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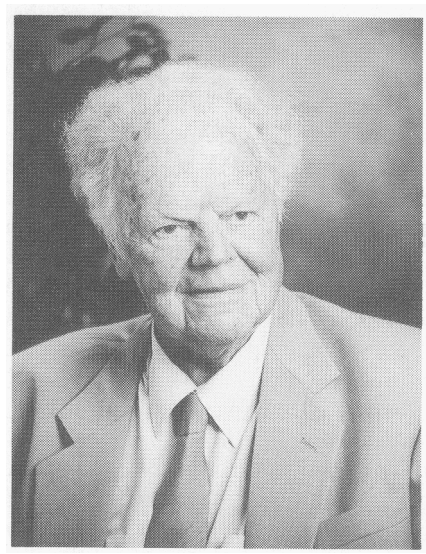
Professor Arthur Wilson FRS and Powder Diffraction

Arthur Wilson, one of the world's leading crystallographers for almost half a century and a pioneer of powder diffractometry, died at his home in Cambridge on 1 July, in his 81st year. Arthur James Cochran Wilson was born in Nova Scotia on 28 November 1914 and started his academic career at Dalhousie University, Halifax, where he obtained an MSc in 1936. He then moved to the Massachusetts Institute of Technology and received a PhD there in 1938. While at MIT he was awarded an 1851 Exhibition Scholarship which enabled him to go to St John's College and the Cavendish Laboratory in 1938, the year in which Sir Lawrence Bragg succeeded Lord Rutherford as the Cavendish Professor of Experimental Physics at Cambridge. During the remaining two years of his Scholarship, Wilson made accurate measurements of the thermal expansion of A1 and Pb, which led to the award of his second PhD in 1942. It was through his work at the Cavendish Laboratory, and the influence of Bragg and Henry Lipson, who was effectively in charge of the laboratory during the war years, that Wilson acquired a life-long interest in powder diffraction and in X-ray crystallography generally.

Wilson's work on thermal expansion involved the measurement of precise lattice parameters which led naturally to a general investigation of experimental and other factors which influence the position, shape and intensity of X-ray powder diffraction lines. Together with Alec R. Stokes, he also became interested in crystal imperfections through a study of stacking faults in Co (1941/2) and in the alloy Cu_3Au (1943), and a general treatment of diffraction effects due to small, distorted or otherwise imperfect crystals followed; his book ***X-ray Optics*** (1949; 2nd edition 1962) has been the starting point for much subsequent research in this field and is still a definitive work on the subject.

Wilson left Cambridge in 1945 to take up an appointment. as lecturer in the Department of Physics at University College, Cardiff. In 1946 he became a senior lecturer and Director of the Viriamu Jones Laboratory and then Professor of Physics and Head of the Department in 1954, a post he held until 1965. Soon after he arrived in Cardiff, Wilson became involved in providing data for the Powder Diffraction File (PDF), an activity which continued there for almost 30 years. Although the database and indexes were then published by the American Society for Testing and Materials (ASTM), they were compiled under the auspices of the Joint Committee on Chemical Analysis by X-ray Diffraction of the ASTM, the American Crystallographic Society and, in Britain, the Institute of Physics, through which the Cardiff work was administered. The Viriamu Jones



Arthur J. C. Wilson (1914-1995)

Laboratory soon became the main centre in the UK for collecting data for the PDF, in those days by means of a Debye-Schemer camera, and for editing data submitted by other laboratories in Britain. Beti E. Lewis was employed to carry out this work from 1947 until she retired in 1975, some five years after the Joint Committee on Powder Diffraction Standards (JCPDS) had been formed to manage and distribute the PDF.

Wilson's abiding interest in powder diffraction originated while working at Cambridge, but prior to that he had developed a life-long friendship with Bill Parrish when both were post-graduate students with Bertram E. Warren at MIT. From this association stemmed their joint work on diffractometry; indeed, Parrish and Wilson were the pioneers of the modem powder diffractometer, Parrish being responsible for its design and characterisation, while Wilson developed the theory of diffractometry and other aspects of powder diffraction. In the late 1940s, after a visit to Parrish at the Philips Research Laboratory in New York, he brought a device to Cardiff which may well have become the first counter diffractometer in the UK. This was a special goniometer developed by Parrish during the War for routine determination of the orientation of quartz oscillator crystals and it was adapted by the department's workshop to serve as a rudimentary powder diffractometer. It was used by John N. Eastabrook, whose thesis, submitted in 1955, was entitled 'Construction and Applications of a Geiger-Counter X-ray Spectrometer'. This work resulted in the publication during the 1950s of a number of papers on various aspects of powder diffractometry, the first of many from the Viriamu Jones Laboratory. Following this early

success, Wilson received support from the Joint Committee to continue development of diffractometry. A commercial vertical-circle diffractometer, again designed by Parrish, was purchased and funds were provided for a succession of Research Assistants - E. Roy Pike (1954/58), later a Fellow of the Royal Society and Clerk Maxwell Professor of Theoretical Physics at King's College, London, Brian W. Delf (1957/1961: MBE 1995), who joined the lecturing staff at Cardiff and J. Ian Langford (1961/66), who subsequently went with Wilson to Birmingham. The first and last of these were principally concerned with the design and construction of a system for programmed control of the diffractometer and for the storage of data on paper tape, the forerunner of the modem Automatic Powder Diffractometer (APD). This resulted in a dramatic increase in the quantity of diffraction data obtained, together with an improvement in quality. All three RAs contributed to the theory and practice of powder diffraction and to the practical implementation of Wilson's use of statistical concepts for a precise determination of the positions and breadths of diffraction line profiles. This work, together with Wilson's own contribution, was published in *The Mathematical Theory of X-ray Diffractometry* in 1963, a companion volume to Parrish's *X-ray Analysis Papers* (1965). Together with H. P. Rooksby and H. S. Peiser, he was editor of *X-ray Diffraction by Polycrystalline Materials* (1955; revised 1960) and MSc lectures he delivered at Cardiff formed the basis of *Elements of X-ray Crystallography* (1970). Thus, over a period of twenty years and due in no small measure to support received from the Joint Committee, the Viriamu Jones Laboratory at Cardiff enjoyed a reputation as one of the principal centres of powder diffraction world-wide. In recognition of his substantial contribution to this field, and also to single-crystal diffraction, Wilson was elected a Fellow of the Royal Society in 1963.

