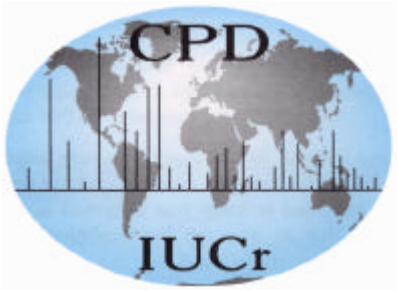

COMISSION ON POWDER DIFFRACTION

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

http://www.iucr.org/iucr-top/comm/cpd/

NEWSLETTER No. 22, November, 1999

http://www.iucr.org/iucr-top/comm/cpd/Newsletters/

NEUTRON DIFFRACTION ISSUE

(Editor R.B. Von Dreele)

In This Issue:

CPD Chairman's Message

The IUCr General Assembly and Congress in Glasgow was a real success, and this is particularly true for Powder Diffraction (PD), that was the main subject of at least 16 microsymposia. Thanks to the efforts of Bob Cernik, untiring work of Lynne McCusker, and other members of the Commission who chaired some of the sessions, Glasgow meeting was the acme of a very important and active triennium for the CPD. I think that we should all thank Bob, Lynne and the other out going members of the CPD for their work, and I really hope that the new commission will continue along this way, even if it will certainly be a difficult task to keep the same level of quality and success in CPD activities.

One of the main jobs of the CPD is improving collaborations among scientists and industrial partners interested in PD and also establishing dynamic relationships with other bodies and scientific organizations. It is therefore important to underline the agreement found between the EPDIC (European Powder DIffraction Conference) committee, chaired by Eric Mettemeijer, and the ECA, the regional associate of IUCr for Europe. During the IUCr meeting Carmelo Giacovazzo, on behalf of ECA, invited the EPDIC committee to form a SIGPD (Special Interest Group on Powder Diffraction) within ECA, in order to better coordinate all the activities and important events concerning PD in Europe. A better organization and close relations are expected for the future, especially for the two main European events regarding PD, i.e., EPCID and ECM. Another important achievement was the elimination of the overlap between future dates of IUCr meetings and Denver X-ray Conference for the next ten years at least. The problem is that both events usually take place in August. Therefore, the DXC committee accepted to anticipate the 2002 DXC to avoid the overlapping with the next IUCr meeting (Israel, 2002), while in the year 2005 the IUCr meeting (Florence, Italy) will not be in August, so the DXC will take place again in its usual date. I think we should be particularly grateful to the DXC committee for this. In this framework of general agreement, I also hope a wide collaboration with ICDD, whose qualified staff organizes a number of interesting activities in the field of PD.

During the 1996-1999 triennium the CPD was particularly active in the endorsement of schools, workshops and congresses on PD and related topics, and in the sponsorship and support of several projects. One of them concerned the Rietveld refinement, and was concluded by the production of a paper by Lynne McCusker, Bob von Dreele, Dave Cox, Daniel Löuer and Paolo Scardi, distributed together with Newsletter No 21. Two Round Robins are in progress and will also hopefully culminate in the production of scientific papers that will be distributed to the large number of Newsletter readers (now of the order of 1500). A further involvement of CPD for the next years will be in the research-industry relations. A set of industrial flyers, illustrating typical PD application to technologically relevant problems is in preparation, and should be used as a sort of *ballon d'essai*, to contact a large number of potential PD users, and also to make aware powder diffractionists of the many applications they can offer to industrial customers.

A final word on the Newsletter. As in the past, each issue will focus on a specific topic, which is neutron diffraction for the present Newsletter, and will report on congresses, school and meetings, plus any additional pertinent information that interested people will submit to the CPD Chairman or to the Editor designed for the issue in preparation. A regular update will be given on CPD projects, like the RR on Size/Strain and on Quantitative Phase Analysis (see below). An important contribution will be the 'Computer Corner', that should be a regular page concerning new PD software developments. Since the CPD Newsletter is not a Journal, and refereeing is not provided, contributions will be conveniently summarized by Lachlan Cranswick, who will present his view on the status of PD software, profiting from his experience and activity as CCP14 Secretary. Web addresses and references to obtain complete documentation and downloadable files will be given. I really wish to encourage readers to send me suggestions on the Newsletter compositions and contributions for next issues.

Paolo Scardi

Unfortunately I must conclude this message with very sad news, recently communicated by Eric Mittemeijer:

Dear colleagues,
This is to let you know that on 23-10-1999 Professor Walter Eysel died. His death was caused by incurable cancer. He knew very well what was happening to him and showed great courage in accepting this. After his illness became clear to him, he spoke openly about it. He tried to maintain contact with a couple of his colleagues by email from his home address, but too soon even that appeared impossible.
Apart from his direct participation in research as a scientist of high quality, his crucial role in the founding of EPDIC and its committee should be recalled here. One cannot forget the straight, sympathetic, and in particular convincing way he used to present his ideas and to approach others to become active in what has become later the EPDIC committee. Of what is clear from what is now history, it follows that Walter Eysel had a strong hand in the shaping of EPDIC.
We will miss him. I do, especially because of his advice I often asked for regarding EPDIC matters.

Eric Mittemeijer, Chairman of The EPDIC Committee

From the Editor of Newsletter No 22

In this issue of the CPD Newsletter we feature some new neutron powder diffractometers that are either currently under construction or are just beginning to become available for users. These new instruments will provide the powder diffraction community with new capabilities in high intensity, better resolution and higher quality neutron powder diffraction data, and we keenly await their coming on line in the upcoming year.

Bob Von Dreele

CPD projects: status of Round Robins supported or endorsed by the CPD

Size/Strain Round Robin

Several commercially available powders were considered as possible candidates for size-broadening or strain-broadening standards. However, preliminary line-broadening analysis has shown strong indications of a multimodal crystallite-size distribution and simultaneous size-strain broadening effects. It was concluded that any commercially available materials are not likely to be suitable for this purpose and that the experts in specimen preparation are needed. I am very thankful to Daniel Louer and Nathalie Audebrand (University of Rennes), who are trying to synthesize an intended size-broadening standard and to David Bish (Los Alamos National Laboratory), who is working on a preparation of an intended strain-broadening standard.
You can learn about the current progress and access the form for your comments or the intent to participate in the Round-Robin at http://www.boulder.nist.gov/div853/balzar or http://www.ccp14.ac.uk/ccp/web-mirrors/balzar/div853/balzar (CCP14 mirror). Both your comments and participation are greatly appreciated.

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Quantitative Phase Analysis Round Robin

The IUCr Commission on Powder Diffraction (CPD) has sponsored a round robin on the determination of quantitative phase abundance. Specifically, the aims of the round robin were (i) to document the methods & strategies commonly employed in Quantitative Phase Analysis (QPA), especially those involving powder diffraction, (ii) to assess levels of accuracy, precision and lower limits of detection, (iii) to identify specific problem areas and develop practical solutions, (iv) to formulate recommended procedures for QPA using diffraction data, and (v) to create a standard set of samples for future reference.

Several samples (exhibiting a wide range of analytical complexity) were distributed to some 120 participants. Sample 1 consisted of a ternary mixture of corundum (Al_2O_3), fluorite (CaF_2) and zincite (ZnO) prepared with eight different compositions in order to test the reliability of analysis at a range of concentration. In addition, these phases exhibit very little peak overlap at low diffraction angle, and thus represent a fairly simple analytical system. Participants could choose to (i) analyse XRD data supplied by the CPD, (ii) collect and analyse their own data, or (iii) both of the above.

The return rate exceeded 60% for the 'compulsory' sample (1G). While most of the participants used conventional X-ray diffraction equipment, a few returns from neutron and synchrotron users were also received.

This report describes some of the preliminary outcomes from the analysis of the sample 1 suite which have been presented at a number of conferences including, (i) the ECM-18 conference in Prague, Czech Republic (Aug '98), (ii) the AXAA-99 conference in Melbourne, Australia (Feb '99), and (iii) the XVIIIth IUCr congress in Glasgow, Scotland (Aug '99).

Figure.1a shows the distribution of phases in the ternary system while Figures 1b and 1c show the returns for the CPD supplied data and the participant collected data respectively.

