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POWDER DIFFRACTION IN INDIA (Centre pages)

Editor Siba Sen-Gupta

More Software for Powder Diffraction

and Glasgow is Coming!

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CPD CHAIRMAN'S MESSAGE

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This issue has been edited by Professor Siba Sen-Gupta who has recently organised a very successful meeting on powder diffraction in Calcutta. The issue contains details of the projects currently underway in India as well as a report on the meeting.

The main IUCr General Assembly and Congress in Glasgow is rapidly approaching. There will not be a satellite meting this year as the powder community has been fully integrated into the main programme. The programme is quite exceptional for powder diffractionists and materials scientists. There are at least 16 microsymposia of direct relevance and a good deal more that are of interest. Specifically the Commission sponsored microsymposia are: 30 years of Rietveld refinement; Optimisation methods; Challenging Rietveld refinements; Industrial on line analysis; in-situ studies using PD; Thick coatings; Line broadening; Non structural aspects of Rietveld refinement; Microporous materials; Structure solution from powder data, molecular compounds; Structure solution from inorganic materials; combined Powder diffraction, XAFS and DAFS; Combinations of electron and powder and finallyab-initio structure prediction. The industrial sessions are clustered around the middle weekend to encourage commercial employees to attend for part of the meeting if they cannot be present for the whole. The powder community will also note that Dave Cox and Carmello Giacovazzo are giving keynote lectures on the topics of materials science and structure solution (respectively) with powder data. The other parts of the programme are more heavily weighted towards materials science than in previous years so I hope to see as many of you as possible in Glasgow.

This newsletter contains a copy of the Rietveld refinement guidelines produced for the Commission on Powder Diffraction by Lynne McCusker, Bob von Dreele, Dave Cox, Daniel Louer and Paolo Scardi and a support cast acknowledged in the text. This was produced in order to give sound advice for Rietveld practitioners, the authors and the CPD hope you find it useful.

Many program authors asked to place details of their programs after the last issue. I am grateful to Lachlan Cranswick for finishing this task.

If you have any comments regarding CPD activity or wish to make suggestions please write or E-mail me on r.j.cemik@dl.ac.uk, Daresbury Laboratory, Warrington WA4 4AD.

FROM THE EDITOR OF THIS NEWSLETTER:

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This newsletter contains more information about what is happening on the Indian subcontinent in recent times. We had International and National Conferences on a large scale. ISPD-98 was a great success. Proceedings have also come out in a nice way which was distributed globally. The IUCR and ICDD supported the meeting; especially our younger scientists. We are now thinking to have this once every two years in a similair way to EPDIC. We expect wider participation also.

We are now looking forward for IUCR-Glasgow meetings.

Best wishes

Siba

Size/Strain Round Robin

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During ECM-18 and EPDIC-6 there were discussions about a need to organize a Round Robin on size and strain diffraction line-broadening effects. As it is widely known, currently there are no standards available that would allow a comparison and calibration of different instruments and methods for diffraction-line-broadening analysis.

It is expected that the Round Robin will result in diffraction-line-broadening standards. An evaluation of different candidate materials could potentially lead to a certification procedure for a new NIST Standard Reference Material (SRM). The Round Robin would be extremely beneficial in achieving this goal.

Quantification of a specimen's size and strain values requires a definition of the analysis method and instrumental-broadening standard. Even a casual user of some of the line-broadening techniques is aware of systematic and significant differences in results obtained through different approaches. Therefore, the intent is to organize the Round Robin in two phases: Methods of line-broadening analysis and broadening standards. These two phases will not be conducted simultaneously.

1st phase: Methods of line-broadening analysis

There are literally dozens of different analysis methods that can yield much different or even physically impossible results. The approaches are broadly divided into two groups: model-independent and model-dependent. The former is mainly identified with the Fourier-deconvolution correction for instrumental broadening (Stokes method), which is followed by the Warren-Averbach approximation for the size/strain-effect separation. The latter mainly contains different integral-breadth methods among which some are more widely used and therefore proposed as a part of the Round Robin. Integral-breadth methods are to be preceded by the instrumental-broadening correction. which will depend on a particular method and will be defined accordingly. Furthermore, as Rietveld-refinement programs build in more and more sophisticated line-broadening approaches. they will be used more frequently as a tool for line-broadening analysis. It would be advantageous to select Rietveld programs with most-effective correction for anisotropic-line broadening.

Hence, the proposed list of methods is as follows:

1. Stokes deconvolution + Warren-Averbach analysis
2. Modified Williamson-HaI1 analysis (Lorentz function for the sizc-broadened profile + Gauss function for the strain-broadened profile)
3. "Double-Voigt" analysis (Voigt function for both size-broadened and strain-broadened profiles)
4. Rietveld-refinement analysis -- modified TCH line-broadening model (GSAS. DBWS. Full Prof. .. ?) and Fourier series profile synthesis (ARIT).

It is planned that the "representative" diffraction patterns be sent to the Round-Robin participants. The "representative" designation has at least twofold connotation: First, diffraction patterns would be collected with different radiation and geometry (sealed and synchrotron x-ray, CW and TOF neutron). Second, it is of utmost importance for a successful Round Robin on methods of line-broadening analysis to have high-quality data without substantial systematic errors. The "representative" diffraction patterns will be collected at the following facilities:

Laboratory x-ray sources:

"Common" instrumental setup: University of Le Mans (Armel Le Bail),
Incident-beam monochromator: University of Birmingham (J. Ian Langford).

Synchrotron x-ray sources:

2nd-generation synchrotron, flat-plate geometry: NSLS. Brookhaven National Laboratory (Peter W. Stephens).
3rd-generation synchrotron, capillary geometry: ESRF. Grenoble (Andy Fitch).

Neutron sources:

Constant-wavelength source: ILL. Grenoble (.Alan Hewat) and NIST, Gaithersburg (Brian Toby)
Spallation source: **ISIS.** Rutherford-Appleton laboratory (Mark Daymond).

2nd phase: Broadening standards

Diffraction-line broadening originates for two main reasons: small size of coherently diffracting domains and crystallic strain Although most frequently these two effects occur simultaneously in materials. it would be beneficial to have separate standards for size-dominant and strain-dominanant broadening. The appropriate materials will be sent to thc Round-Robin participants for the mesurments

Bascd on the results of the 1st phase. the method(s) to evaluate values of domain sizes and crystallite strain will be defined. This will allow for unequivocol quantification of the Round-Robin results.

Invitation for your participation

The intention is to have a "generic" Round Robin, that is, everyone is welcome t o participate. Furthermore, the intent is to include participants with different laboratory instruments and configurations and at synchrotron and neutron beamlines. Not every Round-Robin participant is expected to be a part of both phases. If you wish to participate in either one or both phases, please fill out the form at the following Web addresses:
http://\vww.boulder.nist.gov/div853/balzar/ or
http://www.ccp14.ac.uk/ccp/web-mirrors/balzar/div853/balzar/ (CCP14 mirror).

These pages will also contain an up-to-date information on the Round Robin.

Your participation is greatly appreciated.

The Round-Robin Organizer,

Davor Balzar

Powder Pattern Indexing Based on a Genetic Algorithm Optimisation of a Whole-Profile Fit.

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Structure determination from powders comprises the following steps: (i) determination of the unit-cell (indexing), (ii) space group assignment, (iii) structure solution, and (iv) structure refinement. Step (iii), structure solution, is generally considered the most challenging. However, it is not possible to proceed at all with structure determination unless the correct unit-cell is found in stage (i); and it is becoming increasingly apparent that indexing is often the limiting step. This article briefly describes a promising new technique that may aid the indexing of more challenging problems when other methods fail. The technique is more fully described in [1].

The most widely used programs for indexing are TREOR [2], ITO [3], and DICVOL [4]; and in most cases a combination of these programs works very well. These programs all rely on the extraction of reliable peak positions. However, the inability to assign unambiguously positions due to peak overlap, or the accidental inclusion of peaks from a secondary phase, can be a major obstacle to the successful operation of these programs. It is with this in mind that an approach to indexing, which follows closely the recent developments in structure solution **[1],** has been developed. The method is a combination of full-profile fitting of the observed powder diffraction data and a genetic-algorithm global-optimitation procedure.

The whole-profile approach to indexing is quite simple. A set of trial lattice parameters is chosen. The lattice parameters determine the positions of peaks in the diffraction pattern. Given the peak positions and parameters describing the peak profiles, a Le Bail decomposition is carried out and a proflie R-factor is calculated from the difference between the calculated and observed patterns. The R-factor gives an indication of the goodness-of-fit. Assuming that the R-factor is at its minimum when the lattice parameters are correct, we can proceed with any global optimisation method we like to achieve the minimum R-factor and thus, hopefully, to obtain the correct unit-cell. The use of whole-profile fitting implicitly overcomes the problem of assigning positions to overlapped peaks. Also, the resence of peaks from minority phases does not affect the indexing of the main phase as profoundly as they would affect the other methods.

The use of Le Bail decomposition [5] to carry out the full-profile fit affords certain advantages. No structural model is required---unlike the Rietveld method. Le Bail decomposition is not a least-squares method and so (unlike least-squares) it does not require the calculation of derivatives. This makes the fitting at least an order-of-magnitude faster and also avoids the potential stability problems inherent with least-squares.