In 1965 Wilson was appointed Professor of Crystallography in the Department of Physics at the University of Birmingham. Three years later a high precision powder diffractometer was purchased and this forms the basis of the present high resolution instrument. During his years at Birmingham he was Visiting Professor at the Georgia Institute of Technology, USA (1965, 1968 and 1971) and at the University of Tokyo (1974). He continued to represent the Institute of Physics on the Joint Committee until the mid 1980s regularly attending the Spring and Autumn meetings in Philadelphia, and in 1984 he received the Distinguished Fellow Award from the International Centre for Diffraction Data, successor to the JCPDS. UK representation on the ICDD was subsequently transferred to the British Crystallographic Association, the link being maintained through the Association's Industrial Group. He retired from his post at Birmingham in 1982 and returned to Cambridge. During his retirement he took on the chairmanship of the IUCr's Commission on *International Tables* and was appointed editor of Volume C. He and Parrish provided much of the content of this volume concerned with powder diffraction, as they had for the earlier Volume I1 (1959) which it replaced. At the time of his death, Wilson had in fact been putting the finishing touches to a further revision of Volume C.

Although Wilson's contribution to the field of powder diffraction is more than most of us achieve in a lifetime, he was equally active in other areas of crystallography. Starting with his seminal 1942 paper in *Nature* on deriving absolute from relative X-ray intensities, he published numerous papers based on the statistical properties of weighted reciprocal lattices and he had a leading role in the affairs of the IUCr since its inception. Dr Sidney Abrahams gives a full account of these aspects of Wilson's career in his 80th birthday tribute *[Acta Cryst.* (1994). A50,655-6571.

Ian Langford

CHAIRMAN'S MESSAGE

A major CPD activity during the six months since the last Newsletter was the Business Meeting held immediately after the EPDIC-IV Meeting in Chester. As usual, this was a full day affair with plenty of important matters to be discussed. Some examples of the items discussed and the agreed outcomes are as follows:

(i) Confirmation of generous IUCr sponsorship for four powder diffraction meetings that were supported by the CPD over the last few months - EPDIC-IV in Chester, Size/Strain '95 in Liptovsky Mikulas, Rietveld Summer School in Moscow, and the Oxford Meeting on structure solution from powder data.

(ii) Continuation of the collaboration between the CPD and Dr Syb Gorter on updating and maintaining the World Directory of Powder Diffraction Programs, and exploring ways in which this system might be made available on the network. [Responsibility Deane Smith and Syb Gorter.]

(iii) Negotiation with the IUCr on the possibility of

Members of the CPD at the Business Meeting in Chester.

presenting future issues of this Newsletter as part of the IUCr's Home Page on the World Wide Web.

(iv) Initiation of a search for a standard material for use in Rietveld refinement, and further analysis of the boundaries of accuracy and precision in this method. [Responsibility - Dave Cox and Lynne McCusker.]

(v) Initiation of a new round robin study of quantitative phase analysis using diffraction pattern analysis, as well as other methods of determination. [This new study is being organised by Deane Smith and Rod Hill and we welcome your expressions of interest.]

(vi) Confirmation of the CPD-sponsored Microsymposium on powder diffraction at the Seattle IUCr Congress and General Assembly - Powder Diffraction, An Update.

(vi) Confirmation of the CPD's involvement in the organisation of four technical sessions at the Denver satellite meeting of the Seattle Congress. These are: Phase quantification, Diffraction peak profile analysis, Developments in detectors and other X-ray instrumentation, and Precision and accuracy in structure refinement from powder data.

In summary, it has been another active half-year for the CPD. I encourage you all to contribute articles for the CPD Newsletter, to make its existence known to your colleagues, and to write to me or any other CPD member with your suggestions for CPD projects, activities or meetings.

With best wishes, Rod Hill

CALL FOR CONTRIBUTIONS TO THE NEXT CPD NEWSLETTER

The next issue of the CPD Newsletter will be edited by Dr JAROSLAV FIALA to appear in April of 1996. He would greatly appreciate contributions from readers on matters of interest to the powder diffraction community, e.g meeting reports, future meetings, developments in instruments, techniques and computer programs and news of general interest. Please send articles and suggestions directly to him (the address is shown on page 12).

H. Toraya, Editor, CPD Newsletter 15

Current Powder Diffraction Research using Synchrotron Radiation at the Photon Factory

The Photon Factory (PF) is a dedicated synchrotron radiation facility at the National Laboratory for High Energy Physics in Tsukuba, Japan. It is located at a distance of about 60 km north-east of Tokyo. The storage ring has a circumference of 187 m, circulating usually positrons with an energy of 2.5 GeV through the 28 bending magnets and several insertion devices. The purpose of this report is to introduce the current research activities in powder diffraction at the PF to the readers of this CPD Newsletter. It will cover four topics: 1) a new powder diffractometer with a multiple-detector system (MDS), 2) the use of imaging plates (IP) for the analysis of electron density distribution by the maximum entropy method **(MEM),** 3) activities at the Australian beamline with the multi-purpose diffractometer BIGDIFF, and 4) high pressure experiments.

New Station and Diffractometer with MDS

Beamline 4B was previously shared by a powder diffractometer called PFPD and an IP camera for single crystals of sub-micron size. Until quite recently, the users of PFPD had to replace a heavy machine (2 tons!) by pushing a man-powered forklift when the camera was used before their experiment. However, they will soon be relieved from this heavy work, since during the past summer, the beamline was reconstructed to divide station 4B into two hutches, 4B1 and 4B2. The former is used for the single crystal camera and the latter for the powder diffractometer, although they are still situated on one beamline. When powder diffraction experiments are conducted, the camera is moved to one side by sliding it on rails in order to allow the beam to pass through. The optical elements for the 4B2 station are a bending magnet light source, a water-cooled double-crystal Si (111) monochromator at a distance of 17 m, and a Rh-coated Si mirror (18 m) for focussing the beam in the horizontal direction at the sample position (29.5 m). A monochromatic beam with wavelengths between 0.62 and 2.28, will be obtained without any change in the beam position. The new hutch 4B2 has enough space for a powder diffractometer to be installed.

A new powder diffractometer has been constructed by our group for structural studies with high-resolution powder diffraction data (Fig. 1). The basic concepts adopted in designing the diffractometer include flat-specimen reflection geometry and the use of a crystal analyzer for diffraction scans. The flat specimen is advantageous for accurate measurements of angular positions and intensities, high counting rates and good particle statistics, and the crystal analyzer for high angular resolution and good signal-to-noise ratio. A wide range of angular resolution can be obtained with different analyzer crystals. Application to thin-film diffraction measurements is another aspect of the proposed research. A novel feature of this diffractometer is that a multiple-detector system (MDS) has been adopted for rapid scanning of the entire powder pattern. The MDS has five detector arms, which are attached radially at intervals of 25º on the 2θ axis of the goniometer. Five scintillation counters, each coupled with a flat Ge (111) crystal analyzer on the respective arms can record simultaneously the whole pattern divided into five segments with a single 2θ scan. An asymmetric 2θ scan technique is used for data collection at a fixed incident angle of the beam on the specimen. The MDS will reduce the scan time to roughly one-fifth, and users can expect to avoid the unduly long scan times required with a conventional single-arm diffractometer. Test