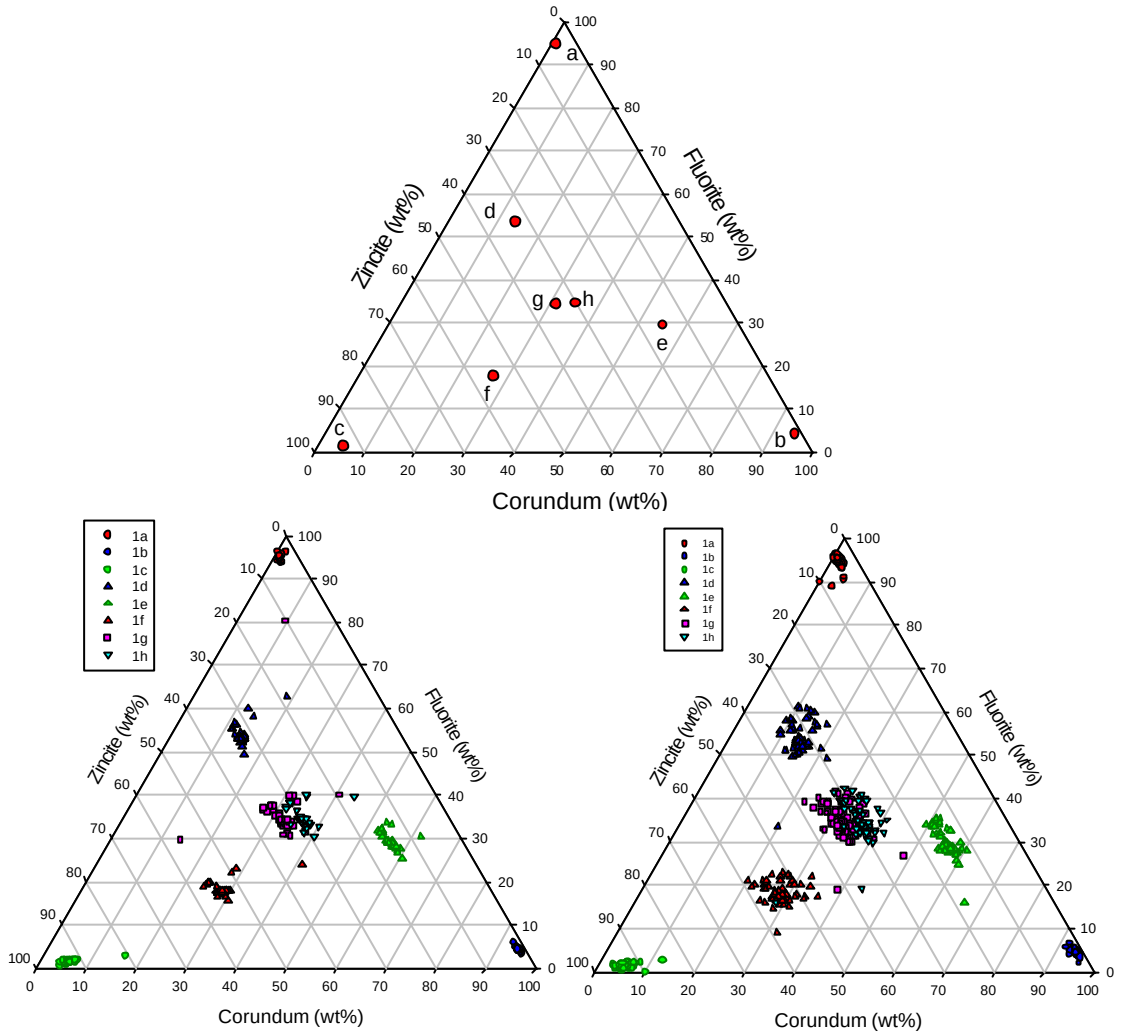

Figure 1. Showing the ternary distribution for sample 1 for (A) the weighed values, (B) the results of analysis for the CPD supplied data, and (C) the results of analysis for data collected by the participants

Table 1 below shows a summary of results for both CPD supplied data and participant collected data for the eight sample 1 mixtures . The values show that there is a wide spread of results when all values are included (even for the CPD supplied data where all participants analysed the same data set). However, the relative errors improve significantly when the 'outliers' are removed from the analysis.

CPD supplied data				
Concn. Range (wt%)	1	50	95	
RSD (%)	10 - 20	4 - 7	0.5 - 2	All results
RSD (%)	3 - 10	1 - 2.5	0.2 - 0.6	25/75 results only
Participant collected data				
Concn. Range (wt%)	1	50	95	
RSD (%)	10 - 50	5 - 9	0.7 - 2	All results
RSD (%)	5 - 20	2 - 5	0.3 - 0.7	25/75 results only

Table 1. Results of analysis of data (i) distributed by the CPD and (ii) collected by the participants for the eight mixtures comprising the Sample 1 suite. The relative standard deviations (RSD) show the variability of results over all values at the specified concentration range. The 25/75 results represent only those values which fall within the 25th and 75th percentiles.

Sample 1G		Weighed	XRF	All	X-ray	Neutron	Synch-rotron
Phase		(wt%)	(wt%)	(wt%)	(wt%)	(wt%)	(wt%)
Corundum	Mean	31.37	31.70	32.25	32.26	31.64	32.83
	Std Dev		0.09	3.29	3.42	1.13	1.86
	Min		31.62	22.40	22.40	29.20	30.80
	Max		31.80	48.60	48.60	32.39	35.20
	N		3	122	111	7	4
Fluorite	Mean	34.42	33.85	34.80	34.84	34.23	34.73
	Std Dev		0.11	3.03	3.14	2.03	0.48
	Min		33.79	19.00	19.00	32.37	34.30
	Max		33.98	41.70	41.70	38.60	35.40
	N		3	122	111	7	4
Zincite	Mean	34.21	34.01	32.97	32.91	34.14	32.48
	Std Dev		0.10	2.30	2.35	0.93	2.22
	Min		33.95	24.70	24.70	32.30	29.40
	Max		34.13	42.00	42.00	35.38	34.60
	N		3	122	111	7	4

Table 2. Results of analysis of data collected by the participants for Sample 1G. The number of determinations (N) includes the replicate values returned by some participants.

A summary of the returns for sample 1G is shown in Table 2. While the means of the participant determinations are in reasonable agreement with the weighed values, there is a large spread in the individual values. The types of analytical issues which have become apparent during analysis of the returns can be divided into a number of groups.

Operator error – these result from inappropriate use of the analysis method and include (i) use of the wrong space group setting for fluorite in the Rietveld method, (ii) omitting phases from the analysis in spite of being told that the samples were three phase mixtures, and (iii) mis-reading of the Rietveld refinement output file – i.e. reading and reporting the wrong number.

Incorrect Rietveld refinement strategy – in many cases, complex analysis software (especially the Rietveld method) is not being correctly applied. Typical analysis problems include (i) insufficient parameters released to ensure effective model minimisation, (ii) incorrect modelling of instrument geometry when transmission samples were used – this results in an incorrect distribution of calculated peak intensities as a function of diffraction angle.

Use of inappropriate RIR values – several participants have used conventional 'single-peak' methods for QPA coupled with the so-called reference intensity ratios (RIR's) for calibration. The spread of RIR values (and hence QPA results) indicates that there exists some confusion regarding the 'correct' values of RIR to use.

Excessive microabsorption correction – many analysis programs have corrections for absorption contrast built in and operators are applying the correction without first investigating whether a correction is required. This can result in severe underestimation of some phases and overestimation of the remaining phases in the sample (especially if methods are used which sum the total content to 100wt%).

The arduous task of completing the collation of results is well advanced with detailed statistical analysis now being undertaken for samples 1A to H. The aim will be to prepare the first draft of a paper, concentrating on sample 1, for publication by the end of 1999. Publication of the results of analysis of the remaining samples will proceed in 2000.

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'HIPPO' A New High Intensity Neutron Diffractometer for Bulk Analysis of Materials

K. Bennett and *R.B. Von Dreele*, Lujan Center, Los Alamos National Laboratory, and *H.-R. Wenk*, Department of Geology and Geophysics, University of California, Berkeley

A new high intensity time-of-flight (TOF) neutron diffractometer for the study of polycrystalline materials (including powders) and liquids at low and high temperature and high pressure will be available in fall 2000 at the Los Alamos Neutron Science Center (LANSCE). The 'HIPPO' diffractometer, named for two of its important applications HIgh Pressure and Preferred Orientation, is being built under the auspices of the United States Department of Energy as part of a $25M facility wide enhancement project. The new instrument is a synergistic effort by both the University of California Campuses and National laboratories to (1) attain scientific excellence and (2) to advance our present knowledge of condensed matter and (3) make neutron diffraction an available tool for younger generation scientists. Of particular interest is the investigation of small ($1mm^3$) and large ($4cm^3$) sample volumes at high (2000K) and low (<4K) temperatures at high pressures (up to 20GPa), and in different atmospheres. With this instrument it will be possible to perform dynamic experiments on bulk anisotropic samples, study kinetics of phase transformations and reactions in situ, and investigate structural and magnetic properties. No existing instrument, world-wide, has this capability.

