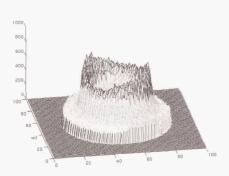


### **COMMISSION ON POWDER DIFFRACTION**

International Union of Crystallography

NEWSLETTER No. 19, Christmas 1997

## INDUSTRIAL APPLICATIONS OF POWDER DIFFRACTION by P. Scardi, A.Gualteri, M. Bellotto



Pole figure diagram during wear testing (see page 3)

Powder diffraction is known as a powerful and versatile analytical technique, whose application ranges from basic science research, to technological studies and industrial quality control. In spite of this huge application field, the connection between people engaged in research and development of the technique, and industrial users is very often unsatisfactory. This can lead to a low-level use of PD, especially when companies do not own a R&D team with specialists in PD, which is more a rule than an exception. The full potential of PD is hardly exploited in the industrial field, and this represents a lost opportunity for the industrial users as well as for research teams **working** at PD.

What is missing is very often the linkage between people **working** in the industry, who currently handle real production problems, and scientists, most of them living in academic institutions and fully engaged in researches apparently far from applications. Therefore, we cannot simply state that industry is not aware of PD uses and potentiality; in fact, we must recognise that many PD researchers are symmetrically not aware of the many practical uses of PD in the technological context, and how near they are to these applications. Moreover, all these people hardly find opportunities to meet and know each other: congresses and scientific meetings are attended by a limited number of industrial users, and scientific literature is regarded (and probably it is) as too complex, cryptic and unoriented to be profitably read by non-specialists.

Initiatives to reduce the gap between research and industrial users are not easy to conceive and to carry out. Nevertheless, the CPD can play an important role, at least in stimulating powder diffractionists to consider practical applications of their techniques. The present issue of the CPD newsletter proposes a few examples, prepared according to the philosophy of showing how common PD methods can be directly used in the industrial context, based on real cases of research-industry collaborations in Italy. The aim was to underline the practical interest of the industrial customers, concerning measurements that can be performed by most PD instruments widely distributed in laboratories all around the world. Only a couple of more 'sophisticated' PD applications, involving non-conventional sources, were proposed. This was to underline the feasibility of many measurements of technological concern, with a correct balance between lab instruments and special facilities. Therefore, the following cards are not all prepared from cutting edge researches in PD (even if they are not so far and obsolete), but show some vital examples of technological transfer of the PD methods.

Industrial awareness of PD is a different and more complex thing. First of all, existing and potential industrial users are a much wider and disperse community with respect to diffractionists. Powder diffractionists can be easily reached

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by the CPD, as well as by other scientific organisations and initiatives: the same is not true for industrial users. PD is not immediately visible to industry.

The present initiative intends to stimulate a large number of powder diffractionists to look around and put themselves forward as reference point for PD applications in technology. The CPD can play the important role of connecting people, but is well aware that the complex problem outlined so far can only be tackled involving the local scientific community. Two points are particularly relevant: **a**) most users wish to work with researchers from the same country, speaking their own language; **b**) PD uses cannot be proposed in the traditional way of the scientific literature. Therefore, it is necessary to create a network of PD scientists, organised in each country, who refer to some technical body or authority, dealing with industrial associations, and produce and spread specifically designed literature to present uses of PD in the industrial context.

### TEXTURE

## HTC SUPERCONDUCTING THIN FILM TECHNOLOGY

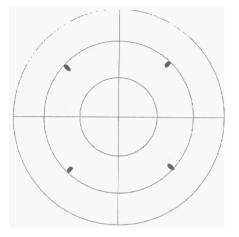


Figure 1.YBCO/NdGa03 (single-crystal) c-axis growth with a high degree of epitaxy ((102) YBCO pole figure.

Besides the well-explored applications in microelectronics, high-Tc superconductor thin films have many other potential applications, including the fabrication of superconducting tapes with high critical current density (Jc) for high field magnets and high current power transmission cables. Jc values above 106 A/cm2 would be requested. Texture analysis is routinely used by scientists and technologists to look for better growth conditions of thin films. Figure 1 shows the (102) pole figure of a YBa2Cu307-d (YBCO) thin film epitaxially grown (c-axis) on a NdGa03 single-crystal [1]; considering that Jc strictly depends on grain structural quality and orientation, it is highly desirable to produce the same type of texture on

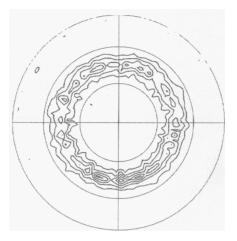


Figure 2. YBCO/YSZ/C-276 (cold-rolled Nibase alloy). c-axis growth, fibre texture ((103) YBCO pole figure.

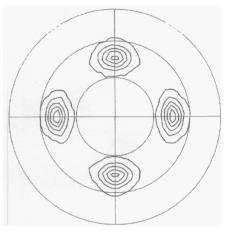


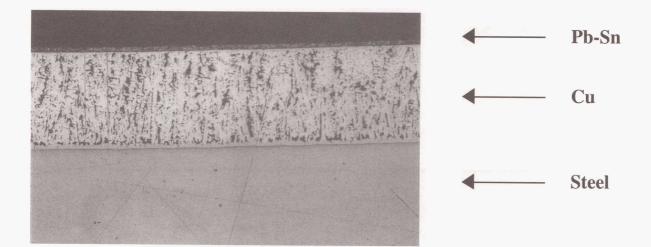
Figure **3.** YBCO/YSZ/Ni (96% cold-rolled Ni foil). c-axis growth and in-plane texture ((103) YBCO pole figure.

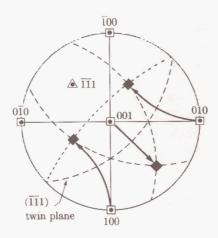
metallic tapes. Texture analysis is crucial in this technological transfer process. As shown in Figure 2, YBCO grown on a cold-rolled Ni-bas alloy is c-axis oriented, but doesn't show the required in-plane order (i.e., it has a fibre texture); this can be achieved by using highly cold-rolled Ni substrates with a Yttria-Stabilized-Zirconia (YSZ) buffer layer. In fact, polycrystalline Ni assumes a strong [200] texture after cold rolling, thus promoting [200] YSZ growth and consequently a c-axis YBCO orientation. As shown in Figure 3, present results are qualitatively good, but further efforts are necessary to improve epitaxy and Jc accordingly [2].

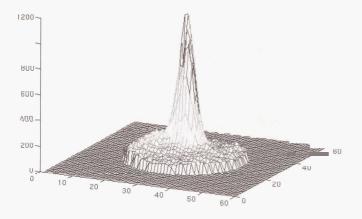
## **SLIDING FRICTION BEARINGS**

Texture analysis is essential to many materials applications in metallurgy and mechanical industry. Here it was used for the design of high performance sliding friction bearings for racing car engines. The aim was to improve the wear resistance of the bearings, acting on the layer deposition process. Fig. 1 shows the (200) pole figure for an asdeposited fcc Pb-Sn top layer, where the main [200] orientation is clearly visible. The evolution of the texture after wear testing (Fig.2) was explained in terms of a deformation twin generation, as shown by the stereographic projection in Fig. 3: the shear stress produced by the sliding friction testing produced a [221] texture, allowing a beneficial energy dissipation mechanism. Therefore it was proposed to make a Ni film, between the intermediate copper layer and Pb-Sn, whose effect was twofold: diffusion barrier to avoid Cu contamination, and buffer layer for a better [200] oriented Pb-Sn growth [3,4].