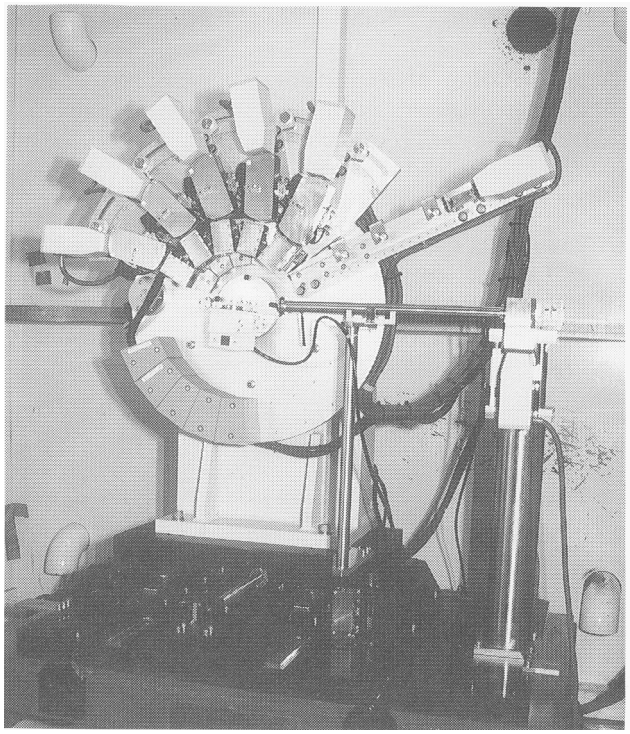


Fig. 1. Powder diffractometer with the MDS.

operations conducted at the old 4B station in May of 1995 demonstrated that only four hours were required to scan the whole powder pattern (28 range = 130'') of Mg_2SiO_4 at a step interval of 0.004''. It may be also noted that only 20 to 30 minutes were needed for alignment of one MDS arm, which includes the tuning of the Bragg angle of the analyzer crystal, the 28-zero position, and the high-voltage/pulse-height-analyzer. Because the instrument is installed at a general user beam-line, a sixth single-detector arm for multi-purpose use is also available. Various kinds of analyzers, such as flat or channel-cut crystals, long horizontal parallel slits with divergences of 0.033 and 0.065°, receiving slits and solid state detectors, can be mounted on this arm for θ-2θ, 2θ, and 8 scans. Station 4B2 will be in full operation from 1996. Software for processing the data obtained with the MDS is now under development.

H. Toraya (Nagoya Institute of Technology)

Imaging Plates and the Maximum Entropy Method

X-ray powder diffraction is an excellent technique for the determination of accurate structure factors for crystalline materials, particularly in the low-angle region. In order to construct real-space images from diffraction data by the maximum entropy method (MEM), it is essential to have accurate and reliable values of the structure factors for the low-Q region where strong Bragg reflections are observed in many materials. Therefore, it is reasonable to conclude that the X-ray powder method is suitable for application of the MEM to the analysis of experimental diffraction data. The biggest disadvantage of powder diffraction is obviously the peak overlap, but by utilizing a synchrotron radiation (SR) source and sophisticated software for profile decomposition, this disadvantage may be overcome to some extent.

In our research group, a series of investigations has been undertaken to produce real-space images of charge density distributions in crystalline materials by MEM analysis. Most of the data analyzed in this way are powder data, either X-ray or neutron. In the X-ray case, as mentioned above, a SR x-ray source has the big advantage over laboratory sources of both much higher resolution and intensity. In order to have reliable data, it is important to collect the data with good counting statistics. In the laboratory, it is not unusual to spend about a week (24 hours operation a day) using an x-ray generator with rotating anode to collect a suitable set of data. At the PF, typically about 20 hours are needed for a step scan in the single-counter mode. Since injection of positrons into the storage ring normally takes place every 24 hours, one set of data can be collected during a given injection, thus avoiding any ambiguities which might result from data obtained in different injection cycles. In the high-angle region, the counting statistics may not be adequate in many cases but it is not practical to allocate more machine time for a single sample.

Valuable machine time can be reduced by a factor of 10 when an imaging plate (IP) is used as a detector. In order to collect whole powder patterns simultaneously in this way, cylindrical specimen are used in Debye-Scherrer geometry. Therefore, this experiment is particularly appropriate for samples composed of relatively light elements unless it is possible to use a very short wavelength, e.g 0.5A. This method can be regarded as complementary to conventional flat-plate reflection geometry, which may not be suitable for samples containing light elements only.

Actual examples of real-space imaging of diffraction data obtained from powder specimens are now gradually increasing. Early investigations were made mostly on simple compounds such as CeO_2[1], TiO_2[2], and simple metals such as Be[3] and Mg[4], but the technique has now been extended to more complicated and topically important subtances such as high T_c superconductors[5] and fullerene compounds[6]). As an example, the electron density distribution in the metallofullerence, $Y@C_{82}$, obtained by the MEM is shown in Fig. 2.

It is possible to further extend the MEM analysis to electron and nuclear distribution; indeed, Bader topological analysis for charge densities[7]) and anharmonic analysis for nuclear densities[8]) have already been made in the case of Be single crystal data. Such analyses may represent one of the future trends of modem crystallography.

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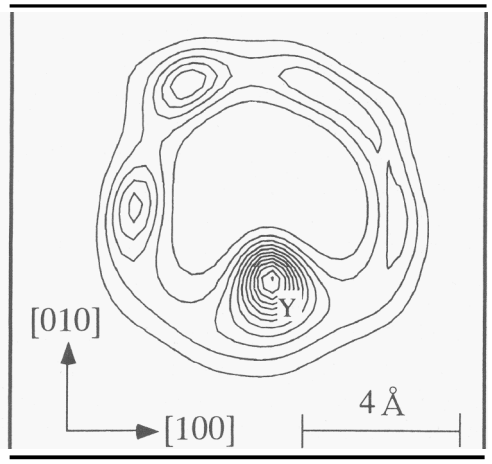

Fig. 2. The charge density distribution in $Y@C_{82}$ obtained by MEM analysis.

Makoto Sakata (Nagoya Univ.)

Australian Beamline with BIGDIFF

Beamline 20B at the Photon Factory is currently operated as the Australian National Beamline Facility (ANBF). The instrument installed there is a high-precision, multi-purpose X-ray diffractometer capable of operating in vacuum. Experimental modes which can be configured include (i) high-resolution powder diffraction, (ii) protein crystallography, (iii) XAFS, (iv) tomography and (iv) topography. This report describes some of the recent work done at the ANBF in the field of powder diffraction.

