COMMISSION ON POWDER DIFFRACTION

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

NEWSLETTER No. 18, JUNE 1997

ABERRATIONS IN POWDER DIFFRACTION AND THEIR CORRECTIONS.

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Aberrations

In the current use of X-ray diffraction the required instrument precision is constantly increasing. With the advent of high-speed computers, more detailed models can be worked out with high qualitative precision. As an example, the reader is referred to the work of Jurgen van Berkum in the Delft University group of Delhez, de Keijser and Mittemeijer on model-based size-strain discrimination. This in turn leads to the objective of extracting model-specific parameters from accurate experimental data. In order for this approach to be successful, a major prerequisite is that the available experimental data form a true projection of the material under study.

Raw (as-measured) X-ray diffraction data are influenced not only by noise, but also by systematic effects. Many of these effects are caused by the imperfectness of the optics in the instrument. Most importantly, the measured data will be blurred. Mathematically, the total of these effects can be written as:

$$\tilde{h}(\theta) = \int_a^b [g(\theta',\theta) f(\theta')]\ d(\theta') + n_i(\theta) + n_S(\theta) \qquad (1)$$

Here $\tilde{h}(6)$ is the measured profile, and $f(\theta)$ is the sample intrinsic profile, The kernel $g(\theta', 6)$ describes the blurring effect of the optics; the range of action of this kernel is over the interval ***[a,b].*** The second deterministic contribution $n_i(\theta)$ is due to the instrument, e.g. scattering of slits. Finally, $n_S(\theta)$ describes all other stochastic effects (statistical noise, ***etc.).***

Another source of nuisance effects is the sample it self. For example, texture renders the accurate determination of the intensities of individual reflections hardly possible. Other effects, which are sometimes hard to detect, are surface roughness and sample inhomogeneity which cause the effective absorption coefficient μ^{eff} to deviate from its actual value μ [I]. Both effects can seriously affect the intensities of the diffraction lines, as demonstrated in Fig.1. To correct for these effects is difficult, because of the dependence on many sample parameters (particle density, packing, particle size distribution).

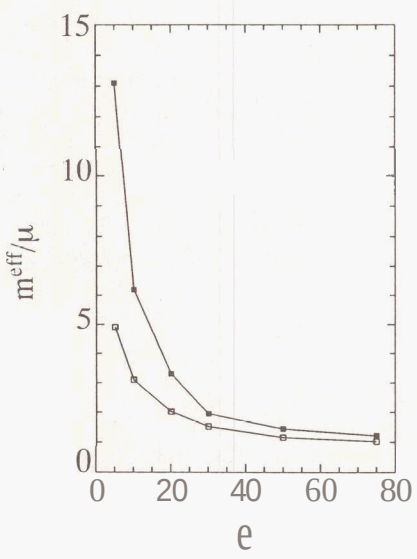

Fig. 1. μ^{eff} ***for a single component sample, as a function of incidence angle 6 (Bragg Brentano geometry). Squares are for medium, triangles for strong absorption.***

Studied already by Alexander and Wilson is the line shape affecting sample transparency. In particular, they made the observation that eq. (1) could well be approximated by a sequence of convolutions (with folding function $g_i(6' - \theta)$), each convolution i representing the aberrations introduced by a single optical element.

Whereas this approach is useful to gain insight in the approximate performance of the instrument, in an accurate analysis the total instrumental aberration for a certain $\omega, 2\theta$ setting is not simply a convolution of individual contributions, and, moreover, the behaviour of the instrument changes over 26. Both these effects are well illustrated by studying the combined effect of sample transparency and horizontal divergence [3].

It appears that this effect is only to first order described by a convolution of the individual effects; even for modest transparencies ($100\ cm^{-1}$) second order effects can be of the order of some 10 %. It also evolved that the area of the folding function changes as a function of 2θ, which can easily change by a factor of 1.3 over 28. Needless to say that this effect can be disasterous for e.g., structure determination or quantitative phase analysis.

Deconvolution

In trying to remain pragmatic, the approximation of a 'piece-wise' deconvolution can be made, where for each 'piece' $\theta' \approx \theta$, a kernel $g(\theta';\theta) \approx g(\theta' - \theta)$ is defined. For many applications in line profile analysis this assumption is justifiable. In such an approach, all the aberrations for a certain $\theta,2\theta$ setting are calculated or measured over a limited range. This range should be small enough to ignore any changes of the instrumental response over this interval.