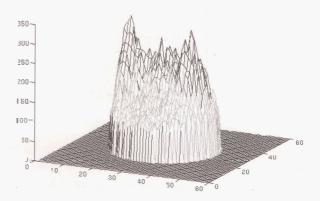


Figure 1. (200) pole figure for an as-deposited fcc Pb-Sn layer

Figure 2. (200) pole figure after wear testing

## SURFACE RESIDUAL STRESS IN TI-ALLOY COMPONENTS DUE TO POLISHING

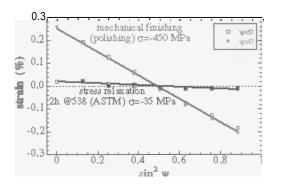


Figure 1. Sin2y plot for a surface polished Ti-alloy component: as polished and after relaxation heat treatment.

Mechanical treatments like grinding and polishing are routinely done on many metal components. The surface of the material is heavily effected, and intense residual stress can be produced. XRD can be used as an effective non-destructive tool for residual stress analysis. The example reported aside, concerns a Ti-6A1-4V alloy component which was polished down to 6 mm diamond paste. A strong compressive stress of ~ -450 MPa was found in the component surface; the XRD technique was also used to follow the stress relaxation process, which was performed by heat treatment in vacuum [4,5].

## RESIDUAL STRESS AT THE INTERFACE OF DIAMOND COATED WC-CO CUTTING TOOLS

One of the main features influencing the reliability of thin films is the adhesion to the substrate, which in turn is strongly dependent by the residual stress field produced during the deposition process or in service. This is particularly important for the application of protective coatings, like those of polycrystalline diamond deposited by Chemical Vapour Deposition on cemented-carbide cutting tools (Figure 1). The traditional XRD residual stress

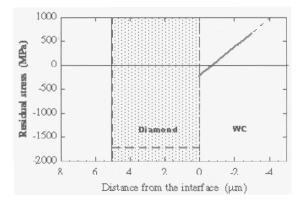


Figure 1. In-plane residual stress in a polycrystalline diamond coating and in the interface region of a WC tool. From data collected at Daresbury SRS, station 2.3.

analysis can be considerably improved by using synchrotron radiation (Figure 2); the possibility to use a perfectly parallel and intense beam with different wavelengths permits to develop suitable models to determine the residual strain gradient through the coating thickness. This is especially important to study the strain field at the coatingsubstrate interface, which is of paramount importance to find out the in-service behaviour [6,7]

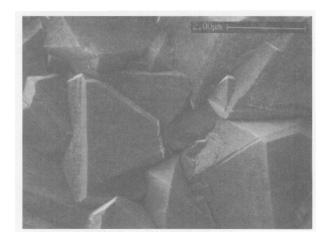
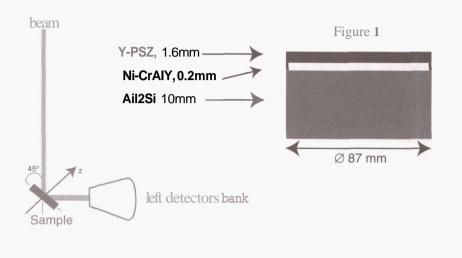


Figure 2. SEM picture of the surface of a polycrystalline diamond coating deposited by Hot Filament CVD. (Courtesy of R. Polini)

## RESIDUAL STRESS GRADIENT IN A AL-ALLOY PISTON HEAD COATED BY Y-PSZ



Another important application field of the residual strain analysis by diffraction techniques concerns thick coatings. In this case, neutron diffraction (TOF data collected at ISIS, on ENGIN) was used to measure the strain field through the entire thickness of an Al-alloy piston head coated by a thick layer of yttriapartially-stabilized zirconia (Y-PSZ) deposited by plasma spray (Figure 1). As shown in Figure 2, it was possible to measure the residual strain along the zdirection, both in the ceramic and in the metal, including a point in the Ni-base bondcoat layer. The measured trend permitted to understand the failure mechanism occurring during the cyclical thermal solicitations typically produced by real service conditions [8].

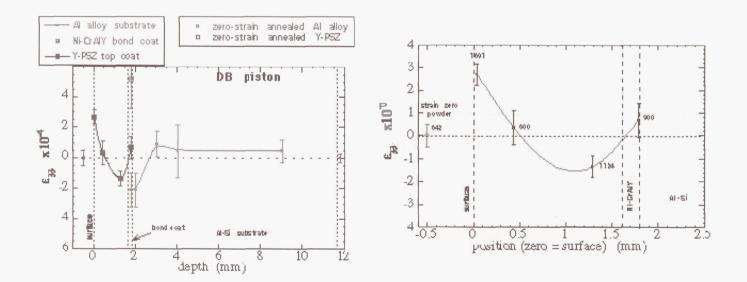


Figure 2.

Residual strain along the axis of the **Y-PSZ** coated piston head (a). A detail of the strain field in the ceramic top coat is reported in (b), together with current data; numbers reported in the plot are current data.

## Surface residual stress in Ti-alloy components due to polishing

The determination of the austenite/martensite phase composition in steel components is among the most frequent and well-known applications of XRD phase analysis in metallurgy. Standard procedures, in use for many years, involved the measurement of peak area from selected reflections from the two phases. As shown in Figure 1, present day approach is based on the Rietveld method, which can be routinely applied to steel components. A typical numerical output is reported in Table 1 and includes, besides phase percentages, information on X-ray density (for each phase and for the sample) and lattice parameters: the former can be compared with other density measurements, to evaluate porosity, whereas lattice parameters may be connected with the alloy content in the

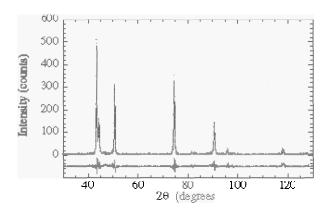


Figure 1. results of whole pattern fitting for a 304 s.s. sample subjected to surface polishing

steel. Recently, a different approach to phase analysis was proposed, which is more appropriate to cases like that illustrated by this example, where the phase distribution in the sample is not uniform. In fact, martensite is likely produced by thermal or mechanical treatments, like in the present case: a surface grinding leads to the formation of a thin layer of martensite on the austenitic steel component. The new algorithm introduced in the Rietveld method [9] permits one to measure the layer thickness directly from the whole XRD pattern refinement; in this way a more interesting information is obtained together with a better agreement with the experimentally measured data.

a) uniform phase mixture:		
Density: 7.9982 g/cm3		
Weight %: 92.7% (1)		
Density: 7.7730 g/cm3		
Weight %: 7.3% (5)		
Density (sample): 7.9818 g/cm3		
۱ I		

*b) two-layer model:* martensite layer thickness (A): 800 (50)

Table I. Results of phase analysis. uniform phase mixture (a) and layer (b) models.

## **GRINDING BURNS IN METAL COMPONENTS**

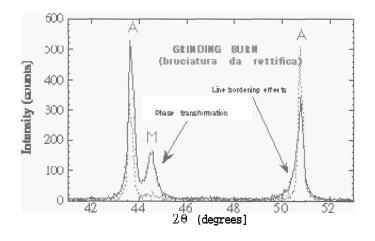


Figure 1. Comparison of XRD patterns of 304 s.s. samples before and after a surface polishing treatment.