The new HIPPO Diffractometer will be located at the Manuel Lujan Jr. Neutron Scattering Center at LANSCE where a unique spallation source (100 μA proton beam and soon to be upgraded to 200μA) produces polychromatic neutrons that are captured in time-of flight (TOF) for fundamental condensed matter research. Refinements of crystal structures, phase proportions, textures and strains can all be performed with the Rietveld method [Von Dreele, 1997, Lutterotti, et al., 1997]. Problems of low crystal symmetry and composites with many diffraction peaks, as is typical for modern materials and for many environmental problems, can be addressed [Wenk, 1993]. For most materials neutron absorption is negligible and large samples can be examined and diffraction signals averaged over large volumes rather than confined to the surface. This provides far better grain statistics than other methods. Also, because of the low absorption, environmental equipment (high temperature, low temperature, and bulk stress/strain) can be used for *in situ* observation of texture changes [Bennett, et al. 1995; 1997].

Until now the major disadvantage of neutrons, compared to X-rays and electrons, is the low source intensity and sample scattering power. The HIPPO diffractometer addresses mainly two experimental issues: (1) A dramatic improvement in intensity by a short flight path (flux at the sample: $3x10^7$ n $cm^{-2}s^{-1}$) and a three-dimensional arrangement of detector banks (six 3-D conical rings, ca. 1400 detector tubes) and (2) flexible sample environments (heating, cooling, high-pressure etc.), while maintaining good resolution. For a detailed description of the diffractometer and the project visit the HIPPO website http://www.seismo.berkeley.edu/~wenk/hippo.htm or search for UCMRD.

The HIPPO diffractometer features a short initial flight path of 9m and an array of 1400 10atm ^{3}He detector tubes covering nearly $4.6m^2$ with five detector banks at scattering angles ranging from backscattering (nominally 150°) to low forward scattering (nominally 10°). Figure 1 shows an exploded view of the HIPPO diffractometer. The detector panels are tilted relative to the scattered neutron paths to give a more constant resolution across their surfaces. Each detector array has an associated FWHM resolution (0.37% in backscattering ranging to 5.0% low angle forward scattering) and associated d-spacing range (0.12- 47.5 A across all banks). A T_o chopper can be used to remove the fast neutron prompt pulse. The collimation views a 12cm diameter round portion of a high intensity ambient water moderator, and converges to a maximum round beam size of 2cm diameter at the sample position. For most applications samples should be fully immersed in the neutron beam and not exceed this size. Smaller beam sizes at the sample position can be produced with adjustable collimation.

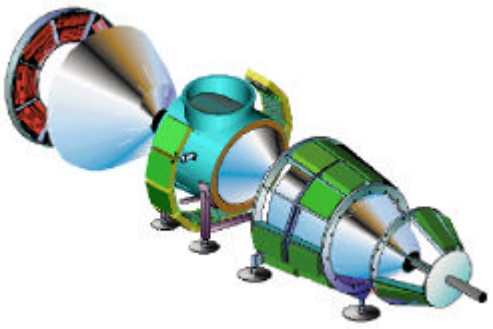

Figure 1. Exploded view of HIPPO diffractometer showing sample chamber surrounded by 5 conical rings of 3D detector tubes. Incident beam travels from left to right of figure, beginning at 150° panels. An argon filled mylar bag is used to reduce incoherent scattering for the secondary flight paths.

It is anticipated that the count rate for some experiments will be approximately 20-60 times what is currently obtained on the present High Intensity Powder

Diffractometer (HIPD) at the Lujan Center, and will enable measurements in as little as 5-10s. The data acquisition will be based on current VME technology and make use of web-based visualization and control software. Experiments can be controlled remotely, e.g. from the laboratory of the user. A 30-sample texture changer will allow quick texture analysis of multiple samples in 5-15 minutes, which is important for larger systematic investigations. A future development for texture studies will include a texture goniometer equipped with a computer controlled X,Y,Z stage and 90deg radial collimators; this will permit the determination of position dependent texture ($2x2x2mm^3$ gauge volume) within the dimensions of an extended sample. A 110–sample changer will allow high throughput crystallographic studies.

A number of sample environments including a cryostat (<4 K), a furnace (>2000K), two texture goniometers, 2 high temperature high-pressure cells (up to 30GPa and 200 K), and a 12 T magnet are among the ancillary equipment for the instrument. This allows applications to a wide variety of disciplines such as materials science and engineering, earth science, physics and chemistry. Figure 2 shows the new high pressure cell TAP-98 with an internally heated furnace that will accommodate pressures of up to 30GPa and temperatures of 2000 K simultaneously (sample size ~$100mm^3$ at 20GPa). [Zhao, et al., 1998].

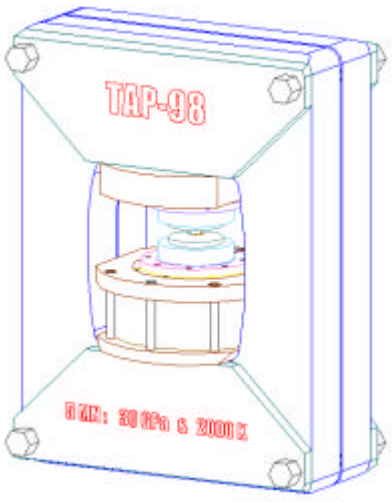

Figure 2. Engineering drawing of TAP 98 (Toroidal Anvil Press) showing composite curved frame, tungsten carbide anvils, sample size ($100mm^3$ at 20GPa). Capacity is 30GPa and 2000 K.

We anticipate that the number of investigations possible over the course of an 8-month annual running cycle will be 100-200, making neutron diffraction not only a method for a few dedicated specialists but also a viable resource for the materials science community. Users can take processed data to their laboratories and process them on their PC with existing user-friendly GSAS or RITA Rietveld codes (workshops will be provided to train the uninitiated). With the vastly improved intensity and data acquisition systems, a fast turnaround of samples is guaranteed. We will have a continuous proposal review system with allocated discretionary time for immediate access for exciting academic or laboratory pilot experiments. Prior to the operations phase two formal workshops are planned: In fall 1999 a first workshop was held at the UC Davis Campus (funded through LANL-UCDRD), in spring 2000 a second workshop is planned at Los Alamos (funded through LANL-IGPP).

To learn more about LANSCE or the Short Pulse Spallation Upgrade project at LANL please see the web site http://lansce.lanl.gov/overview/index_over.htm.

References:

Bennett K., H.-R. Wenk, W.B. Durham and C.S. Choi (1994). Texture analysis of high-pressure low-temperature ice polycrystals: a study by neutron diffraction, In: *Textures in Geological Materials*, H.J. Bunge, S. Siegesmund, W. Skrotzki and K. Weber (eds.). Deutsch. Gesell. Metallkunde, Oberursel, Germany, 251-160.

Bennett K., H.-R. Wenk, W.B. Durham, L.A. Stern and S.H. Kirby (1997). Preferred crystallographic orientation in the ice I-II transformation and the flow of ice II, *Phil. Mag. A.*, 76, 413-435.

Lutterotti L., S. Matthies, H.-R. Wenk, A.J. Schultz and J.W. Richardson (1997). Combined texture and structure analysis of deformed limestone from time-of-flight neutron diffraction spectra, *J. Appl. Phys.* 81, 594-600.

Von Dreele, R.B. (1997). Quantitative texture analysis by Rietveld refinement, *J. Appl. Cryst.* 30, 577-587.

Wenk H.-R. (1991). Standard project for pole figure determination by neutron diffraction, *J. Appl. Cryst.* 24, 920-927.

Wenk H.-R. (1993). Texture analysis with TOF neutrons, In: *Time-of-Flight Diffraction at Pulsed Neutron Sources*, J.D. Jorgensen and A.J. Schultz. (eds.), *Trans. Am. Cryst. Ass.* 29, 95-108.

Wenk H.-R., S. Matthies and L. Lutterotti (1994). Texture analysis from diffraction spectra, *Proc. ICOTOM 10, Mater. Sci. Forum* 157-162, 473-479.

Zhao, Y., I. C. Getting, R. B. Von Dreele (1999). TAP-98 : A New Design of Toroidal Anvil Press for High *P-T* Neutron Diffraction Proc. Structural Study Under Pressure Using Neutron Sources at The ARAPT-17 International Conference on High Pressure Science and Technology, Hawaii, U.S.A; 25-29 July, 1999.

Acknowledgements

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'SMARTS' Spectrometer for Materials Research at Temperature and Stress

Mark Bourke, Lujan Center and Materials Science Division, Los Alamos National Laboratory, *David Dunand*, Northwestern University, *Ersan Ustundag*, California Institute of Technology

Origins

Over the last 15 years the use of neutron diffraction to study deformation in engineering components has increased dramatically because of the unique insights that can be obtained by virtue of the deeply penetrating property of neutrons into most structural materials. The interest is driven by a variety of practical problems: residual stresses in critical components, discrete phase deformation, load transfer in composites, stress evolution during temperature (or pressure) fabrication, and strain development during reduction, oxidation or other phase transformations. All of which impact the structural robustness of components that range from composites containing micron sized reinforcement particles to welds in aerospace components that may weigh hundreds of Kg.