The optimisation method of choice, in this case, is a genetic algorithm (GA). A 'population' of trial sets of lattice parameters is chosen at random from within a given volume range. The genetic algorithm operates on this population according to well defined procedures for mating, mutation and natural selection of the fittest members of the population. The fitness of an individual member (a set of lattice parameters) depends on its value of Rwp (low Rwp corresponds to high fitness). More details of the GA can be found in [1].

The efficiency of the GA method as a global optimisation technique depends largely on the existence of what are known as schemata--i.e. combinations of parameters associated with high fitness. The presence of schemata make it is possible for the GA to recognise that one or more parameters of an individual are close to optimal, even though the rest of the parameters are far from optimal, and thus propagate good genetic information to the next generation. The existence of schemata in indexing is clear and can be understood from the fact that there are subsets of peaks that depend on only one or a few parameters. For example, the positions of the {h00} peaks depend only on the *a* lattice parameter, so that when the *a* lattice parameter is correct the {h00} peaks are fitted corrrectly resulting in a fitness that is higher than the fitness of an individual for which none of the parameters is correct. The Rwp surface shown in Figure 1 reveals several strong local minima connected by deep 'valleys' to the global minimum. These valleys provide an expression of schemata in this surface. The presence of schemata in the indexing problem makes a GA an ideal technique.

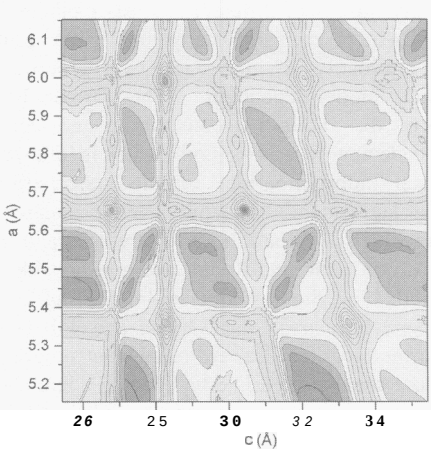

Figure 1: *Contour plot of an R-factor surface around the global minimum of tetragonal Sr (a=5.6533Å, c=3.043Å). The 'valleys' leading to the global minimum show directly the existence oj schemata in this particular R-factor space.*

Figure 2 shows the best fit found by the GA indexing method for orthorhombic GaAs. The observed data are contaminated by peaks from a second phase (arrowed) but despite these extra peaks the program still managed to find successfully the correct unit-cell. The inclusion of the strongest peak from the impurity phase caused other methods of indexing to fail completely. The success of the method in this case demonstrates the utility of our approach, and we expect it will be a useful addition to the currently available indexing techniques.

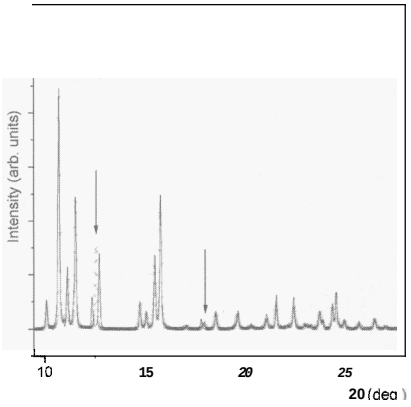

Figure 2: *The Le Bail fit of the calculated data (solid line) to the observed data (crosses) when orthorhombic phase-II of* GaAS *is correctly indexed. The arrows highlight the impurity peaks.*

Extensive testing and development of the new method is currently being carried out and it is hoped that executables of the program will susequently be made available.

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[3] Visser, J.W., J. Appl. Cryst., 2, 89 (1969).
[4] Boultif, A. and Louer, D., J. Appl. Cryst., 24, 987 (1991).
[5] Le Bail, A,, Duroy, H. and Fourquet, J.L., Mater. Res. Bull., 23,447 (1988).

EFLECH/INDEX - a program pair for peak search/fit and indexing

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In the summer 1998 issue of the CPD newsletters, we talked about BGMN: a rietveld program using an unique raytracing fundamental parameters approach. The FPA peak shape model used within BGMN was developed and used firstly for the program EFLECH. EFLECH pursues a simple idea: Having designed an almost true profile shape, one can do much more than only peak fitting. Indeed, an advanced statistical search algorithm should be able to find the optimum decomposition of the whole pattern into a set of peaks, starting from an empty diagram without any predefinition of background or peak parameters. This work is done by EFLECH. Some examples shall demonstrate the success of this program:

Instrumentally caused maximum shifting (eg. by axial divergence) is fully included in the fundamental parameter model and does not influence the calculated peak positions (Fig. 1). The FPA model also includes the wavelength distribution. Therefore, Ka2 separation is not necessary and highly overlapped peaks are found and fitted in automatic mode without user interaction (Fig. 2). So EFLECH delivers a better base for following search/match procedures, lattice refinement or indexing than a conventional maximum search algorithm.

As a part of its statistical approach, EFLECH delivers the whole statistical error information of all parameters calculated. This means not only the errors (diagonal of the curvature matrix) but the whole lower half of the curvature matrix!

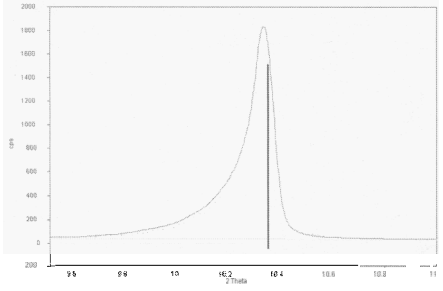

Figure 1: *001 profile and calculated peak position of the SRM 675 mica line position standard, illustra-ting the elimination oj instrumentally caused maxi-mum shifting (without any additionul correction).*

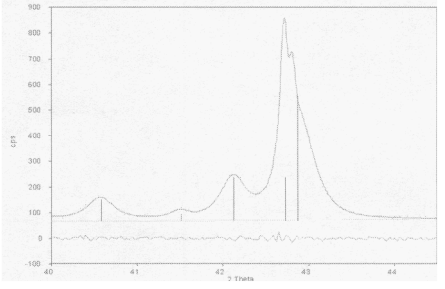

Figure 2: *Part of an automatic fitted diffraction pat-tern and calculated peak positions of a goethite-quartz mixture. No predefinition or constraining of peak number, peak shape parameter or background.*

INDEX was designed for consuming this rich information for indexing. INDEX uses no special artifical method. Instead of, it uses a kind of "brute force" indexing. E.g. while checking for monoclinic solutions, INDEX checks for nearly 100000000 (10**8) different unit cells! For every possible solution, a figure of merit based on the statistical information given by EFLECH is calculated. If the figure of merit of any trial is sufficiently small, then a least square search for the minimum solution follows. For every lattice type, the minimum solution is given, if any was found. The program gains, like EFLECH and BGMN, from many optimizations in data structures/algorithm design. Due to such optimizations, a complete monoclinic scan only needs for nearly two hours, which means more than 10000 (10**4) trials per second!

Until now, INDEX is called to be a beta program. The actual version 2.5.2d is checked to solve ten test patterns, decomposited by EFLECH:

- -two cubic examples: fluorite, magnetite
- -one hexagonal example: corundum
- -one orthorhombic example: anhydrite
- -four monoclinic examples: epidote, gypsum, kyanite, muscovite
- -two triclinic examples: $K_2Cr_2O_7$, plagioclase

All patterns are measured using a setup as used for routine phase analysis. This means medium to low counting statistics plus medium to wide profiles. The total counting time mostly was about three to five hours.

If you are interested, please read the online documentation, download and check out the beta programs from