The many mechanical machining usually performed on steel components also produce remarkable effects on the microstructure, which can be responsible for frequently unwanted changes in the required properties. Diffraction offers a further control tool, which simply consists in the observation of profile changes after treatments. As shown in Figure 1, grinding burns can be easily detected on a simply qualitative way: a quantitative evaluation can also be performed by one of the well-developed methods of Line Profile Analysis [10,11]. In this way, the microstructural effects of machining can be described in terms of crystalline domain size and lattice distortion due to defects.

## QUANTITATIVE PHASE ANALYSIS OF ASBESTOS CONTAINING MATERIALS

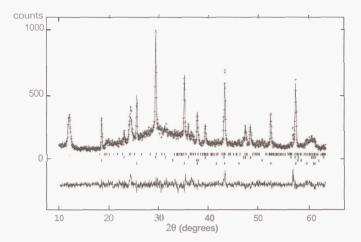
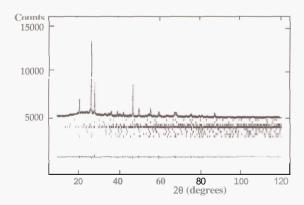


Figure 1. Rietveld refinement [Observed (cross), calculated (full line), and difference curve] of an asbestos containing material from a public parking.

Fibrous asbestos minerals have been identified as priority substances for risk reduction and pollution prevention since their hazardous effects associated with past occupational exposures to asbestos have been definitely demonstrated. In order to limit the exposures of workers and citizens to asbestos, the identification and quantification of asbestos in bulk materials which were utilized in a number of plants and public buildings **is** fundamental for a proper plan of social prevention and general intervention. X-ray powder diffraction is considered as an effective tool of investigation of bulk materials with a highly statistical significance; so far, the application of the combined **Rietveld-RIR** method has been successful for the determination of asbestos minerals in the range 1-50 wt% in bulk materials such as insulating cements, mixed asbestos-slag wools, contaminated soils, and others. The use of the internal standard for the renormalization of the results must be invariably used since most of the materials contain amorphous matter or glass wool. Figure 1 reports the results of a Rietveld refinement of an asbestos material utilized for the insulation of a ceiling in a public parking composed of chrysotile asbestos (11.9(7) wt%), calcite (0.6(1)wt%), brucite (0.6(1) wt%), and glass wool (87(1) wt%) [12].

## QUANTITATIVE ANALYSIS OF CERAMIC MATERIALS



Traditional ceramic components are produced by a single firing process: traditional clay based mixtures are used for wall and floor tile ceramics, oxides mixtures yields pigments, glazes, frits, and glass ceramics. The physical, chemical, and technological properties of these materials are directly related to the phase composition (type of stable and metastable crystalline phases, **crystalline/amorphous** ratio, etc). X-ray powder diffraction has been used since late '50 as the main technique for the identification and tentative quantification of the crystalline phases in such systems; in particular, the variation of the physical properties such as mechanical resistance, water absorption and linear Figure 1. Rietveld refinement [Observed (cross), calculated (full line), and difference curve] of a traditional white paste floor tile ceramic.

shrinkage in temperature is directly related to changes in phase composition and microstructure. An accurate quantitative determination of both crystalline and **amorphous phases** as well as a determination of the some microstructural features is now possible by using the combined **Rietveld-RIR** method. The calculated weights of crystalline and amorphous phases usually display relative errors of -2%.Figure 1 reports the result of a **Rietveld-RIR** refinement of a clay-based white paste floor ceramic where mullite, quartz, albite, and glass have been identified and quantified [131.

## **CLINKER MINERALOGY**

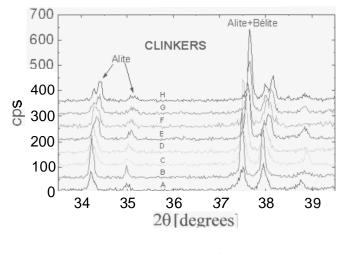
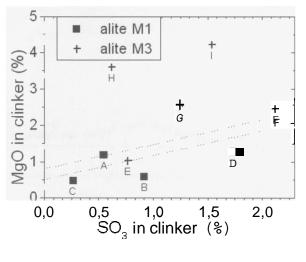


Figure 1

It is nowadays common practice in all cement works to carefully control the chemical composition of the raw feed. This practice is dictated by the strict normative requirements which impose to keep the clinker composition within narrow limits. In some production sites this control is pushed to the limit of bypassing the step of homogenization of the raw feed within specially built silos, and the matter flows directly from the grinder to the kiln. To achieve this an XRF spectrum is recorded each 5 min., and the signal is fed back to the grinder input.

Clinker mineralogy, on the other hand is not routinely controlled, but at most verified 'post mortem' in the case of plant disfunctioning. Yet the XRD diagram of clinker (and even that of the resulting Portland cement) is full of information which can be exploited in the control of the firing process. Differences in the structure of alite from





different production sites (presence of the M1 or M3 polymorph), shown in Fig. 1, are well related to the chemistry of the raw feed as shown in Fig. 2, and to the firing cycle, and have marked influences on the performance of the final product. Similarly the aluminate phases show clear-cut differences between production sites, as shown in Fig. 3.

Push-button Rietveld quantitative analysis of clinker and Portland cement is going to became the best mineralogy control choice, and is going to be transferred to production sites. To do this it is most probably needed to design a specially built acquisition system. The use of the data thus obtained in process control will need a long experience to be acquired, but if successful it will be the first example (to the author's knowledge) of a crystal-structure based feedback control loop.

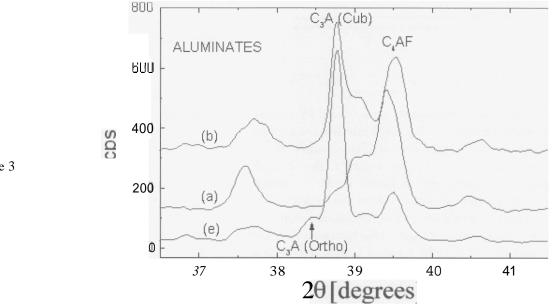


Figure 3

## **GRINDING OF RAW FEED**

In cement production the raw feed grinding stage is of the utmost importance, because the grain size of the raw materials will dictate the reaction **kinetics**. It is commonly agreed that the fraction of quartz coarser than 40 mm should be carefully controlled. **To** do this the dynamic separators are given the desired settings.

The flow sheet of an industrial grinding system is shown in Fig. 1. A check-up of the system is periodically done to

point the sources of coursequartand to define the set points of the separators accordingly. To do this the **XRD** quantitative analysis performed on all the streams, and a mass balance is **finally** established, as **shown** in Table 1. In the case which is illustrated, contrary to all expectations, it has been found that the main source of large quartz grains is not in the sand, but in the limestone, and this would appear to be a side consequence of the different settings **of** the two separate grinding systems.

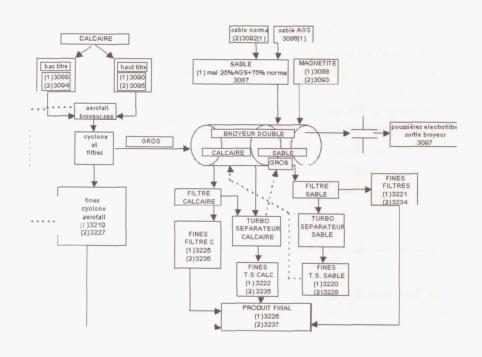


Figure 1

<b>%</b> quartz > 40	) mm
0.3	sortie aero
0.1	fines filter sable
2.8	fines TS calcaire
0.1	fines filter calcaire
3.3	
3.4	
	0.3 0.1 <b>2.8</b> 0.1 <b>3.3</b>

Table 1

People interested in this subject are encouraged to contact CPD members and national crystallography associations. Comments will be welcome on next issues of this newsletter.