In the simplest neutron diffraction strain measurement elastic strains are inferred from changes in interplanar lattice spacings that result from applied or residual stresses. (The interpretation of these data can be complicated by variations in the chemical composition of the sample or systematic problems associated with the experiment setup). By virtue of their weak interaction with matter, neutrons provide a non-destructive, bulk probe that both enhances and is complementary to measurements that are more widely accessible but suffer from greater experimental ambiguities. Seminal neutron diffraction measurements include studies on critical parts like welds in reactor pressure vessels (or NASA rocket boosters), fundamental studies recording co-deformation behavior under a range of conditions in composites like Ti-SiC, W-Fe, Cu-Nb or Be-Al and studies of stress-induced phase transformations in shape-memory alloys like NiTi.

At Los Alamos National Laboratory (LANL), the instrument most commonly used for "engineering" strain measurements has been the neutron powder diffractometer (NPD). Indeed the percentage of beam time used on NPD for studies of engineering materials increased from 30% in 1990 to almost 90% in 1997. Whereas NPD can address many interesting issues, it was designed for conventional powder diffraction measurements, thus, for many engineering problems it is compromised by limited access, neutronic performance and detector configuration. Consequently, in 1997 a spectrometer development team proposed the construction of SMARTS which was subsequently approved and funded by the DOE Office of Basic Energy Sciences through the Short Pulse Spallation Source Enhancement Project at LANL.

Technical description

The attraction of building a dedicated instrument that is optimized for engineering measurements at a pulsed source is the leap that will be achieved in materials engineering by performing these measurements faster and better than before. The optical components of SMARTS are; chilled H_2O moderator, shutter, guide, T-zero & frame definition chopper, guide, incident collimation, sample, get–lost pipe and beam stop (Fig 1). The sample position is 30.75m from the moderator. The functional features that distinguish SMARTS from NPD are the use of a neutron guide to bring a higher thermal flux to the sample, a large accessible sample cave permitting versatile access for ancillary equipment and samples, and a 6 fold increase in detector solid angle focussed at ±90°.

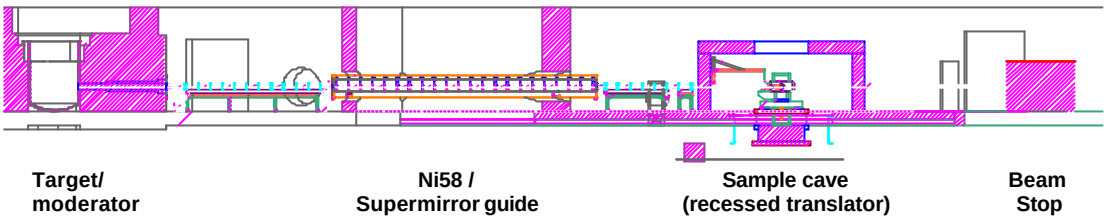

Fig. 1. SMARTS layout (the distance from the moderator to the sample is 30.75m) The location of the T_o and Frame definition choppers (not shown) is 10m from the moderator.

At the heart of the instrument is the sample cave (Fig 2). With approximate internal dimensions of 6x5m, and overhead access through a hatch in the roof it provides enough space to accommodate large objects, as well as allowing the use of permanent theodolites for precision alignment. The translator is recessed below floor level to increase the available height below the beam. The beam enters from the right (in the figure) from the neutron guide. Detector panels are mounted on either side of the translator. The SMARTS load frame-furnace is shown on the translator.

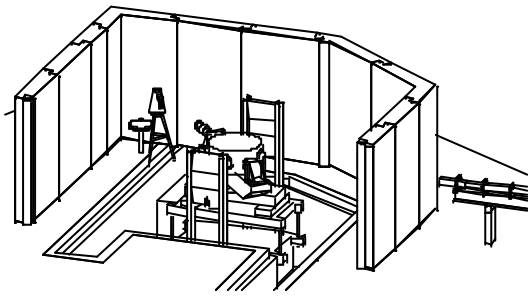

Figure 2; SMARTS cave - cutaway view.

SMARTS team

The concept for SMARTS was initially articulated by Mark Bourke (LANL), David Dunand (Northwestern University) and Ersan Ustundag (Caltech). However a project of this magnitude requires much more input and accordingly a spectrometer development team was formed (Fig 3). The team comprises players from a range of academic and industrial institutions; Bob Asaro (UCSD) Hahn Choo (LANL), Bjorn Clausen (LANL), Mark Daymond (ISIS), Ray Green (LANL), Tom Holden (AECL), Cam Hubbard (ORNL), Bimal Kad (UCSD), Aaron Krawitz (MURR), Phillip Nash (IIT), Cev Noyan (IBM), Mike Prime (LANL), Partha Rangaswamy (LANL), Jim Richardson (ANL), Ravi Varma (LANL), XunLi Wang (ORNL), Andy Winholtz (MURR), Ken Wright (G.E.).

Fig 3 ; The SMARTS – spectrometer development team at the "kick-off" meeting.

Features

Two SMARTS features are worthy of explicit note; the load frame-furnace and the data analysis / acquisition system (called SMARTS –EXPERT).

Performing *in situ* deformation measurements provides insights into strength and failure mechanisms. Moreover by performing measurements at extreme temperatures, neutron diffraction can provide unique insights into regimes that have only been partially studied to date. Accordingly a significant component of the SMARTS design effort addresses a dedicated load frame integrated with a vacuum furnace. The load frame with a 180KN load capacity is currently under design. Specific technical constraints of concern are to provide unobstructed access to the sample by the neutron beam and to minimize the weight of the load frame so that it can be accurately positioned using a translator. The associated vacuum furnace is also under design with an anticipated maximum operating temperature of 1500°C and operating pressures between 510^{-6} torr and 2PSIG. It can also operate in air, utilizing interchangeable heating elements for different atmospheres. The hot zone will be about 100mm x 150mm long.

An engineering strain spectrometer is often used as an industrial tool providing information for materials development. As such the user base is often relatively new to neutron scattering and a principal design goal will be ease-of-use, both for ergonomic experiment set-up and for data acquisition and processing. Consequently we anticipate that SMARTS will use an expert system as a user interface in which a neophyte user can analyze data simply and efficiently in real time, and which also offers a range of options for monitoring the results, from a birds-eye view to a close-up. This system is under design at present under the guidance of Cev Noyan from IBM.

Value and performance

Properties like durability, fatigue, fracture toughness and strength are all affected by the presence, sign and magnitude of residual stresses, thus their measurement and prediction are of great importance. The ability to control, measure and predict residual stresses is critical in processing, stress relief, heat treatment, lifetime prediction and alloy design. Consequently the ability to non-destructively probe the strains in the center of a metallic component, up to an inch thick, is attractive. SMARTS will be installed on flight path 2 at the Lujan Center at Los Alamos. Following the current accelerator upgrade, LANSCE will operate at an average current of 200μA. The increase in available neutron flux, coupled with the refinements described above, imply that SMARTS performance should be qualitatively better than NPD by a factor of 30 to 50. Moreover SMARTS will open up high and low temperature deformation regimes hitherto impossible to study as well as offering $1mm^3$ spatial resolution for macrostrain measurements.

Construction Timeline

At the time of writing (May '99), the SMARTS engineering design is largely complete. The guide has been ordered, and the translator is under contract. Many other components have been ordered. The instrument is projected for a commissioning start early in 2000.

Acknowledgements

Engineering design of a new spectrometer of this magnitude involves many people working in a concerted team effort. Specific recognition is due to; Joe O'Toole, Mark Taylor, Ben Etuk, Cathy Chapman, Joe Balderas, Kathy Lovell, Gene Gould, Bob Catherwood and John Goshen.

OSIRIS: First of a New Generation

David Martin y Marero, ISIS Facility, Rutherford-Appleton Laboratory

The OSIRIS Project was initiated to explore new methodologies using Cold Neutrons on Pulsed Sources, in particular the uncharted territory of long wavelength high resolution diffraction [1]. Designed and built by David Martín y Marero at the ISIS Pulsed Source, OSIRIS constitutes the first member of a new generation of powder diffractometers. It builds on pioneering work by Colin Carlile on the IRIS spectrometer and takes full advantage of the unexpected high levels of cold neutrons on the ISIS Pulsed Source.

The aim of providing a high resolution instrument with enough intensity to study systems as a function of thermodynamic parameters or time evolution, implies the use of a carefully designed neutron guide. The neutron guide has a supermirror multilayer coating of nickel and titanium (m=2) and constitutes the first supermirror guide at ISIS. At the exit, the last metre and a half of the 32 metres guide is a supermirror converging guide with "m" increased from 2 to 3.6 [1]. The OSIRIS primary flight path starts from the same beam hole as IRIS in such a geometry that no reduction in intensity at the IRIS sample position is caused. Figure 1 shows the measured flux.

