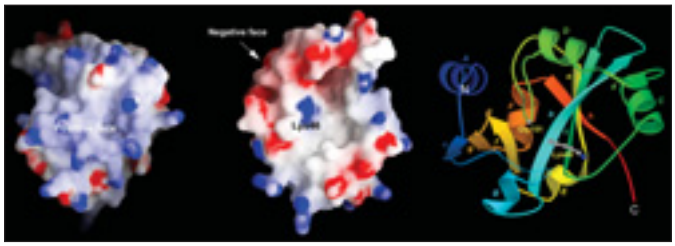
Given that more than 50% of the proteins encoded by any genome are of unknown or uncertain function – to what extent can the protein structures contribute to the discovery of function?

The speakers in the microsymposium, which was chaired by Ted Baker (New Zealand) and Sung-Hou Kim (USA), reflected the global spread of interest in this topic: Bill Shepard (France), Osnat Herzberg (USA), Ray Stevens (USA), Seiki Kuramitsu (Japan) and Al Edwards (Canada, UK). Talks ranged from detailed analyses of a single protein to discussions of broad biochemical and biophysical screening assays.

Bill Shepard described a hypothetical protein from *Mycobacterium tuberculosis* that proved to be a fatty acid binding protein, although its true physiological substrate has yet to be fully identified. Osnat Herzberg showed that time and expert knowledge can be important allies. One hypothetical protein from *Haemophilus influenzae* was almost a "singleton" when the structure was first solved, but is now representative of a family of more than 800 members, with both structure and function (as a tRNA editing domain) established. She also showed the importance of structure in differentiating enzyme functional families through specific structural signatures, even in the presence of high sequence identity.


B. Shepard


O. Herzberg


Structure of HI1434, whose function was unknown when the structure was determined, and is now known to be a stand-alone tRNA editing protein, Cys-tRNAPro deacylase.

Ray Stevens showed that not even nature's thunderbolts can keep a good talk down. When Jerry Joseph, the invited speaker, was delayed by thunderstorms in Georgia, Ray Stevens stepped in at 30 minutes notice, and gave a fascinating account of their SARS structural genomics efforts. It is remarkable how the technological advances of recent years now allow structural biology to address new viral threats with great urgency - although Ray also cautioned that the biology still remains the biggest challenge in such cases, especially where protein-protein interactions need to be elucidated. Seiki Kuramitsu described progress with the RIKEN structural genomics project on an extreme thermophile, which has the ambitious long-term goal of in vitro reconstitution of the organism, as well as characterisation of its proteins.


J. Joseph


S. Kuramitsu

Finally Al Edwards finished the microsymposium in rousing style, with a talk that included a surprising excursion into the mysteries of soccer (revealing to this listener some unexpected physical similarities with ice hockey). The human structural genom-

continued on Page 11

INCOATEC
innovative coating technologies gmbh

Optics for Crystallography

Incoatec produces ultra precise thin films according to client-specific requirements using modern deposition technology. Our main products include the latest generation of multilayer optics for

- **X-ray diffraction**
- **X-ray spectrometry and**
- **synchrotron applications.**

Computerized optics simulation, production of various types of substrates as well as characterization of films round off our service profile.

Simulation

- X-ray optical properties
- complete beam paths using 3D ray tracing methods

Coating

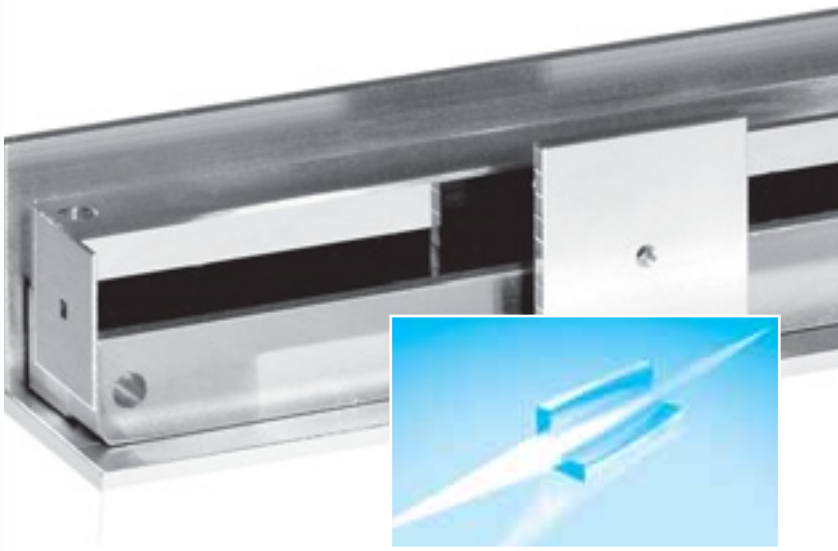
- ultra precise films & multilayers
- more than 50 materials

Characterization

- XRD, XRF, profilometry
- quality testing

Incoatec GmbH
Max-Planck-Str. 2 · 21502 Geesthacht · Germany
Tel.: +49 (0) 41 52 – 88 93 81
Fax: +49 (0) 41 52 – 88 93 83
email: info@incoatec.de

www.incoatec.de



Montel Optics

- 2D collimation and focusing
- More than 10^8 photons/sec with sealed tubes
- More than 10^9 photons/sec with rotating anodes
- Flux density above 10^{10} photons/sec/mm^2
- Cr, Fe, Cu and Mo radiation
- Optics with various lengths, focal distances and divergences
- Client-specific optics

Single-Bounce Mirrors

- 2D focusing with flux densities above 10^{10} photons/sec/mm^2
- Twice the amount of flux and flux density than Montel Optics
- Free choice of apertures for high intensity or high resolution
- The most brilliant optics you can get for your crystals

continued from Page 9

ics project he heads, which now incorporates sites in Toronto, Oxford and Stockholm, and which operates as a public good enterprise, is currently determining 13 new protein structures per month. Importantly, it has developed a range of screening assays, for example to discover enzymatic activity or ligands to assist in crystallization, which are clearly a very important resource for the community.


A. Edwards

Ted Baker

Putting the pedal to the metal: speeding up the structure determination process

One major task of structural genomics is the design of tools that increase the efficiency and speed of experimental structure determination. Such developments will ultimately result in a reduction of the average cost per structure for the more standard protein targets while allowing efficient screening of many hundreds of crystals. The implementation of high-throughput protein expression and crystallization robots has already done much to accelerate the wet-chemistry part of a structure determination. MS23 focused on ongoing efforts to automate the X-ray data collection and phasing parts of the structure determination process. Martin Walsh (France) gave an overview about the hardware and software implemented at the BM14 beamline (ESRF, Grenoble) and the e-HTPX project that will enable users to manage the entire data collection process with a seamless exchange of wet-chemistry and diffraction data over the internet. Wayne Anderson (USA) reported on the Automated Crystallography System (ACrS). The system, which was successfully applied in 75% of all cases, relies on existing software and explores different software combinations in parallel. The application of ACrS was discussed in light of two crystal structures that were solved using the anomalous signal of zinc, since Se-Met MAD phasing was impossible. John Rose (USA) described a 24-hour synchrotron shift during which five structures were determined by SAD using the SCA2 structure pipeline. This pipeline operates either in an automatic hands-free mode or at an expert user level. In contrast to this the HKL2000_ph program combines data reduction and phasing into a single stand-alone program. Wladek Minor (USA) illustrated the capabilities of this program by solving SAD and MAD structures on stage. Keith Wilson (UK) focused on ongoing efforts to streamline the entire structure determination process from the perspective of medium sized structural biology laboratories. Lessons were drawn from a recent workshop on Structural Proteomics in Europe with particular examples of high-throughput structure determinations of *Bacillus anthracis* proteins. These systems are already accelerating X-ray structure determination in an impressive way and facilitate structure determination even by non-expert users.


M. Walsh


W. Anderson


J. Rose


W. Minor


K. Wilson

Peer Mittl and Yvonne Jones

Structure Determination from Powder Diffraction Data (Organics).

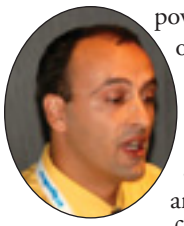
The prevailing methods for structure solution of organic materials from powder diffraction data exploit known molecular structure via a global minimisation in real space, though direct methods remain an essential option.

Vincent Favre-Nicolin (France) gave an expert overview of his freely available FOX program. Originally developed for inorganics, its versatility allows molecular structures to be solved *via* Monte Carlo or parallel-tempering minimisation routines. Molecules are described and manipulated using bond-length, bond-angle and dihedral-angle restraints, providing a very flexible way to define the degrees of freedom that need to be optimised. New features include maximum likelihood which enlarges the hypersurface near the global minimum and is useful when the model is incomplete or has systematic errors. Vincent showed some impressive examples, including two triglycerides from chocolate with up to 57 torsion angles that took two months of computing time to solve.


V. Favre-Nicolin

Many structures are solved from laboratory powder data, and the question of their accuracy can arise, especially if the structure does not agree with the expectations of the synthetic chemist. Vladimir Chernychev (Russia) related such an instance when the organic ligand was clearly tridendate, whereas the chemist believed that it should be bidentate. The controversy was only resolved once a single crystal was finally grown, confirming the powder structure. Further examples were given, corroborated by synchrotron or neutron diffraction data, to demonstrate the veracity of structures determined from laboratory data.

Cikui Liang (USA) explained how direct-space methods can fail if the powder pattern is of inadequate quality, or if there are too many degrees of freedom to be defined. The structure must make chemical sense, so inclusion of potential energy in the minimisation can help, e.g. with a close-contact penalty function and a combined figure of merit. Energy can also be incorporated into the Rietveld refinement provided accurate potentials are known. The relative weight to be given to the diffraction data versus the energy is not intuitive, but can be derived *via* a Pareto optimisation to find the proper balance between fitting the diffraction pattern and minimising the energy. These ideas were illustrated with some nice examples, e.g. (E)-2-(4,6-Difluoroindan-1-ylidene)acetamide, analysed using Materials Studio.


C. Liang

Philippe Fernandes (UK) reported attempts to use direct methods and differential thermal expansion (DTE) to solve the structure of γ-carbamazapene, with 72 non-hydrogen atoms. With powders, data to atomic resolution is difficult to obtain, especially with severe peak overlap, but harnessing DTE can improve things, because peaks overlapped at one temperature may be better resolved at another. Data collection using synchrotron radiation was concentrated at high angles to improve the quality of this crucial part of the pattern. To minimize radiation damage, low temperatures and a wavelength of 0.8 Å were used, automatically translating and changing capillaries to expose fresh sample to the beam. All in all an impressive amount of data, from which a set of intensities was extracted using a multipattern Pawley procedure implemented in Topas. Direct methods have not yet been success-

P. Fernandes

ful, but work is continuing. Using DASH and global optimization, the structure could be solved and refined without additional restraints.

Anders Markvardsen (UK), standing in for Kenneth Shankland, emphasized that computing power is essential for solving complex structures by multisolution simulated annealing (SA). Whereas, small molecules may need only seconds per SA run, and have close to 100% success rates, complex structures need possibly hours per run, and success may fall to below 5%. Implementing a grid system can give access to almost unlimited computing power, by using unused time on other computers. Anders illustrated the impressive performance of this multi-machine approach, combined with the hybrid Monte Carlo search algorithm. The grid does not just give you more, faster: it allows you to attempt the otherwise impracticable.

Andy Fitch and John Faber

Recent Advances in Quasicrystal Research

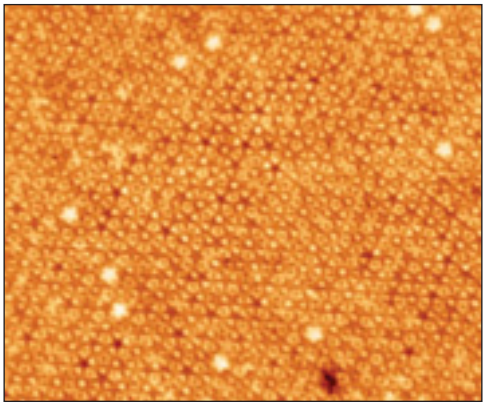
Rónán McGrath (UK) reviewed recent experimental studies of surfaces exhibiting fantastic long-range order on the atomic scale, as can be seen in the beautiful STM image below. He also showed that a vibrant current research theme is the use of quasicrystal surfaces as templates for the growth of novel nanostructured systems. Zorka Papadopolos (Germany) showed how accurate STM data can be used to determine the principles that govern with which surfaces quasicrystals terminate.


R. McGrath


Z. Papadopolos

A common theme of the talks was the increasing quality and accuracy of quantitative information obtained in current experiments. Not only is it possible to reach atomic resolution in real-space images, it is also possible, as shown by Marc de Boissieu (France), to obtain extremely precise data from X-ray diffuse scattering in order to extract quantitative information regarding the role played by phasons in the thermodynamics of quasicrystals. The high precision of current X-ray diffraction experiments allows the study of quasicrystals at extreme pressures and temperatures, as described by Günter Krauss (Switzerland). To the astonishment of all participants, Krauss reported that a number of different decagonal quasicrystals remain stable, without any structural transformation, up to tens of GPa and almost 1000 K. These data are sure to keep theorists busy for some time.


M. de Boissieu


A 200 Å x 200 Å STM image of the five-fold surface of the icosahedral AlPdMn quasicrystal (Courtesy of Rónán McGrath of the U. of Liverpool).


G. Krauss

The microsymposium ended with a presentation by Yushu Matsushita (Japan), who introduced the newest sibling in the family of quasicrystals—a polymeric quasicrystal. The building block of this system is composed of a star-shaped configuration of three polymers. By varying the length of one of the three arms, the system exhibits a variety of long-range ordered 2-dimensional structures with tiles on the order of 100nm. Among these is an approximant of the dodecagonal square-triangle tiling, which with some tweaking may yield an exact dodecagonal quasicrystal in the near future. This possible new addition to the growing number of systems exhibiting quasiperiodic long-range order is yet another indication that quasicrystals will remain in the forefront of crystallographic research for years to come.


Y. Matsushita

Ron Lifshitz and Koh Saitoh

Detectors: Developments and Requirements for X-ray, Synchrotron and Neutron Sources

The first speaker, Burckhard Gebauer (Germany) described several different types of neutron detectors developed in DENTI, using MSGC and Si-MSD. Considerable efforts are being made for ASICS development. Three different types of X-ray area detectors were described. Jules Hendrix (Germany) talked about a Se-based TFT flat panel detector with a diagonal size of 555 mm. Data obtained using synchrotron radiation were presented. He stressed the high spatial resolution due to the use of direct conversion by Se. The detector was to be commercially available for protein crystallography by the end of 2005. Gregor Huelsen (Switzerland) presented the recent status of the PILATUS detector. A detector developed in colloboration with a synchrotron facility, it is a silicon pixel array detector using bump-bonding and modern semiconductor technology. A tiled assembly of the 1M prototype has been tested for protein crystallography. After corrections for inhomogeneity and distortion, an electron density map was successfully obtained. Roger Durst (USA) announced Resistive Microgap Detector, which is a gas detector with a high local counting rate. The readout is through a delay line. For high gain and stability, electrodes were specially designed to avoid sparks. Parallax problem was solved by field shaping. The latter two X-ray detectors are photon counting, and David Laundy (UK) described his analysis of dead-time when such detectors are used with a pulsed X-ray source like synchrotron radiation. This problem will be more serious in future because the proposed next generation x-ray sources are all pulsed sources.


B. Gebauer


J. Hendrix


G. Huelsen


R. Durst


D. Laundy

Naoto Yagi and Christian Broennimann

Structure Determination from Powder Diffraction Data (Inorganics)

Powder diffraction was used primarily for phase identification until the mid nineteen nineties. Recent rapid progress in X-ray sources, instrumentation, computers, software and methodology has made the use of powder diffraction for solving crystal structures realistic.

Textured powder samples can be exploited to resolve the problem of overlapping reflections in powder diffraction. Lars Kocher (Switzerland) showed an improved experimental set-up collecting only a quarter of the full 360° scattering pattern on an image plate system gathering data to higher 2θ values. He presented algorithms which help reduce the disadvantage of poor statistics when using a new linear detector with extremely high resolution.


L. Kocher

Anna Grazia Moliterni (Italy) provided an overview of the "EXPO2004" software package and described new features of EXPO2005 which includes improved methods and algorithms for space group determination, background calculation, estimation of integrated intensities and phasing. Moreover, a new global optimization approach exploiting Fourier maps provided by direct methods has been optimized for organic structures.


G. Moliterni

Robert Dinnebier (Germany) demonstrated that many phases may still be missing in the phase diagrams. He presented powder diffraction studies at variable pressure and temperature conditions. Using a new fast image plate detector he was able to dramatically improve data collection, leading to the solution of the crystal structures for many intermediate phases. Elaborate strategies were adopted for processing large amounts of raw area detector data to obtain the final individual diffraction patterns.


R. Dinnebier

Thierry Bataille (France) talked about the ab-initio solution of crystal structures of products obtained by thermal decomposition. Due to phase transitions during heating/cooling of the samples and the corresponding reorganization of the crystal structures, single crystal data are generally not available for these compounds. He described in situ powder data collection using Bragg-Brentano optics in combination with a conventional X-ray source and presented several new crystal structures.

A special highlight was Pavol Juhas' (USA) description of an elaborate new algorithm to reconstruct the three-dimensional structure of a single-element molecule from its pair distribution function (PDF). Step by step the build-up of clusters starting from individual atoms was demonstrated. New atoms were added to the cluster, controlled by a figure of merit based on the agreement between the calculated and observed PDF. Several trials were ranked according to the figure of merit and a special new algorithm inspired by soccer leagues was applied. The case of a C60 molecule was analyzed.