In the powder diffraction mode, the ANBF instrument can collect data from both flat plate and capillary samples utilising a conventional scintillation counter as well as imaging plates. The image plates allow the collection of a wide angular range of data (±160° **20)** in times as short as a few minutes. The installation of a moving cassette further enhances the capabilities of the instrument for time resolved studies.

A number of workers (Madsen & Bamea, O'Connor et al., Kennedy et al., Sabine et al.) have worked on defining the characteristics of the instrument, including measurement of the width and shape of diffracted peak widths, and variation of diffracted peak position and intensity from theoretical values. Results of this work show that instrumental peak widths of 0.03 to 0.04'' **28** can be obtained routinely with both counter and image plate configuration. This bodes well for the collection of rapid, high-resolution data at ANBF.

B. J. Kennedy and co-workers have carried out Rietveld type refinements of the structures of a number of metal oxides both to assist in the commissioning of the diffractometer and as part of a wider research program. Highlights of this work have included very precise and accurate structural studies of the primitive cubic structures $Bi_3Sb_3MO_{11}$, M = Ga, A1 where the data were collected over 160'' range with incident wavelength of 1Å and the identification of oxygen vacancy ordering in the defect pyrochlores $Pb_2M_2O_{6.5}$.

B.J. Kennedy and C.J. Howard carried out a series of measurements using both flat plate and capillary samples of the pyrochlore $Y_2Sn_2O_7$. The former data have been utilised in a MEM electron density distribution analysis by M. Takata and co-workers (University of Nagoya) to reveal details of the bonding in this material.

E. R. Vance has utilised the facilities at 20B for both high resolution powder diffraction and XANES studies of SYNROC materials including studies of both cubic and tetragonal $BaTiO_3$. A feature of the instrumentation available at the ANBF is the ease with which experimental modes can be changed.

T.M. Sabine carried out extensive measurements on a sample of rutile, TiO_2 in order to fully characterise the performance of the powder diffractometer utilising imaging plates as the detector. Using data collected over a range of wavelengths (0.62 - 1.90Å) an algorithm for the correction of absorption to high μR values has been developed and in collaboration with Dr Brett Hunter (ANSTO) has been implemented into a PC version of the Rietveld program LHPM. This program has been further modified to enable simultaneous refinement of a number of data sets; this is essential since 4 image plates are used to span the 160º angular range.

J. W. White and P. Reynolds have been active in a number of studies including that of ammonia doped Rb_3C_{60} which combined x-ray and neutron powder diffraction studies have shown to disproportionate to RbC_{60} and the new phase $Rb_4C_{60}(ND_3)_2$, highly crystalline samples of the mesoporous zeolite material MCM-41, the nature of alkane adsorption on graphite surfaces, and a molecular cluster of 12 manganese atoms linked by acetate and 0X0 bridges.

The collection of in-situ data to observe the crystallisation of gibbsite $Al(OH)_3$ has been a feature of the work of A. Gearson and J. Counter. They have designed and constructed a cell which allows a liquor of caustic soda and aluminium metal to be continuously pumped at a temperature of 65°C. Under these conditions, the aluminium is converted to gibbsite over a period of about 10 hours. The use of image plates allowed rapid data collection times and continouous monitoring of the conversion process. Understanding of the mechanism of crystallisation of gibbsite and its impact on the extraction of aluminium from bauxite ores is especially relevant to the Australian mining industry.

ANBF has also been used to investigate the use of glass capillaries to focus the incident X-ray beam from about l00μm down to spots of 5 to 50 μm in diameter. The use of total internal reflection provides an increase in beam intensity of 12 times (at 50μm) to 25 times (at 30μm). High resolution XRF data have been obtained from steel and ceramic materials, but future work could be extended to the development of phase mapping using micro-diffraction techniques (Balaic & Barnea).

Information for this report has been obtained from Experimental Reports - Access to Major Research Facilities Program - July 1993 to June 1994.

Ian Madsen **(CSIRO)** and Brendan Kennedy (Univ. Sydney)

High Pressure Experiments

There are two kinds of high pressure apparatus for diffraction studies at the PF; one is the multi-anvil-type apparatus named MAX80, and the other is a diamond-anvil cell (DAC). MAX80 was installed at the PF in 1983 and subsequently moved to the Accumulation Ring (AR) where X-ray energies of up to 150 keV can be utilized'). Using sintered diamond anvils, many studies in the fields of physics, chemistry, materials science, earth sciences etc. have been performed in pressure and temperature ranges up to 20 GPa and 2000°C. A DAC was combined with an imaging plate (IP) for the first time at the PF in 1987[2], and since then techniques for obtaining reliable intensity data have been developed. These data are used for Rietveld refinement and the analysis of electron density distributions by the maximum entropy method. The following are typical experimental results which are of interest from a crystallographic point of view.

Many MX type compounds with the NaC1-type structure (B1) are known to transform to a CsC1-type structure (B2) under high pressure, and there has been much discussion about the nature of the transition mechanism in terms of reconstructive and displacive schemes. Recently, AgCl was found to show successive phase transitions under pressure, which suggests that the transition mechanism is of the latter type[3]. Experiments were performed using MAX80 at the AR in the energy-dispcrsive mode in the pressure and temperature ranges of 18 GPa and 500°C. The first transiton from the B1 phase (LPP) took place at 7.5 GPa and another transition at 9.0 GPa at room temperature. The high pressure phase I (HFPI) was suggested to have the KOH-type structure ($P2_1$), in which the coordination numbers for both Ag+ and C1- are 6+1. The high pressure phase II (HPPII) was found to have thc TII-type structure *(Cmcm)*, in which the coordination number is 7 for both Ag+ and Cl-. A high pressure phase HPPIII with the B2 structure was found at 13.5 GPa and 500°C. The phase boundaries were positive for LPP to HPPI, tcmperature independent for HPPI to HPPII, and negative for HPPI to HPPIII. The crystal structures of the LPP, HPPI, HPPII and HPPIII phases are shown in Fig. 3. They can be represented by a common monoclinic cell, which is just the unit cell of KOH itself (Fig. 3). From changes of the unit-cell dimensions versus pressure, the LPP-HPPI-HPPII-HPPIII transitions can be considered to be consecutive phenomena. Fig. 3 also shows a simple mechanism for the NaCI-CsCl type transition under high pressure. In this process, the [100] and [011] directions of the B1 and B2 structures are interchanged. It is noteworthy that this relation is the same as that found in the B1-B2 transition induced by temperature.