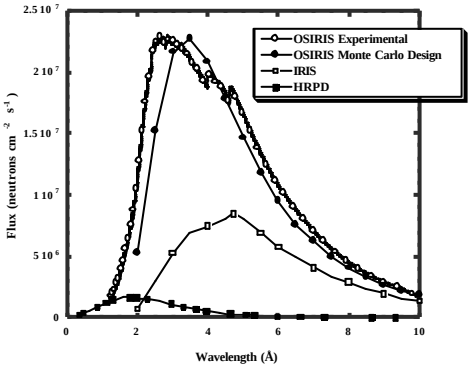

Fig. 1. Flux comparison at ISIS for different instruments.

As is traditional with ISIS diffractometers, one of the first compounds to be studied was FeAsO4 [2] in collaboration with Paul Attfield's group from Cambridge University. We carried out preliminary investigations of the variation of this magnetic structure with chemical doping. Three samples were studied, $FeAsO_4$, $(Ga_{0.08}Fe_{0.92})AsO_4$ and $Fe(P_{0.08}As_{0.92})O_4$, down to temperatures of 2K using a standard orange cryostat. The magnetic structure is incommensurate with a propagation vector of $(k_x,0,k_z)$ in the ac plane of the monoclinic unit cell. Rietveld refinements were carried out which indicate that the propagation vector changes significantly with doping (See figure 2).

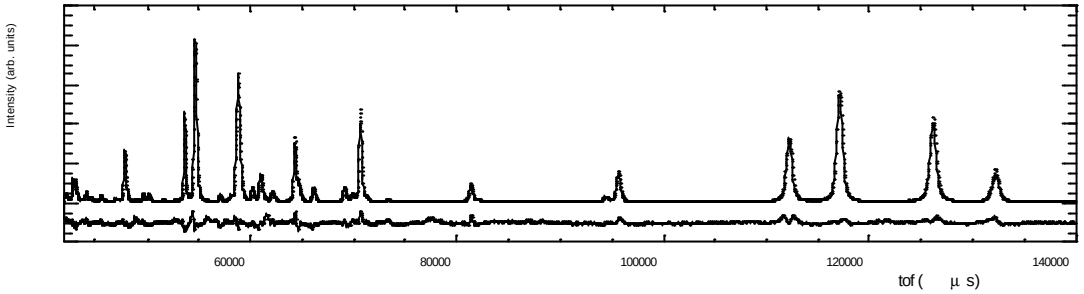

Fig. 2. Rietveld fit using GSAS for $Ga_{0.08}Fe_{0.92}AsO_4$.

Another collaboration, this time with Prof Keith Ross' group from Salford University, concentrated in the technologically important compound $LaNi_5$. This system is the parent compound of a set of AB_5 materials (A: mischmetal, B: Co, Mn or Al) that are currently under study to provide new electrodes material capable of sustaining higher charge/discharge currents/unit mass than its predecessors. We were able to study the change in microstructure and site occupancy as a function of cycle of the deuterium load and as a function of deuterium concentration.

This will help to explain the mechanisms of hydrogen diffusion in the hydride electrode and indicate new avenues to achieve a considerable higher hydrogen absorption rate. Figure 3 shows the diffraction patterns for three different concentrations during the same cycle. Work with the late Prof H. Ikeda's group from KEK, demonstrates the unique capabilities of the instrument as

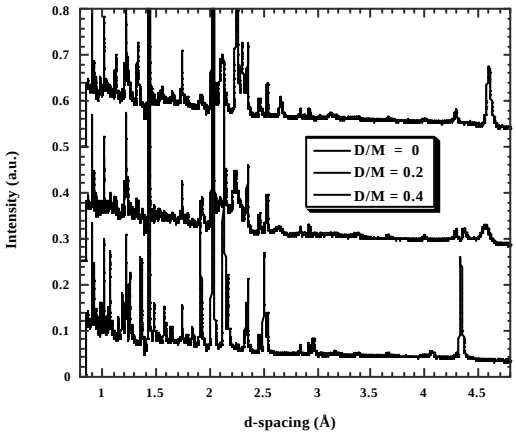

Fig 3. HAK-$LaNi_5$ for different concentrations.

shown in figure 4. Evidence for a crossover from a self-similar fractal structure to a homogeneous structure is revealed by the intensity distribution of the magnetic elastic scattering of neutrons near the superlattice position in the two dimensional diluted Ising antiferromagnet $Rb_2Co_cMg_{1-c}F4$. Only on OSIRIS these dramatic subtleties can be measured. With its combination of broad wavelength range, high resolution and high count rate, OSIRIS constitutes the most powerful neutron diffractometer in the world.

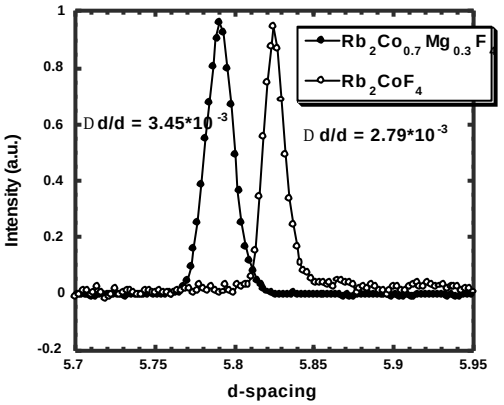

Fig. 4. Crossover from homogeneous to fractal structure.

References:
[1] D. Martín y Marero et al: J. Phys B: Condens Matter, in press (1999).
[2] D. Martín y Marero et al: J. Phys. Soc. Japan 65 (1996), 245-248.
[3] J.B. Forsyth et al: J. Phys B: Condens Matter 11 (1999), 1473-8.
[4] D.K. Ross, Brite-Euram Project Internal Report BE-1403, (1999).
[5] H. Ikeda et al: Phys. Rev. Lett., 64 (1990) 1266.

‘SPODI’ The new structure powder diffractometer at the FRM II in Garching

R. Gilles, University of Technology Darmstadt, *G. Artus*, University of Technology München, *J. Saroun*, Nuclear Physics Institute, Czech Republic, *H. Boysen*, Ludwig-Maximilians-Universität München, and *H. Fuess*, University of Technology Darmstadt

Abstract

SPODI, the Structure POwder DIffractometer, will be installed on beamline SR 8 at the FRM II in Garching. The instrument has been designed to achieve an ideal compromise of good-resolution up to very high 2θ (by using a monochromator take-off angle of 155°) and high-flux with special emphasis on ‘good’ profile shapes and low background. To optimise the parameters of the optical components like coatings of neutron guides, monochromator and soller collimators Monte Carlo simulations were carried out. To check the results of the simulation calculations with two different independent programs (MCSTAS and RESTRAX) were applied. An option for using a Small-Angle Neutron Scattering (SANS) device will eventually be included to perform Bragg scattering, SANS and diffuse scattering simultaneously on the sample.

Introduction

A new powder diffractometer for thermal neutrons will be built on beamline SR 8 at the FRM II in Garching near Munich. It is specifically dedicated for structure determination (including magnetic structure, localisation of light elements and the determination of atomic displacement parameters). Apart from standard powder samples (average particle size diameter a few µm) nanoparticles, polycrystalline sintered compacts or textured materials will be investigated.

Experimental

The main idea of the concept is to optimise the neutron optics of the instrument for the geometry provided in the experimental hall. Fig.1 shows a schematic drawing of the instrument, which is positioned on the left side of the double beam tube SR 8. Two standard monochromator angles 90° and 155°, plus an optional 135° are foreseen. The neutron path from source to monochromator is an evacuated supermirror system with m_v=3 for top and bottom and m_h=2 for sidefaces. The neutron guide is vertically divergent and horizontally parallel. A focusing germanium (551) monochromator with mosaicity 20 ' horizontally and 10 ' vertically will be used to cope with the high monochromator angle of 155°.

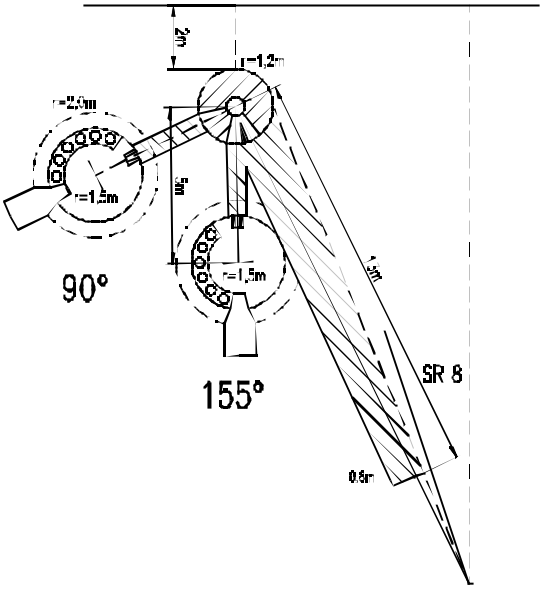

Fig. 1: Sketch of the Structure Powder diffractometer SPODI at FRM II for two optional monochromator angles of 90° and the mainly used angle of 155°.