Several approaches exist to solve the deconvolution equation; see [2] for an overview. Conceptually the simplest is Fourier deconvolution. Fourier deconvolution features several flaws, most notably its high sensitivity to noise when the instrumental profile has a width of the same order as the observed profile. A more stable deconvolution technique is Tikhonov deconvolution. This, however, is at the expense of the maximum gain in resolution. An empirical rule of thumb is that the instrument response should be at most half the width of the diffraction profile in order to obtain sensible results.

An approach which is used in our laboratory is the Maximum Entropy (MaxEnt) deconvolution, where the

$$\text{entropy } S(f) = \int f \log f \, df$$

is used to stabilize the deconvolution.

Experiment shows, that this method is capable of deconvolutions where the width of the instrumental profile is roughly 0.85 times the experimental profile. Moreover, because the approach is non-local (\ie, the intensity at some channel is not dependent on the intensity of its neighbours) it does not artificially influence the shape of the diffraction profile. This, of course, is of utmost importance in line profile analysis

Another desirable property is the possibility to include any prior information in an elegant way (one may, *e.g.*, happen to know the *position* of the diffraction line(s)).

Note, that with this increase in resolution, exact knowledge of the instrument response is vital. Any errors in the latter can cause the deconvolution to fail, or, worse, produce non-sense results.

The MaxEnt approach is flexible enough even to allow removal of the instrumental aberrations over regions where the response is *not* constant any more, which is a requirement set in, *e.g.*, structure determination from powder data. Some promising results are shown in Fig. 2, where a computer-generated profile is shown, together with its reconstruction.

Nevertheless, in spite of the highly promising results, profile reconstruction is still in its infancy, and many obstacles should still be overcome.

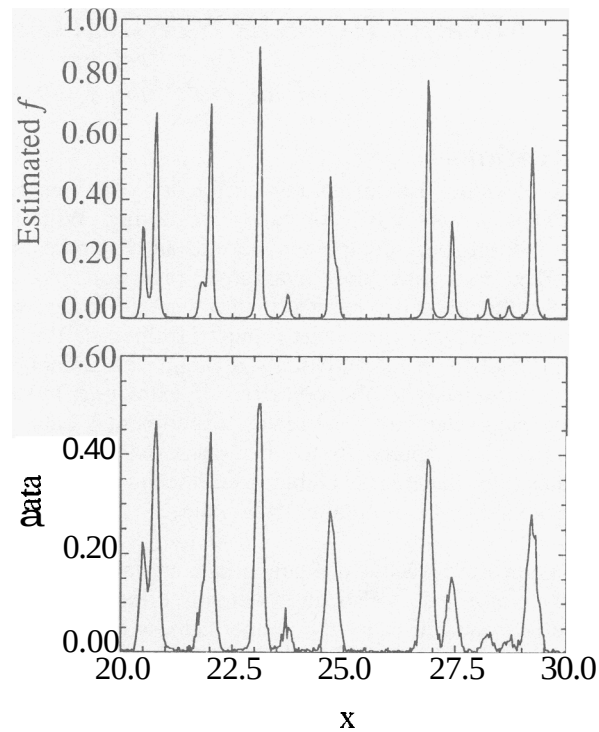

Fig. **2** *Reconstruction example. Bottom: (artificial) data, blurred and with noise added. Top: reconstruction. Note the (correct) reconstruction of the shoulders around x = 22,25.*

References

[I] D. Reefman, "Calculation of the effective absorption coefficient in multi-phase powders", Textures and Microstructures **28** (1996).

[2] D. Reefman, "Towards higher resolution: a mathematical approach", in *"Microstructure Analysis from Diffraction'*, ed. R.L. Snyder, H.J. Bunge and J. Fiala (Oxford: Oxford University Press) to be published

[3] D. Reefman, "Effects of sample transparency in powder diffraction", Powder diffraction **11** 107 (1996).