http://www.bgmn.de/related.html

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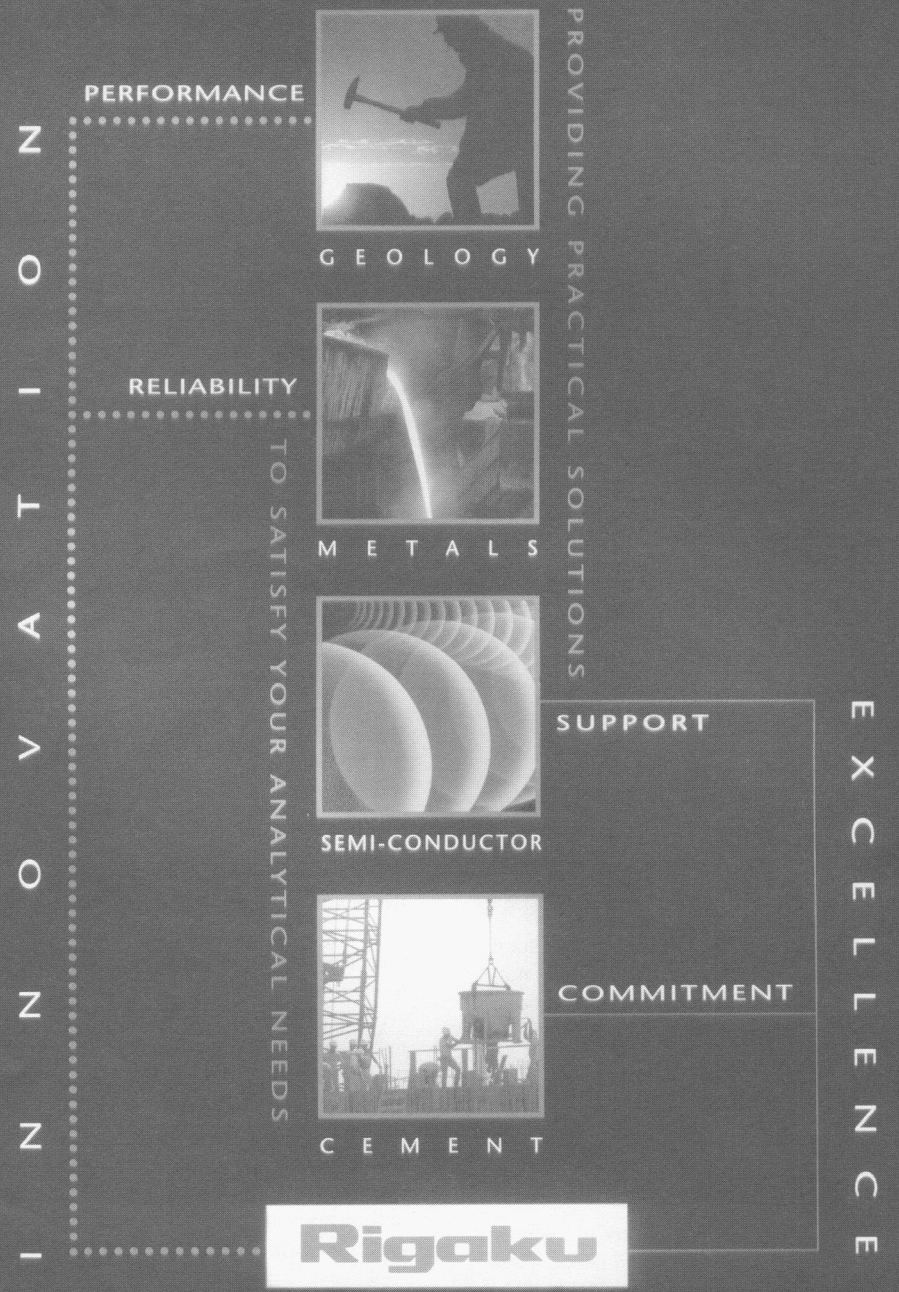

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Ye Computer Fayre at the IUCr Glasgow 99 Congress (4th to 10th August 1999)

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Thanks to the conference organisers and hardware arranged and supplied by Compaq (http://www.compaq.com), there will be an informal non-Commercial Software Fayre at the IUCr Glasgow 99 Congress during the entire event (4th to 13th August 1999 except for 10th which is the day of the conference excursion and the centre is closed).

The Software Fayre presently has 2 SGIs and 5 non-networked Compaq Windows PCs for general usage.

Non-commercial software authors are invited to bring or arrange for their programs to be installed on the computer systems. Software users are invited to bring data and examples that they may like to try out on various systems while interacting with colleagues and software authors. It is also possible for people to book times for computers prior and during the congress if they wish to have a semi-format presentation.

However, please note that software lecture demonstrations are permitted at lunchtime in some lecture theatres. These time-slots are booked through Professor Chris Gilmore (E-mail: iucr99@chem.gla.ac.uk) on a first-come first-served basis.

The computers will be located in an area on the ground floor of the main Conference Centre and people can bring their own computing hardware for specialist demonstrations.

More detailed information (including maps) is available at the Software Fayre homepage at:
http:/lwww.ccp14.ac.uk/projects/iuce99-softwarefayer/

This information will be updated over time as things develop - and hopefully a productive mixture of planned and un-planned interaction will occur over the duration of the congress.

Lachlan.

PowderX - a Windows Program for Powder X-ray Diffraction Data Processing

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A Windows95-based program (PowderX) has been written for powder x-ray data processing and analysis. It can be used for plotting diffraction patterns, data smoothing, background subtraction, a2 elimination, peak search, indexing and zero-angle error correction. PowderX can also be used to prepare the input data for Rietveld refinement and structure determination programs, such as DBWS, FULLPROF, GSAS, SIMPRO and EXPO. It is very helpful for not only routine x-ray data analysis but also ab-initio structure analysis.

PowderX takes full advantage of the graphical interfaces of the Windows95. PowderX uses pull-down menus and mouse to control the program executions. It provides the convenient tools for processing powder x-ray diffraction data. Savitzky-Golay method or other 3 methods can be used for data smoothing and peak search. Background subtraction can be made either automatically by Sonnerveld method or manually by mouse clicking. The a2 elimination can be performed either using previous methods by Rachinger. Ladell or using a new method developed by the program author.

PowderX can read 13 data formats, either angular-dispersive or energy-dispersive, used by various diffractometers made by Mac Science, Philips. Siemens, Rigaku, etc. It uses a new and accurate Cu Ka2 elimination algorithm. With PowderX, zero-angle shift can be corrected automatically before indexing and no internal standard material is required. It can produce the input tile for TREOR90 after peak search automatically, and only minor editing is needed. The newest version of PowderX has built-in ERACEL program for refinement of lattice parameters. This program has more than 100 users in the world now. Online help describes the main features of the program and provides instructions for the users. A user's manual is also available as Word document in rich text format.

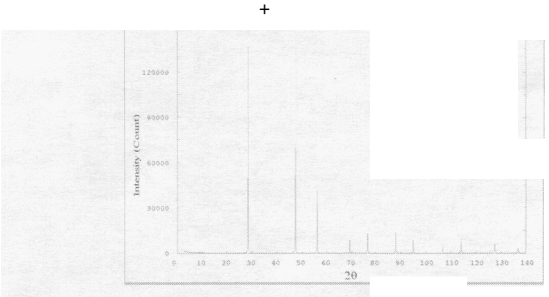

Figure 1: *Cu K-a_2 eliminated laboratory X-ray data of Silicon standard.*

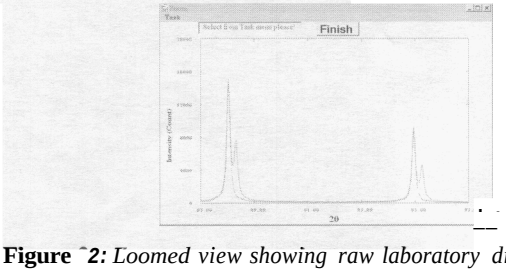

Figure 2: *Zoomed view showing raw laboratory diffraction data overlapped with Cu K-a_2 eliminated data*

The files for standard windows installation of the program and the user's manual document are freely available for academic and non-commercial use. The program distribution may be obtained from the program author by (E-mail: **chengdon@aphy.iphy.ac.cn).** A short tutorial for PowderX is available at the CCP14 website **(http://www.ccpl4.ac.uk/tutorial/powderx/).**

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Savitsky, A. & Golay, J. E. (1964). Anal. Chem. 36, 1627.1639.
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Werner, P. E., Eriksson, L. & Westdahl, M. (1985). J. Appl. Cryst. 18, 367-370.

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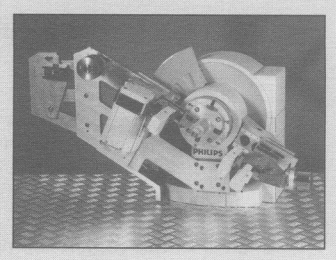

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Program for microsymposium on "Interfaces, Thin Films and Multilayers", IUCr Congress in Glasgow 1999

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The programme for the microsymposium on "Interfaces, Thin Films and Multilayers" to take place at the IUCr Congress in Glasgow 1999 is as follows:

Date: Friday 6 August 1999 from 1500-1730

1500-1530 Hartmut Metzger (Ludwig-Maximilians-Universität, Munich, Germany)
"Analysis of semiconductor quantum-dot systems by grazing incidence x-ray scattering techniques" Authors: T. H. Metzger, I. Kegel, R. Paniago, M.Rauscher, Z. Kovats, V. Holy and J. Peisl.

1530-1600 Roger Cowley (University of Oxford, UK)
"The structure of epitaxial thin films" Author R Cowley

1600-1630 Milan Sanyal (Suha Institute of Nuclear Physics, Calcutta, India)
"X-ray reflectivity and diffuse scattering studies of periodic multilayers" Authors: M.K.Sanya1, J. K. Basu, S.Banerjee, A.Datta and S. Hazra

1630-1700 Ivan Vartanyants (Institute of Crystallography RAS, Moscow, Russia)
"Reconstruction of Surface Morphology from the Coherent X-ray Scattering Experiments". Authors: LVartanyants, LRobinson, J.Pitney

1700-1730 Robert Feindenhans'l (Riso National Laboratory, Roskilde, Denmark)
"Interfacial structures of bonded Si wafers", Authors: R. Feidenhans'l, M. Nielsen, P.B. Howes, S. Weichert, F. Grey and J. Vedde.

I look forward to meeting you all in Glasgow. If you have any problems with these arrangements please let me know. Detailed information concerning the conference is available on the website: **(http://www.iucr.or~iucr-top/congll8/welcome.html)**

Best wishes, Paul F Fewster

For full details of the whole Glasgow programme see httD:l/www.iucr.org/ and the chairman's message (p2)

International School on Powder Diffraction, October 7-10 , 1998, Sponsored by the IUCr Commission on Powder Diffraction

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International School on Powder Diffraction (ISPD'98) held at the Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700 032, India, form October 7-10, 1998.

