



Newsletter

of the ASIAN CRYSTALLOGRAPHIC ASSOCIATION.

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President's Message

The proposed survey of crystallographic facilities in the region has not progressed much beyond where it was six months ago. What appeared at first to be a relatively straightforward and useful project, has turned out to have more facets to it than a dodecahedron! For the smaller countries this information is well known and relatively easy to tabulate. However, for larger countries, gathering this data is much more complex. This is further complicated by the uncertainty about which data is useful, and which is accessible. This aspect of the survey that has to be considered further by the AsCA Executive. Other questions, such as whether industrial, as well as academic and government, facilities should be included in this survey, must also be resolved before a sensible questionnaire can be prepared for circulation. There appears to be little opportunity to decide on these matters before the Executive meets at the 1990 IUCr Congress. If you have have a particular point you would like to make about such a survey, please let me, or your Councillor, know before this meeting.

It cannot be overemphasised that this newsletter is very dependent on the submission of news items. Much more so than for the newsletter of a national society, because of the wide geographic separation of activities. Just being aware of an item of interest in the region is not enough without factual details. For this reason, reporting news should be looked upon as the responsibility

news should be looked upon as the responsibility of all crystallographers in the region, not just the AsCA Councillor. Any item of interest will be gratefully received and gladly included. So if there are some crystallographic goings-on that you think would be of interest (including seminars, meetings, visitors, new or existing research projects, new appointments and national association details) please send me details of them. Many thanks.

Syd Hall

News from Japan

The Executive Office of the Crystallographic Society of Japan (CSJ) is now located at 2-16-13, Yushima, Bunhyo-ku, Tokyo 113, Saito Building 2F, Phone: 03-815-8514, FAX: 03-815-8529.

The President of the 1989 CSJ Executive Committee of the is Professor Nobutami Kasai (Osaka U.). Other CSJ committee members will be decided in April.

The Japanese Society for SOR Research was inaugurated on 1 April, 1988. The Society will act as a forum for the rapid exchange of information both within and outside Japan. Emeritus Professor Kazutake Kohra has been elected as the first President of the Society. For further details please contact: The Japanese Society for Synchrotron Radiation Research, c/o Ionics Publishing CO. LTD., Kawada Building,

2-3-4 Koishikawa, Bunkyo-ku, Tokyo 112, Japan.

The 3rd International Conference on Synchrotron Radiation Instrumentation, SRI-88, was held at the Lecture Hall of Agency of Industrial Science and Technology in Tsukuba, Ibaraki, 27 August - 2 September, 1988. The Photon Factory in the National Laboratory for High-Energy Research acted as host at this conference. There were about 480 participants and 360 papers as posters presented. There were 53 invited papers and 15 oral presentations. An adhoc meeting was also held concerning the "Small Stage Ring". Collected papers will be published as a regular issue in "Review of Scientific Instruments". The next conference SRI-89 will be held at the Daresbury Laboratory in England.

A book on the history of crystallography in Japan (written in Japanese) has been published. For further information please contact: the Executive Office of the Crystallographic Society of Japan.

The 1988 Annual General Meeting of the Crystallographic Society of Japan in conjunction with two symposiums on "Recent Research of Structure Analysis of Biomacromolecules" and "SOR Experiments that Challenge the Limitations of Observation and Measurement" was held at the Hotel Sunroute Minamisenri in Osaka, 7-9 November, 1988. There were more than 300 participants and 117 papers were presented. The CSJ prizes were given to Ayahiko Ichimiya (Nagoya U.) for the development of reflective high energy electron diffraction for studying surface structure of crystals, and to Keiko Nishida (Gakushuin U.), the first woman CSJ prize winner in Japan, for the application of X-ray structure analytical methods to the study of structures of liquids and plastic crystals. The Seiji Nishikawa commemorative talk, entitled "A watch that an organism possesses and its mechanism and physiological meaning", was given by Prof. Hachiro Nakagawa (Osaka U.)

In next July issue, a who's who and some current research topics in Japanese Universities and National Laboratories will be reported in a series of articles.

Tianjin IUCr Summer School

In September of last year an International Summer School for Crystallography and its Teaching was held in Tianjin, Peoples Republic of China. The meeting was organised under the auspices of the IUCr Commission on Crystallographic Teaching, the Chinese National

Crystallographic Teaching, the Chinese National Committee of Crystallography, Tianjin Normal University and Beijing University.