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#### **International Centre for Diffraction Data**

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## J.D. Hanawalt Powder Diffraction Award

The International Centre for Diffraction Data is seeking nominees for the 1998 J.D. Hanawalt Powder Difraction Award. The award is presented every three years for an important, recent contribution to the field of powder diffraction. The award consist of a citation and a cash got of \$1,000. The award recipient is expected to submit an abstract and present a paper on the work being recognized at an appropriate Powder Diffraction/Crystallographic Meeting. Recipient's travel expenses to the meeting will be provided. Work eligible for consideration must have been published after 1 january 1990. The selection committee welcomes suggestions, nominations, and documentation of accomplishments for possible recipients through 15 February 1998.

Contact: Camden R. hubbard Charieman Hanawalt Award Selection Committee c/o Campus Boulevard, PA 19073-3273, U.S.A.

## ANNOUNCEMENT

The International Centre for Diffraction Data and Fachinformationszentrum, Karlsruhe, Germany, (FIZ), have signed an agreement which marks the beginning of an important relationship between the two organizations. As a result of this relationship with FIZ, ICDD will release a significantly enhanced powder diffraction database in September of 1998.

The first enhancement, and the one potentially with the longest term impact, is the cross-correlation of the Powder Diffraction File (PDF) and the Inorganic Crystal Structure Database (ICSD). Today, automated search/match algorithms are limited to listing the best matched phases in order of "goodness of fit". The automated ability to access the atomic coordinates and then generate the calculated patterns for potential phases identified in an unknown mixture opens a new era in phase ID. Least squares refinement of the calculated patterns will permit the next generation of algorithms to test and resolve postulates concerning preferred orientation and solid solution shifting in establishing the match. With this new ability, algorithms will be able to, fully automatically and unambiguously, identify the actual phases in an unknown, when the appropriate information is in both of the databases (DBs). In addition, all of the other information potentially contained in the powder patterns can be readily extracted as part of the phase ID – i.e. semi-quantitative analysis from the calculated I/Ic values, concentration of each of the phases exhibiting line broadening, etc. The integration of the crystal structure information with the PDF will bring on a new era of phase analysis for licensed users of both databases.

For the present, the 1998 release of the PDF will be enhanced by the addition of approximately 40,000 calculated patterns obtained from ICSD. This enhancement does NOT require that users have an ICSD license – the calculated patterns are a permanent addition to the PDF and there will be NO INCREASE IN THE PRICE OF THE PDF. The enhanced database will follow the same format as the previous PDF-2 database. We expect the combination database to contain:

Total number of entries	<del>,</del>	115,000
Number of organic compounds	-	20,000
Number of inorganic compounds	,-	95,000
Total number of entries with I/Ic	-	50,000
Number of unique entries with I/Ic	,-	37,000

Space requirements for the data files and ICDD index files will require approximately 580 MB of space.

We anticipate that this product will be distributed, in the short term, using conventional CD-ROM technology. However, we will rapidly approach the maximum capacity of the CD-ROM. Consequently, we will be exploring the feasibility of alternative distribution media, particularly DVD technology. We will keep you informed of our progress in this area.

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Please visit our web site @ www.icdd.com

## 4th Stockholm School on Electron Crystallography 13-19 June 1998 Topics for lectures and practical sessions

**Electron Microscopy** • Image Formation and Diffraction • Kinematical and **Dynamical** Theory **Crystallography** • The effects of symmetry in real and reciprocal space • The phase problem and ways to solve it **Data Collection, Quantification and Processing** • Film and CCD Cameras, HRTEM, SAED, CBED and

Powder Diffraction

- **Data Processing** HRTEM Images: Fourier processing and extraction of amplitudes and phases Determining and compensating for the CTF SAED patterns: Extraction of intensities CBED
- **Determining symmetry and finding the phases** Symmetry determination from HRTEM, SAED and CBED 3D data merging
- **Phasing Methods** Experimental phases from HRTEM images and CBED Phase extension Phases deduced ab initio by probability; direct methods
- **Constructing a Structure Model in 2D and 3D** Inverse FT of phased data Interpretation of density maps **Structure Refinement and Verification** Image simulations Least-squares refinement

#### Combination of powder diffraction and electron crystallography

- Scattering of X-rays and electrons from microcrystalline powders
- How to use X-ray powder diffraction intensities for structure refinement
- How electron crystallography can help in **Rietveld** refinement by providing unit cell dimensions, space group and unambiguous indices

Structures of Surfaces determined by electron crystallography

#### Applications of electron crystallography

# There are lectures in the mornings and practical sessions on electron microscopy and computing (twostudents per computer) in the afternoons.

The sessions start 9 am on Sunday June 14 and end 15.00 on Midsummer Eve 19 June. All participants are encouraged to arrive on Saturday 13 June, making it possible to buy cheap APEX air tickets.

## Teachers

Dr Giovanni Luca Cascarano Prof Bob J. Cernik	<b>Bari,</b> Italy Daresbury, England	Prof John W Steeds Dr Gunnar Svensson	Bristol, England Stockholm, Sweden
Prof Sven Homöller	Stockholm, Sweden	Dr <mark>Thom</mark> as Weirich	Stockholm, Sweden
<b>Prof Laurence D Marks</b>	Chicago, USA	DrXiaod ong Zou	Stockholm, Sweden

### Fee and Accommodation

The school fee, SEK 3000 (US\$400) includes tuition, written material, lunch, coffee and social events. A limited number of cheap student dormitories will be available. Hotels cost 500-1000 SEK per person and night. We hope to be able to support grants for some students.

The School will be at Stockholm University. The university campus is beautifully situated in the National City Park about 10 km north of Stockholm and 30 km south of Arlanda international airport.

## Applications

Apply before 31 January 1998, using the enclosed form. The number of participants is limited to 40. Priority is given to early applicants as well as to a wide geographical distribution of participants.

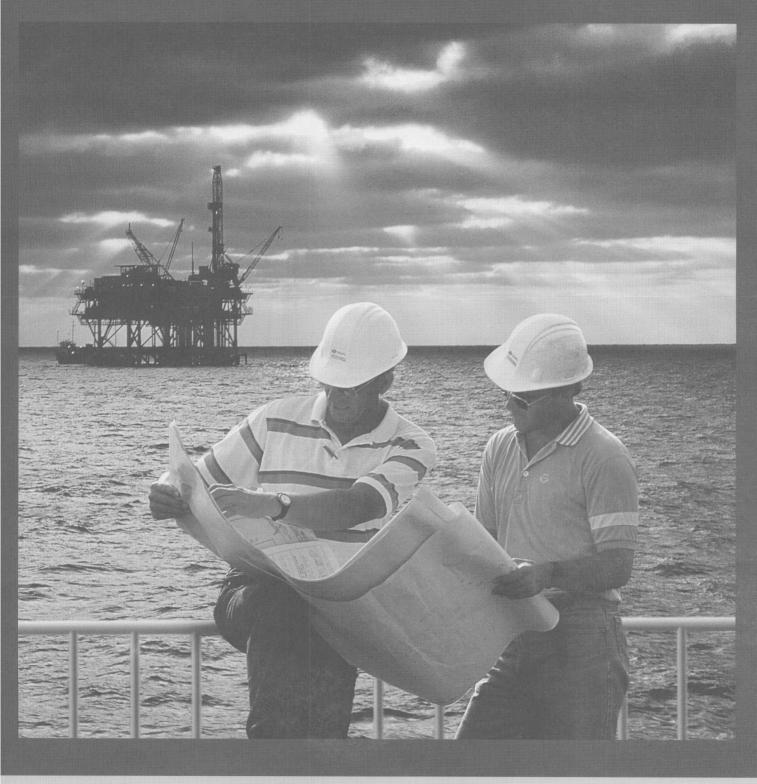
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11.