P. Juhas

Angela Altomare and Holger Putz

Charge, Spin and Momentum Densities in Materials Science

This session presented a wide range of scientific problems that can be favorably addressed with "sub-atomic" crystallography through, for example, very accurate low-order structure-factor measurement. Experimental techniques spanned high energy and high intensity synchrotron X-ray diffraction, through convergent-beam electron diffraction (CBED) to the measurement of magnetic Compton profiles. Thomas Lippman (Germany) opened the session by discussing the virtues of very high energy radiation (> 100 keV) to minimize extinction errors for obtaining charge densities (CDs) on inorganic structures, and he exemplified the vast potential of the technique with a study of charge and orbital ordering in heavy atom oxides. Part of the talk was devoted to describing the new GKSS high energy beam line being constructed at HASYLAB and the great promises of the new PETRAIII ring. Benoît Guillot (France) discussed an amazing study of the 6700 atom human aldose reductase protein, giving a detailed description of how to handle millions of reflections in the multipole model – and it actually worked. Convincing electron deformation maps can now be retrieved even on the inhibitor, and subtle electronic features never before exposed in such large molecules can be analyzed. In an eminently scholarly talk Dietmar Stalke (Germany) then took the audience back to freshman chemistry and challenged the concept of hypervalency. Applying the quantum theory of atoms in molecules on the experimental CDs of a range of formally hypervalent compounds our foundations were shattered and then rebuilt in simple bonding models, which have also led to the development of new types of chemical reactions. Very predictive indeed! Jian-Min Zuo (USA) addressed the problem of data accuracy in vital low order reflections, which can be overcome by CBED using a nanometer probe and perfect crystal theory to avoid extinction errors. A range of "simple" inorganic materials were discussed, and a detailed comparison with state of the art theoretical calculations showed that not far beyond monoatomic crystals, theory gets seriously challenged. Experimental data do in fact have smaller errors than the differences between theoretical models, and CD studies are important for further development of *ab initio* methods. In the concluding talk Yoshiharu Sakurai (Japan) explained about the peculiar material UGe_2, which has coexistence of superconductivity and ferromagnetism. The magnetism in the system was approached by a novel orbital decomposition scheme of the magnetic Compton profiles. The method allows the temperature dependence of the separate orbital populations to be studied, and this led to the conclusion that superconductivity in UGe_2 is mediated by orbital fluctuations. In summary, the session spanned from simple metals to proteins, and from small organics to ultra heavy inorganics on the journey through charge, spin and momentum space. Development of new experimental techniques continues to propel the vibrant field of sub-atomic crystallography, which is clearly a very.


T. Lippman


B. Guillot


D. Stalke


J.-M. Zuo


Y. Sakurai

B. Iversen and J. Spence

Liquid nitrogen free

...but cooler than ever

Introducing the Cobra, the new NON-LIQUID Cryostream from Oxford Cryosystems...

Cryostream-like efficiency and reliability without the liquid: Cobra truly offers the best of both worlds.

The Cobra offers:

- Temperature range 80-500K
- Fast cool down time (30 mins to 100K)
- Complete programmability from a Cryostream-style controller
- Turbo mode (10L/min gas flow) for fast cooldown

The Cobra can be supplied with or without a nitrogen gas generator, so you can use your laboratory dry nitrogen gas supply if available.

We will even offer you a trade-in on your old nitrogen system – just contact us for details.

We look after our technology so you can look after yours!

OxfordCryosystems

Head Office
3 Blenheim Office Park
Lower Road · Long Hanborough
Oxford · OX29 8LN · UK
T. +44 (0)1993 883488
F. +44 (0)1993 883988
E. info@OxfordCryosystems.co.uk

North American Office
7 Jackson Road · Devens
MA 01432 · USA
T. 1-866-OXCRYO-8
978 772 7930
F. 978 772 7945
E. Info@OxfordCryosystems.com

Enzymes and Allostery

This microsymposium was organized through a joint effort of Alexander Wlodawer (USA) and Silvia Onesti (UK). Unfortunately, the latter was not able to attend due to her involvement in an applied genetics experiment, the results of which were due in late October, but both co-chairs were responsible for the difficult decisions involved in choosing only five speakers from among many excellent abstracts. The session was started by Lukasz Lebioda (USA) who presented exciting results on the negative cooperativity of human thymidylate synthase. That enzyme cycles between an active and inactive conformation, both of which may be independently targeted by inhibitors. The inhibitors that stabilize the inactive conformation show positive cooperativity with currently used antifolate cancer drugs. Momoyo Ishikawa (Japan) discussed substrate channeling in a fatty acid β-oxidation multienzyme complex. Large changes in the structure of the enzyme are responsible for sequential presentation of the substrates for several stages of catalysis, without their intermediate release. Pamela Williams (UK), a finalist in this year's Pharma Achievement Award, gave a fascinating talk on structural studies of cytochromes P450, enzymes directly responsible for metabolism of a majority of drugs. Cytochromes such as CYP3A4 and CYP2C9 have been studied as complexes with a variety of marketed drugs and their structures provide novel insights into the principles of substrate binding and allostery. Wojciech Rypniewski (Poland) presented the first structure of a eukaryotic phosphofructokinase 1, describing how catalytic sites could have evolved into allosteric effector sites. The final speaker, Marcus Rudolph (Germany) apologized that his favorite macromolecule, formylglycine generating enzyme, is not actually allosteric, nevertheless the combination of high resolution crystal structure and extensive mutagenesis went a long way towards explaining the molecular basis of multiple sulfatase deficiency, an inherited human disease. Thus the session ended up being 100% enzymes and 80% allostery, a combination that seemed to be of considerable interest to the audience.


L. Lebioda


M. Ishikawa


P. Williams


W. Rypniewski


M. Rudolph

Alexander Wlodawer

Busy Relaxing...

Based on surveys of self-reported time use through the decades, Erik Hurst (U. of Chicago) reported that leisure time rose dramatically for men and women. Because there's been a huge time savings in housework – about 12 hours a week – more women were in the job market in 2003, 74% compared with 48% in 1965. TV watching is devouring two-thirds of the leisure time gained, while time spent reading and churchgoing is down.

SCIENCE, Vol. 311, February 10, 2006

Applications of Synchrotron and Neutron Facilities in Structural Chemistry

In this microsymposium some recent structural highlights obtained by chemical, biological and crystallographic groups worldwide, using both synchrotron and neutron diffraction facilities were reported.

Russell Morris (UK) described fascinating structural studies using a combination of microcrystal X-ray diffraction techniques, carried out on Station 9.8, at the SRS, UK, coupled with laboratory based MAS NMR studies of zeolite structures. Some of these zeolite materials exhibit negative thermal expansion properties, and through structural analyses it has been possible to explain these temperature effects by librational changes in the cage structures.


R. Morris

Wolfgang Scherer (Germany) showed how single crystal neutron diffraction studies, augmented by high resolution X-ray data, could be used to provide an accurate picture of the C-H and M-H interactions in a series of catalytically important metal complexes. The experimental pictures did not always correspond to preconceived predictions and the results shed new light on "agnostic" interactions in a range of main group and transition metal complexes.


W. Scherer

Alberto Albinati (Italy) showed how single crystal neutron diffraction studies, carried out at the ILL, Grenoble, could be coupled with inelastic neutron scattering studies to provide new information on the bonding in classical and non-classical metal hydride complexes. This detailed information could not be obtained by other experimental techniques and contrasted with solid state ^{1}H NMR results. Alberto emphasized the importance of carrying out librational corrections in this type of analysis.

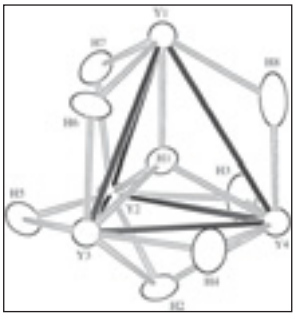

A. Albinati

Bob Bau (USA) presented a "hot off the press" result, the structure of the first complex with a four-coordinate interstitial hydride ligand. This has been one of the "holy grails" of cluster chemistry for three decades, and in a single crystal neutron diffraction study of $Y_4H_8(Cp'_4)(THF)$ [Cp' = $C_5Me_4(SiMe_3)$] one of the hydrides sits in the middle of the metal tetrahedron.


B. Bau

Matthew Blakely (France) emphasized the importance of neutron diffraction in locating hydrogen/deuterium atoms in protein structures and described a method that he and his co-workers had developed for cryo-cooling crystals of a suitable size for neutron diffraction studies to 15K. Structure analysis using data at this low temperature gave much improved structural refinements and provided more information as to the nature of the hydrogen bonding in several systems compared to room temperature data.


M. Blakely


An ORTEP plot on the H8Y4 cluster with the four-coordinate H atom.

Paul Raithby and Trevor Forsyth

Microstructural Properties from Powder Diffraction Data

The first lecture "Subgrain Size Distributions, Dislocation Structures, Stacking- and Twin Faults and Vacancy Concentrations in Crystalline Materials Determined by X-ray Line Profile Analysis" by Tamás Ungár (Hungary) presented many different applications of line broadening analysis based on physically sound models. Especially interesting were new insights into the relationship between measurements of domain/crystallite size, as obtained by X-ray diffraction and transmission electron microscopy, and analysis of vacancy concentrations. Matteo Leoni (Italy) gave an overview of different types of defects and modeling of their influence on diffraction lines. A theoretical overview was followed by several examples treated by the program for modeling line broadening, WPPM. Radomír Kužel (Czech Republic) discussed defect structure obtained by high-pressure torsion and films made of colloidal gold nanoparticles. Line-broadening analysis was complemented by diffuse scattering studies, TEM, and life-time positron annihilation spectroscopy. Nicolae Popa (Russia and Romania) discussed "Size Anisotropy and Lognormal Size Distribution in the Powder Diffraction Whole Pattern Fitting". He proposed a new model that uses ellipsoids to model size anisotropy of crystallites, compared it with the model that employs spherical harmonics, and tested it on a zinc-oxide powder. The last speaker, Nicholas Armstrong (Australia and USA) described the "Development of a NIST SRM 1979 Nano-Crystallite Size Standard for Broadening of X-ray Line Profiles". Especially interesting was the certification process of the standard reference material (SRM), which employed the Bayesian/maximum entropy method.


T. Ungár


M. Leoni


R. Kuzel


N. Popa


N. Armstrong

Davor Balzar and Paolo Scardi

Structures, Phase Transitions and Properties at High Pressure

Structures, phase transitions and properties at high pressure have been the center of high-pressure research for decades, since they provide fundamental structural information that is the basis for all high-pressure science, from biology to cosmology.

In recent years, enormous progress has been achieved in experimental techniques, in particular, in X-ray and neutron diffraction under extreme pressure-temperature conditions. A remarkable example of high pressure single crystal work was presented by Tetsu Watanuki (Japan) on subtle structural modification of a complex Cd-Yb 1/1 quasicrystal approximant. This was clearly seen in his synchrotron X-ray oscillation photographs showing the evolution of superlattice reflections with decreasing temperature at high pressure. This structural change is attributed to the successive orientational ordering of the Cd_4 tetrahedron which is the most inner unit of the four-shell atomic clusters occupying the bcc lattice sites. These four newly found structures, together with two known structures, constitute a complex P-T phase diagram.


T. Watanuki

Nozomu Hmaya

Advances in Computational Methods for Protein Crystallography

This session covered developments in methods, which will be useful in the investigation of more difficult problems not amenable to automated solution and in future high-throughput work.

Randy Read (UK) presented "New likelihood based phasing methods in 'phaser'". He introduced likelihood phasing, in which the best model is the one which is most probable to produce the observed data. This approach has been applied to both molecular replacement and heavy-atom phasing in 'phaser' software.


R. Read

For molecular replacement, this software provides a number of benefits: likelihood-enhanced rotation and translation function provide greater sensitivity; anisotropic data correction helps with some difficult datasets; and modular programming allows the implementation of complex automation strategies which involve the testing of many chains of hypotheses when searching for multiple models. An example was given in which a 4-helix bundle was solved in under a minute by exploring permutations of helical fragments.

Heavy atom phasing for SAD and MAD experiments has also

been implemented, using the conditional probability of the Friedel mate to modify the phase probability distribution for the original reflection. Log-likelihood gradient maps from this approach are very powerful in identifying minor sites, for example in the case of Halide soaks. A high resolution case was presented in which this method allowed the location of Fe, S, and eventually the C atoms within the phasing program.

In the future, it is hoped that molecular replacement and heavy-atom phasing will be combined for difficult problems. Problems still remain in the exploitation of non-crystallographic symmetry in molecular replacement. Asked about the limits of the method, Read said models may be as small as 15% of the total structure, or as low as 20% sequence homology.


M. Schiltz

Marc Schiltz (Switzerland) presented a lecture on 'Broken Symmetries in Macromolecular Crystallography', dealing with cases when multiple measurements of symmetry related reflections give different results.

The first case considered was that of radiation damage, which over the course of the experiment causes changes in the crystal leading to changes in the measured intensities. Others have employed this as a means to determine a model of the changes within the crystal. The focus of this work was the use of this information to enhance phasing. Two parameters are added to each heavy-atom to model change in occupancy during the experiment.

A more unusual application of this approach arises when polarized X-rays are anomalously scattered from heavy atoms with anisotropic density distributions, for example due to bonding effects. In this case, the magnitude of the anomalous effect may be dependent on the incident and diffracted beam direction. Schiltz was asked about the effect of detector size on the diffracted beam direction, and he suggested that the incident beam is more important in this effect.


H. Xu

Hongliang Xu (USA) presented his work on 'Statistical direct methods of phase determination'. Direct methods may be approached by optimizing some target function whose value is minimised by the true phases. The assumption of a uniform random distribution of atoms leads to the result that triplets of structure factors whose normalised magnitudes are large are likely to have phases which sum to zero. This principle has been employed in the tangent formula, and in the minimal function used in the Shake-and-Bake direct methods software. However the effect becomes weaker as the number of atoms increases.

A new approach has been implemented in which phases are shifted to increase the fraction of the triplets whose phases fall within some range from zero. Analysis of data from real problems suggests that the width of this interval should increase as the number of atoms in the problem increases. This approach improves the success rate in determining heavy atom substructures over a range of test cases. It was suggested that the adoption of a linear integer method increases the radius of convergence for the calculation.


P. Skubak

Pavol Skubak (The Netherlands) presented his work on 'Direct use of SAD phase information in automated model building and refinement', implementing model refinement directly against anomalous data in the REFMAC5 software, comparing three approaches. Traditionally, only the estimated non-anomalous magnitudes were used in the refinement.

More recently, phase probabilities have been output from the phasing software, in the form of Hendrickson-Lattman coefficients, and employed in refinement software to provide more information from which to determine the model parameters. There are problems with this approach, in that the heavy atom phase distribution is not updated to include information from the final model, and the dependence between the heavy atom and model phases is ignored.

To address these problems, all of the SAD data is used in the refinement program. The software was tested on a range of problems and was as good as existing methods in every case. It provided a significant benefit, measured by residues built in ARP/wARP, in about 30% of cases.

R. Read and G. Bricogne (UK) suggested that the anomalous phasing information was well described by Hendrickson Lattman coefficients, so the improvements may arise from elsewhere in the process.


R. Grosse-Kunstleve

Ralph Grosse-Kunstleve (USA) presented a lecture titled 'Hybrid Programming in Crystallography: Phenix.refine and phenix.hyss'. The 'phenix.refine' macromolecular refinement software uses components developed in the PHENIX project including bulk solvent model, and restraints on the isotropic B-values. A grid search of bulk solvent parameters avoids some problems of instability in the calculation and restraint of B-factors by proximity is found to be helpful in avoiding extreme values.

The 'phenix.hyss' software is a substructure solution program combining Patterson and direct methods with dual-space recycling. The software is open-source.

Piet Gross and Kevin Cowtan

Chemical Insights from Electron Density Studies and Wavefunctions

This microsymposium ranged from fundamental to applied aspects of the electron density in molecules and crystals. In his keynote lecture, M. Spackman (Australia) showed how the number of publications of charge density studies increases year after year and he enumerated the accurate electrostatic properties that can be derived from high resolution X-ray diffraction experiments for molecules and solid materials. R. Hoffmann (USA) discussed theoretical approaches for the characterization of the molecular bonds by using Bader's topological theory and D. Jayatilaka (Australia) showed how wavefunctions can be fitted to experimental diffraction data. The first speaker in this microsymposium, Richard Bader (Canada), offered deep insight into the nature of chemical bonding and its concept in chemistry. He redefined the basis of quantum mechanics in relation to the properties of atoms in a chemical system through the topological properties of its electron density. He demonstrated how the resulting boundary conditions can be useful for the extension of his theory to open systems. Jean-Michel Gillet (France) showed the possible combination of theory and experiment in a joint refinement to reconstruct reduced density matrices for small to extended molecular systems. Peter Luger (Germany) discussed the use of synchrotron radiation to collect very accurate data suitable for electron density studies. The application to strained carbon ring and cage systems with conformations close to that of fullerenes was highlighted in this presentation. He showed how topological analyses of the electron density for such compounds are powerful tools to characterize even unusual carbon bonds. So-called hypervalent compounds containing Si and Ge atoms were presented by Alexander Korlyokov (Russia). Examples of Si(Ge)...O(N) hypervalent bonds were discussed in the scope of calculated and experimental electron density topological properties at the bond critical points. Anders Madsen (Denmark) showed how accurate electron density determination and rigid-body TLS analyses can be pertinent to reveal physical properties of materials. On this basis, he could explain the observed difference in calorimetric and energetic results of diastereomeric xylicol and ribitol compounds. He illustrated his talk with animated videos showing the harmonic and uncoupled thermal motion of each molecule in the crystal lattice.