THE COMMISSION ON POWDER DIFFRACTION REPORTS

The commission was extremely busy in 1996 with the main IUCr congress in Seattle and the combined powder diffraction satellite and XRD/XRF conference at Denver. The commission played a major role in both events in addition to itc already very ambitious programme of size strain, quantitative analysis and Rietveld refinement evaluation. The mailing list for the Commission newsletter continues to grow and a new home page on the world wide web (http://www.dl.ac.uk/SRS/XRD/IUCR) has been established. The twice yearly CPD newsletter reaches a substantially different audience than the main IUCr newsletter and as such will continue for the next triennium. The CPD plans to make this information available in electronic form for as wide an audience as possible.

Meetings/Workshops/Schools

The preparations for the Denver and Seattle meetings dominated the first half of the year. The commission was

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involved directly with sessions on materials research using powder diffraction and structure determination techniques. The commission was represented on the main programme committee by Dave Cox and Rod Hill. At the combined IUCr satellite and Denver conference the commission organised sessions on peak profile analysis, precision and accuracy in structure, refinement from powder data and phase quantification. The CPD was represented on the Denver programme committee by Deane Smith and Dave Cox. This was in addition to participation by individual members in a large number of other microsymposia. The sessions were so well attended in Seattle that extra seats had to be provided in the lecture theatre. The CPD sessions at Denver were also very successful providing a good balance between the academic and industrial research that characterisesthe Denver meetings. Professor Daniel Louer (Rennes) gave the keynote lecture at the IUCr main congress entitled 'Modern Powder Diffraction in Materials Science'. This was an excellent talk covering all aspects of powder diffraction with particular emphasis on its applications. Professor Louer pointed out just how far the subject has progressed in ten years since the CPD was formed.

The commission has been involved in the European powder diffraction meeting in Parma (EPDIC 5) through the programme committee (Bob Cernik and Paolo Scardi) and by recommending IUCr support for students. The general relationship between the EPDIC meetings and the IUCr is becoming clearer after some discussion. The EPDIC meetings are very successful in their own right and will continue to be independent meetings. They will still attract IUCr support and the CPD will continue to look for informal ways to encourage co-operation. The EPDIC meetings will as far as possible be held one and a half years apart with a break of one year during the IUCr main congress years. The relationship with the ECM meeting is also becoming clearer with the appointment of the CPD chair to the programme committee. The CPD hopes that powder diffraction will play an increasing role in the ECM meetings and that the current excellent relationship with EPDIC will continue. In addition to these major meetings the commission lent its support to the 5th school on X-ray diffraction from polycrystalline materials in Frascati, Italy. The subject of the school was glancing angle X-ray diffraction. There was also a powder diffraction course in Merida, Venezuela, and a meeting on materials structure characterisation in the Czech republic.

Projects

The CPD has continued to help the development of the program exchange bank (PEB) for powder diffraction software and has provided a platform for the launch of an anonymous FTP site. The project to evaluate quantitative phase analysis is being led by Rod Hill and Deane Smith, this is at the stage of calling for interested parties to participate in the programme. The commission is following up the Rietveld refinement comparison study published by Hill et al in 1994 with a set of recommendations. This is being led by Lynne McCusker and Bob von Dreele and will probably appear in one of the IUCr journals this year. The CPD is also actively searching for new standard materials with more refineable parameters for more complex Rietveld comparisons. Retired CPD member Dave Cox has agreed to continue with this project. Later this year the commission wishes to conduct a survey of instrumentation to determine the need for laboratory based high resolution studies.

Newsletters

Two newsletters were produced in 1996, issue 16 was edited by Vaclav Valvoda (Prague) and issue 17 by Lynne McCusker (Zürich). The first of these contained a detailed account of powder diffraction in Prague in the form of ten "post cards". The latter newsletter contains a feature article on powder diffraction at the ESRF by Andy Fitch, the benefits of a small source size are becoming very clear. Both contained many items that one should expect in a newsletter: a series of meeting reports, up to date contact points, meeting calendars. Thus the newsletters provide a vital platform for information exchange for all interested in powder diffraction.