The CPD has had a very active year co-ordinating powder diffraction activities, recommending financial support for meetings, carrying out a wide range of projects including a **QPA** survey and publication of **Rietveld** guidelines, and keeping the powder diffraction community informed of events via the world wide web and *this* newsletter.

One event this year has resulted in the formation of the European Crystallography Association under the presidency of professor Carmello Giacovazzo. This will in the short term take over the functions of the European CrystallographicCommittee (which has replaced) in organising the European Crystallography Meetings. The Association may well expand and people are now discussing whether it would be sensible to have specialist interest groups (SIGs) in various areas, powder diffraction of course being one possible area. I would be very keen to hear your views on the matter, if you have an opinion please let me know by e-mail on r.j.cernik@dl.ac.uk

Another area of great interest for powder diffractionists is EPDIC. Should these meetings have a standing organising committee? If so should a newly formed SIG have some involvement with that committee? Again I would be very pleased to hear from you. theI think that some lirk is necessary to facilitate communication between the various activities and Iamsure that the CPD is right body of people to disseminate this information. However I amalways grateful for suggestions so if you have any ideas about the role of the CPD in thisor any other matter please let me knowl am very keen to demonstrate that the CPD can be flexible and react to the changing needs of the powder diffraction community.

I have included **I this** issue an application pro-forma to the **IUCr** Calendar Committee **fox IUCr** funds to support a meeting. If you have any ideas for workshops of conferences that you would like to **organise** in the area of powder diffraction and you would like financial support please let me know. Photocopies of the pro-forma printed in the **newsletter are quite acceptable**. In the first instance please send a copy of *the* outline programme and pro-forma to me at: **Daresbury** Laboratory, Warrington, WA44AD, UK.

R J Cemik

## **MEETING REPORTS**

## **5th European Powder Diffraction Conference EPDIC** • **V** *Parma, 25-29 May* **1997**

The 5th European Powder Diffraction Conference took place last May in Parma, Italy. **EPDIC-5** was the last of a semi-regularly held series of Conferences on all aspects of powder diffraction: previous editions were sited in Munich (D), Wien (A), Enschede (NL), and Chester (UK). The successful meeting was attended by over 350 scientists from Europe and overseas Countries: the number and quality of the scientific contributions and the lively atmosphere of the Conference, demonstrated that powder diffraction is an attractive research area for a large community of scientists in fields as diverse as chemistry, physics, mineralogy, and biology, and it is a fundamental tool for the characterisation of materials ranging from pharmaceutical compounds to **art** objects.

In spite of the diversity of the contributed studies, the areas of crystal structure solution from powder diffraction data and the one of in situ studies of phase transformations and chemical reactions proved to be of prominent interest, and they seem to be rapidly developing both in the theoretical and in the applicative aspects. The latter field includes the topic of the EPDIC Award lecture, delivered by the recipient of the Award, Malcom McMahon (Liverpool), on the powder diffraction studies of highly-condensed matter, and the use of in situ powder diffraction in the study of reaction kinetics by Dermot O'Hare (Oxford). The area of structure solution was well covered by the plenary lectures of Lynne McCusker (Zurich), reviewing the tools that the smart powder crystallographer ought carry in his structure solution toolbox, and of Yuri Andreev (St. Andrews) and Robert Dinnebier (Bayreuth), who showed specific applications of novel techniques involving simulated annealing and grid search techniques of molecular fragments, respectively.

The present and future role of synchrotron radiation and neutron sources in powder diffraction were described by Andy Fitch (ESRF, Grenoble) and by Steve Hull (RAL, Didcot), while Richard Wagner (Geesthacht) presented some interesting insights on the contribution of neutron scattering in materials science and engineering. Massimo Marezio (Parma) and Bob Snyder (Columbus) brilliantly elucidated the important role of powder diffraction in the characterisation of high Tc superconducting materials. The models used in texture analysis of polycrystalline materials were critically reviewed by Matti Jarvinen (Lappeenranta).

All in all, the Conference touched the most interesting applications and newly devised methods in powder diffraction. The many sessions, held in parallel, offered a variety of topics of interest to a large community of scientists working in Chemistry, Physics, Biology and Material Science. In the following a brief review of the main contributions to the various session is presented; details on each presentation will be soon available in the proceedings of EPDIC-5 to be published in *Materials Science Forum* in a few months.

# Structure solution / refinement / quantitative phase analysis

A large section of the Conference was devoted to the recent advancements in the field of structural crystallography, with particular emphasis on the newly emerging technique of *ab-initio* structure determination from PD data only. Three main lectures were dealing with methodological aspects of the technique, with striking examples in the organic and organometallic chemistry fields (Dinnebier, Bayreuth; Andreev, St.Andrews) and a bright, colourful presentation of the 'Structure Determination Toolbox' by Lynne McCusker (Zürich).

A few ancillary oral presentations and posters completed this program and included interesting talks on new computational methods (Monte Carlo, Kariuki, Birmingham; Direct Methods, Altomare, Bari; Genetic Algorithms, Shankland, ISIS) and the characterisation of solid state reactions in coordination chemistry (Masciocchi, Milan).

(N. Masciocchi, Milan)

#### In situ / HT-HP / kinetics studies

The importance of in situ diffraction both in equilibrium or in dynamic conditions for the understanding of phase transitions, non ambient processes, and reaction kinetics is now well recognised. The large number of papers presented at EPDIC-5 on such topics confirm that in situ diffraction is now a diffuse tool for characterisation of materials in a variety of operating conditions, ranging from cathode oxide materials in fuel cells (Krogh Andersen; Soerby), mineral reactions in geological processes (Balic Zunic), pharmaceutical polymorph compounds (Pfeffer), or zeolite and transformation crystallisation processes in hydrothermal conditions (Stahl; Gualtieri; Norby; Jensen). The results of powder diffraction studies performed under extreme environments were presented, showing the possibilities offered by brilliant radiation sources (McMahon; Tang; Hausermann; Degtyareva).

(G.Artioli, Milan)

#### Catalysts/ disordered structures

The chemical reactivity of many materials used in industrial processes is closely linked with their physical state, and they often show poor crystallinity or extensive structural disorder. The use of modern powder diffraction is especially valuable in the characterisation of catalytic materials (metallic carriers: Moroz; intercalated clays: Capkova; metastables aluminas: Bellotto) and in the interpretation of physical and structural properties by profile modelling (Dupont; Bergmann; Janeba).