The school was attended by 112 scientists from all parts of the world. 86 of the participants were from the Peoples Republic of China. In 10 days the school provided 26 plenary lectures and tutorial sessions on all aspects of Crystallography and its Teaching. There was much interest in the tutorial sessions which were mostly held at the Long Feng Hotel in Tianjin. These were not only theoretical, and participants had the opportunity to do some hands-on computing at Tianjin Normal University Computer Centre. The lecturers were: H. Hauptman (U.S.A.), W. Clegg (U.K.), Th. Hahn (F.R.G.), E. Nordman (U.S.A.), P. Main (U.K.), Yao Jia-Xing (China), Fan Hai-Fu (China), P.T. Beurskens (Netherlands), D. Watkin (U.K.), D. Schwarzenbach (Switzerland), I.D. Brown (Canada), J.P. Glusker (U.S.A.), R. Jenkins (U.S.A.), R. Goddard (F.R.G.), N. Kasai (Japan) and C.L. Kennard (Australia).

The emphasis of the School was on techniques for solving structures and methods of teaching crystallography to students. Topics ranged from accurate data collection from single crystals and powders through to structure refinement and the evaluation of the results, which included an introduction to crystallographic databases. The various methods of solving structures, such as direct methods, Patterson search methods, partial structure expansion were covered in detail, as was least-squares refinement together with constraints and restraints. Participants were also instructed in symmetry in crystallography and the analysis of powder diffraction data.

During the meeting participants were treated to two superb banquets and several dances which were enjoyed by all. For the excursion participants were offered a choice, and those who did not go to Tianjin Zoo went to a local art workshop where hand-printing could be seen. Unfortunately, the Chairman of the Program Committee Henk Schenk was unable to attend the meeting due to illness. Participants were none the less aware of the considerable work that he had put into the preparation of the School. Jenny Glusker stepped into his shoes at the last moment and she and Miao Fang-Ming are to be congratulated on organising a truly successful meeting.

Richard Goddard

News from Australia

Sandy Mathieson will undertake the preparation of "The History of Crystallography in Australia." This should result in a medium-sized book of, say, 300 pages including photographs.

Neil Isaacs has accepted the foundation Joseph Black Chair of Protein Crystallography at Glasgow University. Neil leaves his present position as senior research fellow at St. Vincents Institute of Medical Research in Melbourne for Glasgow in December. Not only is Australia losing a leading crystallographer and medical researcher, but the Society of Crystallographers in Australia (SCA) is losing its Vice President (and hence next President)! However, congratulations and best wishes must go to Neil, and thanks for his services to the Society.

The Australian Journal of Physics has just published two special conferences issues which will be of interest to many readers. The first is "X-Ray Powder Diffractometry" (International Symposium, Fremantle, Australia, 20-23 August 1987), price \$50, and the second is "Accuracy in Structure Factor Measurement" (International Symposium, Warburton, Australia, 23-26 August 1987), price \$45. These journals are available from the Publications Sales Office, CSIRO, 314 Albert Street, east Melbourne, Vic. 3002, Australia. Prices include postage; cheques are payable to 'Collector for Moneys CSIRO.'

On 11th August, Prof. Allan White delivered the RACI Smith Medal Lecture in Melbourne at La Trobe University. Allan began by querying the structure of $\text{Ag}(\text{NH}_3)_2\text{Cl}$, and then led a fascinating journey through a series of far from simple structures of complexes of the coinage metals ($\text{Ag}(\text{I})$, $\text{Cu}(\text{I})$) with various amines and halogens. He concluded with some analogous Group I complexes, and the heresy that the Li ion appears larger than $\text{Cu}(\text{I})$. We were all left with the view that $\text{Ag}(\text{NH}_3)_2\text{Cl}$, if not life itself, is considerably more complicated than we had previously preferred to believe.

At the August 1987 IUCr Congress in Perth, the General Assembly established a Commission on Powder Diffraction. The Australian member of the new Commission is Dr. Rod Hill of CSIRO Division of Mineral Chemistry. The first newsletter of the new Commission was produced in January, and those wishing to receive future copies should write to Dr. J. Langford, Dept. of Physics, University of Birmingham B15 2TT, England.