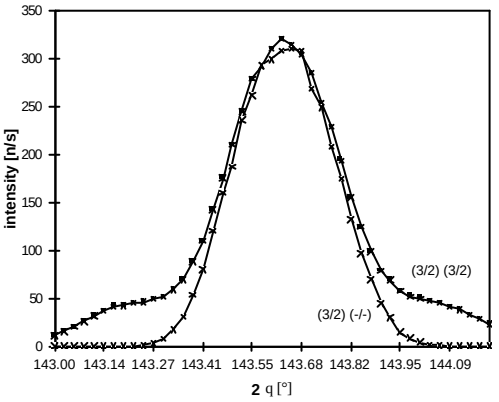

Fig. 2: Influence of secondary guide (monochromator – sample) on profile of Bragg reflection (1 1 15) Al_2O_3.

The monochromator to sample path is equipped with an evacuated beam tube only. As shown in Fig.2 a secondary guide results in a deterioration of the profile quality.
To adjust the resolution, a variable collimator system with 20 ', 10 ' or 5 ' will be installed in front of the sample. The

detector system consists of 64 single He^3 detectors that are position sensitive in vertical direction (300mm height and 25mm wide). This allows a larger part of the Debye Scherrer cone to be included and allows data to be evaluated in selective ways. For example, one can use the middle part of the detector for high resolution or to find exact position of Bragg peaks at small 2θ angles which are normally shifted by the vertical divergence effect (see Fig. 3). Or one can carry out combined fits with several patterns obtained by dividing the detector height into several parts. If good resolution is not necessary the full height with high intensity can be used.

Results and Discussion

For optimization of the neutron optics the programs MCSTAS [2] and RESTRAX [3] based on Monte Carlo simulation techniques were used. To find the compromise of good resolution and high intensity the components of the neutron optics like coating of supermirrors, choice of monochromator crystals, mosaicity of monochromator, divergency range and geometrical space of instrument have been taken into account. Table 1 exhibits an example of flux and intensity calculations up to the sample for a certain instrument configuration. Detailed comparisons of the programs with variations of the neutron optic parameters will be given elsewhere. Small deviations of the results of the programs are mainly caused by different methods used to calculate reflectivity and soller transmission. A flat plateau and homogeneous illumination of the sample results from tilting all single slabs of monochromator crystals in the simulation to optimum values. Bragg profiles of an Al_2O_3 sample were performed to finally optimise all components of the powder diffractometer.

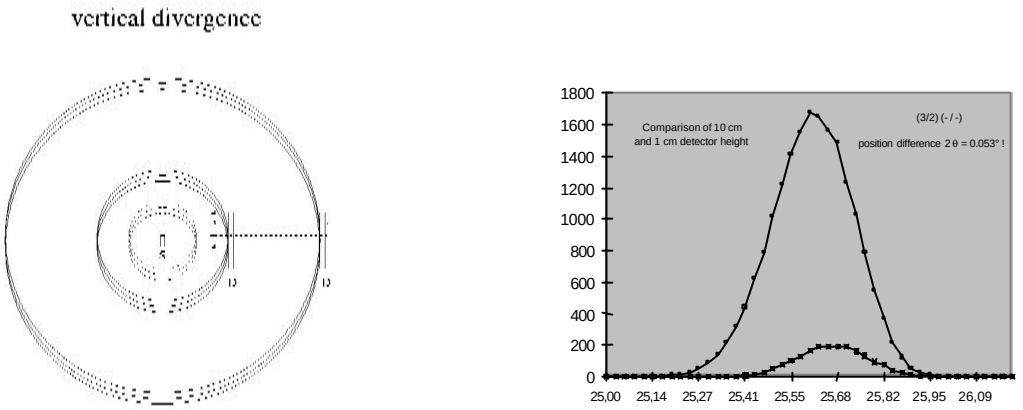

Fig. 3. Shift of Bragg peak position by changing the detector height from 100mm to 10mm resulting from vertical divergence effect.

	MCSTAS	RESTRAX
wavelength λ [Å]	1.5469	1.5469
supermirror (m_v / m_h)	(3/2)	(3/2)
Intensity [n/s]	1.31E+07	1.26E+07
flux [n/s/cm^2]	1.28E+06	1.31E+06

Table 1: Comparison of simulations of intensity and flux in the center of the sample with the programs MCSTAS and RESTRAX for a certain instrument configuration.

Acknowledgement

Financial support of the German BMBF under grant KFZ 03-FU5FRM is gratefully acknowledged. We would like to thank also P. Böni for fruitful discussions of the concept.

References

[1] R. Gilles, H. Boysen, H. Fuess, Proceedings of German Neutron Scattering Conference (1999), Potsdam, 65.
[2] K. Nielsen, K. Lefmann, Neutron Ray-tracing package MCSTAS, Risø National Laboratory, Denmark, (1998).
[3] J. Saroun, J. Kuldar, J. Neutron Research Vol. 6 (1997), 125-133.

WWW SITES OF GENERAL INTEREST TO POWDER DIFFRACTIONISTS

The Commission on Powder Diffraction (CPD)
http://www.iucr.ac.uk/iucr-top/comm/cpd/index.html

The International Union of Crystallography (IUCr)
http://www.iucr.ac.uk/welcome.html

The International Centre for Diffraction Data (ICDD)
http://www.icdd.com

General crystallography:
http://www.unige.ch/crystal/w3vlc/crystal.index.html

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ICDD Fall Meetings

The ICDD Annual Fall Meeting was recently held at ICDD Headquarters in Newtown Square, Pennsylvania. Following a new format, the meeting took place 21–23 October 1999, and assembled the ICDD Board of Directors, the Regional Co-chairs, and the Technical Subcommittee Chairs. The meeting provided an opportunity for these groups to participate in the strategic planning of the organization and to provide input on their respective activities.

ICDD Regional Co-chairs

PPXRD-Pharmaceutical Powder X-ray Diffraction Symposium

On 27–29 September 1999, the ICDD welcomed nearly 100 visitors attending the ICDD's first specialized conference, *The Pharmaceutical Powder X-ray Diffraction Symposium (PPXRD)*. Filled to capacity, ICDD Headquarters' west wing was the venue for scientific interactions, characterized by dynamic discussions and friendly exchanges of ideas among members of the X-ray diffraction and pharmaceutical communities.

Symposium registrations totaled 79; 16 invited speakers contributed to the total attendance of 95. Attendees represented nine countries including France, Germany, India, Israel, Italy, South Africa, Spain, United Kingdom and the U.S.A.

The technical program featured sessions on:

- Acquisition and Use of X-ray Powder Diffraction Data
- Polymorph Characterization by XRPD
- Structure Determination, Indexing and Molecular Modeling
- Pre-Formulation, Formulation, Patent & Regulatory Issues

Following the symposium, 38 of the PPXRD participants attended a workshop on *Structure Determination* on Thursday, 30 September. The workshop featured hands-on use of *Cerius2* and *Powder Solve*, Molecular Simulations Inc.'s software programs for display and determination of structures from powder data. Demonstrations of the Cambridge Structural Database were also included in the workshop.

Due to the overwhelming number of positive responses, the PPXRD will be repeated next year, tentatively scheduled for September 2000 in Europe. Monitor www.icdd.com/ppxrdsymp for updated information.

First International Workshop on Powder Diffraction

The ICDD will sponsor an *X-ray Powder Diffraction Workshop* at St. Helens College, Merseyside, U.K., 6–8 December 1999. The first in a series of international workshops, the seminar will focus on the basis of X-ray powder diffraction, ways of obtaining good quality experimental data, the role of the ICDD and the Powder Diffraction File®, qualitative and semi-quantitative analysis, the use of reference intensity ratios, and exercises using PCPDFWIN® and PCSIWIN®.

Awards and Presentations

The Distinguished Grantee Award was presented to Professor Ekkehart Tillmanns at the ICDD Spring Meeting in March for his contributions to the Powder Diffraction File® as a grantee and ambassador for the ICDD. Information about the ICDD's Grant-in-Aid Program is available at www.icdd.com or e-mail info@icdd.com.

The ICDD recently elected Professor Doctor Walter Eysel to join the astute group of ICDD Distinguished Fellows, in recognition of his sustained, outstanding contributions to the International Centre for Diffraction Data.

The 1999 Barrett Award was presented to Howard F. McMurdie at the 48th Annual Denver X-ray Conference, 4 August 1999, in Steamboat Springs, Colorado. The Barrett Award is presented biennially at the Denver X-ray Conference (DXC) to recognize scientific achievements and contributions to the field of powder diffraction. DXC information can be obtained at www.dxcicdd.com.