R. Bader


P. Luger


A. Korlyokov


A. Madsen

N.E. Ghermani

Protein Interactions with Other Biological Macromolecules

E. Yvonne Jones (UK) discussed strategies to produce X-ray-quality crystals of components of the extracellular region of the receptor protein tyrosine phosphatase mu. These strategies have recently led to the structure of the full-length protein including four fibronectin domains which are seen to adopt an extended "beads-on-a-string" conformation.


E.Y. Jones

Chris Hill (USA) discussed so-called molecules of mass destruction, i.e. protein-degrading complexes. He focused on various activators of proteosomes and how they regulate access to proteolytic sites within the proteosome interior.


C. Hill

The RecBCD protein is a multifunctional enzyme complex that provides one mechanism for the repair of double-stranded breaks in DNA. Dale Wigley (UK) discussed the large and complicated, yet modular interdependent, structure of the enzyme. The RecBCD structure explains the regulation of nuclease digestion and also suggests how the protein can recognize single-strand DNA sequences as they pass through the complex.


D. Wigley

Yong-Seok Heo (Korea) discussed the structures of different scaffolding proteins (JNK1, 2 and 3) that assemble components of the c-jun N-terminal kinase signaling pathway. Complexes of human JNK1, JNK2, and JNK3, with their appropriate activating peptide, provide a structural rationale for the specificity of peptide recognition and how associated hinge motion allosterically modulates ATP binding.


Y.-S. Heo

Hanna Yuan (Taiwan) described a number of structures bearing the so-called H-N-H motif that forms the core of the active site of many endonucleases involved in restriction, repair and degradation of DNA. One of these proteins is the bacterial toxin ColE7. The structures of the nuclease domain of this protein in complexes with various DNA duplexes were described. The results show how the H-N-H motif is bound in the minor groove and primarily contacts phosphate groups rather than ribose groups or bases. The His-metal fold of the active site suggests a universal mode of DNA recognition and interaction.


H. Yuan

B.W. Matthews and Z. Rao

Topology of Crystal Structures: Nets, Knots and Surfaces

Interest in coordination polymers, metal-organic frameworks, and supramolecular networks is rapidly expanding not only for their potential properties as functional solid materials but also for their intriguing architectures and topologies. Indeed, many examples have evidenced structural types and topological features unprecedented in the world of inorganic compounds and minerals, but a unified view of the observed complex topological phenomena is still lacking. Mike O'Keeffe (USA) illustrated the natural tiling approach to describe nets and that the self-dual tilings show the full catenation of the most frequently interpenetrated nets and the relation to the five genus-3 minimal surfaces was shown. Stephen Hyde (Australia) explored in depth the relation between the minimal surface and the hyperbolic plane showing results from the "Epinet" project (Euclidean Patterns in Non-Euclidean Tilings). 3D euclidean networks are formed by a process of projection onto triply periodic minimal surfaces. Interpenetrated nets arise from 2D hyperbolic tilings by infinite tiles. A possible definition of "knottedness" in 3D nets was proposed. A different view of nets is possible via sphere-packings graphs as shown by Elke Koch (Germany) with some exceptional cases including interpenetration of 3D nets, catenation of 2D layers and pairs of


M. O'Keeffe


E. Koch


V. Blatov


S. Batten

packings showing self-catenation. All the above apparently abstract results have been shown to exist with many examples taken from crystal structures that have been collected in a very useful web page by Stuart Batten (Australia). The experimentalist and crystallographer can find the tools to handle the complexity of all the above topologies in TOPOS as illustrated by Vladislav A. Blatov (Samara State U., Russia) where a complete classification of 3D nets has been illustrated by analyzing CSD and ICSD.

Davide M. Proserpio and Jean-Guillaume Eon

Non-ambient Powder Diffraction and Kinetic Studies

Peter Chupas (USA) gave an excellent overview of how rapid PDF information can be gained from samples using data collections as short as one second, opening up the possibility of studying both short and long range structure of materials as a function of time, temperature or during chemical reactions. Karena Chapman (Australia) illustrated the importance of considering both local and average structure in an excellent presentation on a variety of CN-bridged framework materials showing negative thermal expansion. Karena presented a comprehensive collection of data on a large family of these materials and gave clear insight as to the origins of this unusual effect. The importance of *in-situ* powder diffraction studies across a range of technological areas was nicely exemplified by the talks of Raj Suryanarayanan (USA) and Gilberto Artioli (Italy). Suryanarayanan showed how the kinetics of molecular polymorphic and desolvation reactions can be determined from lab data. These studies are of crucial importance for assessing the storage life of pharmaceuticals. He also showed how one can follow the crystallization of a material as a function of time and then deduce the amorphous-to-crystallize starting ratio, allowing quantitative analysis without internal standards. Artioli showed how *in-situ* studies allow one to follow important processes including the removal of template molecules from zeolites and hydrogen production from methane. René Guinebretière (France) described a new high temperature attachment for thin film diffraction studies and how its intrinsic thermal expansion can be automatically corrected to allow accurate determination of key sample microstructural parameters under non-ambient conditions.


P. Chupas


K. Chapman


R. Suryanarayanan


G. Artioli

Ivana Radosavljevic Evans

Structural Biology of the Immune System

This microsymposium reported recent advances in understanding the structure and function of molecules of the immune system, the line of defense of evolved organisms against pathogens. The number of high-resolution structures of antibody fragments, antigen-presenting molecules and their complexes with T-cell receptors, costimulatory molecules, and other proteins involved in this process is growing rapidly. These models are instrumental both for a more complete definition of the synergistic role of macromolecules in the immune response, and for opening new avenues for development of compounds with therepeutic potential. The session was opened by Ian Wilson (USA), who summarized the results deriving from the structural characterization of HIV-neutralizing antibodies, and the use of the antibody structures in a retro-vaccinology process. Of particular interest was the domain-swapped, carbohydrate-specific 2G12 antibody, that allowed the development of novel strategies for anti-HIV vaccines using rationally engineered antigens. Annette Shrive (UK) described the role of the Ca^{2+}-dependent collectins in interacting with bacterial cell surface oligosaccharides, one of the mechanisms of antigen uptake by cells. Victor Streltsov (Australia) presented the structure of the unique IgNAR from the shark, the most primitive animal that has an adaptive immune system to fight infections. These antibodies differ from their mammalian counterparts since they are monomeric, and are substantially lacking a CDR2 region. Two structures of IgNARs, both unliganded and in complex with lysozyme, elucidate how these novel molecules can achieve the necessary hypervariability to interact with a broad spectrum of antigens. Michelle Dunstone (Australia) added another piece to the puzzle of the full-fledged, signaling-competent T cell receptor complex by presenting the structure of the CD3 εγ heterodimer in complex with the therapeutic antibody OKT3. The final talk from Piet Gros (The Netherlands) described the first structure of the C3 complement protein, the plasma protein with a central role in the cascade of events that leads to the formation of the membrane-attacking complex. The extremely complex, intertwined architecture of this member of the α2-macroglobulin superfamily of proteins is paralleled by a dramatic conformational change that occurs upon proteolytic activation.


I .Wilson


A. Shrive


V. Streltsov


M. Dunstone


P. Gros

Massimo Degano and E. Yvonne Jones

Structural Knowledge and Catalysis

This microsymposium focused on the relevance of structural knowledge in designing new catalysts, and studying their mechanism of operation. Agustin Galindo (Spain) described how oxy and thiodiacetate manganese complexes could be used as catalyst precursors in model oxidation reactions. Tsuneo Imamoto (Japan) lectured about high to almost perfect enantioselectivity using rhodium complexes and optically pure P-chiral diphosphine in some asymmetric hydrogenation reactions. He explained that enantioselectivity which is determined by the catalyst structure, also allows one to predict the mechanism of migratory insertion.


A. Galindo


T. Imamoto

Antonio Mezzetti (Switzerland) addressed the issue of stereo selectivity in reactions of atom transfer in chiral ruthenium complexes, and

continued on Page 22

marresearch

High-performance X-ray data collection systems

mardtb/csc

- Advanced goniostat with integrated automatic cryogenic sample changer
- Easy manual or automatic sample mounting and centering
- Fully automated alignment to the X-ray beam
- Ideal laboratory screening station with mar345 or marccd
- Complete state-of-the-art high-throughput beamline endstation with marmosaic CCD detector

marmosaic

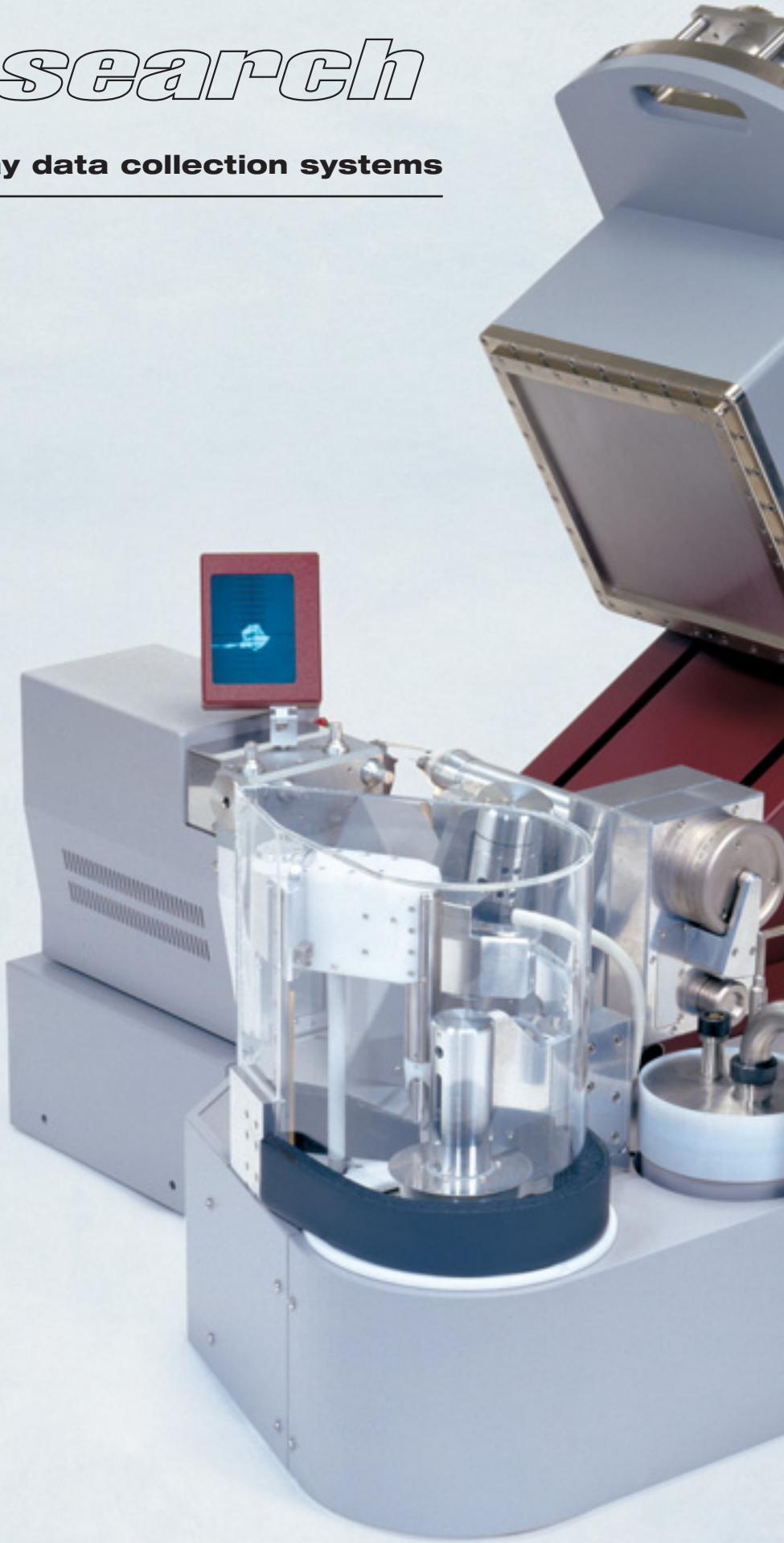
- Seamless multi-element CCD technology
- 225mm × 225mm or 325mm × 325mm active area
- Multichannel readout in 1 second
- Low noise, low dark current design for fully usable 16-bit dynamic range

marccd

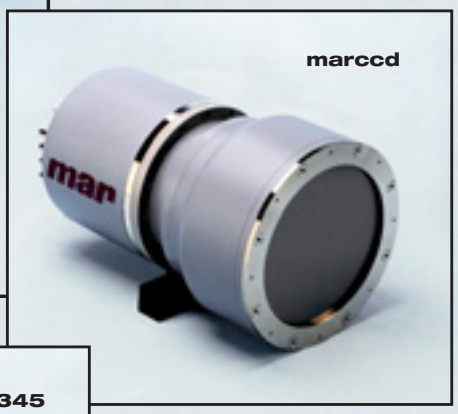
- Largest available single chip design: 165mm diameter
- Based on 4k × 4k CCD with four parallel readouts
- Low noise, low dark current design for fully usable16-bit dynamic range
- Versatile detector for rotating anode and synchrotron beamlines

mar345

- Calibrated image plate
- Fast spiral readout
- Ultralarge 345mm diameter
- Perennial standard for accuracy and reliability



The marmosaic 225 with mardtb goniostat and cryogenic sample changer is a complete endstation for high-throughput crystallography.



marusa

www.mar-usa.com

1880 Oak Avenue
Evanston, IL 60201 USA

Toll-free: 1-877-MAR-XRAY (1-877-627-9729)

From outside the U.S.: 1-847-869-1548

Fax: 1-847-869-1587

E-mail: info@mar-usa.com

marresearch

www.marresearch.com

Hans-Boeckler-Ring 17
22851 Norderstedt Germany

Telephone: +49 40 529 884-0

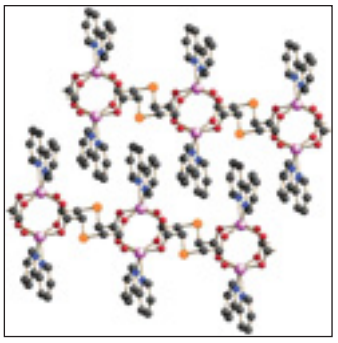
Fax: +49 40 529 884-20

E-mail: info@marresearch.com

continued from Page 19


A. Mezzetti

stressed the role of molecular modelling studies and the need of crystallographic analysis to validate the method used. The theoretical point of view was emphasized by Walter Baratta (Italy) who spoke about agostic interactions studied with the help of X-ray and neutron diffraction techniques. He remarked that electron poor ruthenium (II) and platinum (II) complexes, stabilized by agostic M–η^3 CH_2 interactions, could be used as highly active transfer hydrogenation catalysts. Finally, Graeme Gainsford (New Zealand) presented recent advances in calculations based on Density Functional Theory (DFT) and attempts to predict the enantiomeric excess by means of those calculations.


Picture of the manganese complex.


W. Baratta


G. Gainsford

J.C. Daran and P. Gómez-Sal

Time-resolved Powder Diffraction for Materials Production and Processing

This session produced wide ranging descriptions of technique, and equally wide ranging, interpretations of their applications. Instrumentation included laboratory, neutron and synchrotron sources involving time resolutions ranging from seconds to hours. Another notable theme, was the wide range of sample environments needed, including several challenging experiments involving aspects such as "one-shot" gas hydrate/clathrate formation, self-propagating reactions, single grain analysis during annealing/tensile stressing, high pressure (autoclave) acid-leaching, calcination/sintering up to 1500°C, and hydrogen gas-flow. The concluding message that emerged from this seesion is that the field has reached a stage that fast diffraction and *in-situ* capabilities are now the expectation and that current practitioners have to be continually ready to meet and cope with new requests.

Paul Barnes


Lodovico Riva di Sanseverino (Italy) was awarded the IUCr Award for Exceptional Service to Crystallography for his organization of the Erice School.

Programming Robust CIF and XML into Crystallographic Software

CIF is the Crystallographic Information File [www.iucr.org/iucr-top/cif/] which has become the standard for submission of crystallographic data sets of small molecules for archiving and publication. XML is the Extensible Markup Language that has become the standard for web-based data management. For many years these have seemed to be very distinct and incompatible frameworks for the management of data. The most important lesson of the microsymposium is that the differences are less important than the commonalities of the two frameworks and the complementary support these approaches offer to structural studies. In addition there was strong acceptance of an open source approach to software development, and the use of abstraction of data to aid in translation.

In the first talk, Peter Murray-Rust (UK) discussed conversion from CIF to XML in the form of CML (the Chemical Markup Language) and the use of XML tools to process information from CIF data sets. To quote from the abstract, "… Open source and Open data provide a robust high-throughput crystallographic semantic web …".


P. Murray-Rust

The theme of interoperability of CIF and XML was continued as Syd Hall (Australia) explained the importance of ontologies (dictionaries with relationships) in the management of data. Syd and Nick Spadaccini (Australia) gave a very convincing demonstration of a faithful translation between CIF and XML and explained the power of embedding validation logic into ontologies.


S. Hall

The third talk addressed some of the practical issues related to recent changes in the CIF format. G. Todorov (USA) began the talk, setting the general context and discussing some of the issues in moving smoothly between CIF and XML, such as the need to extend the character set used in CIF to agree with that in XML. Kostadin Mitev (USA) continued with a detailed explanation of a new open source utility that is being created for the IUCr publication process.


K. Mitev

Joerg Kaercher (USA) discussed the automatic generation of data in multiple alternate formats from a database. The abstraction of the data as something distinct from its presentation is a very helpful way to move among formats and is one of the key concepts in easing the transitions among formats. In the last talk, Ganesh Jawahar Swaminathan (UK) extended the theme of database use to abstract data and showed its powerful use at EBI for support of the wwPDB and other initiatives requiring complex data management with data in multiple formats. In this case XML was the central format used. It was heartening to see an emerging consensus in an area that in past meetings has been contentious.