News from Taiwan

A crystallography meeting was held in Taipei on July 23, 1988 with 100 participants. The meeting started with a plenary lecture "Electron Diffraction Analysis of Thin Films" given by Prof. L. J. Chen of National Tsing Hua University. He gave an introduction to various techniques used in electron diffraction analysis, including convergent electron beam EM, high resolution EM and their applications to the structure determination of thin films. After coffee, there were five oral presentations on structure determinations of cluster phosphates, AlN substrate material, micell and disulfides using X-ray diffraction methods and neutron small-angle scattering. Work on the quantitative phase determination using 3-beam interference was also presented. After lunch, four oral and 21 poster presentations were given. These covered many aspects in crystallography.

This is the first annual meeting since the formation of a study group in crystallography. There will be seminars every three months covering specific topics, and an annual meeting covering general topics each summer. The success of this meeting suggests that the next will be even more popular.

Access to Synchrotron Radiation Facilities for Australian Scientists

(Extracted from the SCA Newsletter)

Background

For about three years discussions have been held between Australian and Japanese scientists with a view to the provision of an Australian experimental hutch on a beam line at the synchrotron radiation source at the Japanese Centre for High Energy Physics, Tsukuba, Japan.

An Australian Research Grants Committee proposal (Creagh, Barnea & O'Connor, 1986) was not funded but funds were made available to hold a workshop on synchrotron radiation. This was organised by Stephen Wilkins (Melbourne, 1987). It was attended by a number of eminent users of synchrotron radiation from England, U.S.A., Japan and Germany as well as local users and potential users of synchrotron radiation sources.

As a result of this workshop two courses of action have been followed. In the first, another

Australian Research Committee proposal for funding has been made (Barnea, Creagh & Sabine, 1988). This proposal seeks funding to investigate a number of issues connected with the future use of synchrotron radiation sources. For example, what sort of instrumentation is required, where might our instrument be sited, and what costs might be involved?

The second was a decision to keep up discussion with our Japanese colleagues on the beam line proposal so that we might best be able to formulate a proposal which serves Australian requirements and fulfils a need to the Photon Factory. A description of the present status of this project forms the bulk of this article.

Unrelated to this is a decision by the National Committee on Crystallography of the Australian Academy to investigate the need for the use of overseas "big science" facilities. Members of the SCA will be aware of the circular letter and questionnaire which Hans Freeman has recently had sent to all members.

The Australian-Japanese Proposal

For any proposal to build an instrument at a synchrotron radiation source to succeed it is necessary to determine what instrument is deemed most desirable by the host institution.

After considerable investigation it has been established that the Japanese lack a versatile high-resolution powder diffraction system.

The emphasis here is on the words "versatile" and "high resolution". Each beam station has to provide a proportion of its time for other users and the Japanese believe that its construction would considerably enhance the range of options open to their own researchers. By the same token Australian scientists would have right of access to all the others stations at the Photon Factory.

Expertise exists in Australia for the design of such an instrument and the preliminary design considerations have been addressed by Stephen Wilkins and myself. Sabine (1987) has proposed a design to be implemented at HASYLAB.

The key to versatility in an instrument is the design of the monochromator system. This system must optimise the flux incident on the specimen at a particular wavelength and have provision for the tailoring of the incident beam cross section. At the Photon Factory the beam line we would be offered is beam line 18C which emerges from a bending magnet. The optimum scattering plane from this line is the vertical plane since the beam is linearly polarised in the

plane since the beam is linearly polarised in the horizontal plane. This implies that the axes of the principal monochromator elements are horizontal. The monochromator consists of a primary and a secondary stage.

The operational range of the primary monochromator system would be 5 to 25 keV with good harmonic rejection and an energy resolution of better than 2 eV. A choice of silicon or germanium diffracting elements would be available. A schematic diagram of the primary monochromator (available from the author) indicates that by moving the primary axis out of the beam the white beam can pass through into the experimental hutch. This enables experiments such as X-ray topography to be undertaken. Axes 1 and 2 can be rotated and translated under computer control setting the monochromator elements to the appropriate positions for selection of the desired photon energy (Creagh, 1988).

When the beam emerges from the second monochromator it is well collimated in the vertical plane but somewhat divergent in the horizontal plane. Slit systems are usually used to reduce the horizontal divergence. This is a cheap expedient but there is a loss in photon flux. An extension to the design would enable the ability to condense the horizontal divergence of the beam either by totally reflecting mirrors or by sagittal Bragg reflecting collimators.