Trivalent lanthanides are known to show a common crystal structure sequence hcp → Sm-type → dhcp → fcc as a function of incrcasing pressure. This sequence is generally accepted to be the result of an increase in electron transfer from s to *d* bands with pressure. Reports of a second-order like transition of La and Pr based on resistivity measurements were followed by an x-ray diffraction study of a new high pressure phase having a distorted structure. Recent systematic investigations revealed that this distorted structure is quite common as a *fifth* structure for lanthanides, and rhombohedral crystal structures *(R3m)* were successfully determined for Pr, La and Nd[4]. These diffraction data were collected at BL-6B with a combination of DAC and IP, and analyzed by the Rietveld method. The transition from fcc to rhombohedral structures took place continuously for each of the three elements. The distortion of the fcc lattice could be explained in terms of the amplitudes of the atomic displacements derived from a linear combination of three TA phonon modes with equal amplitudes and wave vectors at the L point of the Brillouin zone of the fcc lattice. This interpretation is consistent with the fact that the unit-cell volume of the rhombohedral phase is eight times larger than that of the undistorted fcc phase. These facts imply that the fcc-rhombohedral phase transition is associated with the softening of the TA phonon mode at the L point of the Brillouin zone. The same pressure dependence for the static atomic displacements has been found for La and Nd.

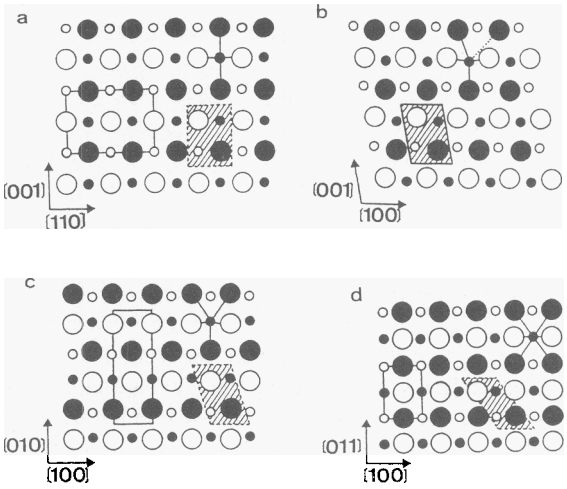

Fig. 3. The crystal structure of the (a) LPP (b) HPPI (c) HPPII and (d) HPPIII phases. Small and large circles denote Ag+ and C1-, respectively. Open and solid circles indicate the different layers. Solid lines show the unit cells, and hatched parallelograms represent the corresponding monoclinic unit cell for the KOH structure.

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Osamu Shimomura **(Photon** Factory, **KEK)**

MAILING LIST FOR NEWSLETTRS

If you would like to be added to the mailing list for the Commission on Powder Diffraction, or you have changed your address, please contact the CPD Secretary, Dr Daniel Louer at the address shown on page 12.

MEETING REPORTS

EPDIC IV, Chester, UK, July 10-14th

The Fourth European Powder Diffraction Conference was held July 10-14th at Chester College in Chester, a very attractive and well-preserved city which dates back to Roman times (and has an abundance of fine pubs, a fact which did not go unnoticed by many participants!). The meeting was organized by the Daresbury Laboratory and a local committee chaired by Bob Cemik assisted by several of his Daresbury colleagues, who did an admirable job of keeping events running smoothly and efficiently (including the unexpected task of chartering a bus at short notice on the last day when British Railways were paralyzed by a strike). Substantial and much-appreciated sponsorship was provided by the IUCr via the Commission on Powder Diffraction, the British Crystallographic Association, and several industrial companies, especially Philips, Siemens and Seifert. The meeting attracted about 350 participants from 33 different countries, including eight of the ten members of that august body known affectionately as the CPD. The social program included a reception held at the Town Hall, hosted by the Lord Mayor of Chester resplendent with his traditional silver chain of office, a conference dinner and trips to nearby places of interest.

Acknowledging the fact that powder diffraction nowadays covers an extremely wide field, the program committee singled out three broad themes for the major non-parallel oral sessions: structure solution and refinement, dynamic studies, and industrial applications. Thirteen invited lectures were presented in these sessions, which were followed later in the day by three parallel oral sessions involving a total of 57 talks drawn from contributed papers in more specialized categories: non-ambient studies, microstructure and quantitative analysis, data analysis, dynamic studies, texture and preferred orientation, magnetic materials, residual stress, minerals, disordered systems and microporous materials. The rcmainder of the contributed papers (about 180 in all) were displayed in poster sessions in the early afternoon, in close juxtaposition to the commercial exhibits, allowing participants easy access to both events.

The main conference was preceded on July 10th by an open meeting of the Collaborative Computational Project in powder diffraction (CCP14), which has the goal of developing and making available an integrated suite of programs for the powder diffraction community, ranging through analysis of samples, peak-fitting of raw data, indexing and structure solution, and graphical display. This is an ambitious and very worthwhile project which should be publicized as widely as possible, and about 100 participants took advantage of the meeting to hear talks by A. Holland (Daresbury), C. Giacovazzo (U. of Bari), K. Harris (University College, London) and J. Cockcroft (Birkbeck College, London), take part in a hands-on demonstration and generally find out more about the current status of the project.

The conference started on a sad note with the announcement of the recent death of Professor A. J. C. Wilson, one of the stalwarts of powder diffraction for many decades and the author of a book on its mathematical aspects which is still a foundation of the field. The next item was a much happier one: the presentation of the ICDD Distinguished Fellow Award to Professor P. M. de Wolf for lifetime achievements in powder diffraction, followed by the presentation of the Philips EPDIC Award honoring an outstanding accomplishment by a young scientist to L. Petras (Vienna) for his work on developing a high-temperature x-ray furnace with very precise temperature control.

The first major session of invited lectures was centered

Bob Cernik and Tom Ryan in conversations at the conference dinner in Tatton Park.

Prof. P. M. de Wolf with the ICDD distinguished fellow award presented during EPDIC IV.

around structure solution and refinement and provided an eclectic menu. R. von Dreele (Los Alamos) spoke about the determination of orientational distribution functions from multiple time-of-flight neutron data sets, M. Rodriguez-Carvajal (Saclay) discussed systematic errors and structural complexity in Rietveld refinement (a matter of increasing concern as the number of refined parameters continues to set new records), P. Attfield (Cambridge) described the application of resonant synchrotron x-ray powder techniques, M. Harding (Liverpool) dealt with structure determination from very small single crystals (bravely suggesting that such methods might even replace powder diffraction one day!), and C. R. Catlow (Royal Institution) reviewed the rapidly advancing field of computational techniques for modelling structures. The second main session was devoted to dynamic studies utilizing respectively conventional laboratory X-rays, synchrotron X-rays and neutrons. P. Benard (Rennes) spoke about the thermal decomposition of unstable compounds such as nitrates, A. Ryan (Manchester) described techniques for collecting simultaneously both small-angle and wide-angle x-ray patterns during the melting and crystallization of the polymer polypropylene, and J. Pannetier (Institut Laue-Langevin) discussed electrochemical insertion reactions in battery materials, a currently important environmental topic. In the final major session, some more applied aspects of powder diffraction with technological and industrial implications were covered. P. Webster (Salford) reviewed x-ray and neutron techniques used for the measurement of strain, J. van Berkum (Delft) described the development of a strain-field model and the corresponding simulation of line profiles, H. Göbel (Siemens) gave an account of graded multilayer optics developed for conventional laboratory x-ray equipment which can be used to give parallel or highly-focused beams and greatly extend the range of possible experiments, P. Fewster (Philips) discussed some applications of high-resolution powder diffraction on a laboratory diffractometer equipped with a four-crystal monochromator, and T. C. Huang (IBM Almaden) described the characterization of iron-oxide films used for magnetic recording by grazing-incidence laboratory and synchrotron x-ray techniques.