J. Kaercher


G.W. Swaminathan

Herbert J. Bernstein and Brian McMahon

Electronic Excitations

Electron Excitations can be measured with a number of probes. They can be probed with inelastic X-ray scattering (IXS) or X-ray Raman Spectra. The field is undergoing rapid progress due to experimental and theoretical advances and spawning, a growing number of workshops, symposia, and new theory networks, e.g., NanoEXC in the EU and the DOE Computational Materials Science Network in the USA.


W. Schuelke

The physics of electronic excitations goes beyond the ground state, one-electron properties of a material, as reviewed by W. Schuelke (Germany), a pioneer in the field. Schuelke noted that such excitations can be characterized in several equivalent ways, e.g., by the dynamical structure factor S, which is the Fourier transform of the density-correlation function, and is directly related to the fundamental dielectric response of a material. The same physical properties can also be measured with fast electrons using electron-energy loss spectra (EELS). The theory requires a quasi-particle description that goes beyond the independent particle approximation. Shuelke reported that a cumulant expansion model for the self-energy yields more accurate results.


J. Soininen

Many body theoretical descriptions can be computationally intensive. Juha Soininen (Finland) reviewed detailed calculations of non renosant IXS (NRIXS) based on the (two-particle) Bethe-Salpeter equation and discussed a new multiple-scattering approach, which has the potential to give much faster calculations over a wide energy range, and can be used to analyze NRIXS.

The nature of IXS can also be used to elucidate the many-body response of a system. John Hill (USA) reviewed how resonant IXS has been used to study the Mott-Gap, and the electronic excitations in transition metal oxides, Pedro Montano (USA) then discussed how magnetic IXS (e.g., magnetic Compton scattering) can be used to understand the physics of Manganites and to resolve the various theories responsible for large magnetoresistance in these materials. Finally T. Colson reviewed correlations in IXS using the low-loss plasmon dominated spectra.


J. Hill


P. Montano


T. Colson

The field of electronic excitations demonstrate that the synergy between theory and experiment have made it possible to interpret the experiments quantitatively and in terms of important dynamical physical properties of a system's response.

K. Hamalainen and J.J. Rehr

Crystallographic Knowledge in Drug Design Strategies

The aim of this microsymposium was to give an overview of the use of structural data at atomic resolution in the rational drug design of new molecules with therapeutic and diagnostic applications.


A. Yonath

Ada Yonath (Israel) described how the analysis of high resolution structures of complexes of antibiotics with ribosomal particles has helped shed light on antibiotic selectivity and has provided a fair degree of understanding of some of the processes involved in antibiotic action (from reducing of decoding accuracy, *via* limiting conformational mobility, to interference with substrate binding and hindrance of the progression of growing proteins). Knowledge of such common principles is crucial and, when combined with genetic, structural and biochemical investigations, can be instrumental in structure-based approaches. She also suggested that combination treatment might be an efficient way to avoid drug resistance. Another interesting approach to overcome drug resistance was presented by Kalyan Das (USA). Structural and modelling studies of HIV-1 Reverse Transcriptase (RTs) in complex with potent dyaryl-pyrimidine nonnucleoside inhibitors showed that the conformational flexibility of these inhibitors appears to allow them to retain their potency against a wide range of drug resistant HIV-1 RTs, thereby providing a means to design drugs effective against rapidly mutating targets. Some of these newly discovered potent inhibitors are currently in clinical trial.


K. Das

In computer-aided design, the limitations of crystal structures selected to perform docking experiments are often ignored and the reliability of the docking results can therefore be questionable. Interestingly enough, Noriaki Hirayama (Japan) showed, using the recently developed docking algorithm Ph4Dock, that Cruickshank's Diffraction-component Precision Index can be used to evaluate the reliability of the docking results.

Franck Leveiller and Michele Saviano


Dancing at the Congress banquet

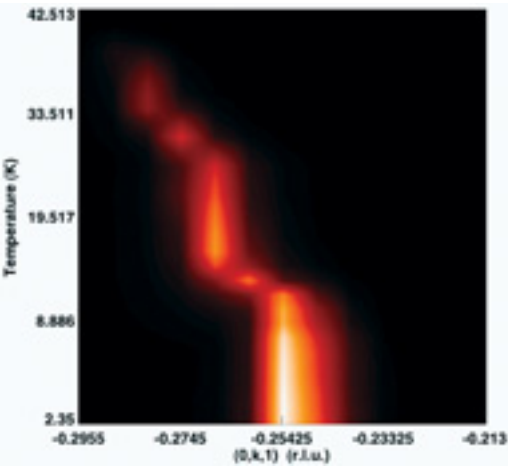
Advanced Functional Materials

This session focused on the interplay between structural features and physical and chemical properties in materials science with applications involving molecular crystals and inorganic oxides. The first presentation concerned electrical conductivity in ionic polymers and electronic metal complexes. Two important breakthroughs have been recently achieved: (i) the discovery of ionic conductivity in crystalline rather than amorphous polymer electrolytes, and (ii) the synthesis of molecular metals based on a single active molecule, rather than on two different interacting units. Yuri Andreev (UK) described the elucidation of the relationships between lithium ion mobility and ordered polymeric structure and methodological aspects of single-crystal and powder techniques for establishing the structure. Minoru Mitsumi (Japan) showed how semiconducting behavior in single-component molecular conductors may be coupled to trimerization or even hexamerization, depending upon the temperature of the active molecules within the linear chains building up the crystal structure. This highlights the details of the structural configuration of such important molecular materials.

Y. Andreev

Two talks focused on the emerging field of magneto-ferroelectrics. In these materials the frustration of parameters such as orbital ordering leads to complex spiral magnetic structures which break inversion symmetry and cause a ferroelectric lattice response. Tsuyoshi Kimura (USA) used this behavior as a search criterion for new magneto-ferroelectric materials and presented measurements illustrating the relationship between frustration, complex magnetic structure and ferroelectricity in $CuFeO_2$ and $Ni_3V_2O_8$. What is unusual and exciting about many of these materials is that the magnetic field couples strongly to ferroelectricity and can be used to manipulate the ferroelectric polarization as demonstrated recently for $TbMnO_3$. Nadir Aliouane (Germany) showed that the polarization flop in $TbMnO_3$ arises from a field induced incommensurate to commensurate magneto-structural transition. This transition is preceded by a change in the magneto-elastic coupling from quadratic (as suggested by spiral magnetic ordering) to linear with applied field. In fact the behaviour of these materials under magnetic field is rather complex, as highlighted by the devil's staircase like behaviour in $TbMnO_3$ shown in the figure.

T. Kimura



Variation of the incommensurate magnetic wavevector (0,*k*,0) as a function of temperature in $TbMnO_3$ under a magnetic field of 5 T applied parallel to the *b*-axis. This data was measured on the E4 diffractometer at the Berlin Neutron Scattering Center, Hahn-Meitner-Inst. (*courtesy of N. Aliouane*).

N. Aliouane

Michele Catti and Dimitri Argyriou

BIOMAC OCM

Open Commission Meeting on Biological Macromolecules

Some years ago the Commission established clear guidelines for the submission of crystallographic data associated with the publication of macromolecular structures. The compliance within the community has been very good with structure factors now accompanying 90% of Protein Data Bank Depositions. The members of the Commission now felt that it was time to discuss the need to capture all available data associated with a protein structure determination. The underlying principle enunciated by Howard Einspahr (USA), Editor, *Acta Crystallographica* Section F, was the need to provide all data necessary for replication of the experiment in another laboratory. For a typical structure biology report, this might include details of the cloning, expression, purification and crystallization of the target protein. Zbyszek Otwinowski (USA) addressed the issue of which data needs to be deposited and, if so, in what format. He questioned the need to deposit all the computational steps along the way to a refined structure despite the ready availability of these data in most of the commonly used software packages. Tom Terwilliger (USA) illustrated how in macromolecular experiments, the final result does not always provide sufficient information about choices made in reaching the model. Harry Powell (UK) stressed the need for an audit trail and that it should be automatic and not an option. Data harvesting needs to commence at the start of the experiment. Howard Einspahr concluded the session with summary of the work he has been doing with the PDB and the *Acta Crystallographica* staff in Chester to expand the mmCIF dictionary to include all the new data items for the complete description of a structure analysis and the tools to extract these data in a form suitable for tabulation for presentation in a publication.

Mitchell Guss

COMCIFS OCM

Open Commission Meeting on COMCIFS

The strength of CIF lies in its dictionaries which provide precise descriptions of the ontology (i.e., the collection of concepts) that define crystallography. In the form approved by COMCIFS, these dictionaries can be found on the IUCr website. Their content can also be given in other representations such as the eXtensible Mark-up Language (XML). Zukang Feng (USA) described how the Research Collaboratory for Structural Biology (RCSB) in the US uses the mmCIF dictionary together with the CIF syntax to produce the archival form of the Protein Data Bank. RCSB receives macromolecular structure reports in a variety of formats which must be converted into CIF before they are added to the archive. An XML version of the Protein Data Bank (PDBML) developed to assist data transfer between the partners collaborating in the World-Wide PDB was described by Haruki Nakamura (Japan). PDBML augments the information received from the Protein Data Bank with further biological and experimental details extracted from the literature with the intention of making PDB content available on-line with a variety of search and display options. Kim Henrick (UK) described how the Protein Data Bank is made available in the UK through the Macromolecular Structure Database.

Ralf Grosse-Kunstleve (USA), speaking from his experience in working with the Phenix project, pointed out that the lack of CIF software tools is the main reason many people prefer to work in XML: writing code for reading and writing CIFs is not a trivial exercise. A solution to this problem was described by Heping Zheng (USA) who is constructing a CIF translation dictionary to provide the link between the internal memory of a program and the CIF that is to be written. To assist in the automatic production of publication-quality CIFs Zheng and his colleagues are adding routines to the HKL2000 suite of programs for macromolecular structure determination to produce a draft CIF and to allow the user to make final adjustments by hand. Ethan Merritt described a Python program library designed to import, manipulate and export macromolecular structure models written in CIF. He described the program TLSMD which analyzes the thermal motions of a protein, looking for the optimum way of breaking the molecule into rigid segments.

Brian McMahon (UK) described the use of CIF for reporting protein structures in the new Acta Crystallographica F. Structure reports of biological macromolecules are deposited in the usual way with the Protein Data Bank, which then provides the author with an mmCIF representation suitable for onward transmission to the journal where it is used for automatic generation of the experimental tables. Frank Allen (UK) reported that, in contrast to the Protein Data Bank, the Cambridge Structural Database now receives 96% of its structure reports in the form of CIFs, an achievement made possible because most small-molecule refinement programs are able to write their output in CIF format. The Cambridge Crystallographic Data Centre, which produces this database, uses CIF syntax internally and has recently released enCIFer, an editor and browser designed to allow people to create CIFs that conform to any given CIF dictionary.

I. David Brown.

Overview of the Banquet, which was held in the "Meridiana" courtyard of Palazzo Pitti

Crystallography in Australia and New Zealand

Collated and edited by Jennifer L Martin

The beginnings of crystallography in the region can be traced back to the turn of the 20th century when Sir William H Bragg was appointed Professor of Mathematics & Physics at the University of Adelaide, a post he held from 1886 to 1908. There he experimented with ionizing radiation, which had then only recently been discovered by Roëntgen in Germany. WH Bragg's son, William Lawrence Bragg, was born and educated in Adelaide and the two Braggs - who moved to the UK in 1908 - were awarded a unique father-and-son Nobel prize in 1915 for "their services in the analysis of crystal structure by means of X-rays". Another well-known pioneer of crystallography, Lindo Patterson, of Patterson function fame, was born in Nelson, New Zealand, in 1902. His family moved to Canada when he was 18 months old, and later to London when he was 14. Equally famous is Maurice Wilkins, who shared the 1962 Nobel Prize with Watson and Crick "for their discoveries concerning the molecular structure of nucleic acids and its significance for information transfer in living material". He was born in the small town of Pongaroa, New Zealand, in 1916 and moved with his family to England when he was seven.

Crystallography in New Zealand and Australia has blossomed during the last century, reflecting the lasting influence of a small group of outstanding researchers in the early days who, in Australia, referred to themselves as 'the Bush Crystallographers'. Their legacy is a vibrant and growing research community representing all aspects of the field. Major research groups are based at universities, medical research institutes, the Australian Government Commonwealth Scientific and Industry Research Organisation (CSIRO), the Australian Nuclear Science and Technology Organisation (ANSTO) and the New Zealand Government Crown Research Institutes.

Synchrotron Activities

The Australian Synchrotron Research Program (ASRP)

In response to the recommendations of reports to the Australian Government from the Australian Science and Technology Council and the National Committee for Crystallography of the Australian Academy of Science, a consortium of government agencies and universities was formed in 1990 to fund the construction of the Australian National Beamline Facility at the Photon Factory in Tsukuba, Japan. This beamline, opened in 1993, gave Australian scientists guaranteed access to overseas synchrotron research facilities for the first time, and catalysed a rapid growth in the Australian synchrotron user community.

A further expansion occurred in 1996, with the formation of the Australian Synchrotron Research Program (ASRP) which added access to six sectors of the Advanced Photon Source (APS) in the USA. The ASRP now supervises and facilitates Australia's off-shore synchrotron activities, including the employment of Australian beamline scientists, the peer-review of proposals, and the promotion of an extensive post-doctoral research fellowship scheme. Access to the National Synchrotron Radiation Research Centre, in Hsinchu Taiwan, was added to the ASRP programs in 2003.

ASRP at the Photon Factory, Japan

The Australian National Beamline Facility (ANBF) is a general-purpose hard X-ray beamline at the Photon Factory. It is equipped for X-ray absorption spectroscopy, high-resolution high-speed powder diffraction, solid surface grazing incidence diffraction, small angle scattering, and X-ray imaging and fluorescence. Two resident ASRP beamline scientists provide expert assistance in the operation, maintenance and development of the facility. The diffraction and scattering experiments are performed in a large vacuum diffractometer combining a Debye-Scherrer geometry with image-plate detectors. This unique instrument was constructed in Australia and can record high-resolution powder patterns in 5-10 minutes.

PhD student Jonathon Morton (Curtin University), using the ASRP diffractometer in its Debye-Scherrer configuration

ASRP at the Advanced Photon Source, USA

ASRP subscribes to three beamline groups at the Advanced Photon Source at the Argonne National Laboratory in the USA; X-ray Operations Research, BioCARS and ChemMatCARS. ASRP beamline staff are stationed at all three. This arrangement gives Australian researchers access to six sectors at the APS with facilities for X-ray physics, X-ray microscopy, X-ray fluorescence mapping, micro-XANES, polarization studies, macromolecular structure analysis, static and dynamic condensed-matter chemistry, small- and wide-angle X-ray scattering, micro-crystallography, reflectrometry and time-resolved laser-excited single-crystal diffraction.

ASRP at the National Synchrotron Radiation Research Center, Taiwan

This 1.5 GeV synchrotron light source in the Hsinchu Science-Based Industrial Park, Taiwan, provides access for Australian scientific and industrial research in the vacuum ultra-violet and soft X-ray spectral regions. Applications include photoemission and near-edge X-ray absorption spectroscopy, micro-machining (deep X-ray lithography), infra-red microscopy, scanning photoemission microprobe measurements, and photoemission microscopy.

The Australian Synchrotron, Melbourne

An Australian Synchrotron light source (pictured) is currently being constructed adjacent to Monash University in Melbourne. It will be a 3-GeV third-generation source with a circumference of 216 m, 12 usable straight sections and the potential for over 30 beamlines. Commissioning first light of the ring is scheduled for April in the first quarter of 2007 when 4 of the initial 9 beamlines are planned to begin operations.

The first 4 beamlines will serve macromolecular crystallography

(MAD bending magnet), powder diffraction (bending magnet), X-ray absorption spectroscopy (wiggler), and soft X-ray spectroscopy (helical undulator). The next 5 beamlines will be for macromolecular micro-crystal and small-molecule diffraction, SAXS/WAXS, infra-red spectroscopy, micro-spectroscopy and imaging/medical therapy. For more information see www.synchrotron.vic.gov.au

A New Australian Neutron Source

In its day, the 1950s HIFAR reactor near Sydney provided state-of-the-art facilities for neutron diffraction. This reactor has now been de-commissioned. Its place will be taken by OPAL, the Australian replacement research reactor, which is due to begin operating in August 2006. A large liquid-deuterium cold neutron source and super-mirror guides will feed into a modern guide hall, in which most of the planned 18 instruments will be placed. Notable features will include a commercial radiography/tomography station and facilities for the neutron irradiation of radio-pharmaceuticals, transmutation-doped silicon and activation analysis samples. The

Photo courtesy of the Australian Synchrotron. Photographer Daniel Mendelbaum

initial instruments will provide facilities for both high-intensity and high-resolution powder diffraction, residual-stress measurements, quasi-Laue diffraction, thermal 3-axis spectroscopy, polarization analysis, small-angle neutron spectroscopy and time-of-flight reflectometry. For more information see www.ansto.gov.au/opal/.

Chemical Crystallography

Small-molecule X-ray crystal structure analysis has been an important component of research in university chemistry departments and government agencies in Australia and New Zealand since the early 1950's, a large number of groups being established during that time and subsequently. [1-18] The first group to be recognized internationally was located at the CSIRO Division of Chemical Physics near Melbourne. Its leaders were A. McL. ("Sandy") Mathieson, Barrie Dawson and David Wadsley. A remarkably collegiate group, they generously shared their expertise and instruments with younger researchers starting work in the universities.