A secondary monochromator of the condensing Bragg optics type (Wilkins, 1987) would be able to be located in the beam for those applications in which highly collimated beams with small cross-sectional area are required. Such experiments include high-resolution powder diffractometry and small-angle X-ray scattering.

For the X-ray diffractometer system a high capacity Huber theta-2theta diffractometer (type 422) would be chosen since these are the basic building blocks on which most experimental systems at synchrotron radiation sources are constructed. Both high- and low-temperature specimen holders would be available for use.

A variety of methods for the detection of the scattered intensity would be made available. For high-resolution powder diffractometry the choice would be between the following:

- 1) the Fuji X-ray plate system (Miyahara et al., 1986), data from which can be extracted digitally by use of a laser-diode detector flying spot scanner system;
- 2) a curved position-sensitive detector system (Shushiguchi et al, 1986)

- 3) a conventional sodium iodide detector mounted on the 2theta arm; and
- 4) a solid-state detector system (for use primarily in energy-dispersive white beam experiments).

In the small-angle X-ray scattering mode, the choice would be either a Fuji plate system or a linear position-sensitive detector system.

The overall system is extremely versatile and should enable experiments to be undertaken in all fields of scientific endeavour. Those involved in the study of ceramic materials (high T_c superconductors, SYNROC etc.) would find the system equally as useful as those involved in the study of biological materials (oncology, biology, etc.). A brief summary of the fields of research which could be undertaken by use of such a system has recently been given (Creagh, 1988).

The cost of the proposal is not astronomical. I expect that the total cost, inclusive of all Photon Factory demands, would not be more than \$900,000. There would be no charge for beam use. The cost of the installation is considerably less than the per annum running cost in the Photon Factory of a beam line.

Conditions which may be encountered by visitors to the Photon Factory are first rate; accommodation is excellent and living costs are quite low. The differences in language and culture are apparently great, but in all my visits I have not yet encountered any difficulty in these respects. Also one suffers no "jet lag" on the trip. It is possible to commence work on arrival, a situation which does not easily occur with any other synchrotron radiation facility.

References

- Creagh, D. C. (1988) *Aust. J. Phys.*, **43**, 2
Miyahara, J., Takahashi, K., Amemiya, Y., Kamiya, N., and Satow, Y. (1986) *Nucl. Instrum. Meth.*, **A246**, 572.
Sabine, T. (1987) *J. Appl. Cryst.*, **20**, 173.
Shushiguchi, S., Minato, L., and Hashizume, H. (1986) *J. Appl. Cryst.*, **19**, 420.
Wilkins, S; (1987) patent pending.

Dudley Creagh

ACA Newsletter Extracts

ACA Officers 1989:

President: Bryan M. Craven, University of Pittsburgh; Secretary: Vivian Cody, Medical Foundation of Buffalo, Inc.; Vice President: David J. Duchamp, The Upjohn Company, Kalamazoo; Treasurer: Catharine M. Foris, E.I. Du Pont de Nemours, Wilmington; Newsletter Editor: Jenny P. Glusker, Institute for Cancer Research; Polycrystal Book Services: Mert Adams, Dayton, Ohio.

1989 ACA Annual Meeting, University of Washington Seattle, Washington, July 23-29.

In addition to the wide range of contributed topics, a special symposium on Molecular Recognition and Carbonhydrate-Protein Interactions, and workshops on Rietveld Analysis and Molecular Dynamics have been arranged. Contributed papers related to any of the above special sessions or to any area of interest to structural scientists are invited. The Abstract deadline is April 1, 1989.

Economical double and single accommodation is at the University of Washington residence halls. The food and lodging packages include five nights, five breakfasts and five lunches for \$170.00 (single) and \$145.77 (double).

The Program Chairperson is Penelope W. Coddington, Institute of Science and Technology, Biophysics Research Division, University of Michigan, 2200 Bonisteel Boulevard, Ann Arbor, MI 48109-2099, U.S.A.. The Local Chairperson is: Elinor T. Adman, University of Washington, School of Medicine, Dept. of Biological Structures, SM20, Seattle, WA 98195, U.S.A..

For further information and abstract forms contact Maria Vair, ACA Administrative Secretary, P.O. Box 96 Ellicott Station, Buffalo, NY 14205-0096, U.S.A. .