Professor S.P.Sen Gupta, Secretary of the Organising Committee for ISPD'98, being a member of the Commission on Powder Diffraction (CPD) of the International Union of Crystallography(IUCr), took the responsibility to organise this International School for the first time in this Sub-continent with great success. The School was sponsored by the IUCr with a financial grant of US$5000, and co-sponsored by the International Centre for Diffraction Data (ICDD), USA with a financial support of US$4000, the Indian National Science Academy (INSA) through its National Committee on Crystallography, DST, CSIR, DAE(BRNS), IACS, SINP, S.N.Bose Centre, Jadavpur University.

ISPD98 was well-attended by nearly 250 participants from all over India and abroad including a strong representation from Bangladesh. The importance of the School was reflected from the presence of Prof. E. N. Baker, who as a President of International Union of Crystallography (IUCr), came all the way from New Zealand to inaugurate the School on October 7 , morning at the MLS Hall of IACS. Dr. R. Chidambaram, Vice-president of IUCr Executive Committee could not attend due to his busy schedule. But, he sent his message and best wishes to ISPD'98. Dr. K.Lal, Director-grade Scientist of NPL gave the key-note address in the inaugural session highlighting the role of materials characterisation studies through various techniques including multi-crystal diffractometry for epitaxial films, powder diffractometry etc. Prof. Sen Gupta in his address emphasised the importance of organising such School for the Young Participants of this subcontinent. He then welcomed the foreign Scientists and participants for attending ISPD98. Prof. J. K. DattaGupta of SINP, Calcutta presented his views from the standpoint of National Committee on Crystallography.

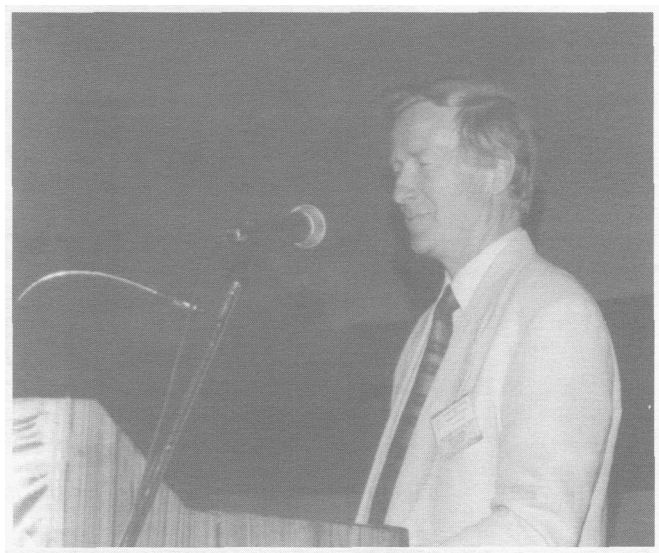

Figure 1: *Prof. Baker inaugurating ISPD'98 on Oct7 1998*

Figure 2: *Prof. and Mrs Baker with Prof. Sen Gupta during dinner (ISPD'98)*

There wcrc nine Technical scssions apart from Nine Hands-on Computer Session mentioned separately for applications of Computer Programs to deal with structure determination. Structure refinement from powders through Rietveld technique which evoked large interests. In the Computer sessions. faculty members cxplaincd the program details to the participants in several batches. Several soft-wares were also copied by the participants. As regards Technical sessions I4 speakers from several disciplines delivered their lectures. Those took part in the deliberations are : Professor Izumi(Japan), Tellgren (Sweden), Guru Row (IISC, Bangalore), John Faber(ICDD, USA), S. Mazumdar(BARC), A. K. Singh(NAL, Bangalore), K. V. Krishnan(Nagpur), M. K. Sanyal(SINP), B. N. Dev(IOP), S. P. Sen Gupta(IACS). From Philips. Dr. Celeste Reiss(Hol1and) and from Brucker AXS, Dr. Arnt Kern(Germany) took part in the recent development of instruments with applications. Philips and Brucker also exhibited their high- resolution instruments. Dr. Faber(1CDD) demonstrated the role of Data-base and ICDD activities. A visit to Science City was also arranged for the participants. A valedictory session was arranged on 10th where speakers and participants interacted with a request to organize such schools in future was made. The proceedings of ISPD'98 are now available from Allied Publishers(New Delhi) for purchase. A free copy to all participants has been given.

Hands-on Computer Session

In the hands-on session around 180 participants took part. The whole session was divided into three batches. Twelve computers was given to each batch so that maximum possible computer time could be allotted. In the computer session following programs were demonstrated

1. FULLPROF for Structure Refinement using Neutron Data - conducted by Prof. Roland Tellgren.
2. GSAS for Structurs refinement using X-ray data - conducted by ProfT. N. Guru Row
3. Powder Data Base and its applications(1CDD) - conducted by Dr. John Faber
4. SIMSAS for analysis of small-angle xray scattering - by Dr S. Mazumdar.
5. TRACES (Diffraction Technology) for routine data analysis. - by Mr. Gautam Bhattacharyya.
6. Several other programs like INDEXING etc were also demonstrated.

Programs were also distributed free of cost to the participants.

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Publishers: Allied Publishers Limited,New Delhi INDIA

Prof S. P. Sen Gupta
Secretary ISPD98

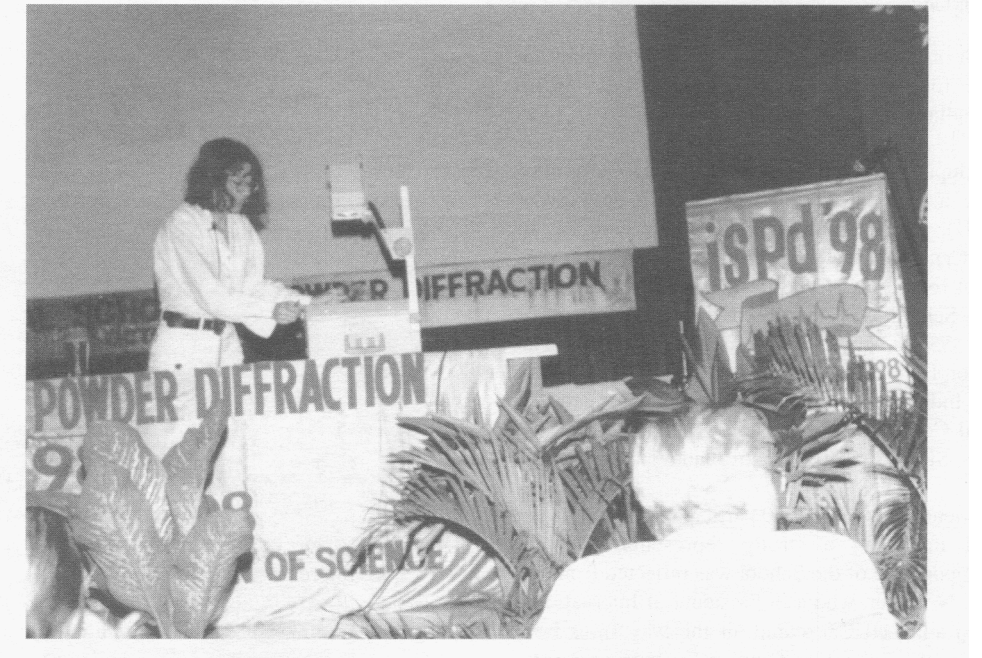

Figure 3: *Dr C. Reiss (Philips Holland) delivering her talk in the Technical Session during ISPD'98*

India-Italy Workshop on Utilisation of Elletra Synchrotron held at the Saha Institute of Nuclear Physics Calcutta, India, November 10-13,1998

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The India-Italy Workshop which was sponsored by the Department of Science & Technology, Govt. of India and Ministry of Foreign Affairs, Govt. of Italy, and organised by Prof. M. K. Sanyal of Surface Physics Division of SINP, Calcutta, was highly sucessful from all aspects. There were selected speakers from India as well as from Italy and was attended by nearly 100 participants from all over India. The inauguration was done by Dr. V. S. Ramamurthy, Secretary to the Department of Science and Technology, Govt. of India and was addressed by Mr. G. Zucconi (Ambassador of Italy in India) and Dr. A. Savoia, Director of Experimental Facilities ELLETRA, Trieste, Italy. There were 11 Technical Sessions apart from Poster Sessions. In the technical Session the following topics were covered: Elettra Synchrotron and INDUS Synchrotron(Indian), Surface structures, Protein Crystallography, Soft X-ray Microscopy, X-ray Standing Wave, Photoemission and ESCA, High pressure XRD and Structure from Powders, EXAFS, SAXS, Novel Materials etc. Prof. S. P. Sen Gupta chaired one of the Technical sessions on Powder Diffraction. A session on 'Synchrotron Experiments carried out by Indian Scientists' was interesting. Italian scientists presented in a detailed manner various possibilities and future experiments which can be carried out at Elettra in Italy. As Indian Synchrotron Facilities are under construction process (to be available in 2-5 years time), this collaborative workshop opened up a new phase in Indo-Italy co-operation in future,

S. P. Sen Gupta

National Conference on Nanomaterials: Physics/Devices held at the Institute of Physics(IOP) Bhubaneswar, India, March 18-20,1999

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The National Conference on Nanomaterials was organised in the sprawling campus of IOP in Bhubaneswar(Orissa) amongst selected participants and invitees. This was a well-focussed conference with chosen lecture topics on the new exotic materials. The inaugural address was given by Professor S N Behera, Director of IOP. He also delivered the first lecture on 'Clusters and cluster assembled nano-materials: A one-dimensional model study of the electronic structure.' Various speakers dealt with different aspects on materials synthesis, characterization by TEM, AFM, XRD etc. and device applications. Prof. S. C. Agarwal (IIT, Kanpur) spoke on metastabilities in porous silicon. Pushan Ayyub (TIFR, Bombay) described a versatile sputtering technique for producing atomic clusters and nanomaterials. Prof. S P Sen Gupta dealt with microstructural characterisation in Nb, Ti and V205 ball-milled powders by X-ray line profile analysis. Dr. S N Sahu(IOP) presented an interesting study on one-dimensional quantum confinement and aging effect innano-crystalline semiconductors. Visits to ion-beam laboratory where Pelletron accelerator is working and X-ray diffraction laboratory for standing wave and glancing angle measurements were arranged. Sight seeing tour to the 11th Century Konark (Sun) temple near Bay of Bengal seacoast was refreshing.