OPAL, photo courtesy of ANSTO

At the outset, research tended to be focussed on the protagonists' own interests, but, with the growing recognition of the capabilities, as well as the cost, of the technique, and the constraints of obtaining funding, most groups broadened their activities to provide a service to a wide range of investigators in the chemical and materials sciences. The field burgeoned during the 1960's when computer-controlled diffractometer installations supplanted Weissenberg and precession camera X-ray facilities and the use of computers became widespread. As elsewhere, the technique became an important ingredient in the characterization and identification of crystalline substances across the chemical, materials, natural product and mineralogical sciences, and many antipodean practitioners feature with distinction in the various data-base compilations. The published work includes very small organic molecules (typical of the 1950's, when hand calculators restricted calculations to projections down short axes), simple transition metal salts and hydrates, leading into more complex ones (as coordination chemistry gained popularity in the 1960's and computers enabled three-dimensional calculations), broad front attacks on chemical problems through many chemically related structures (as computing became more straightforward and data acquisition more automated throughout the 1970's) to the very much larger molecules containing hundreds of atoms. Rationales for these analyses range widely from bio- and pharmacological, to underpinning the understanding of physical effects such as magnetism and electrical properties, and to the understanding of chemical reaction paths, as well as an appreciation of the symmetry and elegance of these structures and processes, to solving structures for more fundamental reasons associated with theoretical and computational development.

With the advent of powerful CCD instrumentation, increasing access to synchrotron facilities in the 1990's, increasing costs, and increasing competition for research funds, the proliferation of facilities has decreased. Major facilities serve the institutions in a large area and neutron studies will be concentrated at OPAL and there is anticipated access to the Australian Synchrotron (see above).

References

[1] Queensland, Les Power (James Cook Univ.), Colin Kennard (Univ. of Queensland), Peter Healy and Graham Smith (Griffith Univ.)
[2] New South Wales, Hans Freeman (Univ. of Sydney), Neville Stephenson (Univ. of New South Wales), 'Blue' Barclay (Macquarie Univ.)
[3] Australian Capital Territory, Glen Robertson (Australian National Univ.)
[4] Victoria, David Wadsley and 'Sandy' Mathieson (CSIRO, Vic), John (CB) White and Bernard Hoskins (Melbourne U), Bryan Gatehouse (Monash Univ.) and Maureen Mackay (La Trobe Univ.)
[5] South Australia, Harry Medlin, Mike Snow (Adelaide Univ.), Max Taylor (Flinders Univ.) and Ted Radoslovich (CSIRO, Adelaide).
[6] Univ. of Western Australia, Ted Maslen, 'Judge' Bevan and Brian Figgis
[7] Univ. of Auckland NZ (F.J. Llewellyn, David Hall, and Neil and Joyce Waters)
[8] Massey Univ. NZ (Sylvia Rumball)
[9] Univ. of Canterbury NZ (Bruce Penfold and Ward Robinson)
[10] Chemistry Division, Department of Scientific and Industrial Research NZ (Peter Williams, Kevin Brown & Graeme Gainsford)
[11] James Cook Univ., Queensland (sharon.ness@jcu.edu.au)
[12] Sydney Univ., New South Wales (p.turner@chem.usyd.edu.au)
[13] Australian National Univ., Canberra (Rae@RSC.anu.edu.au)
[14] Melbourne Univ., Victoria (j.white@chemistry.unimelb.edu.au)
[15] Monash Univ., Victoria (stuart.batten@sci.monash.edu.au))
[16] Univ. of Western Australia (bws@crystal.uwa.edu.au)
[17] University of Auckland NZ (g.clark@auckland.ac.nz)
[18] University of Canterbury NZ (ward.robinson@canterbury.ac.nz)

Precision Density Studies

Charge density research is actively conducted in two locations: the University of Sydney and the University of Western Australia. For the past few years, the group in Sydney [1] has used the Crystal Structure Analysis Facility of the School of Chemistry, and the HIFAR research reactor, to gain insight into drug-related organic molecules through X-ray and neutron diffraction studies. A group, which at the University of New England in Armidale conducted

model studies analyzing the possibilities for determining molecular properties from X-ray diffraction data, has recently moved to the University of Western Australia [2] where their research will focus on extracting information on nonlinear optical properties from X-ray diffraction data, through a series of combined experimental and theoretical [3] studies. The experimental work will make use of single crystal X-ray diffraction facilities in Perth and Sydney, and new instruments at the OPAL reactor in collaboration with ANSTO [4].

Charge density research is now a major activity of worldwide modern crystallography, but its development was fostered by pioneering studies in Australia. These included early work on the multipole refinement model by Barrie Dawson in Melbourne in the 1960s, detailed charge density studies on materials ranging from organics to rare earth oxides and low-T superconductors by Ted Maslen and co-workers at the University of Western Australia, and combined X-ray and polarized-neutron charge and spin density studies on transition metal complexes by Brian Figgis and colleagues using a 10 K diffractometer, also at the University of Western Australia, in the 1990s.

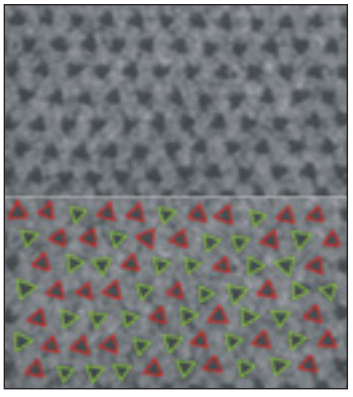
References
[1] University of Sydney, New South Wales, Dai Hibbs d.hibbs@chem.usyd.edu.au
[2] University of Western Australia, Mark Spackman mas@cyllene.uwa.edu.au
[3] University of Western Australia, Dylan Jayatilaka dylan@theochem.uwa.edu.au
[4] ANSTO New South Wales, Wim Klooster wim.klooster@ansto.gov.au

Fibre Diffraction

Fibre diffraction analysis is concerned with obtaining detailed structural information from fibrous specimens: specimens that are oriented and rotationally disordered. The molecules usually have helical symmetry and the rotational disordering leads to cylindrical averaging of the X-ray diffraction intensities in reciprocal space. The challenge is to determine structures from this limited data.

Fibre diffraction has a significant history in Australia, dating back to cutting-edge research by Bruce Fraser and Tom MacRae in the 1950s in Melbourne [1]. In the context of a large laboratory serving the Australian wool industry, this work produced important structural results on collagen and keratin. An early collaborator on this work continues research on fibrous proteins in New Zealand [2].

A group at the University of Canterbury [3] uses fibre diffraction together with the theory of diffraction by disordered lattices to study systems that are both rotationally disordered and subject to various forms of lattice or substitution disorder within the constituent microcrystallites. Diffraction from these specimens consists of Bragg diffraction with amplitudes that are modulated by the disorder and diffuse diffraction between the reciprocal lattice points. Such problems arise in a variety of contexts including artificially prepared fibre specimens, such as nucleic acids and polysaccharides, and naturally occurring assemblies such as in vertebrate muscle. A current collaborative project [3, 4], analyses the rotational disorder of myosin filaments in myofibrils of higher vertebrate muscles, which is critical for the rigorous application of fibre diffraction analysis to muscle. Electron microscopy allows direct observation of the disorder and current efforts are aimed at modelling the disorder and developing a description of the diffraction.



(Top) Small section of frog muscle micrograph and (Bottom) classification of myosin filament orientations.

Other activity in fibre diffraction and disordered materials includes studies of cellulose microfibril orientation in wood [5], use of reflection high-energy electron diffraction to study crystal orientation and growth in compound semiconductor thin films [6], and a variety of industrial applications to cement, fertilisers and soils.

References
[1] Wool Textile Research Laboratory, CSIRO, Victoria. Bruce Fraser and Tom MacRae
[2] Massey University, NZ, David Parry (d.parry@massey.ac.nz)
[3] University of Canterbury, NZ Rick Millane (rick@elec.canterbury.ac.nz)
[4] Imperial College, UK, John Squire (j.squire@ic.ac.uk)
[5] University of Canterbury, NZ, Ward Robinson (ward.robinson@canterbury.ac.nz)
[6] University of Canterbury, NZ, Steve Durbin, (s.durbin@elec.canterbury.ac.nz)

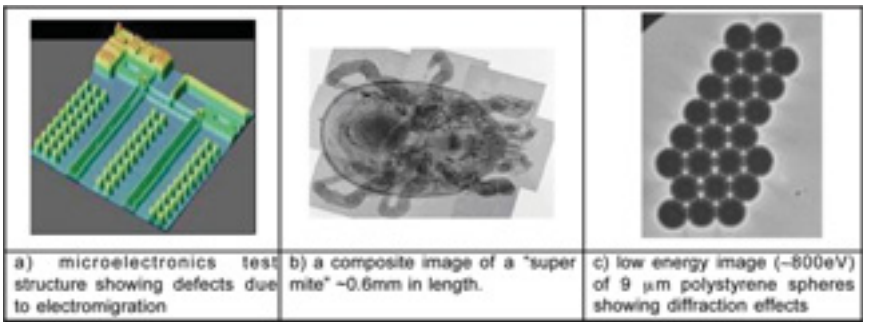
X-ray Phase-contrast Imaging and Microscopy

Phase-contrast X-ray imaging exploits the phenomenon of Fresnel diffraction. By comparison with conventional absorption-type X-radiography, it includes an additional contrast mechanism in image formation that arises from the effects of refraction by the sample. This provides complementary information and is of particular value for weakly- and/or non-absorbing samples.

Early work at CSIRO [1] into the development of methods for phase-contrast imaging was based around a "double crystal" technique (now called Diffraction Enhanced Imaging - DEI). However, this had practical limitations and a more practical and robust method was developed that did not rely on optics and could use broadband polychromatic radiation from a conventional microfocus source. This method, termed In-Line phase contrast imaging, is now widely used in many conventional laboratories. It was developed independently [1] of a related synchrotron-based approach outlined elaborated by Anatoly Snigirev and co-workers at the ESRF. CSIRO [1] also developed a very high spatial resolution X-ray ultramicroscope (XuM) which used an SEM as host and exploited phase contrast. This instrument has achieved sub-100 nm resolution (on semiconductors) and provides very high spatial resolution tomography. Examples of processed XuM images recorded on this instrument are presented below.

Pioneering research into the development of theoretical methods for extracting quantitative information from phase-contrast images

continued on Page 30



a) microelectronics test structure showing defects due to electromigration

b) a composite image of a "super mite" ~0.6mm in length.

c) low energy image (~800eV) of 9 μm polystyrene spheres showing diffraction effects

oxford diffraction
driving X-ray innovation

Why wait?
X-ray through the plate!

NEW
PX Scanner

- Screen for crystals in the crystallisation plate
- The only optical ***and*** X-ray imager in one system
- Plug and play desktop system for the crystallisation lab

sales@oxford-diffraction.com www.oxford-diffraction.com

Oxford Diffraction Ltd 68 Milton Park, Abingdon, Oxfordshire OX14 4RX Tel: +44 (0)1235 443630 Fax: +44 (0)1235 443631
Oxford Diffraction Inc 300 Baker Ave, Suite 150, Concord, MA 01742 USA Tel: +1 (866)371-5506 Toll Free
Tel: +1 (978)371-5506 Fax: +1 (978)369-8287
Oxford Diffraction Poland Sp. z o. o. Rogowska 117B, 54-440 Wrocław Tel: +48 71 7835380 Fax: +48 71 7835381

THE QUEEN'S AWARDS FOR ENTERPRISE: INTERNATIONAL TRADE 2006

continued from Page 28

has been carried out at the University of Melbourne [2]. This involved the development of phase-retrieval algorithms with application to visible light optics, X-rays, neutrons and particle beams. A collaboration between CSIRO [3] and Monash University [4] investigates multi-energy and polychromatic approaches to phase retrieval as well as hybrid approaches combining DEI and in-line imaging. A unified conceptual framework for the whole multiplicity of phase-contrast imaging techniques is provided by the idea of virtual (software based) optics that has been developed both at Melbourne University [2] and more recently, for the specific case of X-ray phase-contrast imaging, by CSIRO/Monash [3,4].

Researchers at Monash University [5] have a particular emphasis on biomedical applications of DEI (which enables images based on absorption or refraction to be separately obtained and also removes parasitic scattering). Conventional laboratory based applications of phase-contrast imaging to biomedical studies have also been extensively carried out at CSIRO [6].

Several of these groups [1,2,5,6] are collaborating on the design of a unique imaging beamline for the Australian synchrotron. This is intended to facilitate a wide range of applications and aims to provide optimized implementations of In-Line phase contrast imaging as well as DEI.

References
[1] CSIRO Victoria, Steve Wilkins (Steve.Wilkins@csiro.au)
[2] Melbourne University, Victoria, Keith Nugent, k.nugent@physics.unimelb.edu.au)
[3] CSIRO Victoria, Tim Gureyev (tim.gureyev@csiro.au)
[4] Monash University, Victoria, David Paganin (david.paganin@spme.monash.edu.au) and Konstantin Pavlov (konstantin.Pavlov@spme.monash.edu.au)
[5] Monash University, Victoria, Rob Lewis (Rob.Lewis@sync.monash.edu.au)
[6] CSIRO, Victoria, Andrew Stevenson (Andrew.Stevenson@csiro.au)

X-ray Absorption Spectroscopy (XAS)

XAS was pioneered in Australia by Hans Freeman [1] in the early 1980s. His XAS experiments were designed as a complement to crystal structure analysis of metalloproteins and included the first XAS studies of oriented metalloprotein crystals. A by-product of this work was the XFIT software for single- and multiple-scattering fits to XAFS data. The software is still in use today. XAS studies expanded rapidly in the mid 1990s after the ASRP was established and it has since grown at a rapid rate.

The largest concentration of XAS users is at the University of Sydney, covering areas as diverse as structures of the active sites of metalloproteins, intracellular XAS for studying biotransformations of toxins and drugs, characterization of drugs, coordination complexes, homogeneous and heterogeneous catalysts, network materials, etc [2,3]. At the Australian National University (ANU) [4], research is conducted into the structures around metal ions in minerals and melts of relevance to the formation of minerals. Studies in this area are also conducted by groups at ANSTO [5] and CSIRO [6]. In the semiconductor area there is extensive research expertise at ANU [7]. The University of New South Wales is the centre of the soft X-ray XAS community in Australia [8] where semiconductors are also a major research theme along with studies on other materials. Spectro-electrochemical XAS experiments are performed by research groups at the Universities of Sydney [2] and Melbourne [9] and the ANU [10]. The University of South Australia [11] applies XAS techniques to problems in mineral processing, forensic chemistry and industrial materials. Groups at the University of Queensland [12] conduct a variety of studies on surfaces, coordination complexes and metalloproteins.

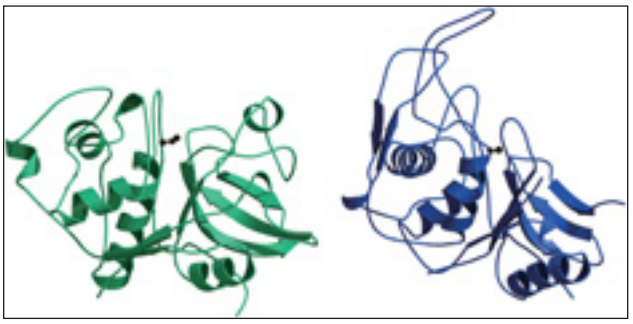
In New Zealand, XAS activity has been concentrated at the University of Auckland, the Victoria University of Wellington, and two Crown Research Institutes, Industrial Research Ltd. and Geological and Nuclear Sciences. Major applications have been in the areas of semiconductor thin films, [13] Lithium Ion Battery cathode materials [14,15] and High Tc Superconductors [16]. Recently, emphasis has shifted increasingly to soft X-ray XANES, with speciation studies on electrode impurities [15] and studies of semiconductor materials [15,17,18]. The earliest XAS studies by New Zealand researchers utilized the LURE facility in France, while more recent XANES work has used the SRC in Madison, Wisconsin and the NSRC in Taiwan.

Through the ASRP, Australian researchers have access to world-class XAS instrumentation: ANBF operates a dedicated bending magnet beamline at the Photon Factory, Micro-XAS on biological tissues and materials can be performed on the XOR sector at the APS and at the NSRRC in Taiwan the main XAS focus is on soft X-rays. The first suite of nine beamlines for the Australian Synchrotron will include a dedicated XAS beamline and a microprobe XAS beamline.