***Collaboration with other** commissions*

With the expansion of the number of IUCr commissions the CPD wishes to form new links with other commissions in order to promote new areas of co-operation. The CPD hopes to form strong links with the commissions for high pressure, electron and neutron diffraction, XAFS, small angle scattering and synchrotron radiation. At present these collaborations are at a very early stage although there are some very promising avenues such as structural characterisation with electron crystallography followed by Rietveld structure refinement. The commission is actively pursuing the possibilities for scientific co-operation as well as ideas for shared meeting sessions.

New membership

The commission bade farewell to Dave Cox, Daniel Louër, Shao Fan Lin, Rod Hill, Jaroslav Fiala, and Dr Ludo Frevel as ICDD representative. However the CPD will keep on the services of Rod Hill and Shao Fan Lin as consultants, firstly to supervise the QPA programme and secondly to provide a service to translate the newsletter into Chinese. The new members of the commission are Rob Delhez (Netherlands), Jean Pannetier (France), Paolo Scardi (Italy), Siba Sen Gupta (India) and Bob Snyder as ICDD representative.

MAILING LIST FOR NEWSLETTERS

If you would like to be added to the mailing list for Newsletters of the Commission on Powder Diffraction of the IUCr or you have changed your address, please contact Prof. R.J. Cernik, Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK.

A USEFUL REVIEW OF POWDER DIFFRACTION, OBTAINABLE FROM THE WEB

A paper by Ian Langford and Daniel Louer reviewing most aspects and applications of powder diffraction appeared in the February 1996 issue of the Institute of Physics' Reports on Progress in Physics (Vol. 59, pages 131-234). After introductory sections on basic principles, modelling of powder-diffraction patterns, instrumentation and experimental considerations, the following topics are reviewed:
crystallographic databases and phase identification, structure refinement, ab initio structure determination, resonant diffraction (anomalous dispersion), quantitative phase analysis, line-profile analysis and microstructural properties, dynamic and non-ambient diffraction. Additionally, there are over 500 references to relevant papers and other publications.
From January 1996, full electronic access on the World Wide Web to all 31 Institute of Physics journals has been included in the price of an institutional subscription. Anyone wishing to read the review via the WWW, or print a copy, must first ensure that their librarian (or other authorised person) has registered the site for access to electronic IoP journals. A registration form for this can be obtained from custserv@www.iop.org or can be downloaded from http://www.iop.org. Full information on browsing a journal or accessing a particular paper is given via the IoP home page. Readers whose institutions have, or are eligible for site registration are encouraged to obtain copies of the review in this way; producing and mailing copies is expensive and time-consuming! It should be noted that there are discrepancies in page breaks between the hard-copy and electronic versions of the review, though the total number of pages is the same. This occurred in a few of the first articles in Rep. Prog. Phys. published electronically and both versions are now produced from the same files.

CRYSTALLOGRAPHY SCHOLARSHIP AWARDS GRANTED BY INTERNATIONAL CENTRE FOR DIFFRACTION DATA

The International Centre for Diffraction Data is pleased to announce the awarding of four Crystallography Scholarships for 1997.
They are Ms. Nathalie Audebrand from the Universite de Rennes in France, Mr. Savvas Savvides from Cornell University in New York, U.S.A., Mr. David Teter from the Carnegie Institution in Washington, D.C. U.S.A., and Mr. Hongwu Xu from Princeton University in New Jersey, U.S.A..
Nathalie Audebrand will perform "Structure, Microstructure and Temperature Dependent Diffraction Studies on New Cerium-based Precursors and Related Oxides".
Studies of "Structure Determination of the flk2/flt3 Ligand" will be conducted by Savvas Savvides.
David Teter's research focusses on "Superhard Carbon Boronitride Alloys: A Rational Approach to Design and Synthesis".
Hongwu Xu will continue his studies entitled "Structural Analyses of Stuffed Quartz Phases Along the $LiAlSiO_4$-SiO_2 Join".