COMPUTER CORNER

Updates on Freely Available Crystallography and Powder Diffraction Software

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WWW: http://www.ccp14.ac.uk

Software presented in this section is a selection and a minor subset of freely available programs that can be evaluated at anytime by downloading off the internet using the given internet address and CCP14 software mirrors. The 'Computer Corner', which is meant to be a regular submission to the CPD newsletter, is dedicated to short reviews of new software and updates of existing one. Readers are invited to submit to the CPD Chairman or directly to the Computer Corner Editor, Dr. L. Cranswick, new software updates or information not covered here already.

LMGP suite for Windows by Jean Laugier and Bernard Bochu

This new GUI (graphical user interface) based suite contains **"OrientExpress"** Laue crystal alignment software; **"Equiv"** and **"Indx"** spacegroup software, **"Wulff"** wulff net generation software, **"Dispano"** anomalous scattering factor software, **"Celref"** unit cell refinement software and **"Poudrix"** powder pattern calculation software. Celref is a graphical unit cell refinement program that can read in a variety of raw data and peak profile formats, calculate peak positions based on the space group and has automatic matching of observed to calculated peaks making it very easy and quick to start performing unit cell refinements on new samples. It's ability to generate lines based on the spacegroup also means it can be use to help identify a spacegroup after indexing of an unknown powder.

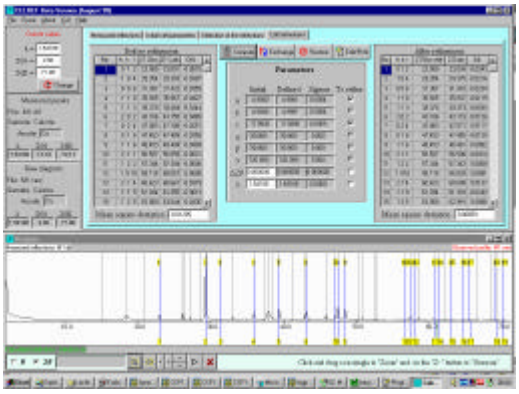

Fig 1: Celref unit-cell refinement interface.

The Poudrix simluates powder diffraction patterns and can open Shelx, ICSD and Powder Cell structure files. It can also use in-built databases of "Brenann and Cowan or Sasaki" Anomalous Dispersion data to calculate the contribution of f' and f" and the user can include parasitic Beta or Tungsten lines for laboratory instruments. Raw or previously calculated data files can compared with calculated profiles and patterns can also be displayed in Q space. While PowderCell for Windows software by Krause and Nolze (refer: *http://www.ccp14.ac.uk/tutorial/powdcell/*) can quickly put a structure through classical phase transitions and multiple phase situations, Poudrix can accurately simulate synchrotron X-ray powder patterns where f' and f" are important. Evaluating both freely available powder pattern simulation programs is highly recommended as you may find both extremely useful. The LMGP homepage is at *http://www.inpg.fr/LMGP/* while software tutorial and download information is at:
http://www.ccp14.ac.uk/tutorial/lmgp/

Fig 2 : Poudrix powder diffraction pattern calculation interface

Powder v2.0 (Sequel to "Convert") for Windows by Nita Dragoe

The website for Powder has moved recently to *http://www.chem.t.u-tokyo.ac.jp/appchem/labs/kitazawa/dragoe/software.html* (as well as being mirrored on the CCP14). The new "Powder" not only does powder data conversion but GUI based unit cell refinement (including Energy Dispersive Diffraction Data), powder pattern processing (background strip, alpha 2 strip, peak find) setup input files for common indexing programs as well as extra functionality.

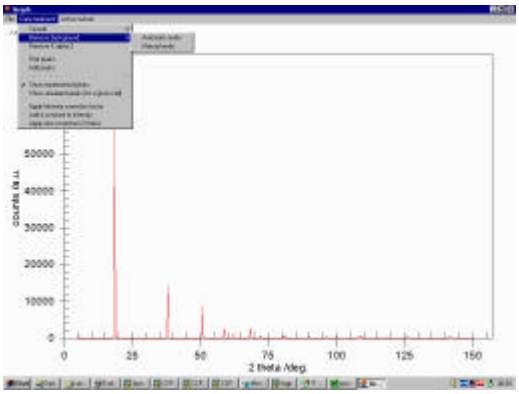

Fig 3: Powder v2.0 powder diffraction toolkit in action.

Beta version of GFOUR for Windows Fourier Map plugin for Fullprof Rietveld by Javier Gonzalez and Juan Rodriguez - Carvajal.

A new plugin for Fullprof is the GFOUR Fourier Map for Windows generation and viewing program which can be downloaded from its home site at *ftp://charybde.saclay.cea.fr/pub/divers/progs_pc/fourier/*, or CCP14 mirrors. Amongst its abilities, GFOUR can overlay atom labels on the Fourier map and pan through the slices using the GUI icons. As Juan mentioned during the ILL Powder Diffraction workshop earlier this year, these types of programs can be used with any Rietveld that supports the basic formats used by these software packages.

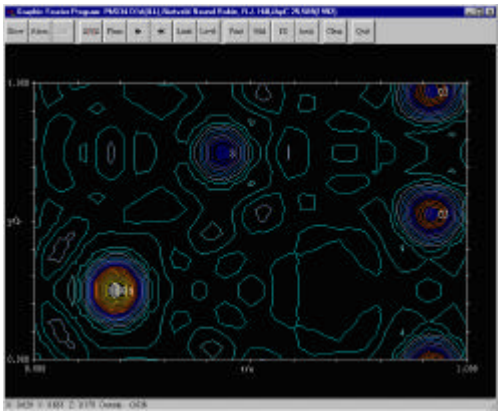

Fig 4: Example of GFOUR program panning up through Fourier slices.

CRYSFIRE (CRYS2RUN of old) Powder Indexing Suite Update by Robin Shirley

By the time this newsletter gets to print, there should be an update of Robin Shirley's CRYSFIRE Powder Indexing Suite for PC at *http://www.ccp14.ac.uk/tutorial/crys/*. Crysfire now links into 8 different indexing programs, **ito**, **dicvol**, **treor**, **lzon**, **taup**, **kohl**, **fjzn** and **losh** and can summarize in a single file, one result per line from all the above indexing programs. The update version will now permit 200 observations, has more appropriate defaults for **dicvol,** a new version of **losh**, better pattern editing for creating subsets of peaks and minor bug fixes. People at the CRYSFIRE demonstration at the Software Fayre during IUCr Glasgow 99 would have seen it successfully index some protein powder diffraction data provided by Bob von Dreele.

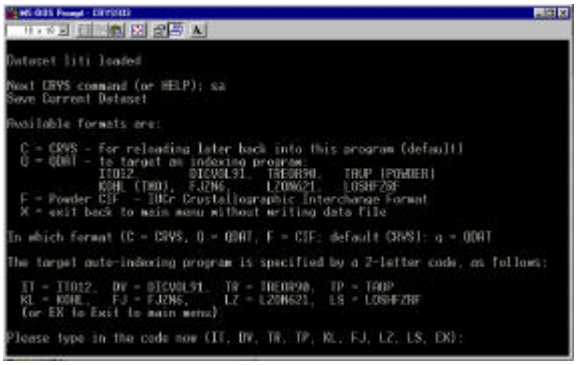

Fig 5: While in CRYSFIRE, about to target and run one of the 8 supported indexing programs.

Cryscon for Windows Shareware by Eric Dowty

Cryscon is a new piece of shareware software that will import and export structures in different structure formats such as Shelx, GSAS, DBWS, CIF, ICSD, Fullprof, Rietan,

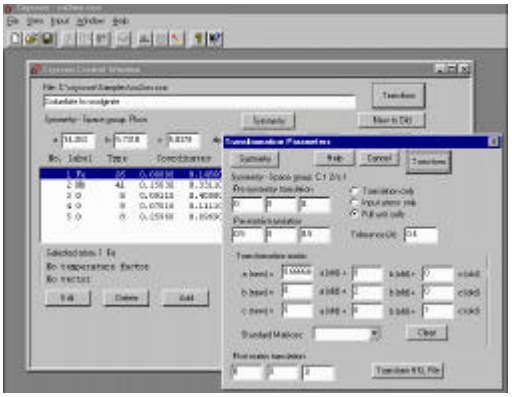

Fig 6: Cryscon structure interconversion and transformation interface

etc. It will also perform structure transformations via a GUI interface; but still allowing complete control on such parameters as pre and post translations. If going from a lower to higher symmetry space group, Cryscon has the option to merge atoms within a user specified distance and to populate the unit cell in various ways making it a very useful tool for generating trail models based on known structures. Cryscon can use the structures to calculate powder patterns and single crystal precession simulations. It is downloadable from *http://www.shapesoftware.com/#anchor_cryscon*.