References
[1] University of Sydney, New South Wales, Hans Freeman (freemanh@chem.usyd.edu.au)
[2] University of Sydney, New South Wales, Peter Lay (p.lay@chem.usyd.edu.au)
[3] University of Sydney, New South Wales, Trevor Hambley (t.hambley@chem.usyd.edu.au), Tony Masters (a.masters@chem.usyd.edu.au), Thomas Maschmeyer (t.maschmeyer@chem.usyd.edu.au), Cameron Kepert (c.kepert@chem.usyd.edu.au), Hugh Harris (h.harris@chem.usyd.edu.au), and Marjorie Valix (mvalix@chem.eng.usyd.edu.au)
[4] Australian National University, Canberra, Andrew Berry, (Andrew.Berry@anu.edu.au)
[5] ANSTO Victor Luca (vlu@ansto.gov.au) and Anton Stampfl (aps@ansto.gov.au)
[6] CSIRO - Land and Water, Enzo Lombi, (Enzo.Lombi@csiro.au), Exploration and Mining, Barbara Etschmann, (Barbara.Etschmann@csiro.au), and Health Sciences & Nutrition, Victor Streltsov (victor.streltsov@csiro.au)
[7] Australian National University, Canberra, Mark Ridgway (Mark.Ridgway@anu.edu.au)
[8] University of New South Wales, New South Wales, Rob Lamb (r.lamb@unsw.edu.au) and Alan Buckley (a.buckley@unsw.edu.au)
[9] University of Melbourne, Victoria, Stephen Best (spbest@unimelb.edu.au)
[10] Australian National University, Canberra, Graham Heath (graham.heath@anu.edu.au)
[11] University of South Australia, South Australia, Andrea Gerson (Andrea.Gerson@unisa.edu.au) and Ivan Kempson, (Ivan.kempson@unisa.edu.au)
[12] University of Queensland, Mark Riley (m.riley@uq.edu.au) and Ian Gentle (i.gentle@uq.edu.au)
[13] Victoria University of Wellington, NZ Joe Trodahl (Joe.Trodahl@vuw.ac.nz)
[14] Pacific Lithium Ltd, NZ, Brett Ammundsen (brett@pacificlithium.co.nz)
[15] University of Auckland, NZ, Jim Metson (j.metson@auckland.ac.nz)
[16] Industrial Research Ltd. NZ, Jeff Tallon j.tallon@irl.cri.nz
[17] Victoria University of Wellington, NZ Ben Ruck (Ben.Ruck@vuw.ac.nz)
[18] Institute of Geological and Nuclear Sciences. NZ, Andreas Markwitz (a.markwitz@gns.cri.nz)

Biocrystallography

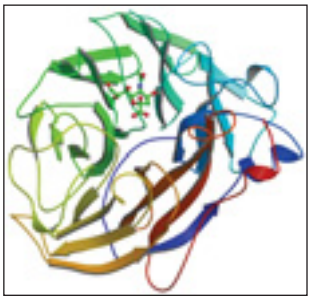
Protein crystallography in Australia and New Zealand has developed rapidly over the past thirty years. In New Zealand, there are structural biology research centres at three Universities. The first was established by Ted Baker [1] (a recent IUCr President) at Massey University in Palmerston North. An early milestone from this group was the structure determination in 1977 of the cysteine protease actinidin and later work on the iron binding protein lactoferrin attracted significant US funding that fully established the laboratory. The Baker lab moved from Massey to the University of Auckland in 1997, where it has grown to encompass several other groups [2] and more than 40 researchers. The lab is now part of one of New Zealand's national Centres of Research Excellence. Its research



Two unlikely evolutionary neighbours: the kiwifruit enzyme actinidin (left), solved in 1977, and the bacterial "flesh-eating" protease SpeB (right), solved 23 years later

focus is on structural genomics, particularly of TB proteins, structure-based drug design, viral crystallography and protein engineering. At Massey University there are four research groups [3,4] working on metalloproteins and enzymes, particularly those of importance in the dairy industry. There is emphasis [3] on twinning, ultra-high resolution structures and solving "difficult" crystal structures. The third centre, and arguably the southernmost crystallography laboratory in the world, is based at Otago University in Dunedin [5] where "wet" biochemistry and crystallography are combined in investigations of enzyme structure and mechanism.

In Australia, structural biology research centres are based in the major cities of Sydney, Melbourne, Brisbane, Canberra and Adelaide. The first laboratory was established by Hans Freeman [6] at the University of Sydney in the early 1970s, specialising in the structures of metalloproteins. The structure of the copper protein, plastocyanin, was determined in 1977, and (in collaboration with colleagues at the Stanford Synchrotron Radiation Laboratory) the first MAD analysis of a metalloprotein structure, using the intrinsic metal atom as the anomalous scatterer, was reported in 1988. The laboratory moved from the School of Chemistry to the Dept. of Biochemistry of the University in 1994, with Mitchell Guss [7], a long-time colleague of Hans Freeman (and currently co-editor of *Acta Cryst.* D and joint editor of *Acta Cryst.* F) as director. Metalloprotein structures continue to be a major theme of the research. Several other groups have been established at Sydney with interests in antibiotic resistance and DNA-drug interactions. [8]



The original beta-propeller: Crystal structure of subunit of influenza virus neuraminidase with product, sialic acid.

Peter Colman established a protein crystallography group at CSIRO in Melbourne in 1978. Five years later his team [9,10] determined the structure of neuraminidase, one of the two major coat proteins of the influenza virus. The structure, reported to be the first to be solved by cross-crystal electron density averaging, led to the development of the anti-flu drug Relenza™, one of the earliest examples of successful structure-based drug design.

Peter Colman now heads a structural biology department at one of Australia's foremost medical research institutes, the Walter and Eliza Hall Institute (WEHI) [9]. There, his research focuses on viral proteins and proteins involved in cancer. Other groups at WEHI pursue structural studies of hormone receptors such as those for insulin-like growth factor and epidermal growth factor [11] and membrane proteins including ion channels and mitochondrial proteins [12]. Research groups at CSIRO [10, 13] work on the structural biology of receptors and viral proteins.

At the same time that Peter Colman was establishing his laboratory in Melbourne, Neil Isaacs founded a protein crystallography unit at the St. Vincent's Institute of Medical Research also in Melbourne. In Dec 1988, Neil left Australia to take up the Chair of Protein Crystallography at the University of Glasgow in Scotland. The St Vincent's unit was re-established by Michael Parker in 1991 [14] with research on pore-forming toxins, glutathione transferases and protein kinases. The unit's current structural interests are relevant to problems in neurobiology, cancer and infection.

In the early nineties there was rapid growth in biocrystallography in Australia, with new laboratories in Canberra, Sydney and Brisbane. In Canberra, a group was set up at the Australian National University [15] with research interests in protein engineering and more recently in receptors. At the University of New South Wales in Sydney, protein crystallography was developed in the School of Physics [16], with recent research into cold adaptation proteins and proteins that function both in water-soluble and chloride channel forms. Queensland's first protein crystallography laboratory was at the University of Queensland [17] with a focus on structure-based drug design, protein folding and more recently high throughput crystallography applied to macrophages [17,18]. In addition, the University of Queensland now has two other structural biology groups studying protein kinases, protein-protein interactions, nuclear import proteins [18] and a variety of enzyme drug targets [19].

The rapid expansion of protein crystallography in Australia in the early 1990s has been repeated in this century. There are new groups in Melbourne [20,21,22], Queensland [23], Canberra [24] and South Australia [25,26]. From small beginnings in the 1970s, the protein crystallography community in Australia and New Zealand has grown to over thirty groups. It is expected that the completion of the first phase of the construction of the Australian synchrotron in Melbourne in 2007, with two proposed PX beamlines, will attract even more structural biologists to the region. The growth and development of the field make this an exciting time for structural biologists 'down under'.

References

[1] University of Auckland, NZ, Ted Baker (ted.baker@auckland.ac.nz)
[2] University of Auckland, NZ, Peter Metcalf (peter.metcalf@auckland.ac.nz), Vic Arcus (v.arcus@auckland.ac.nz), Sean Lott (s.lott@auckland.ac.nz), Richard Kingston (rl.kingston@auckland.ac.nz)
[3] Massey University, NZ, Geoff Jameson (g.b.jameson@massey.ac.nz)
[4] Massey University, NZ, Gillian Norris (g.norris@massey.ac.nz), Bryan Anderson (b.f.anderson@massey.ac.nz), Andrew Sutherland-Smith (a.j.sutherland-smith@massey.ac.nz)
[5] Otago University, NZ, John Cutfield (john.cutfield@stonebow.otago.ac.nz) and Sue Cutfield (suemc@sanger.otago.ac.nz)
[6] University of Sydney, New South Wales, Hans Freeman (freemanh@chem.usyd.edu.au)
[7] University of Sydney, New South Wales, Mitchell Guss (m.guss@mmb.usyd.edu.au)
[8] University of Sydney, New South Wales, Charles Collyer (c.collier@mmb.usyd.edu.au), Adrienne Adams (a.adams@mmb.usyd.edu.au)
[9] Walter and Eliza Hall Institute, Victoria, Peter Colman (pcolman@wehi.edu.au)
[10] CSIRO Health Sciences and Nutrition, Victoria, Jose Varghese (Jose.Varghese@csiro.au)
[11] Walter and Eliza Hall Institute, Victoria, Tom Garrett (tgarrett@wehi.edu.au)
[12] Walter and Eliza Hall Institute, Victoria, Jacqui Gulbis (jgulbis@wehi.edu.au)
[13] CSIRO Health Sciences and Nutrition, Victoria, Mike Lawrence (mike.lawrence@csiro.au)
[14] St Vincents Institute of Medical Research, Victoria, Michael Parker (mparker@svi.edu.au)
[15] Australian National University, Canberra, David Ollis (ollis@rsc.anu.edu.au) and Paul Carr (carr@rsc.anu.edu.au)
[16] University of New South Wales, Paul Curmi (p.curmi@unsw.edu.au)
[17] University of Queensland, Jennifer Martin (j.martin@imb.uq.edu.au)

[18] University of Queensland, Bostjan Kobe (kobe@uq.edu.au)
[19] University of Queensland, Luke Guddat (guddat@mailbox.uq.edu.au)
[20] Monash University, Victoria, Jamie Rossjohn (jamie.rossjohn@med.monash.edu.au), Matthew Wilce (matthew.wilce@med.monash.edu.au), Ossama El-Kabbani (el-kabbani@vcp.monash.edu.au)
[21] St Vincents Institute of Medical Research, Victoria, Galina Polekhina (gpolekhina@svi.edu.au)
[22] Austin Research Institute, Victoria, Paul Ramsland (p.ramsland@ari.unimelb.edu.au)
[23] Griffith University, Queensland, Helen Blanchard (h.blanchard@griffith.edu.au)
[24] Australian National University, Canberra, Aaron Oakley (oakley@rsc.anu.edu.au)
[25] Flinders University, South Australia, Ian Menz (ian.menz@flinders.edu.au)
[26] University of Adelaide, South Australia, Maria Hrmova (maria.hrmova@adelaide.edu.au)

Powder Diffraction

Powder diffraction research has been heavily influenced by the availability of facilities at the Australian "HIFAR" reactor and, over the past decade, by access to the Debye Scherrer diffractometer at the Photon Factory in Japan. Extensive use is also made of major facilities in Europe and the USA.

Many crystallographers at the School of Chemistry, University of Sydney, routinely use powder diffraction methods. A major collaborative effort with ANSTO, looking at the fundamentals of structural phase transitions in perovskite based oxides, has focused on combining parametric studies, very high resolution neutron and synchrotron X-ray diffraction and group theory to understand the nature of the observed crystallographic phase transitions [1]. A second group at Sydney [2] uses PXRD to monitor the structural consequences of desorption and sorption of guest molecules from nanoporous molecular hosts. Studies of the thermal expansion properties of molecular frameworks has seen the discovery of a broad family of negative thermal expansion (NTE) materials. Others study phase-separation in 'electron-doped' colossal magnetoresistive (CMR) manganite perovskites [3] using the complementary techniques of synchrotron X-ray and neutron powder diffraction, as well as small-angle neutron scattering and polarised neutron scattering. A fourth group at Sydney in the School of Chemistry [4] analyses modulated structures by PXRD. When bismuth oxide is doped with transition metals such as niobium or tungsten, its high-temperature cubic polymorph can be stabilised to room temperature. These doped phases are of interest because they preserve the high ionic conductivity of the cubic form and are being studied through a combination of electron diffraction, synchrotron XRD and neutron powder diffraction.

Elsewhere in Sydney, researchers at the new Bragg Institute at ANSTO [5], in collaboration with Australian National University researchers, are studying a wide range of perovskite-based rare earth cobaltates. A phase boundary exists between compounds containing large and small rare earths. Powder neutron diffraction has been used in conjunction with other diffraction techniques to reveal cation and oxygen vacancy ordering within these materials. Others in the Bragg Institute are exploiting recent developments in powder diffraction techniques to solve and refine structures of natural and synthetic mineral specimens whose structures had previously been intractable. The Materials & Engineering Science unit at ANSTO [6] uses powder diffraction in research related to Synroc, a material for the long-term encapsulation and storage of radioactive waste. Powder diffraction is used to monitor materials preparation and to study rutile and perovskite variants.

At the University of Newcastle, north of Sydney [7], crystallographic and diffraction techniques have been applied to a variety of Materials Science problems. Perhaps the most spectacular is the study of combustion synthesis reactions using very fast in-situ neutron powder diffraction. Studies of the structure and phase transitions of giant piezoelectric effect material as both a function of temperature and of applied electric field have also yielded insights into the large piezoelectric response.

In Canberra, researchers at the Australian Defence Forces Academy [8], investigate the crystal and magnetic structures of rare-earth intermetallic compounds as well as iron oxides and ferrites. The crystal structures of some 70 compounds in a new family of quaternary rare earth intermetallics – $R_3Co_{29}M_4B_{10}$ (M=Si, Ge, Al) – have also been determined along with the magnetic structures of some compounds in this series. The crystal and magnetic structures of strontium ferrites have been delineated as has the behaviour of zinc ferrites with particle sizes in the range ~ 8-50 nm.

In the West Australian Capital, Perth, powder diffractionists at Curtin University apply diffraction techniques in materials science, chemical and geological research, often related to primary resources [9]. Examples include the study of ceramic materials, particularly alumina and zirconia based ceramics for wear and corrosion resistant applications in engineering and cement processing, and the development of alumina matrix ceramics from bauxites to which additives from mineral sands are included. Other active areas are inorganic polymers (geopolymers), nanochemistry, crystallisation and biomineralisation.

At the South Australian Museum in Adelaide [10], researchers use powder X-ray and neutron diffraction for quantitative phase analysis in kinetic studies on the transformation of metal sulfides. The work aims to follow the course of reactions that occur in the formation and alteration of base metal deposits. Extensive use is made of PXRD in the identification and characterization of new mineral species.

Finally, in the AD Wadsley Minerals Laboratory [11] at CSIRO in Melbourne, researchers use in situ XRD studies to follow mineralogical changes during mineral processing. The research includes the study of the mechanism and kinetics of formation of the iron ore sinter phase, the pressure acid leaching of nickel laterite ores, and the mechanism and kinetics of Portland cement clinker hydration. The expertise developed in these in situ studies is being used to develop instrumentation for on-line PXRD measurement of mineralogy in industrial processes. This group has been active in the IUCr Commission on Powder Diffraction and coordinated the CPD Round Robin on quantitative phase analysis.

In New Zealand, powder diffraction is used principally within the universities and Crown Research Institutes. Of the Crown Research Institutes, Industrial Research Limited [12] has major research efforts in ceramic high-temperature superconductors, non-oxide ceramics (sialons and carbide cermets), and mesoporous materials. Landcare Research and Institute of Geological and Nuclear Sciences (GNS) Limited [13] have a shared interest in soil science, clay and rock mineralogy. Recent powder diffraction research at GNS has focused on geothermal studies, oil exploration, and massive sulphide deposits from undersea hydrothermal vents – the famous "black smokers". At Victoria University of Wellington [14] nano- and micro- particles in glass ceramics for applications in radiation imaging are studied.

The future for powder diffraction in the region looks extremely bright, with two diffractometers under construction at OPAL and a high resolution instrument to be installed at the Australian Synchrotron.

References

[1] University of Sydney, New South Wales, Brendan Kennedy (b.kennedy@chem.usyd.edu.au)
[2] University of Sydney, New South Wales, Cameron Keppert (c.kepert@chem.usyd.edu.au)

[3] University of Sydney, New South Wales, Chris Ling, (c.ling@chem.usyd.edu.au)
[4] University of Sydney, New South Wales, Siggi Schmidt (s.schmid@chem.usyd.edu.au)
[5] Bragg Institute, ANSTO New South Wales, Mike James (mja@ansto.gov.au or kiw@ansto.gov.au)
[6] Materials Division, ANSTO New South Wales, Chris Howard, (cjh@ansto.gov.au)
[7] University of Newcastle, New South Wales, Erich Kisi (erich.kisi@newcastle.edu.au)
[8] University of New South Wales, Australian Defence Force Academy, ACT Stewart Campbell (stewart@phadfa.ph.adfa.edu.au)
[9] Curtin University of Technology, Western Australia Arie Van Riessen (a.vanriessen@curtin.edu.au) or (B.O'Connor@curtin.edu.au)
[10] South Australian Museum, South Australia, Allan Pring, (pring.allan@saugov.sa.gov.au)
[11] CSIRO Minerals, Victoria, Ian Madsen (ian.madsen@csiro.au) or Ian Grey (ian.grey@csiro.au)
[12] Industrial Research Limited, Wellington, New Zealand (martin.ryan@irl.cri.nz)
[13] Institute of Geological and Nuclear Sciences Limited (GNS Science), New Zealand. Raymond Soong (r.soong@gns.cri.nz)
[14] Victoria University of Wellington, New Zealand. Andrew Edgar (andy.edgar@vuw.ac.nz)

Interfacial Structure by X-ray & Neutron Reflectivity

There is widespread interest in measuring the structure of surfactants, polymers, proteins, electrochemically produced species and chemical reactions at the air-water, oil-water and solid-liquid interfaces using the reflection of X-rays and neutrons. The only X-ray reflectometer in the region for the air-water interface was completed in 1996 at the Research School of Chemistry, ANU [1, 2] and made available to the community.

Research at the University of Canberra [2] has included the development of methods for electrochemical and grazing incidence studies on surfactant interfaces and semiconductors as well as considerations of the use of reflectivity for the determination of the real part of the anomalous dispersion correction f ', and the problems with this as a technique. Together with the Surface Chemistry Group at the University of Queensland [3] a focussing monochromator and image plate camera was developed and research performed on time resolved studies of film growth.