(G.Artioli, Milan)

#### Instruments & Methods / Database & Software

The considerable interest in the development of new instruments and techniques was witnessed by the several interesting papers presented at the Conference. Andy Fitch reviewed some recent advances in XRD using synchrotron radiation, and in particular he reported on the new high resolution ESRF beamline, whereas Bob Cernik discussed how to achieve more brilliant sources. A really amazing presentation was that of T. Wroblewski, who described a new imaging method using micro-channel plate and PSD at DESY. X-ray optics were the object of several interesting presentations (Göbel; Kogan; Xiao). Progress in neutron powder diffractometry were reported by Wagner, Hauback and Tellgren. Finally, several papers on new software and databases were presented (Hewat; Cherepanova; Holzel; Leoni; Zorina)

(P. Scardi, Trento)

#### Accuracy / size-strain / texture / thin films

Two interesting talks addressed Standard Reference Materials (SRMs): Jim Cline reported on the status of the certification of SRM 640c, whereas Ian Langford presented some new interesting advances in **SRMs** for Line Profile Analysis (LPA). The overall interest in applications of LPA was remarkable, as demonstrated by the many contributed lectures and posters (Otto; Vaughan; Ben Haj Amara; Bor; Garber; **Guinebretiere**; Paiva-Santos; **Skala**): in particular, **Tamas Ungar** described a dislocation model for strain broadening, whereas Bob Von Dreele and P.W. Stephens reported their work on size-strain algorithms for the Rietveld method.

Besides the fundamentals of texture analysis in powder diffraction, reviewed by M. Järvinen and by H.J. Bunge, contributions were presented by Derk **Reefman**, on the effect of texture on quantitative phase analysis, H.-G. Brokmeier and W. Schäfer, and N. Herres on high resolution texture analysis in thin films.

Thin film analysis by grazing incidence diffraction (GID), reflectometry (GIXR), as well as traditional Bragg-Brentano diffractometry, was discussed in several papers (Jergel; Mattern; Klimke; Smigiel; Bassas; Kurt; Maixner; Maximovskiy; Quade; Singaletti): an interesting review on multilayer structures was presented by V. Valvoda.

(P.Scardi, Trento)

#### Materials: inorganic & organic

The state of the art of structural and **microstructural** study has been reported for a number of materials. In particular, Marezio showed in his lecture the complementary use of synchrotron radiation X-ray and neutron powder diffraction techniques in the field of high Tc superconductors. **This** approach was proposed also by Wagner and Kampmann as a tool for assessing the microstructure in materials science and engineering. Moreover, the numerous advantages for the study of polycrystalline materials, using high resolution powder **diffraction** facilities at ESRF, were elucidated by Fitch. In his plenary lecture Snyder highlighted the importance of the dynamic characterisation in the development of advanced materials and manufacturing. Examples were reported with reference to the field of high Tc superconductors.

Peculiar structural and microstructural characterisations were reported by Berar, Mazza, Cerny, Chiari and Dunlevey in their oral presentations. In addition, seventy posters collected the most recent advancement in the characterisation of materials. They were reported in the various sections: *Mineral, Inorganic, Organic, Metal and Ceramic, Disordered and Amorphous Materials, Nanocrystalline materials, Magnetic Materials and Catalysts and Microporous Materials.* 

Stimulating discussions among authors and interested people in the above topics were numerous and useful.

#### (V. Massarotti, Pavia)

The lovely town of **Parma** and the warm Italian climate did encounter the favour of the participants to EPDIC-5, as did the typical culinary tradition of the area and the social programme: the **Verdi** arias sung in the splendid surrounding of the church of **S**. Giovanni will most likely be a longlasting memory of everyone present.

The simultaneous presence at the Conference of most distinguished powder diffraction experts, and of a large number of students and young scientists, made EPDIC-5 an ideal place for the exchange and discussion of recent results **and developments:** as in the past, future **EPDIC** Conferences will undoubtedly represent a reference point for all workers in the field. The chairman of EPDIC-5 (Gilberto Artioli, Milano) warmly invites all scientists to the next edition of EPDIC, to be held in Budapest next year.

Gilberto Artioli and Paolo Scardi

## **46th Annual Denver X-ray Conference** *Steamboat Springs, 4-8 August 1997*

he 1997 Denver X-ray Conference, 46th in the series was held August 4-8 1997, in Steamboat **Springs** Colorado, in conjunction with the 1997 **US** X-TOP Symposium on High Resolution Diffraction and X-Ray Topography. The first two days of the conference were devoted to tutorial workshops on a number of topics. Those of interest to the diffraction community are listed below (with the organizers in parentheses):

- Applications of Microfluorescence & Microdiffraction (M.Eatough)
- Amorphous Scattering (A.C.Wright and G.R.Mitchel1)
- Specimen Preparation for XRD (D.Smith and R.Jenkins)
- Composition Depth-Profiling by Combined Grazing-Incidence XRF and Reflectometry (K.K.Bowen)
- Applications of Neutron Diffraction (C.R.Hubbard)
- Heteroepitaxial Layers & Semiconductor Substrates I,

IL\_(M.Halliwell and ICBassignana)

• Crystal Chemistry applied to XRD Phase Identification I & II (G.J.McCarthy, D.K.Smith, P.W.Wallace, R.L.Snyder)

The remaining three days were devoted to special sessions, contributed sessions and poster sessions on a variety of topics. In particular, the Plenary Session on X-Ray Analysis and Characterization of Thin Films, organized by I.C. Noyan, IBM, Yorktown Heights, NY, which was held in the upper gondola terminal on Mt. Werner was a highlight of the conference, featuring the following invited papers:

- High Resolution X-Ray Diffraction Applied to Strain Relaxation of Lattice Mismatched Semiconductor Films-P.M. Mooney and J.L. Jordan-Sweet, IBM Research, Yorktown Heights, NY
- High Resolution X-Ray Diffraction and Process Control of InP-Based Long-Wavelength Lasers - J.M. Vandenberg, Lucent Technologies, Murray Hill, NJ
- Synchrotron White Beam X-Ray Topography Studies of Semiconductor Substrate Crystals M. Dudley, SUNY at Stony Brook, NY
- characterization of Thin Films by Grazing Incidence X-Ray Scattering - D.K. Bowen, M. Wormington and C.R.Thomas, Bede Scientific, Englewood, CO

The 1997 Barrett award for X-Ray Diffraction was presented to James D. Jorgensen of ANL, Argonne, IL, and ICDD special awards were presented to G.J. McCarthy of North Dakota State University, Fargo, ND and P.K. Predecki, University of Denver, Denver, CO.

Other special sessions, (with the organizers shown in parentheses) of interest to diffractionists were as follows:

- Analysis and Characterization of Thin Films 1I, XRD and XRF (T.C. Huang and P.-W. Wang)
- X-Top-1: High Resolution Diffraction and X-Ray Topography (M. Goorsky and R. Matyi)
- Polymers I: Time-Resolved SAXS/WAXS Investigations (B.L. Farmer and B.S. Hsiao)
- Applications of Rietveld Analysis (R. Von Dreele)

- Applications of Microfluorescence and Microdiffraction I & II (G. Havrilla and B.R. York)
- X-TOP-2: High-Resolution Diffraction and X-Ray Topography (M. Wormington and P. Moran)
- Polymers 11: Polymer Structure and Morphology (G.R. Mitchell and N.S. Murthy)
- X-Top-3 High-Resolution Diffraction and X-Ray Topography (M. Dudley and W. Beard)
- Polymers III Amorphous Materials (R. Barton and A.C. Wright)
- Neutron Diffraction Applications (J. Richardson and T. Lorentzen)
- Strain and Stress Determination By Diffraction Methods (B. Clemens)
- X-TOP-4: High-Resolution Diffraction and X-Ray Topography (R. Armstrong)

The conference proceedings will be published in CD-ROM form by the ICDD. Exhibits of X-ray and related equipment by 32 companies were available for perusal during the conference week.