APPLICATION FOR CRYSTALLOGRAPHY SCHOLARSHIP AWARDS GRANTED BY INTERNATIONAL CENTRE FOR DIFFRACTION DATA

The science of crystallography has played a key role in the development of X-ray diffraction, electron diffraction and neutron diffraction for the elucidation of the atomic structure of matter. Crystallography is an interdisciplinary branch of science taught in departments of physics, chemistry geology, molecular biology, metallurgy and materials science. To encourage promising graduate students to pursue crystallographically-oriented research, the International Centre for Diffraction Data (ICDD) has established a Crystallography Scholarship Fund. While the Ewald Prize is awarded every three years to an internationally recognized crystallographer, little effort has been made by science departments to cultivate aspiring crystallographers. Convinced of the beneficial, scientific impact of the proposed scholarships for crystallographically-oriented research, the ICDD has solicited funds from private and industrial sectors to support this program. The ICDD has awarded two scholarships in 1992, two in 1993, three in 1994, three in 1995, four in 1996 and four in 1997. Applications for the 1998 awards must be received by ICDD no later than 31 October 1997.

Qualifications for the applicants: The applicant should be a gradute student seeking a degree with major interest in crystallography e.g. crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification and materials characterization. There are no restrictions on country, race,

age or sex. The term of the scholarship is one year. Application for one renewal may be made by the recipient at the end of the first year. Because a limited number of scholarships are awarded, renewal applications will be considered on a competitive basis in conjunction with all applications that have been submitted up to the closing date.

Submit:

a. Curriculum Vitae, listing degree(s) held and degree(s) sought,

b. A one-page proposal by the graduate student describing the type of crystallographic research to be partially supported by scholarship.

c. A supportive letter from the sponsoring professor of an accredited university or an institute of technology on institution letterhead.

Restrictions on the scholarship fund

a. The scholarship stipend of $2,000 is to be used by the graduate student to help defray tuition and laboratory fees. A portion of the stipend may be applied to registration fees to accredited scientific meetings related to crystallography.

b. No more than one scholarship will be awarded to applicants at any one institution per year.

c. The funds of the scholarship are not to be used for travel.

The awarding of the scholarships shall be administered by a committee consisting of the ICDD Chairman, the Chairman of the ICDD Technical Committee, the Chairman of the ICDD Education Subcommittee, and one or two individuals without conflict of interest. One or more professors (with no conflicts of interest) may be invited to assist in the selection of successful candidates.

Applications must be received by 31 October 1997.

Please mail to:
Secretary, International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, PA 19073-3273 U.S.A.

MEETING REPORTS

Keeping up-todate on the many advances in powder diffraction instrumentation, data analysis and application is a difficult task Just how active the powder diffraction community is, can be seen in the number of workshops, symposia and conferences that are devoted to the subject each year. To give our readers an impression of the current interests in powder diffraction, reports from various meetings, many of which were sponsored and/or organized by the CPD, are given below.

European X-ray Powder Diffraction Standardization: Past and Present Needs of XRPD at the Centenary of the Discovery of X-rays

Palazzo della Sapienza, Pisa, Italy
7 - 8 October 1996

This short conference was organized by G. Berti and colleagues from Pisa University and it was held in conjunction with a meeting of Ad-Hoc Group 2 (AGH-2) of Technical Subcommittee 138 of the Comité Européen de Normalisation (CEN). The task of AGH-2 is to draft standard methods and practices in X-ray powder diffraction (XRPD) which, after approval by CEN, will eventually control procedures in European research and industrial laboratories.

The conference, which commemorated the centenary of the discovery of X-rays by Röntgen, opened with a lecture by J.I. Langford on the substantial contribution of A.J.C. Wilson, FRS, to powder diffraction. Wilson developed much of the basic theory associated with diffraction effects from imperfect structures and, together with W. Parrish, was a pioneer of powder diffractometry. He also devoted considerable time and energy to statistical analyses of both powder and single-crystal data.

The general theme of the remainder of the meeting was standardization in XRPD and the introductory lecture was followed by the second 'round table' discussion on this topic, the first having been held at EPDIC-4 in 1995. G. Berti introduced the discussion by stating the aims of AGH-2 and outlining progress to date. The discussion centred on three main areas: *(a)* terminology, general principles and experimental procedures, (*b*) standard reference materials for instrument calibration and procedures for sample preparation and (*c*), instrument characteristics. The first day concluded with a paper by C. Martinelli on problems associated with the analysis of airborne asbestos and silica and the need for standard procedures for sample preparation and data collection and analysis in this field.