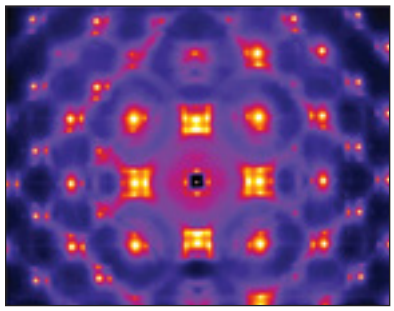
The Surface Chemistry Group [3] also uses neutron reflectivity measurements at ISIS in the UK. The films of interest are either on an air-water interface or on an air-solid interface. Recent work has shed light on the mechanism of action of a lung surfactant protein crucial for the breathing process in humans and animals. At ANU [1], time dependent studies of the growth of inorganic films (using surfactant templates at the air water interface) have shown the nanometre by nanometre build up and composition of the interfacial layers. The structure development has been followed from a simple surfactant surface excess through to a highly crystalline mesoporous film thousands of layers thick. A key initial insight was obtained using constrained refinement fitting to X-ray and neutron reflectometry data collected on self-assembled mesoporous silicate films growing at the air-liquid interface.

New facilities for reflectometry research include the construction of a world class time of flight reflectometer for the neutron beam guide hall of the OPAL reactor.

[1] Australian National University (jww@rsc.anu.edu.au)
[2] University of Canberra (Dudley.Creagh@canberra.edu.au)
[3] University of Queensland (gentle@chemistry.uq.edu.au)

Diffuse Scattering

Diffuse scattering research is represented through the work of researchers at the Australian National University in Canberra. One group [1] combines diffuse X-ray scattering methods with computer simulation to deduce the arrangement of atoms and molecules in disordered crystals. Diffuse scattering gives information on how neighbouring atoms or molecules interact with each other and the techniques have been applied by this group to disordered molecular crystals, guest/host systems such as urea inclusion compounds, non-stoichiometric inorganic materials and minerals, flexible framework structures such as silica polymorphs and their analogues, zeolitic materials, ferroelectric materials, alloys, and quasicrystal phases.



Diffuse scattering in Wüstite, $Fe_{1-x}O$, viewed down [001], recorded at the Advanced Photon Source at Argonne, USA. Wüstites are of considerable importance as they are thought to be a major constituent of the Earth's lower mantle. The diffuse scattering is due to the formation of a complex distribution of defect clusters which contain both Fe^{2+} vacancies and Fe^{3+} interstitial ions.

Another group at ANU [2] aims to understand and exploit the factors that determine structure and function in the crystalline solid state. Here, the interest is in the balance between local crystal chemistry, strain and order in a wide range of compositionally and/or displacively flexible crystalline solids. On the theoretical side, group theory, lattice dynamical calculations and bond valence sum analysis are the principal techniques. Crystalline systems investigated include non-stoichiometric solid solutions, displacively flexible zeotypic framework structures, ferroic phases, solid electrolytes, dielectric materials and incommensurately modulated structures. There is also a strong interest in determining the shapes of observed diffuse distributions in reciprocal space and then relating this back to multi-body correlations in real space. Systems to which this approach has been applied include the study of oxygen/fluorine ordering in metal oxyfluoride systems and various zeotypic microporous molecular sieve materials.

References

[1] Australian National University, Richard Welberry (welberry@rsc.anu.edu.au)
[2] Australian National University, Ray Withers (withers@rsc.anu.edu.au)

Crystallographic Software and Data Definition

Australian scientists are active in the development of crystallographic software and processes for the definition, validation and publication of crystallographic data. Software packages currently available includes:

- *CRYSTAL_EXPLORER* to display Hirshfeld surfaces and related graphics for molecular crystals [1] (to be distributed on www.theochem.uwa.edu.au/crystal_explorer);
- *DIFFUSE* for calculating X-ray diffuse scattering from model disordered crystals [2];
- *DISCUS* for defect structure simulation [3]; and
- *XTAL* a general structure analysis package distributed as GNU software by Source Forge (xtal.crystal.uwa.edu.au) [4].

There is also close involvement in the definition and validation of electronic crystallographic data. In 1987, the Australian delegation to the General Assembly at the Perth IUCr Congress proposed that an approach should be developed for the electronic publication and archiving of structural data. This led to the development of the crystallographic information file (CIF) now in wide use for data exchange. Perhaps more importantly, the CIF approach focused the

crystallographic community on the need for precise identification and definition of the myriad of data items used in the discipline. The subsequent adoption by the IUCr of a series of data dictionaries means now that CIF data may be automatically and comprehensively validated and checked when submitted electronically to journals and databases. This approach was initially introduced for manuscripts and data submitted to *Acta Crystallographica* C while Syd Hall (University of Western Australia) was Editor. Its success subsequently led to the creation of Acta E, a fully electronic journal, and more recently its macromolecular equivalent Acta F (Mitchell Guss, University of Sydney, joint Editor). The pivotal role now played by ontologies in data exchange has resulted in the compilation of International Tables Volume G entitled: Definition and exchange of crystallographic data (Syd Hall, joint Editor). Currently a new data definition language (StarDDL) is being prototyped at the University of Western Australia [5] in collaboration with researchers at Rutgers University in the USA.

References

[1] University of Western Australia, Mark Spackman (mas@cyllene.uwa.edu.au) and Dylan Jayatilaka dylan@theochem.uwa.edu.au

[2] Australian National University, Richard Welberry (welberry@rsc.anu.edu.au)

[3] Currently Los Alamos National Laboratories, Thomas Proffen (tproffen@lanl.gov)

[4] University of Western Australia, developed by many researchers, coordinated by Syd Hall (syd@crystal.uwa.edu.au)

[5] University of Western Australia, Syd Hall and Nick Spadaccini (nick@csse.uwa.edu.au)

Crystallographic Organizations

Crystallographers in Australia and New Zealand are represented by three separate but equally important organisations. The first two are the New Zealand and Australian National Committees for Crystallography. In New Zealand, the membership (see below) represents all the centers where crystallography is practised. In Australia, the committee is formed by the Australian Academy of Science which is the adhering body to the various International Unions and hence the International Union for Crystallography (IUCr). For example, it is the National Committee that nominates the Australian delegates to the General Assembly of the IUCr. In New Zealand, the affiliation to IUCr is through the Royal Society of New Zealand.

The third organization is The Society for Crystallographers in Australia and New Zealand (SCANZ), which has membership open to any scientist or student with an interest in crystallography. Originally the Society of Crystallographers in Australia, there has been regular participation over many years by New Zealand crystallographers and this led in 1999 to the formal incorporation of New Zealand in the society, which thus became SCANZ. The Society organises scientific meetings, awards student travel scholarships and nominates the Australian representatives on the council of the Asian Crystallographic Association (AsCA), one of the three regional associates of the IUCr. SCANZ is run by a council which is elected by the membership. Meetings of SCANZ are held regularly (about every 18 months) but with uneven frequency so as not to clash with IUCr congresses or major meetings of AsCA. The last meeting was held in Marysville, Victoria in March 2005 and the next SCANZ meeting will be held in 2007, hosted by Sydney, New South Wales.

Following the successful IUCr Congress and General Assembly held in Perth, Western Australia in 1987, residual funds from the meeting were invested for the purpose of supporting the travel of young crystallographers from Australia and New Zealand to meetings of SCANZ, AsCA and the IUCr. In addition, "1987 Fellowships" are awarded to leading crystallographers to present their work at a SCANZ meeting. The Scholarships and Fellowship have been named for Ted Maslen, who played a leading role in the establishment of SCANZ and in the successful organization of the 1987 Congress. His untimely death at a relatively young age was a loss to crystallography everywhere, and it is fitting that he be remembered by the Scholarships and Fellowship that bear his name.

Contributors (in alphabetical order)
Ted Baker, Peter Colman, Hans Freeman, Graeme Gainsford, Richard Garrett, Ian Gentle, Mitchell Guss, Syd Hall, Chris Howard, Geoffrey Jameson, Brendan Kennedy, Shane Kennedy, Peter Lay, Jennifer Martin, Jim Metson, Rick Millane, Michael Parker, Rob Robinson, Ward Robinson, Mark Spackman, Andrew Stevenson, Richard Welberry, Allan White, John White, Steve Wilkins

Current New Zealand NCCr Members

Convenor: ..... Ted Baker (U. of Auckland)
Secretary: ..... Eddie Davis (RSNZ)
Members: ..... Brian Nicholson (Waikato)
Geoff Jameson (Massey U.)
Graeme Gainsford (Industrial Research Ltd)
Ward Robinson (Canterbury U.)
Jim Simpson (Otago U.)

Current Australian NCCr Members

Chair: ..... Peter Colman (Walter and Eliza Hall Inst.)
Members: ..... Syd Hall (U. of Western Australia)
Jennifer Martin (U. of Queensland)
Brendan Kennedy (U. of Sydney)
Jose Varghese (CSIRO)
Ray Withers (Australian National U.)
Rob Robinson (ANSTO)

Current SCANZ council Members

President: ..... Brendan Kennedy (U. of Sydney)
Vice President: ..... Steve Wilkins (CSIRO)
Past President: ..... Jennifer Martin (U. of Queensland)
Secretary & Newsletter Editor: ..... Geoff Jameson (Massey U.)
Treasurer: ..... Bostjan Kobe (University of Queensland)
Councillors: ..... Brian Skelton (U. of Western Australia)
Ray Withers (Australian National U.)
Jose Varghese (CSIRO)

Contributers to this Issue

A. Altomare, D. Argyriou, J. Arthur, T. Baker, D. Balzar, P. Barnes, H.J. Bernstein, Ul. Bismayer, D. Bourgeois, C. Broennimann, I.D. Brown, M. Catti, P. Colman, K. Cowtan, J.C. Daran, M. Degano, J.-G. Eon, J. Faber, G. Ferraris, A. Fitch, T. Forsyth, H. Freeman, G. Gainsford, R. Garrett, I. Gentle, N.E. Ghermani, P. Gómez-Sal, S. Gorfman, P. Gross, M. Guss, S. Hall, K. Hamalainen, N. Hmaya, C. Howard, B. Iversen, G. Jameson, M. Jaskolski, E.Y. Jones, B. Kennedy, S. Kennedy, P. Lay, F. Leveiller, R. Lifshitz, J. Martin, B.W. Matthews, B. McMahon, E.A. Merritt, J. Metson, R. Millane, P. Mittl, M. Parker, J.M. Perez Mato, D.M. Proserpio, H. Putz, I. Radosavljevic Evans, P. Raithby, Z. Rao, J.J. Rehr, R. Robinson, I. Robinson, K. Saitoh, M. Saviano, P. Scardi, J. Spence, K. Stahl, B.H. Toby, T. Tschentscher, I. Turowska-Tyrk, A. van der Lee, M. Weil, A. Wlodawer, N. Yagi.

Louisa Gross Horwitz Prize to Yonath

Each year, the Louisa Gross Horwitz Prize has been awarded by Columbia U. for outstanding basic research in the fields of biology or biochemistry. The purpose of this prize is to honor a scientific investigator whose contributions to knowledge in either of these fields are deemed worthy of special recognition.

Ada Yonath is the director of the Helen and Milton A. Kimmelman Center for Biomolecular Structure and Assembly of the Weizmann Inst. of Science and a Professor in the Dept. of Structural Biology. Her research focuses on the mechanisms underlying protein biosynthesis by the ribosomey, a research line she pioneered over twenty years ago despite considerable skepticism by the international scientific community. She has determined the complete high-resolution structures of both ribosomal subunits. She showed that the ribosome is a ribozyme that places its substrates in stereochemistry suitable for peptide bond formation and for substrate-mediated catalysis. Two decades ago she visualized the path taken by the nascent proteins, namely the ribosomal tunnel, and recently revealed the dynamic elements enabling it's involvement in elongation arrest, gating, intra-cellular regulation and nascent chain trafficking into their folding space.


Ada Yonath

Ada elucidated the modes of action of over twenty different antibiotics targeting the ribosome, illuminated mechanisms of drug resistance, deciphered the structural basis for antibiotic selectivity and showed how it plays a key role in therapeutic effectiveness.

To enable ribosomal crystallography Ada introduced the novel technique of cryo biocrystallography, which has become routine.

She is a member of the National Academy of Sciences, USA; the American Academy of Arts and Sciences; the Israel Academy of Sciences and Humanities; the European Academy of Sciences and Art and the European Molecular Biology Organization. Her awards and honors include the Israel Prize, the first European Crystallography Prize, NIH Certificate of Distinction, the Harvey Prize, the Kilby Prize, the Cotton Medal of the US Chemical Society, the Anfinsen Award of the International Protein Society, the Datta Medal of the Federation of European Biochemical Societies, and the Fritz Lipmann Award of the German Biochemical Society.

Bochtler receives Pienkowski Award

The Stefan Pienkowski Award of the Faculty of Physics, Warsaw U., Poland, went in 2005 to **Matthias Bochtler**, a protein crystallographer holding a Group Leader position in the International Inst. of Molecular and Cell Biology in Warsaw, supported jointly by the Polish Academy of Sciences and the Max-Planck-Institute for Molecular Cell Biology and Genetics. The Award was established to promote research in natural sciences that is of particular importance for the scientific community in Poland, and to commemorate Prof. Stefan Pienkowski, a prominent experimental physicist of the first half of the XXth century, also interested in the use of X-rays in structural studies, founder of the Warsaw school of physics. The Award recognizes achievements in broad experimental physics, including applications in chemistry and biology. Matthias is a physicist by education but he received his PhD in chemistry (1999) for biostructural work on proteasome model HslV, carried out with Robert Huber in Martinsried, Germany. Matthias came to Warsaw in 2001 and in this short span of time he not only created a young, vibrant, and competitive protein crystallography group, but has also marked his position by an outstanding record of achievement and publication. Among his accomplishments are crystal structure determinations of novel amidases and their inhibitors. The citation on the Diploma highlights "Dr. Matthias Bochtler's achievements in crystallographic studies of protein structure". The award ceremony was held in connection with a Symposium, during which Matthias presented a lecture about "Physics in Biology: Protein Crystallography".


Matthias Bochtler

Mariusz Jaskolski, Poznan

Seeman Receives World Technology Award

Nadrian Seeman, a chemist at New York U., has been named winner of the 2005 World Technology Award for Biotechnology by the World Technology Network. He was named the recipient after the organization stripped the initial winner, Woo Suk Hwang, of the honor after Hwang's research on stem cells was found to be falsified.

Seeman and his colleagues at NYU developed the field of DNA nanotechnology. The systems they have produced enable the specific organization of a variety of other chemical species that are relevant to nanoelectronics, photonics, and drug design. They have also built machines that work on the nanoscale, such as a device that allows for the translation of DNA sequences, thereby serving as a factory for assembling the building blocks of new materials.

C&EN, March 6, 2006

Max Perutz ECA Prize to Dodson

The European Crystallographic Association has awarded the second Max Perutz Prize to **Eleanor J. Dodson** for developing, implementing, teaching and applying the best tools available to produce macromolecular structures of highest quality.

Eleanor Dodson is an unusual scientist who has made a number of remarkable contributions. Since the early years of working on insulin together with Dorothy Hodgkin, she has been at the center of the mathematical side of macromolecular crystallography and has been developing, implementing, teaching and applying the best tools available to produce science of highest quality.

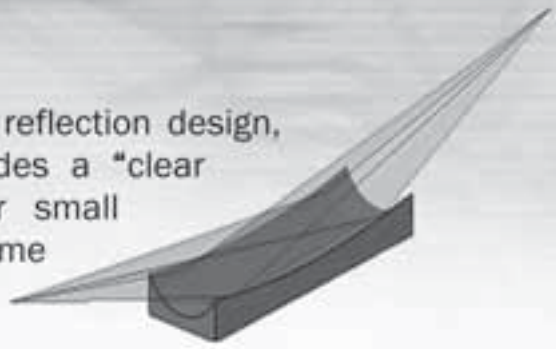

Eleanor J. Dodson

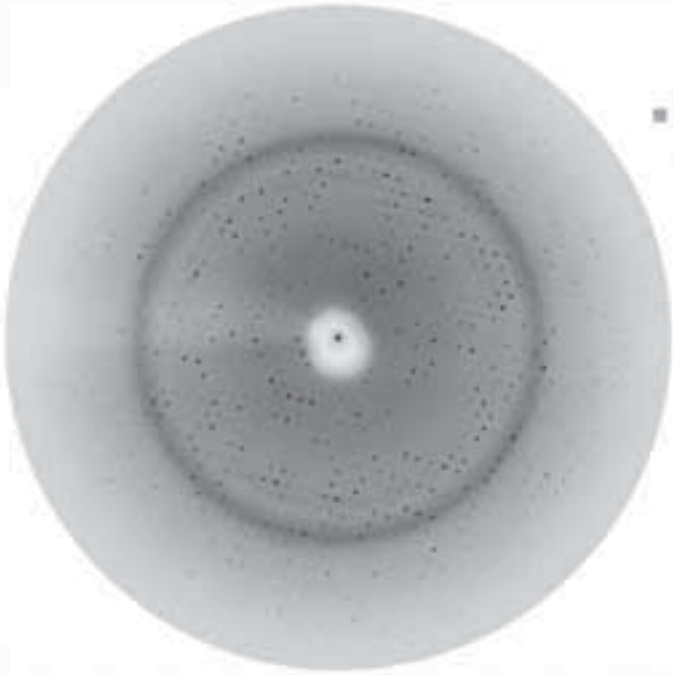
FOX2D CU 25_25P

focusing x-ray optic...

... simply brilliant !

Based on Xenocs' innovative single reflection design, the new *FOX2D CU 25_25P* provides a "clear improvement in data quality for small crystals" even with your existing home lab x-ray source.





- enhanced useful flux with low background
- improved data quality
- enhanced lifetime
- lower cost of ownership
- easy alignment and integration
- compact mechanical design adaptable to all X-ray generators

Data Courtesy of Dr. Andrew GW Leslie
MRC Laboratory of Molecular Biology, Cambridge.