S. P. Sen Gupta

AsCA'98 - Report on the microsymposium MS-05. Structure refinement by powder diffraction

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The microsymposium was held as a part of the third conference of the Asian Crystallographic Association (AsCA'98) at hotel Equitorial, Bangi, Malaysia on Tuesday October 13th at 16:00 hrs. The chairman of the session was Professor B.H.O'Connor with Professor H.Toraya as co-chairman. There were six presentations by experts from different parts of the globe.

I. B.J.Kennedy, School of Chemistry, University of Sydney.
16:00-16:30
I3B2-1 X-rays or Neutrons or X-rays and Neutrons? Structural refinements of metal oxides.
This discussed the current status of powder diffractometry with special reference to the spectacular developments in the last decade. Recent studies of different metal oxide structures studied by this group were presented with the necessity of combining neutron diffraction data with high quality X-ray diffraction data.

2. S.FLinn et. a1 Centre laboratory Nankai University, Tianjin, 300071, P.R.China
13B2-2 Crystal Structure Studies of Organic Compounds From Powder Diffraction Data.

The author presented two methods one based on combined use of molecular mechanics with crystal structure and another using maximum entropy considerations. In the first case of the crystal structure of ethyl hydrazo dicarboxylate was solved by generating the trial structure based on molecular mechanics calculations. Refinements were done using the Rietveld approach. The second structure of (15 crown-5) manganese (II) di-isothiocynate was determined using maximum entropy technique which refines the intensity of the indexes in the extended range with a trial structure generated using Shelxs-86.

3. M.Hikam et. al. Department of Physics, Faculty of Mathematics and Science, University of Indonesia. Depok, 164224, Indonesia.
13B2-3 The influence of carbamide peroxide and stannous fluoride on crystallite size and microstrain of tooth enamel.

This article evaluated the influence of microstrain in the tooth enamel with addition of 10% carbamide peroxide and 0.4% stannous fluoride. The crystallite size and lattice parameters however do not change.

4. H.Toraya, Ceramics Research Laboratory, Najoya Institute of Technology, Japan.
13B2-4 Improvement of the accuracy of structural parameters in Rietveld Refinements using a new weight function.

The accuracy of structural parameters are generally not enough for a detailed chemical discussion even on simple structures like alpha-Si02. This new weight function gives importance to higher order reflections and statistically a better fit. The refined positional parameters of Mg2Si04 using 1.2Ang. high resolution synchrotron data improved substantially. Several applications were highlighted.

5. TN. Guru Row, Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore.
13B2-5 Studies on inclusion Complexes Via Powder Refinement and computer simulations

The basic idea is to locate the guest molecule in a zeolite-like structure using molecular dynamic simulations at that temperature and identify the resulting electron density on a difference Fourier map based on powder data.

6. J.Faber et al. ICDD, U.S.A.
13B2-6 Application of crystallographic databases to materials.

Two databases PDF maintained by ICDD and ICSD were reviewed. Combining data from PDF and ICSD it was demonstrated that new structural features could be obtained.

In all this microsymposium highlighted the recent advances made in structure determination and refinement using powder diffraction data. In conclusion Professor. B.H. O'Connor from Australia gave his chairman's remarks with emphasis on the future advances in powder diffraction, particularly for abinitio structure solution.

With best regards,
Guru Row.

Report on XXIX National Seminar on Crystallography held in the University of Madras, India, 21st-23rd Dec 1998

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The XXIX National Seminar on Crystallography was conducted at the Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai-600025 from 21st-23rd Dec 1998. 270 papers were presented during oral and poster sessions. The topics covered included crystallographic applications to biomedicine and materials science, biocrystallography, organic, inorganic, inorganic structures, physical properties, crystal growth and characterisation etc. Dr. Krishan Lal, treasurer, Asian Crystallographic association, inaugurated the meeting in the place of Dr, R. Chidambaram, Vice President IUCr, as Dr R. Chidambaram had to cancel his visit at the last moment. The highlight of the meeting was the conference talk delivered by Prof. C. N.R. Rao FRS on 'Crystallography in the Study of Chemistry of Materials'. Sessions on weak interaction and Synchrotron Radiation applications were organised for the first time in a National Seminar this year. Designing of the polymeric network, Supramolecular structures using metal organic coordination complexes, smart materials etc. was discussed. A session on publishing in the ACTA was also scheduled, but it had to be dropped as the Indian Co-editors could not make it to the meeting. Diffraction effects form graphite nanotube formation and nanoparticles, high temperature, high pressure studies of materials were other topics which were presented during the meeting

Figure 1: *XXIX National Seminar (Madras) Prof. GN.R.. Rao (3rd from left) with participants*

Vasantha Pattabhi
(Convenor)

WinMProf : a visual Rietveld software

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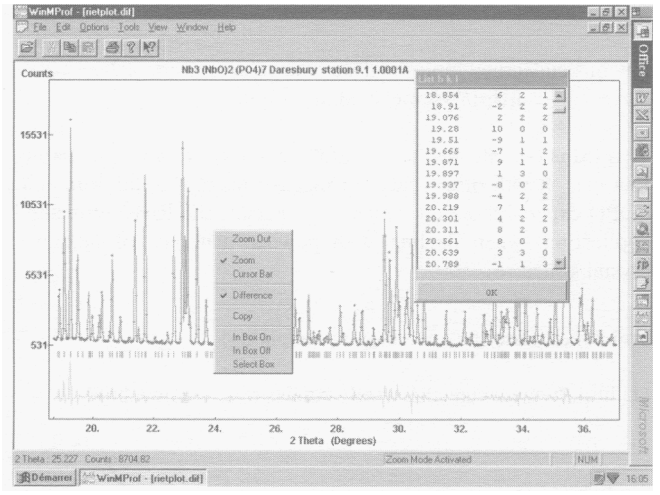
WinMProf is a Windows 95/98 and Windows NT based program developed in combined Visual C++ and Visual Fortran. WinMProf is both a general GUI for MPROF Rietveld profile refinement program and a viewing software for experimental or calculated powder diffraction patterns. It can also be used as GUI for other associated programs (Fourier difference, bond distances calculation). WinMProf has all the features of a conventional Windows application using the mouse to select menus, tools in the toolbar, to resize and to move windows etc...

When a powder diffraction pattern is displayed in the graphic window, several options are available in the menus bar (Options) as well as by clicking on the right mouse button to call a context menu : zoom, copy, selection of background points, visualisation of (hkl) indices etc... This is illustrated on the opposite figure which typically displays a calculated pattern. Context menu and (hkl) list dialog boxes are also opened.



An internal text editor (Wordpad class) is included in WinMProf, which allows to create or edit the input control file (*.pro) required for executing the MPROF Rietveld program, as well as to display the output text files (*.lis and others).

The actual version of MPROF is extensive modification of the initial routine by Murray & Fitch (1989). Numerous modifications have been made for more flexibility, easy-to-use and better performances. New options, corrections, peak-shape functions have been included. MPROF can be used to refine conventional X-rays, synchrotron, neutron (nuclear and magnetic) diffraction data collected at constant wavelength. Some of the MPROF features are:

- Le Bail decomposition method implemented.
- Several choices of peak-shape function for each phase.
- Phenomenological Stephens model of anisotropic peak broadening implemented.
- Qualitative account for anisotropic broadening (FWHM and shape).
- Absorption (and micro-absorption) correction available for various geometries.
- Asymmetry correction.
- Cheminal slack contraints and strict constraints.
- Bond distances and angles calculation.
- Output files can be produced for various other programs (SHELX, EXPO, STRUVIR...).