G. Will opened the proceedings on the second day, by considering the evolution of X-ray diffractometry, highlighting some of the problems which can influence the results of XRPD experiments. A. Haase then reviewed 100 years of X-ray instrument manufacture by Richard Siefert & Co. and D. Louër covered modern indexing methods. B. Rebours considered the need for standardization in industrial laboratories where modem XRPD is practised, based steps taken in her own laboratory to meet this requirement. V. Valvoda then reviewed progress in studies of texture by means of XRPD and the meeting concluded with a series of short papers on a variety of topics related to standardization. The proceedings of the meeting will be published in due course and information on these and on AGH-2 may be obtained from Dr G. Berti, Department of Earth Sciences, University of Pisa.

SECOND ANNOUNCEMENT FOR CPD ROUND ROBIN

Initiated and Organized by the IUCr Commission on Powder Diffraction

The International Union of Crystallography - Commission for Powder Diffraction intends to conduct a Round Robin focusing on quantitative phase analysis using powder diffraction data. This message is a reminder for those who may have missed seeing the first announcement and call for expressions of interest.

Aims of the Round Robin:
The round robin will focus on the use of laboratory X-ray, synchrotron X-ray and neutron diffraction data for the derivation of quantitative phase abundance. However, other methods may be used to validate the diffraction results (e.g. FTIR, normative analysis, etc.). These additional methods will be at the discretion of the participant.

The general goals of the round robin will include the following:

- To document the methods & strategies commonly employed in Quantitative Phase Analysis (QPA), especially those involving powder diffraction
- To assess (i) levels of accuracy & precision, and (ii) lower limits of detection
- To identify specific problem areas & develop practical solutions
- To formulate recommended procedures for QPA using diffraction data
- To create a standard set of samples for future reference

The samples used in the study will consist of mixtures of major and minor components covering a wide range of analytical complexity and include sample related phenomena such as preferred orientation, microabsorption and amorphous content. The samples will be comprised of synthetic mixtures, natural mineralogical specimens as well as pharmaceutical materials. The involvement of participants in the round robin can vary depending on the amount of time available to each individual/laboratory. This may range from the analysis of supplied data to the preparation of samples along with the subsequent data collection and analysis. However, since the success of the round robin will depend on the number of results returned, full participation is encouraged.

Since the purpose of the round robin is to assess the methods of quantification, and not identification, the identity of each of the component phases will be supplied. For those participants using Rietveld based methods for the analysis, full structural information for each of the phases will also be supplied.

How to participate
Potential participants can register their interest in the round robin by sending an Email message containing the full contact information to the address given below. Details should include

Name
Affiliation
Address, including organisation, postal address, post code and country.
Phone number (including country and area codes)
FAX number (including country and area codes)
Email address

Respondents will be sent a questionnaire request information about which of the samples they wish to analyze plus the amount of sample required (i.e. are they an X-ray or neutron user).

Operating Team

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Rod Hill	CSIRO Minerals, Australia
Edward Groleau	Eli Lilly & Co, USA
Lachlan Cranswick	Melbourne, Australia

Advisory Team

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Grants-in-aid from the International Centre for Diffraction Data