Overall, both the main and parallel oral sessions were of a high standard and provided a topical and informative view of the current state-of-the art in the various fields. A survey of the contributed papers revealed a strong emphasis on structural characterization, with structure solution or refinement accounting for about *35%*, and 'non-ambient' studies 20% (phase transitions and equilibria, reaction kinetics, dynamic and high-pressure studies). Roughly 15% dealt with microstructure and related topics (line-shape analysis, texture and preferred orientation, residual stress), 10% with thin films, 10% with instrumentation, *5%* with quantitative analysis and *5%* with data analysis. Another interesting statistic was the relatively large proportion of papers in which synchrotron or neutron diffraction techniques were used; about 17% and 10% respectively, indicative of a steady growth in the user community at major facilities of these types.

Some personal observations are as follows: the increasing emphasis on the *ab-initio* solution of quite complex structures (up to 50 positional parameters with laboratory diffractometers, 100 or so with current synchrotron instruments and conceivably many more at third-generation sources), not only in the 'traditional' areas of materials science but also for organic molecules of pharmaceutical interest. High-resolution neutron diffraction has benefitted from recent advances in monochromator fabrication and will undoubtedly play an important complementary role in these structural studies. However, more attention will need to be given to improved accuracy in data collection (at the 2% level?), better peak-shape models (anisotropy, asymmetry), better goodness-of-fit criteria, and improved techniques for structure solution and refinement (maximum entropy methods?). "on-ambient' structural studies are becoming increasingly important and sophisticated, examples being the characterization of phase transitions involving extremely subtle changes in symmetry, and precise structure determination at high pressure in diamond-anvil cells. Residual stress has become an important area with many technogical applications, as rcflected by the steady growth of dedicated instruments at many neutron centers throughout the world. High-energy synchrotron X-rays may well have an increasing role in this area. There has also been considerable progress in the application of grazing-incidence techniques to the study of thin films, which will surely accelerate with the ready availability of parallel-beam optics for laboratory diffractometers.

The last event in the program was the conference dinner at one of England's stately homes, Tatton Park, where part of the very successful TV series 'Brideshead Revisited' was filmed. Dining in the great hall (watched over by a huge collection of animal trophies shot in Africa by one of the family ancestors in an era when such activities were not politically incorrect) provided a memorable finale to EPDIC IV!

Dave Cox

Structure Determination from Powder Data, Oxford, UK, July 16-20th

Structure determination from powder data has been carried out since the early days of crystallography.The method was a combination of logical arguments and trial and error. Today, through the advances of computers and programmes, very powerful methods are available to solve a crystal structure *ab-initio* from powder data. A workshop to show the state of the art was organised at Wadham College, Oxford by Bill David and Kenneth Shankland with a never failing support from the staff at the Rutherford-Appleton Laboratory.

During four long and well-planned days about 120 participants from 21 different countries were guided from sample preparation, indexing and powder pattern decomposition to Bayesian statistics and direct methods.

The mornings were devoted to common lectures and the afternoons to demonstrations and discussions in smaller groups. The lecturers were competent and enthusiastic which can be illustrated with a few quotations from the lectures: 'Recovering maximum information in the overlapping lines is a central problem in *ab-initio* structure determination' (D. Louer in 'Laboratory X-rays and structure determination'), 'Probability is nothing but common sense reduced to calculation' (D.S. Sivia in 'Intensity Extraction'), 'Everything should be made as simple as possible but not simpler' (G. Bricogne in 'Baysian Approach to Structure Solution') and 'It is nothing better than an experiment to find out how it really is' (L.B. McCusker in 'Chemical Intuition').

The nice and pleasant atmosphere of Wadham College and social events like a dinner in Lane Barns and a concert of 18th century music in Holywell Music Room contributed to the great success of the workshop.

Roland Tellgren

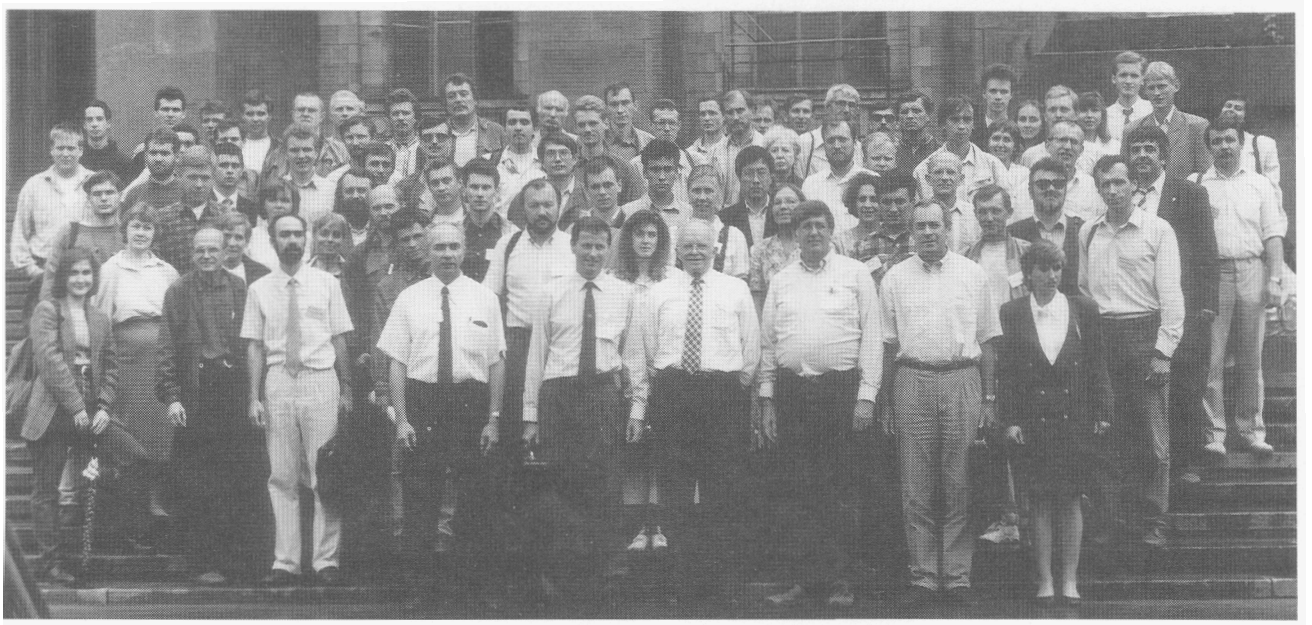
Rietveld Summer School (RSS95-RS), Moscow, Russia, July 20-22th