WinMProf is freely available via the web at **http://pecdc.univ-lemans.fr/WinMProf/WinMProf.htm**, and is mirrored at the CCP14 (http://www.ccp**14.ac.uk/ccp/web-mirrors/winmprof/WinMProf/** WinMProf.htm)

Solving structures by reverse Monte Carlo from scratch

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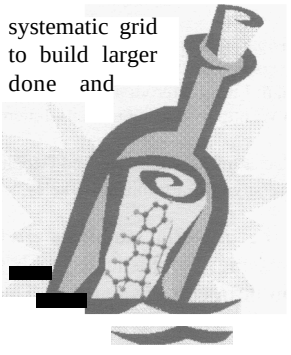
Trying to locate a guessed fragment in a crystalline cell while matching to either extracted "IFobsl" or the full powder pattern or the Patterson function (or...), has become a very active topic since about 15 years, though less than 50 experimental cases were truly undertaken. Methods use either systematic grid search, Monte Carlo, simulated annealing, genetic algorithm (...), as already listed in recent review papers [1,2]. Regretfully, a problem is the lack of availability of many software, with notable exceptions like *DIRDIF; PATSEE, PROMET* (public domain) and *POWDER SOLVE* (commercial).

When no fragment is previously known and if the classical approach (Patterson and direct methods) fails, then the crystallographer does not dispose of so many tools. Independent translation of dominant X-ray scatterers through the unit cell were attempted, for instance by Monte Carlo (with up to 2 different atoms in ref [3]) as well as by systematic grid search. Recent efforts in order to build larger models from scratch were done and implemented in several available software: *FULLPROF* [4] able for instance to locate Pb in $PbSO_4$ by Monte Carlo, *ENDEAVOUR [5]* working by simulated annealing and/or using potential functions, and *ESPOIR* [6] using a reverse Monte Carlo (RMC) approach applied on extracted "IFobsl".This last possibility was claimed to be impossible in ref. [7], in which the author declares : **"RMC modelling will certainly not enable ab initio crystal structure models to be obtained starting from random initial structure".** On the contrary, ESPOIR shows that this is possible by using the pertinent strategy. Indeed, structures with up to 15-30 independent atomr can be solved from scratch. The structure of the SDPD Round Robin [8] sample I, $[Co(NH_3)_5CO_3]NO_3ïH_2O$ [9], for



which no participant proposed a model, can be solved by *ESPOIR* (15 independent non-hydrogen atoms in $P2_1$ space group). Essentially, the (not so clever) strategy consists in trying again and again, jumping quickly to a new starting configuration if a model is frozen (false minima). Then, it is understandable that the main problem of those programs, when dealing with the more complex cases, is computer time. The direct methods find 30-100 independent atoms (though 50 were never attained from powder diffractometry data till now) in a matter of minutes on a PC (100-500MHz), and less than 30 atoms in a matter of seconds. The millions of moves and atom permutations, necessary for finding 30 atoms with *ESPOZR* from a set of 500 hkl reflections, require one night, at least, if you are lucky. So that, testing for larger configurations was not already done, due to lack of easy access to faster computer. Fortunately, the Moore's law is still expected to be applicable for many years, so that some hope may be placed on ESPOIR and the other above mentioned software. As a matter of fact, "espoir" (in french) means "hope" in english, suggesting that you should not lose it. Moreover, the source code (Fortran) is delivered with the package, allowing you to add your own stones to the building.

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[9] J.H. Zhu, H.X. Wu and A. Le Bail, *Solid State* ***Sciences*** **1** (1999) 55-62

SDPD (Structure Determination by Powder Diffractometry) E-mail Discussion List

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It is a pleasure to announce the birth of the Structure Determination by Powder Diffractometry (SDPD) Mailing List. Details on the obvious concerned topics and ways to subscribe arc gathered at

http://www.cristal.org/sdpdl

This list is not intended to substitute to the Rietveld Users Mailing List (1). It will offer space for discussions that could bore non-SDPD experts about all which may precede the Rietveld method application, when dealing with powder materials of unknown crystal structures.

Welcome, subscribe and enjoy participating!

(1) **http://www.unige.ch/crystal/stxncws/riet/wc~comc.htm**

MAUD: a friendly Java program for Material Analysis Using Diffraction

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In the material analysis field, researchers arc demanding increasingly sophisticated tools to obtain the required information from diffraction techniques. The latter has been evolved from the past and actually very powerful apparatus arc available to collect in a short time an enormous amount of data. All these data arc difficult to process in the traditional way also by modern computer. In short, the process time by a new generation computer is decreasing by a factor of two any year. Nevertheless the number of data to process is increasing also noteworthy, but the time available to the user or researcher working on the analysis is always the same. This will lead to the conclusion that a lot of data and/or information collected by the actual instruments arc lost and never used. Two solutions may arise. The first is to increase the number of researchers while the second is to develop new analysis tools that can process more data and requiring less time and experience by the user. The latter must not be forgotten because it can led to the result of enlarging the user basis and reducing the number of mistakes that only the diffraction expert can avoid.

Based on the experience with the program Rietquan [1] (Rietveld program for quantitative analysis featuring an automatic mode of refinement for non-expert Rietveld users) and on the new methodologies for Rietveld texture/stress analysis [2-7], we started a project to build a program easy to use, expandable and of general applicability, to help the end user in obtaining more information from data collected by traditional and new instrumentation. In the first implementation, we chosen to address users of the material field due to the potentialities of this approach for their needs.

Following an object oriented programming approach we have implemented the MAUD program and actually is available has a beta release [10]. The program is written in Java, so it can run virtually in any computer environment supporting the Java Virtual Machine. At the present installers arc available for the Macintosh and Windows platform but some testing has been done also on Unix without problems.

The principal features of Maud can be summarized in:

- Simultaneous crystal structure refinement, line-broadening, texture (stress under implementation) and quantitative phase analyses.
- Multiple samples, phases, diffraction spectra, and instrument geometries usable and analyzable at one time.
- X-ray normal tube, synchrotron, neutron constant wavelength and time of flight patterns analyzable also at the same time.
- Wizard or manual mode of refinement; the wizard mode allows the user to select what kind of analysis he needs to perform between (at the present): quantitative phase analysis, crystal structure analysis or texture analysis.
- Plug-in structure. Different methodologies can be added to the program by the user without the need to recompile it or to know the internal structure of the program. The plug-in structure involves also: instrument geometries and correction/calibrations, data formats, line-broadening methods, texture algorithms, peak intensity extraction, etc.
- Database support for crystal structures (phases), instruments, sets of data etc.
- CIF friendly program; the program uses, imports and supports CIF (Crystal Information File) formats.
- Multiple data format for input files (only ASCII): Philips, Rigaku, Siemens, GSAS, DIB etc.
- Easy addition by the user of other input file formats trough the plug-in structure.
- Quantitative analysis of crystalline fraction for silicate-glass containing materials or polymers.
- Unlimited number of data file, phases, instruments, wavelength and other objects. The only real limit is the computer memory. Up to now some analysis have done loading simultaneously more than 1000 datafiles (from the SKAT diffractometer at Dubna).
- Space group and symmetries relationships computed using SgInfo [13] linked as a native library to the package. In the future also this part will become pure Java to allow the program to run in web browsers over internet.

The latter is based on the method reported in reference [9]; no internal or external standard is necessary and the accuracy attainable is the standard Rietveld accuracy.

In the present implementation, the supported methodologies for the crystallite-microstrain separation are the theory developed by Delhez et al. [11] and the recently published method of Popa [12], including the anisotropic crystallite shape by harmonic expansion. Figure 1 reports a screen shot were is visible the 3D model for the crystallitc shape as refined by the program for the Y_2O_3 sample of the CPD Round Robin. The texture includes the classical March-Dollasc formula for a simple correction or the WIMV method [3] that permits to obtain the entirc orientation distribution function if a sufficient number of spectra at different tilting angles are available for the refinemcnt.

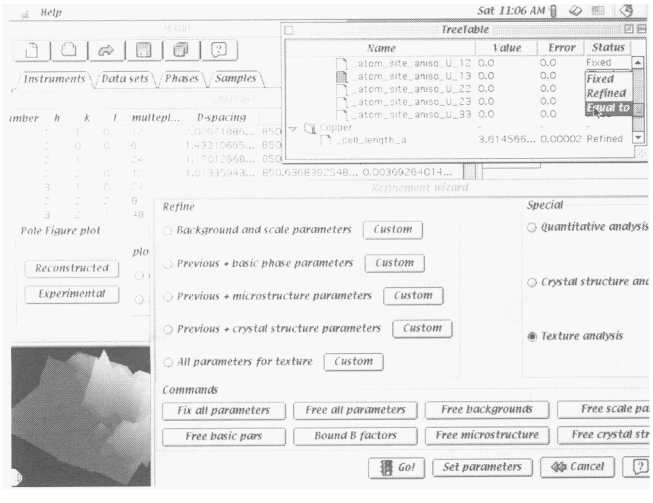

Figure 1: *Screen shot of Maud after refining the Y_2O_3 CPD Round Robin sample. The powder was found not a perfect instrumental profile and the analyzed crystallite shape using the Popa model is shown in the center:*

Any single parameter or data is available trough the interface as recognizable in Figure 2. More example shots are available in the Maud web page [10] along with the installers for the actual beta version.

The program has been successfully applied to analyze the texture of multiphase samples, to refine spectra with anisotropic peak broadening, quantitative analysis of polymers and samples containing silica glass. In many cases, the simple automatic mode of refinement has been used by the wizard panel and only in very few cases it was necessary to complete the analysis in manual mode for better results.