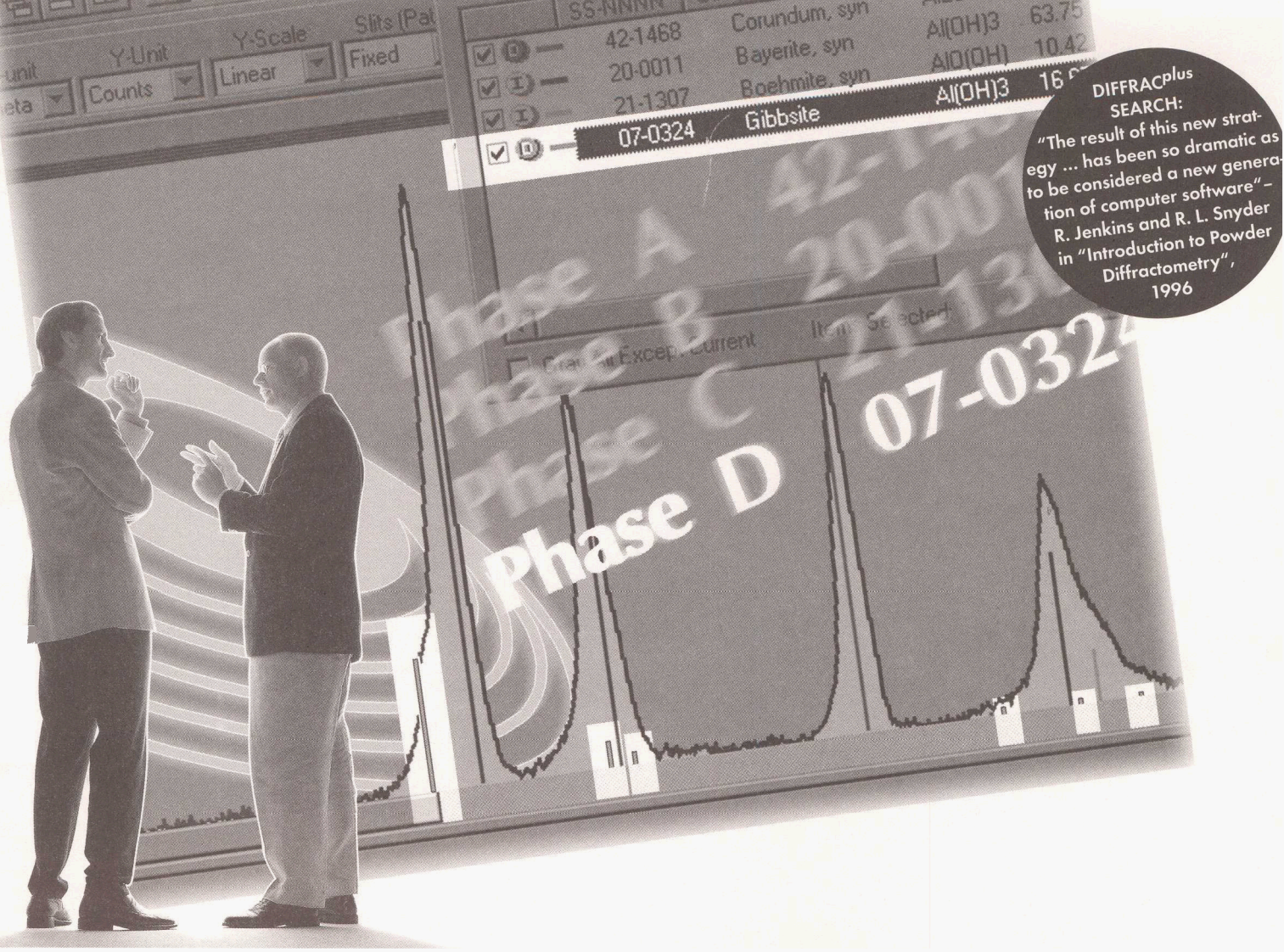
"Let us help each other"

The ICDD (International Centre for Diffraction Data) needs more high quality powder diffraction patterns to add to its database, the PDF, which is used worldwide. Perhaps you could use a little additional financing. If you had that small financial help, could you produce some high quality X-ray powder diffraction patterns, in the needed format, for materials not now represented in the PDF? Then you might be interested in applying for an ICDD Grant-in-Aid.

Proposals addressing current opportunities to extend and improve the usefulness of the PDF are given highest priority.

The duration of a Grant-in-Aid is 12 months.

Deadlines for receipt of Grand-in-Aid proposals at ICDD Headquarters are 31 December, 1996, 31 July I997 and then 31 January and 31 July thereafter. Detailed guidelines for the proposals and proposal forms are available from Ms. Therese Mauchline, International Centre for Diffraction Data, 12 Campus Blvd., Newtown Square, PA 19073-3273, USA (Tel: (610) 325 9814, Fax: (610) 325 9823, E-mail: Mauchline@ICDD.com)



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THE IUCr COMMISSION ON POWDER DIFFRACTION

The CPD was formed in 1987, and since then a large number of people have worked very hard on behalf of the Commission. I would like to thank everyone who has helped in this respect, especially Rod Hill, the out going chairman. Rod has done a great deal to put the Commission in its current healthy state and he will be a hard act to follow.