The Peter Debye Award in Physical Chemistry of the ACS will be presented to Prof. Gabor A. Somorjai at the Society meeting in April. The award, sponsored by the DuPont Company, recognizes the University of California, Berkeley professor's pioneering work and continuing leadership in surface science and heterogeneous catalysis research involving, among many other activities, the characterization of clean single-crystal surfaces and the determination of surface structures of ice, alkanes and amino acids grown epitaxially on metal single-crystals. In current investigations, Somorjai is using scanning tunneling microscopy to study surface structure of cataysts.

BCA Newsletter Extracts

The Chemical Crystallography Group of the BCA will conduct a Second Intensive Course in X-ray Structural Analysis of Small and Medium Sized Molecules at Aston University, Birmingham, 7-13 April 1989.

The lectures will be on: basic maths and space group theory; data collection; direct methods; maximum entropy methods; Fourier methods; Patterson methods; least squares, theory and methods; refinement, theory and methods; data bases; analysis of results; and interpretation of results. Contact: David Watkin, Course Director, Chemical Crystallography, 9 Parks Road, Oxford OX1 3PD, England.

The Biological Structural Group Session at the British Crystallographic Association Meeting in Oxford will take place on Friday, 7 April 1989 and will be devoted to: "The Crystallography of Viruses - Polio Virus Structure"; the main speaker will be James M. Hogle, Scripps Clinic & Research Foundation.

There will also be a Symposium on "Developments in Structure Solution" on 5 April. Invited speakers are: P. Beurskens (Nijmegen) - "Developments and Automation of Patterson Methods", C. Gilmore (Newcastle) - "A Hitchhiker's Guide to Maximum Entropy", P. Main (York) - "Image Processing Techniques in the Improvement of Protein Maps."

Invited speakers for the Industrial Group Symposium, BCA Spring Meeting, 6 April 1989 include: R. W. Joyner (Liverpool) - "In situ EXAFS investigations of Catalysis Materials"; J. Thomas (Uppsala) - "Aspects of Micro-Ionics in Industrial Applications". and D. Dingley (Bristol) - "On-line Micro-Texture Determination in Metals and Mineralogical Materials".

The Physical Crystallography Group will have a symposium at the 1989 BCA Oxford Meeting on Diffraction by Weak Potentials. Invited speakers are: W. Lovesey (Rutherford Appleton) - "Introduction to the magnetic scattering of photons and the charge scattering of neutrons"; P. J. Brown (Institute Laue Langevin, Grenoble) - "Neutron studies of bonding in III-V compounds"; and M. J. Cooper (Warwick University) - "Synchrotron studies of magnetic structure."

Meeting Diary

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| 13-15 Jun | International Workshop on the Rietveld Method. <i>Petten, The Netherlands.</i> |
| 2-7 July | IX International Conference on the Chemistry of the Organic Solid State (ICCOSS IX), <i>Como, Italy.</i> |
| 2-7 July | XXVII International Conference on Coordination Chemistry, <i>Gold Coast, Australia.</i> |
| 9-14 July | 4th International Conference of STM/ESCA. <i>Ooarai, Ibaraki.</i> |
| 23-29 July | ACA 1989 Meeting, <i>Seattle, USA.</i> |
| 7-11 Aug | Gordon Conference on "X-Ray Physics." <i>New Hampshire, USA.</i> |
| 20-25 Aug | 9th International Conference on Crystal Growth, <i>Sendai, Japan.</i> |
| 20-29 Aug | 12th European Crystallographic Meeting. <i>Moscow, USSR.</i> |
| 26-31 Aug | 7th International Summer School Crystal Growth. <i>Yamagata, Japan.</i> |
| 10-15 Sep | IXth International Hydrogen Bond Conference. <i>Zeist (Utrecht), The Netherlands.</i> |
| 11-15 Sep | International Conference on "Drug-DNA Interactions". <i>Cambridge, UK.</i> |
| 22-25 Sept | 3rd International Symposium on Defect Recognition and Image Processing for Research and Development of Semiconductors (DRIP-III). <i>Mejiro, Tokyo, Japan.</i> |
| 22-24 Nov | 1st European Conference on Material Science and Technology (EUROMAT'89). <i>Aachen, FRG.</i> |
| 27-29 Nov | CSJ Annual General Meeting, <i>Yokohama, Kanakawa, Japan.</i> |