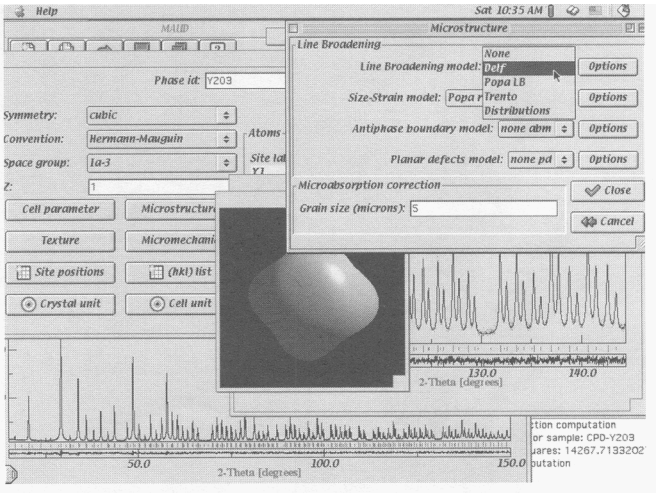

Figure 2: *The wizard panel for fast refining strategies is visible in this picture. Refinable parameters can be specified also manually one by one. In the background a reconstructed polefigure, as result of the texture analysis, is reported in a 3D plot.*

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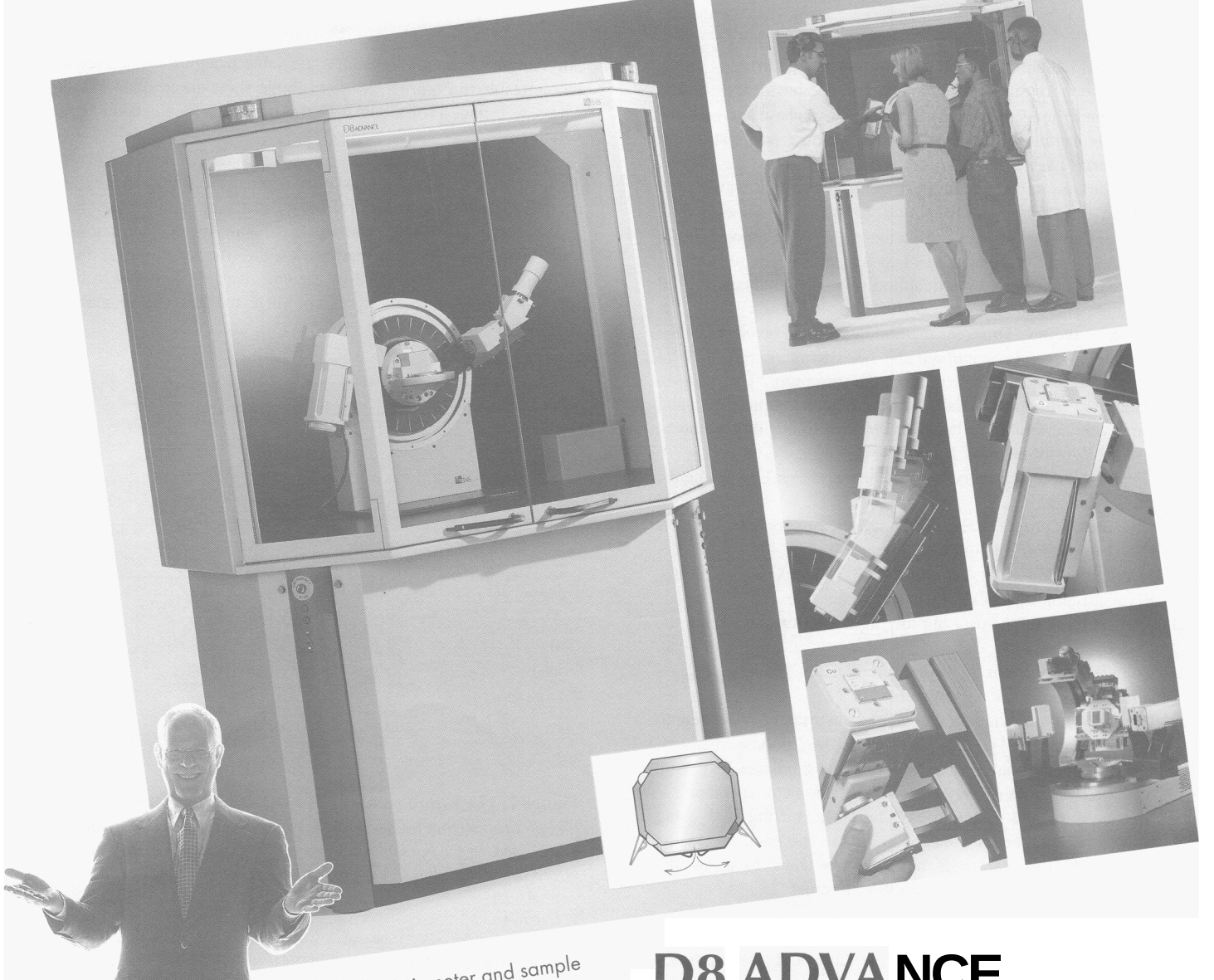

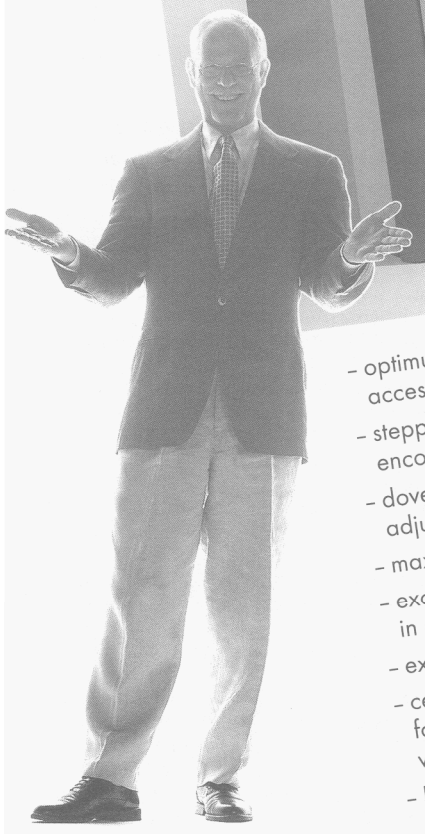

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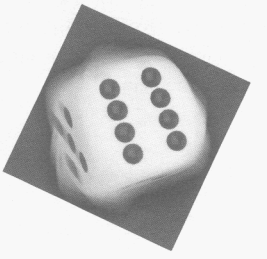

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What's New with ICSD-for-WWW?

Alan Hewat,
ILL Grenoble, France
E-mail : hewat@ill.fr - Web : http://www.crirtal.org/

The site-server version of the Inorganic Crystal Structure Database (ICSD) is now distributed by FIZ Karlsruhe on CD-rom together with ILL'sWWW interface. A number of features have been added of special interest for powder diffraction (see **http://barns.ill.fr/dif/icsd/**).

Following suggestions from Lachlan Cranswick, ICSD-for-WWW data files can now be exported in many formats including CIF, Shel-X, GSAS, FullProf, PowderCell, CCSL and Lazy PulverIx. This makes it easy to start refining your new powder data if an isomorphous structure already exists among the almost 50,000 in the database.

You can also display an indexed profile plot of any of these structures using ICSD-for-WWWs built-in Lazy PulverIx, or export this profile for display with your favourite profile plotter. Other new features include the display of ORTEP-like thermal ellipsoids in interactive 3D (VRML), and the calculation of Brown-Shannon valence sums.

The latest demonstration version of ICSD-for-WWW for SGI, HP and Sun servers can be downloaded from **ftp://ftp.ill.fr/pub/dif/icsd/**but already the full ICSD-for-WWW database is available to academic users in several countries:

France: ILL/ESRF Grenoble at **http://barns.ill.fr/dif/icsd/**
UK: CDS at Daresbury **http://www.dl.ac.uk/CDS/llicsd.html**
UK: CCP14 at Daresbury **http://icsd.ccp14.ac.uk/icsd/**
USA NIST Washington **http://www.ncnr.nist.gov/-toby/icsd/**
USA Oak Ridge National Laboratory **http://quintus.ssd.ornl.gov/dif/icsd/**
Spain: Scientific Research Council CICS: **http://xsg0.roca.csic.es/difksd/**
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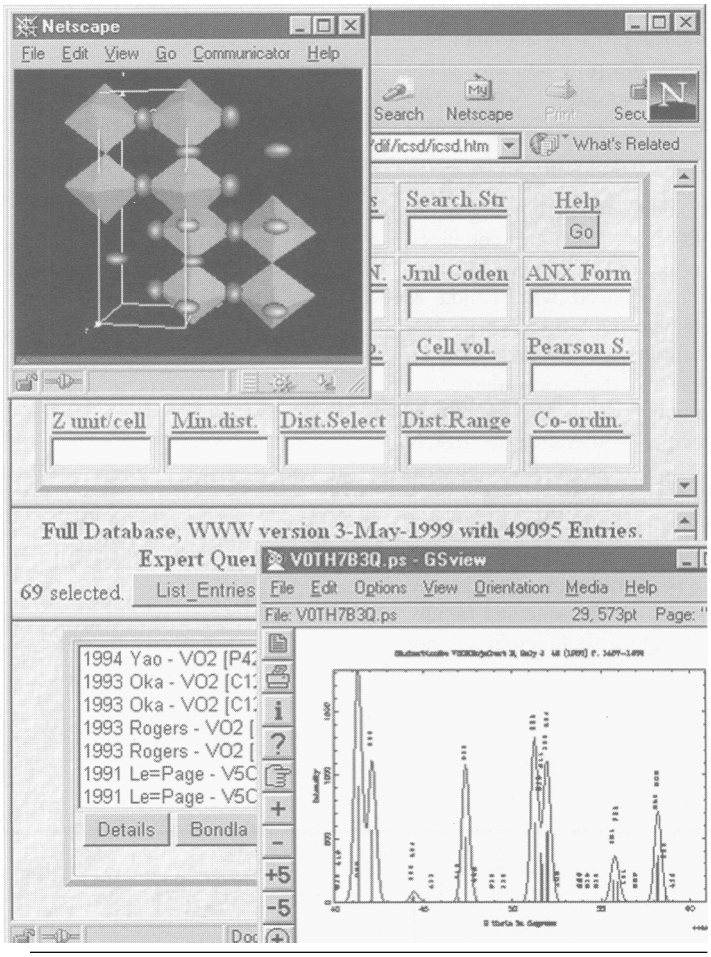

Practical Advances in Automatic Powder Indexing: CRYS2RUN, LZON and the Indexer's WorkBench Project.