Resources on the Web for Bob von Dreele and Alan Larsen's GSAS

A large number of resources based around GSAS are available off the internet via *http://www.ccp14.ac.uk/solution/gsas/*. This includes the availability of the new beta version of GSAS released in July 1999. Resources include structure viewing programs that import GSAS files (such as GUI WinOrtep and GUI WinStruplo). There are multiple programs to convert GSAS plot files into ASCII formats suitable for scientific graphing. There is also a link to Brian Toby's Tcl/Tk based GUI interface for GSAS which works on UNIX and PC.

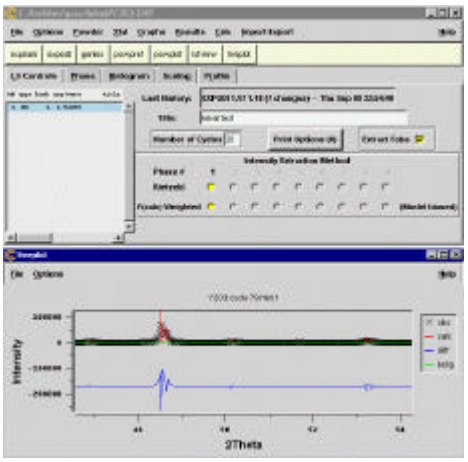

Fig 7: EXPGUI GSAS interface with "liveplot" window open while starting on a Le Bail extraction.

Platon/"System S" Structure Checking and Single Crystal Suite by Ton Spek

A program that should be part of any crystallographer's toolkit is the Platon software by Ton Spek at *http://www.cryst.chem.uu.nl/platon/*. Platon functionality includes the addsym algorithm to check for extra symmetry in the structure; automatically generating CSD Cambridge Database queries to check if the structure has been solved already or vet related structures, ORTEP plots and Povray output for generating photorealistic images of crystal structures.

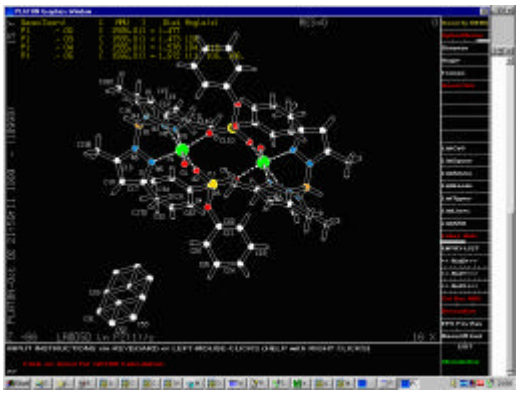

Fig 8: Interactively investigating a structure in Platon and interactively obtaining bond length and angle information by clicking on atoms of interest.

For Any program that can output a legitimate Shelx, CIF or native Platon file can immediately have access to this functionality. Basic run throughs on Platon are available at the above Platon site or in the CCP14 tutorials area at *http://www.ccp14.ac.uk/tutorial/platon/*The UNIX version of Platon also has "System S", a structure solution and refinement suite that links into 5 structure solution packages (Shelx97, Shelx86, Sir, Crunch and Dirdif) which can be highly useful for people trying to solve structures from powder data. If already a Windows PC user, it is not that difficult to get a dual boot Windows/(freeware UNIX: Linux or BSD UNIX) system installed. Webpages on creating dual boot PC systems for crystallographic usage are available via *http://www.ccp14.ac.uk/solution/linux/* and *http://www.ccp14.ac.uk/solution/bsdunix/*. Linux is probably the best option at the moment for a client based UNIX style operating system on PC but the BSD based UNIX's are a very credible alternative and have a much better reputation for security to limit hacker intrusions.

Useful non-Crystallographic Utility Software

Whether it is grinding through a thousand or so energy dispersive powder patterns, watching refinement cycles go by or setting up complex constraints, the hours, days, months spent on these activities can seem more pleasant when listening to some music. Most modern computers give the option of listening to a music CDs via the CD-ROM (using earphones if sharing an office or slumming it in an open plan area). A very nifty bit of free software is the "EasyCD" audio CD player by Linas Purinis and is downloadable from the internet at *http://www.is.lt/linas/easycd/*.

EasyCD is the Platon of Windows audio CD players; not only allowing complete control of playing order, keyboard hot keys for those who dislike computer mice, different "skins" interfaces, and the ability to connect to a CDDB (CD Audio Database) server on the internet to automatically grab the CD title and track information for a new audio CD.

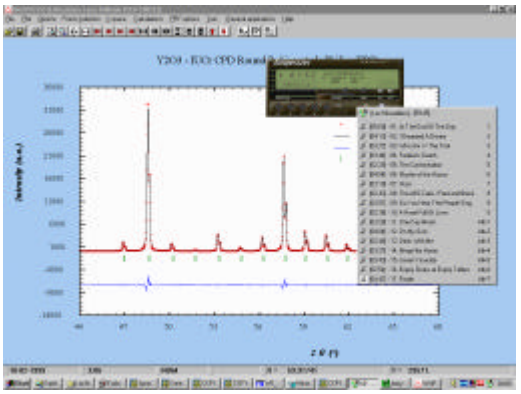

Fig 9: Optimising the EasyCD play list while Winplotr/Fullprof'ing away in the background

Lachlan (E-mail: L.Cranswick@dl.ac.uk)

WHAT'S ON

Structural Characterization of Amorphous and Nanocrystalline Materials, Ismailia, Egypt, 22-27 January 2000.
http://biohome.aucegypt.edu/cnfrnce2000/conf2000.html

21st meeting of the Society of Crystallographers in Australia (SCA), Thredbo, New South Wales, 1st-4th February 2000
http://rsc.anu.edu.au/~welberry/crystal21/

NOBUGS-III (New Opportunities for Better User Group Software) conference, Chester, UK, 12th - 14th April 2000
http://srs.dl.ac.uk/nobugs/nobugs3/

EPDIC-7, 7th European Powder Diffraction Conference, Barcelona, Spain, 20th-23th May 2000.
http://icmuix.icmab.es/epdic7/

A Short Course on Rietveld Analysis, Atlanta, GA, USA, 14-16, June, 2000.
http://www.chemistry.gatech.edu/~angus/short_course/frame_set.html

ACA2000 - American Crystallographic Association Annual Meeting, St. Paul, Minnesota, 22-27 July, 2000.
http://www.hwi.buffalo.edu/ACA/ACA-Annual/StPaul/StPaul.html

The 49th Annual Denver X-Ray Conference, ***X-ray Analysis in the 21st Century*** Denver, CO, USA, 31 July-4 August, 2000
http:// www.dxcicdd.com

ECM 19 - 19th European Crystallographic Meeting, Nancy, France, 25th - 31st August 2000
http://www.lcm3b.u-nancy.fr/ecm19/

20th Conference on Applied Crystallography, Hotel "Stok", Vistwa, Poland, 4-7 September, 2000
http://www.us.edu.pl/uniwersytet/konferencje/2000/cac/tekst/index.shtml

International Workshop on Rietveld Refinement, Hotel "Stok", Vistwa, Poland, 8-10 September, 2000
http://www.us.edu.pl/uniwersytet/konferencje/2000/cac/tekst/index.shtml

IWPCPS-1 1st Int. Workshop on Physical Characterization of Pharmaceutical Solids, Lancaster PA USA, 24-29 Sept., 2000
http://www.assci.com/~marekz/IWPCPS-1.htm

VII Workshop Structure Determination and Refinement from Powder Diffraction Data, Bayreuth, Germany, 4-8 Oct., 2000
http://www.uni-bayreuth.de/departments/crystal/workshop2000

ICDD Clinics:

X-ray Powder Diffraction Workshop, St. Helens College, Merseyside, U.K., 6–8 December 1999
http://www.icdd.com/education/clinics/

Advanced Methods in X-ray Fluorescence Spectrometry, ICDD, Newtown Square, Pennsylvania, U.S.A., 8-12 May 2000
http://www.icdd.com/education/clinics/

Fundamentals of X-ray Powder Diffraction, ICDD, Newtown Square, Pennsylvania, U.S.A., 5-9 June 2000
http://www.icdd.com/education/clinics/

Advanced Methods in X-ray Powder Diffraction, ICDD, Newtown Square, Pennsylvania, U.S.A., 12-16 June 2000
http://www.icdd.com/education/clinics/

Call for contribution to the next CPD Newsletter (No 23)

The next issue of the CPD Newsletter will be edited by Bob Cernik and Ian Madsen, to appear in May of 2000. They 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 news of general interest. Please send articles and suggestions directly to one of the Editors. Software developments can be directly addressed to Lachlan Cranswick or to the Editors (addresses are given below)

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