The fifth Summer School on the Rietveld Method to be co-organized by the IUCr's Commission on Powder Diffraction was held in Moscow on 20-22 July 1995 at the Moscow State University. There were 86 registered students from 10 countries (Germany, France, The Netherlands, the U.K., Bulgaria, Latvia, Ukraine, Byelorussia, Russia, and the U.S.A.). The format was, as before, lectures in the mornings, hands-on experience with the method on PC computers in the afternoons, and additional availability of the 37 computers in the evenings for students who wanted to extend their computing time. Many did.

Student interest remained high throughout. The ages of the students ranged from 19 years to 60+. Many of the 'students' had substantial experience with single-crystal crystallography. Some of the students had experience with the Rietveld method, including programming for it, though not much with the programs used. Others had none. The prepared computer exercises were based on the two most widely distributed Rietveld refinement programs, DBWS and GSAS (which has just become avairable in a PC version). The students were asked to concentrate on just one choice of program, but many found they had enough prior experience to benefit from trying out both programs.

As in the previous RSS's, the three main lecturers were **A.** K. Cheetham, R. B. Von Dreele and R. A. Young. Dr Vladimir Chernyshev, of Moscow State University, provided needed language balance with a lecture in Russian about considerations in writing computer programs for the Rietveld method. All four lecturers also served as very busy guides and tutors throughout the computer sessions.

To enable more persons to participate, the registration fee was kept very low *($5)* and low-cost housing was arranged. The low registration fee was certainly appreciated by many attendees. Partially offseting that appreciation was the fact that the low fee and the high cost of photocopying made it impossible to supply each student with a photocopy of the manual (User's Guides) for each of the two Rietveld programs offered (DBWS-9411 and GSAS) and the monograph of 'Using the Rietveld Method' written for use in such schools. Nonetheless, the students did seem to get a lot out of the course, as was evidenced by their concentrated attention to the lectures and their diligence in the computer sessions. We will see from the literature and meeting reports during the next few years whether, as has been the case with the previous RSS's, RSS95-RS has actually provided the expected stimulus to productive use of the Rietveld method in Russian and other countries from which the students came.



Participants in the RSS95-RS.

The organizing Committee, under the able and very active chairmanship of Prof. L. A. Aslanov (Chemistry Department, Moscow State University), did a phenomenal job of arranging the needed confluence of space, computers, housing, meals, and supporting services under difficult circumstances.

RSS95-RS was organized by the IUCR Commissions on Powder Diffraction and on Crystallographic Teaching, the European Universities Association, Moscow State University, the Frank Laboratory of Neutron Physics (Dubna), and the St.-Petersburg Institute of Nuclear Physics, Gatchina.

Sponsorship with money or 'in kind' contributions, or both, was given by the International Union of Crystallography (general expenses and Young Scientist grants), the Russian Fund for Fundamental Investigations, the Netherlands Organization for Scientific Research, Nonius B.V. (including some Young Scientist grants), the Frank Laboratory of Neutron Physics, and the Moscow State University.

As is now an RSS custom, in the closing ceremony Tony Cheetham spoke breifly on behalf of the three main lecturers expressing their thanks and appreciation of a job well done by the organizers and of the diligence of the students .... in the language of the host country. This always amazes and amuses the audience because Tony's pronounciation and intonation are excellent: the jokes also come across well, even though he had never spoken the language before arriving at the RSS. He attributes his sucess with these talks to his dedication to the RSS program. We also note that the young women he always chooses to help him prepare these talks are both native speakers of the language and participants in the RSS.

R. A. **Young with L.** A. Aslanov

Denver X-ray Conference, Colorado Springs, USA, July 31-August 4th

The 44th annual Denver Conference on Applications of X-ray Analysis was held in Colorado Springs, Colorado 31 July to 4 August. There were 386 attendees for the two days of workshops and three days of technical sessions on both diffraction and fluorescence analysis. The meeting was one of many that recognized the 100th anniversary of the discovery of X-rays.

The Charles S. Barrett award in X-ray Diffraction was presented to Paul K. Predecki for his many activities in the measurement of physical properties of bulk materials as well as his leadership of the Denver Conference for over ten years.

The highlight of the meeting was the plenary session which was devoted to a historical review of X-ray analysis including topics on the early development of instrumentation 1950 - 1970 by Dr J. L. de Vries. Other topics included later instrumentation, software from 1950 to present, development of X-ray fluorescence, and a general history of analytical techniques for diffraction analysis. The afternoon was the Ben Post Commerative Session where the manufacturers also described early developments in instrumentation including how and why some companies entered the business of X-ray instrumentation. One interesting revelation was the request of Rontgen to Siemens for a discount on some manufactured tubes because he thought the price was too high.

Other sessions at the meeting included: Developments in the analysis of powder diffraction data: Stress and strain determination by diffraction methods: Conditioning of X-ray beams: Characterization of amorphous materials; Polymer applications; Characterization of thin films, XRD and XRF: Developments in X-ray instrumentation; XRF Quantitative data interpretation, and Unusual applications, XRD and XRF. There were also 29 posters on XRF topics and 41 posters on XRD topics.

The next Denver Conference will be a joint meeting with the Commission on Powder Diffraction scheduled for Denver, Colorado 3-8 August 1996.

Deane K. Smith

X-ray Powder Diffraction Analysis of the Real Structure of Matter Liptovsky Mikulas, Slovakia, August 21 - 25th

The conference was organized by the Commission on Powder Diffraction of the IUCr jointly with the Czech and Slovak Cryst. Assoc. and the Military Academy of Liptovsky Mikulas in Eastern Slovakia. P. Sutta chaired the local committee and R. L. Snyder was the program chairman assisted by J. Fiala and others. It was an international meeting for people working in the field of powder diffraction who are interested in the problems of the real structure of materials (size, strain and texture).

There were 25 invited lectures, 11 short oral contributions, and 81 posters presented at the conference covering the whole range of real structure analysis by X-ray and neutron diffraction. The scientific program was complemented by commercial exhibitions and software presentations.

Invited lecturers agreed to prepare texts based on their presentations which will be organized into an authoritative book on powder diffraction. R. L. Snyder, H. J. Bunge and J. Fiala will serve as Editors. This book will be aimed to serve as a comprehensive tutorial and reference work on microstructure analysis by diffraction techniques for crystallographcrs and materials scientists.