Robin Shirley,
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The classic programs for finding unknown unit cells from powder diffraction patterns of single solid phases in any symmetry, ITO(8), DICVOL[3, 4, 5] and TREOR[9, 10] date back some 20 years. Each program (sometimes all three) may well not yield a convincing solution using its default settings, and their expert deployment remains an art. Data problems, sometimes unavoidable, and the intractability of indexing solution space, make the development of effective indexing a demanding task that tends to get little support, despite its increasing importance with the growth in ab-initio powder structures. Some attempts to address this are reported here: by making existing programs easier for non-specialists to use; by adding a fourth program to the above list; and by promoting a co-operative project to address future needs in this field.

1) CRYS2RUN is a simple script-based system for making existing indexing facilities more accessible to non-specialists, that runs with minimal demands under MSDOS or Windows. The CRYS program (currently v9.28) forms an interactive front end and offers data enhancement facilities such as self-calibration for detecting and correcting 2theta-zero errors[6]. From CRYS, a target indexing program is selected and a data file written for the format-translator QDAT. On exit, the run proceeds automatically using nested scripts via QDAT to the indexing program, leaving the user looking at indexing output in a file-editor. Reruns with adjusted parameters are supported by a family of associated scripts.

2) LZON (currently v6.21) forms an addition to the set of general, automatic indexing programs for PCs, based on the combined Shirley, Louer & Visser mainframe program LZON v6L [7]. It (a) performs an ITOv6 zone-search@), enhanced with Ishida & Watanabe's PM algorithm[1], (b) completes Q(A,B,C,F) basis sets using Shirley's dominant-zone heuristic, (c) seeks Q(D,E) solutions for each basis set using exhaustive dichotomy algorithms from Louer & Shirley's LOSH program[7], and finally (d) returns to Visser's ITOv6[8] for solution refinement and evaluation. LZON is best for low-symmetry monoclinic and triclinic phases, particularly the pathological dominant-zone cases that can spawn hundreds of pseudo-solutions. Typical running times are 2-15 minutes on a 200MHz Pentium. If impurity lines are suspected, up to "N" spurious unindexed lines can be ignored, though this may increase run times. Specified basis sets can be searched rapidly with the associated LOSHFZRF[7] program (both programs are supported by CRYS2RUN).

CRYS2RUN, LZON and LOSHFZRF are distributed free for non-commercial use via the CCP14 website. For a tutorial, see http:l/www.ccp 14.ac.uk/tutorial/crys/ and the latest version of the suite is available via http:l/www.ccp14.ac.uk.uMccp/web-mirrors/crys-r-shirley/.

3) Looking to the future, the "Indexer's WorkBench" is a proposed co-operative project to integrate available mature indexing programs into a single easy-to-use facility accessed from an interactive, graphical front end, in two parallel versions - for 32-bit Windows and for Linux. It is hoped to include newer methods such as genetic algorithms(l), [2] and to support both line-position and profile data[2]. Its implementers will form a virtual project team working via the Internet. Those interested in taking part are invited to contact the author at R.Shirley@surrey.ac.uk.

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What's On (Conferences and Workshops)

Wednesday 4th to Friday 13th August 1999,
SECC, Glasgow, Scotland.
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.iucr.org/iucr-top/cong/l8/

Wednesday 4th August 1999,
SECC, Glasgow, Scotland
Structure factor phase determination in electron crystallography
Ways of solving the phase problem in electron diffraction will be discussed including: extraction of structure factor phases from high resolution election micrographs; direct methods applied to electron diffraction intensity data; phase invariants from dynamical effects in convergent-beam electron diffraction (CBED); coherent CBED. Application to structure determination will be dealt with as well as the problems and possibilities associated with dynamical diffraction.

WWW: **http://www.iucr.org/iucr-top/cong/l8/sat/workshop.html**

Questions and comments regarding this workshop should be directed to:

Professor Sven Hovmoller	or	Professor Jon Gjonnes
Structural Chemistry,		Centre for Materials Science,
Arrhenius Laboratory,		University of Olso,
Stockholm University		Gaustadallen 21,
S-10691 Stockhom, Sweden.		N-0371 Oslo, Norway
E-mail: svenh@tom.fos.su		E-mail: jon.gjonnes@fys.uio.no

Wednesday 4th August 1999,
SECC, Glasgow, Scotland.
Structure Determination from Powder Diffraction Data
The aim of this workshop is to give an overview of the state of the art of structure determination (and refinement) from powder diffraction data by some of the worlds leading experts in this field. The ab initio determination of structures from powder diffraction data is a brand new but rapidly growing field which has seen exciting progress during the past few years. Besides the adaptation and improvement of traditional structure solving tools, many new methods have been developed, some of which will be presented here in detail. The workshop will concentrate on the practical aspects of structure determination from powder data and will show the possibilities as well as the limitations of the different methods.

For further information regarding this workshop consult the following web site:http://btakx3.kri.uni-bayreuth.de/-btako3/

Questions and comments regarding this workshop should be directed to:
Dr. Robert E. Dinnebier
Laboratory of Crystallography
Fax: + 49 921 553770 University of Bayreuth
D-95440 Bayreuth
Germany
E-mail: robert.dinnebier@uni-bayreuth.de
Phone:+49921 553880
Fax: +49 921 553770

Wednesday 4th August 1999,
SECC, Glasgow, Scotland.
30 Years of Rietveld Analysis: The Next Generation - Organised by Bruker AXS
This workshop gives an overview of the latest developments in the field of Rietveld analysis. The techniques presented will dramatically extend the possibilities of all profile analysis methods, starting from single line analysis and ending up with ab-initio structure solution from powder data.

The workshop will emphasize the following topics:
1. A new fundamental parameters approach for describing X-ray line profile shapes
2. Rietveld refinement without the need of a parameters turn-on sequence
3. **Ab-initio structure solution from powder data as part of the Rietveld refinement process**

In the below referenced webpage, a more detailed description of the workshop contents is provided. The procedures presented lay the foundation for the next generation of Rietveld analysis.

Organzer: Dr. A. Kern, Dr. A. Coelho & Dr. M. Winter, Bruker AXS

For further information please email to arnt.kern@bruker-axs.de or refer tohttp://www.brucker-axs.com/Events/glas**1**.htm (which includes the registration form)

Date: August 4th, 1999 10 am - 4 pm

Workshop site:Lecture Theatre G29, The Gilbert Scott Building, University of Glasgow

Workshop fee: 30 GBP (standard rate) / 20 GBP (student rate)
Fee includes workshop materials and luncheon

Wednesday 11th August 1999,
Computer Science Cluster, Glasgow University, Glasgow, Scotland.
Simulating Crystals as a Teaching Tool and to Analyse Defect Structures
IUCr Congress, Glasgow - additional workshop
Workshop under the auspices of the DGK (German Crystallographic Association)

When: During the IUCr Metting Glasgow, Aug **11**, 1998; l0am through 5pm

Where: Computing Science CLuster at Glasgow University

For registration please fill out the format at http://www.uni-**wuerzburg.de/mineralogie/crystal/workshop.** html

For further information contact:
Reinhard Neder or Thomas Proffen
E-mail:reinhard.neder@mail.uni-wuerzburg.de or proffen@pa.msu.edu

28-30 September; 1999
ECRSS: the Fifth European Conference on Residual Stresses,
Congress Centre "Leeuwenhorst", Noordwijkerhout, The Netherlands
Deadline for Abstracts: 1 Februari, 1999
Contact: Mrs. G. van Galen, Netherlands Society for Materials Science, P.O.
Box 390, NL-3330 AJ Zwijndrecht, The Netherlands
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CALL FOR CONTRIBUTIONS TO THE NEXT CPD NEWSLETTER

The next issue of the CPD Newsletter will be edited by Bob von Dreele to appear in late 1999. 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 Bob von Dreele, Los Alamos National Laboratory, MS H805 LANSCE-12 : LUJAN, CENTER, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA , Fax: +1 505 665 2676, E-mail: vondreele@lanl.gov)

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