The conference was marked by the usual exceptionally friendly atmosphere engendered by the attendees and the exhibitors. The latter are to be congratulated on the opulence and quality of their receptions which did much to further the spirit of camaraderie and cooperation.

The hotel put on a wonderful conference dinner, which was followed by a memorable performance by the Barbershop quartet: The Powdermen (Ron Jenkins, Jim Kaduk, Greg McCarthy and Walt Schreiner), with contributions from various national groups in the audience. An enjoyable and informative time was had by all.

This year marks the last year that the conference will be organized and sponsored by the University of Denver, Department of Engineering, with P.K. Predecki as conference chairman. These tasks will henceforth be assumed by the ICDD, with Ron Jenkins as Conference chairman.

Paul K. Predecki

## Workshop on Advanced Neutron Powder Diffraction Instrumentation and Data Analysis Techniques

August 22, 1997, Toronto, Ontario, Canada.

This Workshop was a satellite meeting of the International Conference on Neutron Scattering held in Toronto on August 17-21. The Workshop was organized by J. Jorensen (USA) and attracted about 40 participants from many countries. The Workshop was split into two components: the morning consisted primarily of a review of instrumentation, with a focus on resolution, larger multidetectors and design of new focusing monochromators, most of which were based on deformed Ge technology. It was proof that, while powder diffractometers are getting ever more expensive, they are still capable of impressive improvements in resolution and intensity. This will allow applications of neutron powder diffraction to new areas of science and technology.

P. Radaelli (ILL, France) gave an overview of the D2B multi-Soller powder diffractometer at the ILL. The D2B vertically-focusing Ge monochromator is constructed from 15 plastically deformed Ge wafers, from which 7 wavelengths can be extracted. He suggested that complicated experiments could be performed, by switching between the multiple collimator options available, and different wavelengths to change the position of the minimum in the resolution functions. Vertical focusing and very large multidetector arrays also lie behind the design of the D20 high-flux two-axis instrument at ILL. P Convert (ILL, France) described the 160" microstrip detector design, composed of 1600 separately addressed detectors, pre-amps and amplifiers. The parallelism inherent in the detector electronic design yields an impressively fast data collection. Combined with the high-flux from focusing monochromators, the instrument should yield a very high throughput, with applications in kinetic studies, stroboscopic measurements, and phase transitions.

Two American contributors dealt with differing approaches to focusing monochromator design. A description of the Brookhaven vertically-focusing monochromator and H1A diffractometer was given by T Vogt (BNL, USA). The Brookhaven monochromator uses 24 aligned composite wafers of Ge(115) and is 30 cm high. The complex deformation technology and the importance of the resulting symmetric line shape were discussed. M Popovici (Missouri University, USA) gave a description of the Missouri University Research Reactor (MURR) design of vertically-focusing monochromator and powder diffractometer. In contrast to the more expensive Getechnology, **MURR** has focused (excuse the pun) on using deformed perfect Si wafers used in strongly asymmetric reflection. An extra gain, in addition to the vertical focusing, comes from the beam compression/condensation from the asymmetric cut of the wafers. The MURR method precludes the use of in-pile collimators used in some other designs. Impressive gains in intensity and resolution were demonstrated, with examples from their experience at MURR.

The use of focusing monochromators to push the limits of sample size was the topic of I. Goncharenko, (Kurchatov Institute, Russia). From measurements at the LLB, Saclay, he cited several successes with sample sizes down to «1 mm3, achieved with the aid of doubly-focusing monochromators.

Developments at the new Swiss national source, **SINQ**, were covered by L. Keller (PSI, Switzerland). DMC (Double-axisMulti-Counter) has been re-installed at the end of a cold neutron guide, giving a dedicated long-wavelength

powder diffractometer with high-intensity and **high**resolution modes, equipped with 400 BF3 detectors. The other powder diffractometer, HRPT (High Resolution Powder Diffractometer for Thermal Neutrons), is located on a thermal beam line and is equipped with 1600 3He detectors spanning 160°. Again, high-intensity and highresolution modes are available, and a 11-element verticallyfocusing Ge-wafer monochromator may be used.

I. Swainson (NRC, Canada) gave a brief overview of the C2 DUALSPEC diffractometer and program at Chalk River, Canada. The 800-wire BF3 detectors span 80° 2q. He claimed that the wide variety of monochromators, take-off angles, and collimations makes the instrument very flexible in terms of wavelengths and resolutions.

Time-of-flight instrumentation was also discussed. The upgrades to the instrument Vega and the new higherresolution instrument Sirius both at KENS, Japan, were described by T. Kamiyama (Tsukuba, Japan). Both machines rely on 3He detectors arrayed in two-dimensions to cover the largest possible solid angle. The new highintensity diffractometer GEM at ISIS, UK, is being designed to measure experiments under constrained sample environments, small sample volumes (ca. 1mm3) and kinetics with time scales of the order of minutes, with a wide-Q range and good resolution. R. Ibberson (ISIS, UK)described its capabilities and how it is envisioned to fit into the existing instrument suite at ISIS. The highresolution Fourier diffractometer at the Dubna pulsed reactor, was described by A. Balagurov (Frank Laboratory, Russia), with a brief history of the development of such techniques.

Data refinement and handling was the topic of the second component of the workshop. F. Izumi (Tsukuba, Japan) covered the development of RIETAN-96T and its application to the Vega diffractometer at KENS, Japan. With an increase in resolution, the line shapes become harder to fit, and so a new profile relaxation approach has been successfully implemented. The merits of maximum entropy methods for the analysis of powder data were propounded by *S*. Kumazawa (JAERI, Japan) with examples of possible applications.

W. David (ISIS, UK) described the analysis of time-of-flight data using the Cambridge Crystallographic Subroutine Library, and its extension into synchrotron X-ray and constant wavelength neutron and laboratory X-ray data analysis. He emphasized to the treatment of sample-induced line broadening as observed on HRPD, symmetry adapted spherical harmonics for disordered molecules, and Bayesian methods of Fourier map analysis. Referring to R. Ibberson's talk, he said the new GEM diffractometer would be capable of collecting 100Gbyte of data/day, requiring rapid on-line data reduction. R. Von Dreele, (LANSCE, USA) described the recent additions to the powder analysis components of GSAS, and to the virtual reality modelling output now available from the PC version, together with his view of the path data analysis would take.

At the end of the day, the floor was opened to discussion on future directions both of instrumentation and data handling/refinement. The liveliest discussion was centred around the smallest sample volumes that people had successfully used and features available in various refinement packages. The workshop proved itself to be a highly successful forum for the exchange of ideas and discussion of the latest developments.

Ian. Swainson

## Spanish Workshop on Synchrotron Powder Diffraction

Universidad de Malaga, 25-26 September 1997

Spanish scientific authorities have taken the decision to design and built a mutidisciplinary and multipurpose beamline at ESRF. The Spanish CRG beamline "SPLINE" is planned to cover the needs of the Spanish Synchrotron Radiation Users Community and it will consist of two independent experimental hutches one of them dedicated to HRPD and EXAFS. The above mentioned workshop has been organised at Malaga to mobilise the Spanish powder diffraction community. The workshop included talks dealing with recent advances of synchrotron powder diffraction and two round tables to discuss technical aspects directly related to the planned diffractometer.