The conference accommodated also a meeting of participants of the international round-robin test on crystallite size and microstrain determination organized jointly by the JCPDS-International Centre for Diffraction Data and the Commission on Powder Diffraction. The results of nine laboratories (U.S.A., Netherlands, Germany, France and Israel) which measured the samples of glass ceramics supplied by R. L. Snyder were

Participants in Size/Strain '95 at the Military Academy, Liptovsky Mikulas, Slovakia

evaluated, and future plans of this project were discussed.

More than 120 attendees from 23 countries enjoyed conference facilities of the Military Academy at Liptovsky Mikulas in the Carpathian Mountains-An active social program, organized by the local committee, included a concert of local folk music, a visit to a major limestone cave, and an excursion to local antiquities and the Tatry Mountains. The abstracts of all contributions were published as a special issue of the journal 'Materials structures in Chemistry, Biology, Physics and Technology', Vol.2, No.1 (1995) (79 pages, 288 authors) which was supplied to all participants at registration.

P. Sutta and J. Fiala

WHAT'S ON

22-24 November 1995
Second Conference of the Asian Crystallographic Association (AsCA'95), Bagkok, Thailand. Contact: Prof. Y. Ohashi, Dept. of Chemistry, Tokyo Institute of Technology, Ohokayama, Tokyo 152, Japan, FAX +81-3-3720-6206, YOHASHI@CHEM.TITECH.AC.JP

18-25 January 1996
International School and Conference on X-ray Analytical Methods - 100 Years of X-rays, Univ. of New South Wales, Sydney, Australia. Contact: AXAA 96 Secretariat, GPO Box 128, Sydney, New South Wales, 2001 Australia. Tel. +61-2-262-2277, FAX +61-2-262-2323, LDALEY@TOURHOSTS.COM.AU

4-6 June 1996
Fourth European Conference on Residual Stresses, Cluny, France. Contact: Societe Francaise de Metallurgie et de Materiaux -SF2M-ECRS4, 1 rue Paul Cezanne, 75008 Paris, France. FAX +33-1-49-53-71-00.

3-9 August 1996
Satellite Meeting on Powder Diffraction associated with the IUCr Congress on Crystallography and Denver X-ray Conference, Denver, Colorado, USA. Contact: Prof. Paul K. Predecki, Dept. of Engineering, University of Denver, Denver, CO 80208, USA. FAX +1-303-871-4450, DENXCON@DIANA.CAIR.DU.EDU

8-17 August 1996
17th IUCr General Assembly and International Congress of Crystallography, Seattle, Washington, USA. Contact: Prof. R.F. Bryan, Dept. of Chemistry, Univ. of Virginia, Charlottesville, VA 22903, USA.

World Directory of Powder Diffraction Programs, Release 1995

The World Directory of Powder Diffraction Programs is a continuing project with the goal to identify and catalogue all the programs available for powder diffraction analysis. It is a joint project of S. Gorter of the Netherlands and D. K. Smith of the USA and is sponsored by the Commission on Powder Diffraction. The 1995 list of programs contains 670 program listings categorized into 22 areas of activity and 6 subgroups. The program listing includes information on the language, platform, distribution and cost where known. In addition there is an Appendix with the addresses of the program authors and an extensive list of references. E-mail addresses and Fax/Phone numbers are included where known. This list will continue to be maintained with the help of program authors and users. There are forms available to supply program information for additional entries for the WDPDP. All the information requested on the form should be supplied for the entry to be complete and usefull to others. The completed forms should be sent to S. Gorter to the address below. In addition to the maintenence of the WDPDP, S. Gorter operates the Program Exchange Bank where many of the programs in the WDPDP are available on request. Programs currently available by this route are indicated in the WDPDP by 'PEB' in the author column. Programs may be acquired by ftp or on some specific media. For the latter way a

charge has to be paid to cover the costs. The cost of the WDPDP95 is US$50 covering printing, mailing from the Netherlands (air mail) and currency exchange. When payment is in cash a discount of US$15 is available. Your address on file at the PEB will assure you of information on updates. An order form will be sent on request. Payment should accompany the order form. An invoice will be enclosed on delivery. Direct orders may be made at any time to the PEB.

Send orders to: Drs Ing. S. Gorter 43 van Lennepdreef, NL-2353 NJ Leiderdorp, the Netherlands Fax +31-71-274537, e-mail **GORTER-S@rulgca.LeidenUniv.nl.**

Syb Gorter and Deane K. Smith

NEWS FROM ICDD

The readers of this CPD Newsletter will be pleased to learn that in March 1995 Dr Jan W. Visser was honored as a Distinguished Fellow of ICDD in recognition of his many years of dedicated efforts on behalf of ICDD. Although retired from TNO-Delft, he continues to be active in chairing ICDD subcommittees, being a European Consultant of the Board, and representing ICDD at trade shows in Europe. At EPDIC IV in Chester, U.K., he presented Prof. Pieter M. de Wolff with a plaque commemorating Dr de Wolff's public recognition as a Distinguished Fellow of ICDD for the many starred patterns contributed by him through the Grant-in Aid program.

A meeting of the Crystal Data Management Board was held at NIST on 8 March at which John Rumble, the principal management leader of the CDIF project from NIST, had the opportunity to meet Dan Richardson. The meeting provided a good forum for ICDD and NIST to interact and discuss the future operation of CDIF. Production schedules were mutually agreed upon for EDD and CDIF. At a database conference at Gaithersburg, MD. on 29 and 30 August, the status of the various crystallographic databases was discussed: ICDD (PDF), FIZ (ICSD), NRCC (CRYSTMET), NIST (CDIF), and Cambridge File (organics).

The ICDD clinics on XRD and XFR held during June at Headquarters, were well attended and much appreciated by the participants. For the XRD sessions, 45 students were instructed by 13 teachers; for the XRF sessions there were 30 students and 10 instructors.

Dr T. C. Huang, Chairman of the Technical Committee, has mailed out a questionnaire to several members of a task group, asking 'what X-ray wavelength for copper should be used in ICDD publications?'. There will be more in the Technical Committee Newsletter, and discussion at the October meeting, but just within three ICDD products the following values for Cu$K\alpha_1$ are given: 1.5401, 1 54056, 1.54060Å, while in ***Powder Diffraction***, various authors use: 1.54051, 1.54056, 1.540598, 1.5406Å. Recommendations from CPD are hereby solicited.

Set 45 printed products are now in-house and ready for the September 1st release of new products. The Publications Dept. deserves a well done for completing this leg of production on time and within budget. Set 45 CD-ROM, the final phase of Set 45 production, is on its way to the manufacturer and is also on schedule.

Ludo Frevel (ICDD Representative)

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