One of the most fundamental arguments for the formation of the commission was the unique position of international research using powder diffraction. In the field of crystallography represented by the main body of the IUCr there is more activity from academic institutions than from industry. This position is exactly reversed in the field of powder diffraction, and it is one of the major purposes of the commission to provide an information link between the very large industrial community and the more academic, less applied aspects of the subject. The commission will continue to do this through the IUCr by endorsing large and small meetings, by encouraging collaboration between groups working in similar fields, by enhancing mobility of students to attend CPD events, and by undertaking specific projects designed to improve standards and research practices in powder diffraction. A particular aim of the CPD that I am very keen to continue is to encourage the teaching of powder diffraction in developing countries

The CPD has a mandate from the IUCr to collaborate with other commissions, this is especially important given the number of new and exiting areas of research using crystallography. I very keen to try to open up links that might be of interest to powder diffractionists in the areas of electron diffraction, XAFS, high pressure research, neutron and synchrotron research and small angle scattering.

The CPD has a very close relationship with the International Centre for Diffraction Data. The ICDD have over 15,000 people on their circulation list which illustrates the huge number of scientists engaged in powder diffraction. These people would not normally describe themselves as crystallographers but as materials scientists or chemists. It is the job of the CPD to draw together these groups, to encourage co-operation and collaboration, to accelerate the already phenomenal growth of the subject and to make new information available to everyone.

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WHAT'S ON

4-8 August 1997
46th Annual Denver X-ray Conference
Steamboat Springs, Colorado, USA
Contact: Dr Paul Predecki, Engineering Department, Uiversity of Denver, Denver, CO 80208, USA
E-mail: denxrcon@du.edu

17-21 Augllst 1997
International Conference on Neutron Scattering (ICNS 97), Toronto, Canada
Contact: Phyllis Geen, Solid State Division, Oak Ridge, Nat'l Laboratory, POB 2008, Oak Ridge, TN 37831-6033
Fax: 423-574-4143; E-mail phg@ornl.gov.

24-28 Augllst 1997
17th European Crystallographic Meeting (ECM-17) Lisbon, Portgual
Contact: ECM17 Secretariat, Departamento de Engenharia
Quimica, Instituto Superior Technico, Av Rovisco Pais, 1096 Lisbon, Portugal: Fax: +I351 (I) 442 1161
E-mail: qteresa@beta.ist.utl.pt or romao@itqb.unl.pt
WWW: http://alfa.ist.utl.pt/ecm-17/

31 August - 4 September 1997
17th Conference on Applied Crystallography, and *4-7 September 1997*
3rd Rietveld Summer School
Wisla-Jawornik, Hotel "Stok" Poland
Cntact: Prof. H Morawiec, Institute of Physics and Chemistry of Metals,
University of Silesia, Bankowa 12,40-007 Katowice, Poland, Tel/Fax+48(32) 59 69 29
E-mail: dana@usctouxl.cto.us.edu.pl.

16-22 August 1998
18th European Crystallographic Meeting (ECM-18) Prague, Czechoslovakia
Email: hasek@imc.cas.cz

22-25 August 1997
6th European Powder Diffraction Conference (EPDIC -6), Budapest, Hungary.
Contact: Professor Tamas Ungar, Dept of General Physics, Etvs University, Budapest (Chairman), or Dr Erzbet Svb, Central Research Institute of Physics of the Hngarian National Academy of Sciences (Scientific Secretary).

4-13 August 1999
18th Congress and General Assembly of the International Union of Crystallography
Glasgow, Scotland, UK
Contact: Dr C Gilmore, Dept of Chemistry, University of Glasgow, Glasgow. G12 8QQ, UK
fAX: +44 (41) 330 4888: E.mail: iucr99@chem.gla.ac.uk
WWW: http//www.chem.gla.ac.uk/iucr99

CALL FOR CONTRIBUTIONS TO THE NEXT CPD NEWSLETTER

The next issue of the CPD Newsletter will be edited by Prof. P. Scardi to appear in October of 1997. 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 (address is given on page 12).

Rob Delhez, Editor, CPD Newsletter 18

WWW sites of General Interest to Powder Diffractionists

The International Centre for Diffraction Data: **www.icdd.com.**
The site contains links to many other useful diffraction and diffraction-related sites.
/index.html

The Commission on Powder Diffraction: **http://www.dl.ac.uk/SRS/XRD/IUCR**