The crystal belongs to space group C222 with cell dimensions a=72.1Å, b=97.4Å, c=191.0Å. Images were collected with an oscillation angle of 0.4°.
The crystal was a thin plate with approximate dimensions 200x75x50 µm³.
The generator was a Rigaku RuH3R running at 50kV, 100mA (300 µm focus) and the data were collected on a Mar345 image plate detector.

	classical confocal multilayer system	Xenocs *FOX2D CU 25_25P*
Exposure time per frame	4 min	4 min
R_{merge} (22.7-2.43A)	8.8%	6.4%
R_{merge} (2.57-2.43A)	44.1%	26.2%
<I>/<sigI> (22.7-2.43A)	12.1	15
<I>/<sigI> (2.57-2.43A)	2.5	4.1
Mean multiplicity	3.3	3.3

Xenocs
Reflecting Future Technology

www.xenocs.com info@xenocs.com
phone +33 4 76269540 fax +33 4 76269549

Xenocs - A spin off company from Institut Laue Langevin

X - Ray Fluorescence at BCA 2007

Kent, Canterbury, April 17-19, 2007

A comprehensive XRF program is planned at the British Crystallographic Assn Spring Meeting. There will be a £50 cash prize and champagne for the best poster! Bursaries will be available for the meeting to BCA members of 6 months standing who present a poster at the meeting.

There will also be a commercial Exhibition and XRF vendors are encouraged to attend. There will also be a XRF Exhibitors' Forum, organized by Dave Taylor. Exhibitors will be able to give presentations aimed at encouraging delegates to visit their exhibition stand for further information. The followinng XRF Sessions are scheduled:

A Tutorial / Workshop Session "XRF: where are we now?" is being organized. There will be two talks (speakers to be selected): XRF: What instruments have we got, or are likely to get soon and XRF: What can we do with it?

Two sessions on Semiquantitative analysis and calibration samples. Semiquantitative - what on earth is this sample? The production of Calibration Samples - sometimes none are available, sometimes they can be bought.

An XRF / XRD joint session on thin films, designed to give delegates an insight into what can be achieved by using XRF and XRD to investigate thin films and coatings.

XRF Applications - including Cultural Heritage. If you have an interesting XRF application, come and tell us about it! Both short and long talks will be welcome; and both wavelength-dispersive and energy-dispersive techniques will be included. Talks relating to cultural heritage topics will be particularly welcome.

A Keynote Lecture "Environmental Issues" will be followed by presentations on the same topic.

Further information is available at http://img.cryst.bbk.ac.uk/bca/ig/XRF/Meetings/meet07.htm.

AsCA'06 and CrSJ Joint Conference

Tsukuba, Japan, November 20–23, 2006

A Joint conference of the Asian Crystallographic Association (AsCA) and the Crystallographic Society of Japan (CrSJ) will take place in Tsukuba, Japan, November 20-23, 2006. This conference includes all aspects of materials science related to crystallography, such as nano and biological materials, and encompasses X-ray and neutron scattering/diffraction, electron microscopy, XAFS, NMR and so on. Crystal growth studies are also welcomed at the conference.

Further information is available at www.asiancrysassn.org/.

Theoretical Crystallography and Materials Science

Tsukuba, Japan, November 18-19, 2006

A satellite conference on Theoretical Crystallography and Materials Science will be held prior to the AsCA'06/CrsJ conference at the same venue, November 18-19. This conference is being organized jointly by the IUCr Commission on Mathematical and Theoretical Crystallography (MaThCryst) and by the IUCr Commission on Inorganic and Mineral Structures (CIMS).

The satellite is addressed to young scientists as well as to all those who wish to learn more about the application of theoretical crystallography to the solution of concrete problems of materials science.

Invited lectures include Mois I. Aroyo (U. of Bilbao, Spain), Andrew G. Christy (Australian National U.), Santiago Garcia-Granda (U. of Oviedo, Spain), Masanori Matsui (U. of Hyogo, Japan) Yoshio Matsui (National Inst. for Materials Science, Tsukuba, Japan), and Dhananjaj Pandey (Banaras Hindu U., India). Contributed oral presentations as well as poster presentations are encouraged

Further information is available at www.lcm3b.uhp-nancy.fr/mathcryst/asca2006.htm. Inquiries should be sent to mathcryst.satellite@lcm3b.uhp-nancy.fr

Engineering of Crystalline Materials Properties

Erice, Italy, June 7–17, 2007

The 39th crystallographic meeting, Engineering of Crystalline Materials Properties: State-of-the Art in Modeling, Design and Applications, course aim is to revise the state-of-the-art in design of new materials with properties of technological interest, to allow a faster progress towards the rational design of these materials in academia and industry. The course will attempt to establish a common language between disciplines that are not traditionally in close contact (materials chemistry, solid state reactivity, nanotechnology and biotechnology). The scientific program is focused on the modelling, design, synthesis and applications of crystalline solids and on the methods to understand and to exploit the resulting collective properties. Top notch scientists will cover the most relevant aspects on molecule-based materials, and discuss frontier problems for applications in magnetism, conductivity and superconductivity, non-linear optics, drug delivery, bio- and nano-technology. The course aims mainly at showing the potential developments of molecule-based materials (magnetic, conducting, superconduction, non-linear optical, bioltechnological…) and to foster new lines of research aimed at the rational synthesis of these materials.

Invited speakers include: Joanna Aizenberg (USA), Alessia Bacchi (Italy), Patrick Batail (France), Joel Bernstein (Isreal), Neil Champness (UK), Eugenio Coronado (Spain), Roger J. Davey (UK), Patricia M. Dove (USA), Peter Erk, (Germany), Paul Fenter (USA), G Fabrizia Repioni (Italy), Louis W. Hobbs (USA), Reiko Kuroda (Japan), Leslie Leiserowitz (Isreal), Joel S. Miller (USA), Sarah (Sally) L. Price (UK), Susan Reutzel-Edens (USA), Concepció Rovira (Spain), Urszula Rychlewska (Poland), Janet Scott (Australia), Samuel I. Stupp (USA), Jennifer Swift (USA), MaryJane Tremayne (UK), and Joseph Zyss (France).

Since June 2003, Erice Crystallography lectures have been broadcast on the Internet. For information on the virtual course, visit http://erice2007.docking.org/vcourse/.

For furhter information on the Erice courses, visit www.crystalerice.org/.

23rd European Crystallographic Meeting

Leuven / Belgium / 6-11 August 2006

Visit the website: **http://www.ecm23.be**

Organising Committee ECM23

L. Van Meervelt (*Chair ECM23*), P. Bombicz (*ECM22*), J-P. Declerq, J. Elsen, H. Fuess (*ECA*), B. Goderis, A. Jonas, D. Maes, K. Michel, D. Poelman, H. Reynaers, D. Schryvers, M-R. Spirlet, A. Thalal (*ECM24*), B. Tinant, J. Van Beeumen, G. Van den Bossche, J. Van Landuyt, J. Wouters

Programme Committee

L. Van Meervelt (*Chair ECM23*), B. Tinant (*Programme Secretary*), D. Maes, D. Schryvers, H. Fuess (*ECA ExeComm*), M. Teresa Duarte (*ECA ExeComm*), D. Viterbo (*IUCr ExeComm*), A. Liljas, H. Graafsma, G. Chapuis, Th. Weirich, W. Depmeier, J. L. Hodeau, R. Boese, J. Rius, T. Spek, M. Kovalchuk, A. Polian, P.A. Thomas, Ch. Wilson

Programme

Tue - Fri, 1-4 August:	Satellite School X-EI2006
Fri - Sun, 4-6 August:	Satellite Symposium MathCryst
Sun, 6 August:	CCDC Workshop
	Registration
	Opening ceremony
	Welcome Reception
Mon, 7 August:	Meeting and exhibition day
Tue, 8 August:	Meeting and exhibition day
Wed, 9 August:	Meeting and exhibition day
Thu, 10 August:	Meeting and exhibition day
Fri, 11 August:	Excursion day

Other important facts

- Scientific programme includes
  - ✓ 16 plenary lectures
  - ✓ 230 oral and more than 400 poster presentations in two poster sessions with free Belgian beer tasting
- Social programme includes concert with Kolacny brothers, special lecture on Belgian beers, congress dinner and excursion 'Brussels discovery'
- The MARResearch Party takes you to the upper sphere of the Atomium in Brussels!

Topics of Microsymposia

- Controlled nucleation and growth of crystals of a variety of materials
- Structural genomics, high-throughput crystallisation and visualisation
- Pipelining in macromolecular crystallography
- Nucleic acids
- High quality diffraction data and high quality structural information
- Macromolecular assemblies
- Hot structures in protein crystallography
- Membrane proteins
- Structural enzymology
- New X-ray sources and new possibilities
- Molecular recognition in biomolecular systems
- Interface of nano and bio-systems
- Understanding molecular interactions
- Structure determination of modulated crystals
- Quantified TEM for crystallography
- Local structure determination by electron imaging
- Structures by electron crystallography
- Crystallography in art and archeological sciences
- Phase transitions in inorganic and mineralogical materials
- Topological aspects of inorganic crystal structures
- XAS: EXAFS and XANES
- Industrial mineralogy
- Instrumentation and experimental techniques for applications to symmetry, charge and orbital studies
- X-ray tomography
- Crystal design and functional crystals
- Inclusion compounds and solvates
- Supramolecular compounds and assemblies
- Advanced methods for computer simulation of molecular crystals
- Advances in powder diffraction: structural aspects
- Advances in powder diffraction: microstructural aspects
- Advances in computational macrocrystallography
- Advances in computational small molecule crystallography
- New crystallographic software
- X-ray optics, guides, focussing
- Crystallography under extreme conditions: state of the art
- SAXS and SANS
- Crystallography of nanotubes and fullerenes
- Natural and synthetic organic-inorganic systems
- Battery and fuell cell materials
- Structural coordination chemistry
- Structure-property relationships in molecular crystals
- Molecular crystallography under non-ambient conditions
- Neutron diffraction in structural chemistry
- Communicating crystallography to young people and the public
- Multiferroics

All further information and details on **Oral and Posters Contributions, Exhibitors, Satellite Meetings, Registration, Accommodation and Social Programme** can be found on the congress website at **www.ecm23.be**

We look forward to welcoming you in Leuven!

Crystallographic Meetings Calendar

A selection of future meetings. A more complete list is available at www.iucr.org. Corrections and new listings are invited by the Editors.

September 2006

1-4 ♦ EPDIC-10 - European Powder Diffraction Conference. Geneva, Switzerland. http://www.sgk-sscr.ch/EPDIC10/EPDIC10.html.

October 2006

25-27 ♦ 2nd Meeting of the Assn Argentina de Cristalografía. Puerto Madryn, Chubut. www.tandar.cnea.gov.ar/~vega/.

November 2006

18-19 ♦ Theoretical Crystallography and Materials Science. Tsukuba, Japan. www.lcm3b.uhp-nancy.fr/mathcryst/asca2006.htm.

20-23 ♦ AsCA'06 / CrSJ Joint Conf. Tsukuba, Japan. www.asiancrysassn.org/.

January 2007

14-19 ♦ Int'l School on Mathematical and Theoretical Crystallography. Havana, Cuba. www.cristalografia.net/havana2007/.

February 2007

19-22 ♦ 6th Pharmaceutical Powder X-ray Diffraction Symposium. Barcelona, Spain. www.icdd.com/ppxrd/.

April 2007

2-6 ♦ Latin American Workshop on Applications of Powder Diffraction and Satellite Workshop - Methods of Powder Diffraction. Campinas, SP, Brazil. www.lnls.br/.

17-19 British Crystallographic Assn Spring Meeting. Southern England. http://bca.cryst.bbk.ac.uk/bca/welcome.htm.

June 2007

7–17 Engineering of Crystalline Materials Properties: State-of-the-Art in Modelling, Design, and Applications, the 39th crystallographic course at the Ettore Majorana Centre. Erice, Italy. www.crystalerice.org/.

July 2007

21-26 ♦ ACA 2007 - The American Crystallographic Assn Annual Meeting. Salt Lake City, UT, USA. www.hwi.buffalo.edu/ACA/.

August 2007

13-17 ♦ BSR2007 - 9th Int' Conf. on Biology and Synchrotron Radiation. Manchester, UK. www.srs.ac.uk/bsr2007/.

August 2008

23-31 ♦ 21st General Assembly and Congress of the IUCr. Osaka, Japan. www.congre.co.jp/iucr2008/greeting.html.

The logo of IUCr2008 is the image of the Osaka Castle, which is symbolic of the architecture in Osaka.

The pattern of the stones in the Castle's foundation was taken from the crystal structure of 'spinel' that was solved by S. Nishikawa in 1919 by applying space group theory for the first time. This structure was used on the cover of the *Journal of the Crystallographic Society of Japan* for a number of years.

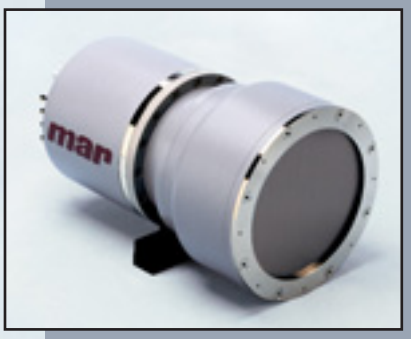
The logo was originally designed by T. Hosoya, a PhD student of Tokyo Institute of Technology.

Index to Advertisers

If you would like to see a copy of the *IUCr Newsletter* in your college or university library, send the address to the Newsletter office so that we can add it to our mailing list.

marusa

High-performance X-ray data collection systems



marccd

- Largest available single chip design: 165mm diameter
- Based on 4k × 4k CCD with four parallel readouts
- Low noise, low dark current design for fully usable 16-bit dynamic range
- Versatile detector for rotating anode and synchrotron beamlines

marmosaic

- Seamless multi-element CCD technology
- 225mm × 225mm, 300mm × 300mm, or 325mm × 325mm active area
- Multichannel readout in 1 second
- Low noise, low dark current design for fully usable 16-bit dynamic range
- 35 frames per minute at standard resolution

The marmosaic 225 with mardtb goniostat and cryogenic sample changer is a complete endstation for high-throughput crystallography.

marusa

www.mar-usa.com

1880 Oak Avenue, Evanston, IL 60201 USA

Toll-free: 1-877-MAR-XRAY (1-877-627-9729)

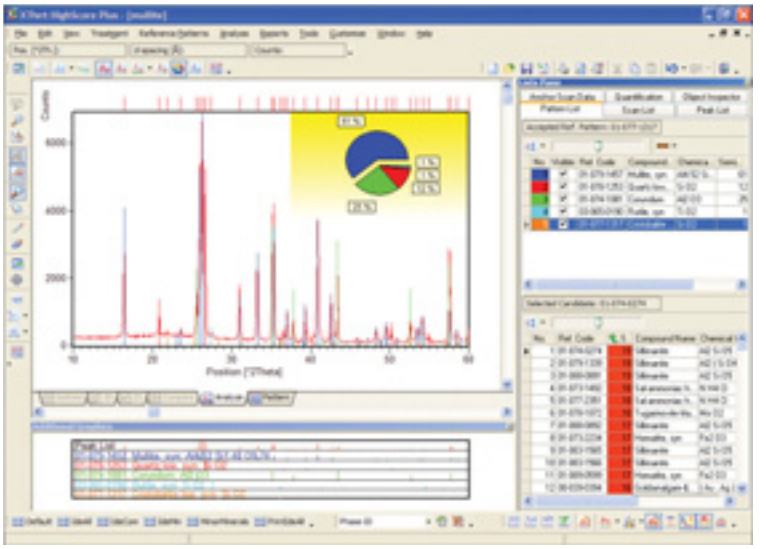
From outside the U.S.: 1-847-869-1548

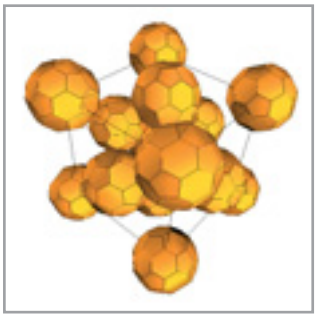
Fax: 1-847-869-1587

E-mail: info@mar-usa.com

X'PERT HIGHSCORE PLUS

Total X-ray powder pattern analysis





With **X'Pert HighScore and X'Pert HighScore Plus**, the analysis of powder diffractograms is easier than ever. Novel algorithms for phase identification have been integrated with crystallographic and Rietveld routines in one user interface, so the software is easily used by specialists and students alike.

X'Pert HighScore is a comprehensive phase identification program, while **X'Pert HighScore Plus** is an integrated package for phase identification, Rietveld, crystallographic, and extended cluster analysis. Both deliver high performance for research scientists and analysts, for identifying complex phase mixtures, performing standardless quantitative analysis using Rietveld or RIR analysis, or simultaneously analyzing a large number of scans for similar composition, or clustering.

X'Pert HighScore and **X'Pert HighScore Plus** use Microsoft Windows® XP.
The interface can be customized by each individual user. Analysis procedure batches can be saved to toolbar buttons for one-touch, fully automated data analysis and subsequent reporting - in Microsoft® Word for example. And for those working in a regulated environment, audit trail functionality for GLP and 21 CFR Part 11 compliance is available as an option.

PANalytical software licensing is designed to support the way you work. Multiple software installations allow you to transfer data from the lab to your office or laptop – wherever is most convenient. Whatever the hardware used for data collection, these powerful software packages help to optimize analytical performance. Find out how by contacting:

PANalytical
PO Box 13
7600 AA Almelo
The Netherlands
Tel. +31 (0) 546 534 444
Fax +31 (0) 546 534 598
info@panalytical.com
www.panalytical.com