Firstly, German Castro, the scientist responsible of SPLINE, gave us a talk about the planned Spanish CRG at ESRF with special emphasis on the optics and planned performances of the beamline. Then, Ake Kvick spoke about materials science at ESRF. After some technical aspects of the ID11 beamline, he showed us an outstanding example of real-time crystallography: the polymerisation of S2N2 to (SN)x. Several other topics such us single microcrystal diffraction and very high energy experiments were also covered. After a Spanish lunch, Andy Fitch avoided "siesta" of the participants with a stimulating talk about some technical aspects and the extraordinary performances of the HRPD installed at BM16 (ESRF). Some key examples about ab initio powder diffraction determination were given. It was, plainly spectacular, the crystal structure determination of two previously unknown phases in "(CH3)2SBr2" metastable sample. Proper credit to Gavin Vaungahn's strategy to index the pattern was given.

Next day, Bob Cernik talked about powder diffraction at Daresbury. Technical information about stations 9.1,2.3 and 9.7 and ancillary equipment was very welcome. Some admirable examples of high pressure and high temperature experiments were presented. He finished his talk with some details about the new curved MWL detector. J. Louis Hodeau introduced us in the fascinating world of new detectors. After technical information of the multi-analyser detector at BM16, he delighted us with some DAFS studies. He also showed the electrochemical Li intercalation in the industrially important Li-Co-0 and Li-Mn-0 systems followed by powder diffraction which illustrated the advances in synchrotron diffraction to characterise chemical reactions. Several examples with 2D detectors were also presented. Finally, Juan Rodriguez-Carvajal spoke about new trends in powder diffraction. Latest data from D20 neutron diffractometer (ILL) in the subsecond time scale were presented which raised much excitation. Combined Rietveld refinements with several data sets also open discussion about the related statistics and the way to weigh the patterns. Several talks of Spanish users were intercalated in the program to induce as much exchange as possible between participants. Our community is in the synchrotron diffraction track !

> Miguel A. G. Aranda, Malaga Secretary of the organising committee

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### STATUS OF THE CPD ROUND ROBIN ON QUANTITATIVE PHASE ANALYSIS

This report provides a brief summary of the status of the quantitative phase analysis round robin sponsored by the CPD.

#### Participants

Response to the call for expressions of interest has been very gratifying with some 140 people requesting the questionnaire. At the time of writing about 90 of the questionnaires have been returned requesting that the samples and/or data be sent. The participants are predominantly X-ray diffraction users with about 10 participants indicating that they have access to neutron diffraction facilities.

#### Design

In their response, many participants have requested that the samples supplied for the round robin cover a wide range of compositions so that standardless least squares methods (which rely on the variation of phase content) could be applied. To assist in this, the CPD will be supplying multiple mixtures for many of the sample suites to those participants who require them. While this increases the number of data sets to be collected, there should not be a large increase in analysis time.

#### Time-frame

The original time frame has been modified slightly and the

## WHAT'S ON

3-7August 1998

#### 47th Annual Denver X-ray Conference

Colorado Springs, Colorado, USA. Contact: Dr Ron Jenkins, International Centre for Diffraction Data Postal Address: ICDD, 12 Campus Boulevard, Newtown Square, PA 19073-3273 U.S.A. Tel: +1 610 325-9810, Fax: +1 610 325-9823 E-mail: jenkins @icdd.com WWW: http://www.dxcicdd.com

#### 16-20 August 1998

#### 18th European Crystallographic Meeting (ECM-18)

Prague, Czechoslovakia Contact: Dr R. Kuzel, Postal Address: Faculty of Mathematics and Physics, Charles University, 121 12 Praha 2, Ke Karlovu 5, Czech Republic. Tel: +420 21911394, Fax: +42 24911061 E-mail: kuzel@karlov.mff.cuni.cz WWW: http://krystall.karlov.mff.cz/ecm/ecm.htm

#### 22-25 August 1998

#### 6th European Powder Diffraction Conference (EPDIC-6)

Budapest, Hungary Contact: Dr Erzsebet Svab, Research Institute for Solid State Physics Postal address: H-1525 Budapest,POB 49, Hungary, Tel:+36 1 3959220lext 1418, Fax: +36 1 3959162 E-mail: epdic6@power.szfki.kfki.hu (Dr. Svab) ungar@ludens.elte.hu (Prof. Ungar) WWW: http://www.kfl<i.hu/-epdic61

#### 13-15 October; 1998

#### **3rd Conference of the Asian Crystallographic** Association (AsCA'98) Hotal Equatorial Panari, Salangar, Malausia

Hotel Equatorial Bangi, Selangor, Malaysia. Contact: Prof. A. Hamid Othman Jabatan Kimia, University Kebangsaan, Malaysia 43600 Bangi Malaysia Fax: +6-034258828 E-mail: hamie@pkrisc.cc.ukm.my Int. Org. Com. Chairman: Prof. Shin-Lin Chang (slchang@phys.nthu.edu.tw) Int. Prog. Com. Chairman: Prof. T. Yamanaka (b61400a@center.osaka-u.ac.Jp) WWW:http://gandalf.otago.ac.nz:800/rweavers/ASCA/ asca98.htm

#### 4-13 August 1999 18th Congress and Cenera

# 18th Congress and General Assembly of the International Union of Crystallography,

Glasgow, Scotland, UK Contact: Dr. C. Gilmore, Department 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.uMuiucr99/

#### 18 May 1998

**1998 NSLS Annual Users' Meeting and Workshops, Structure solution from powder diffraction data** Brookhaven National Laboratory, Upton NY 11973, USA Contact: D E Cox Tel: 516 344 4818, Fax: 516 344 2739 E-mail: cox@bnlx7a.nsls.bnl.gov

#### 1998 ICDD X-ray Clinics

ICDD Clinic	on X-ray Fluorescence Spectrometry	
April 20-24	Fundamentals of X-ray Fluorescence	
	Spectrometry	
April 27-Ma	y 1 Advanced Methods in X-ray	
	Fluorescence Spectrometry	
ICDD Clinic	on X-ray Powder Diffraction	
June 1-5	-5 Fundamentals of X-ray Powder Diffraction	
June 8-12	Advanced Methods in X-ray Powder	
	Diffraction	
Contact:	Manager, Schools and Conferences	
	International Centre for Diffraction Data	
	12 Campus Boulevard, Newtown Square,	
	PA 19073-3273	
Phone: (610) 325-9814; FAX: (610) 325-9823		
E-mail: CLINICS@ICDD.COM		

#### 47th Annual Denver X-ray Conference

August 3-7 1998 Antlers Doubletree Hotel, Colorado Springs, Colorado

Contact: Manager, Schools and Conferences International Centre for Diffraction Data 12 Campus Boulevard, Newtown Square, PA 19073-3273 Phone: (610) 325-9814; FAX: (610) 325-9823 E-mail: CLINICS @ICDD.COM



Paolo Scardi Editor, CPD Newsletter 19

# CALL FOR CONTRIBUTION TO THE NEXT CPD NEWSLETTER

The next issue of the CPD Newsletter will be edited by R J Cernik to appear in May of 1998. 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 22) by the end of April '98.