

Errata

QPDA – A User-Friendly, Interactive Program for Quantitative Phase and Crystal Size/Strain Analysis of Powder Diffraction Data

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Abstract

Recent developments in the Rietveld method for the analysis of powder diffraction data have seen the method evolve from its original purpose of crystal structure refinement to include the determination of phase abundance in polycrystalline mixtures and the estimation of crystal size and strain parameters. However, the Rietveld method is not easy to use and may deter many powder diffractionists, who are not interested in structure refinement *per se*, from using the method in its non-structural applications.

In order to overcome the difficulties in using the Rietveld method, a program, QPDA (for Quantitative Powder Diffraction Analysis), has been written that sets the condi-

tions necessary for a single or multi-phase refinement, runs the Rietveld program and extracts phase abundance and size/strain information from the refined parameters. The program comprises a user-friendly, default-driven system of subroutines, written initially in VAX Fortran, and operates from a database of inorganic materials frequently encountered in a wide range of minerals and materials science industries.

Equations (3) and (5) should be corrected to read as follows:

$$e_{\text{rms}} = \pi (U-U_i)^{0.5} / 720 (2\ln 2)^{0.5} \quad (3)$$

$$D = \lambda (180/\pi) / (\gamma - \gamma_i) \quad (5)$$

The following citation should be added to the reference list:

Donnay, J.D.H. & Le Page, Y. (1978). *Acta Crystallogr.* A34, 584.

International Report

A word from the editor . . .

Dr. Jaroslav Fiala has submitted a report on the meeting on Advanced Methods in X-Ray and Neutron Structure Analysis of Materials which was held in Prague, Czechoslovakia, last August. His historical introduction is very interesting. I think you will enjoy it. I did.

Helein D. Hitchcock, Editor

Calendar of Meetings	53
Correspondents Reports	54
Book Reviews	57
Short Courses and Workshops	58
Computer Comments	59

Regional Correspondents

Australia

Mr. Tony Raftery, Dept. of Physics,
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Czechoslovakia

Dr. Jaroslav Fiala, Central Research Inst.,
ŠKODA, 31600 Plzeň, Czechslovakia

Calendar of Meetings

1991

First European Powder Diffraction Conference (EPDIC)

March 14-16, 1991

Munich, West Germany

This new meeting was initiated as a forum for all European powder diffractionists to discuss recent developments and applications in all fields of science and technology. This first meeting is scheduled in conjunction with the annual German Crystallography Meeting (March 11-13, 1991) at the Ludwig-Maximilian University of Munich. The official language of the conference be English. There will be oral papers and posters presented, as well as a half day workshop on data bases and methods presented by the International Centre for Diffraction Data. The Scientific Programme Chairman is Dr. Jan Visser.

Contact: Siemens AG, ZFE ME AMF 12, Dr. H. E. Göbel, P.O. Box 830952, D-8000 Munchen 83, West Germany

Third Intensive Course in X-Ray Structural Analysis of Small and Medium-Sized Molecules.

March 14-16, 1991

Aston University.

Contact: David Watkin, Chemical Crystallography Laboratory, 9 Parks Road, Oxford, OX1 3PD, UK.

International Centre for Diffraction Data Spring Technical Meetings and Annual Meeting March 19-21, 1991

Concordville, Pennsylvania, USA.

Contact: Ms. Josephine Felizzi, JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081, USA. Phone (215) 328-9403.

British Crystallographic Association Spring Meeting March 25-28, 1991

Sheffield, UK

Contact: Dr. A. J. Smith, Department of Chemistry, University of Sheffield, Sheffield S3 7HF, UK.

Materials Research Society Spring Meeting April 29-May 4, 1991

Anaheim, California, USA

Contact: M. Geil, Materials Research Society, 9800 McKnight Road, Suite 327, Pittsburgh, PA 15237, USA. Phone (412) 367-3003; FAX (412) 367-4373.

3rd European Conference on Crystal Growth May 5-11, 1991

Budapest, Hungary

Contact: E. Lendvai, Research Institute for Technical Physics, Hungarian Academy of Sciences, POB 76, H-1325, Budapest, Hungary.

Third International Conference on Progress in Analytical Chemistry in the Iron and Steel Industry May 14-16, 1991

Luxembourg

The aim of the conference is to bring together chemists from all over the world, working in connection with iron and steel, for an exchange of experience covering the different analytical techniques used in their laboratories. Analysts working in the iron and steel application sector, in affiliated research institutes, universities and in government control bodies are also encouraged to participate. The conference languages will be English, French, German, Italian and Spanish. Simultaneous interpretation between all these languages will be provided.

Contact: Presidium of Cetas, Mrs. M. R. Posch, PO Box 185, NL-1940 Ad Beverwijk.

Synchrotron - Perspectives and Applications Summer 1991

France

Joint meeting of French, Italian, German and English physical chemistry sections of chemical associations.

Contact: Dr. C. Troyanowsky, Societe Chim. Phys., 10 rue Vauquelin, 75231 Paris 05, France.

ICDD Clinic on X-Ray Powder Diffraction June 17-21, 1991 Fundamentals

June 24-28, 1991 Advanced Techniques

**The Pennsylvania State University
University Park, PA, USA**

The ICDD X-Ray Clinics are the continuation of the SUNY Clinics which, for some twenty-five years, were held at the State University of New York at Albany. The ICDD assumed responsibility for these clinics in 1990. The Clinic is presented in two separate week-long sessions, each of which stands alone as a complete course.

Contact: Mario Fornoff, ICDD X-Ray Clinic, International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081, USA. Phone (215) 329-9400, FAX (215) 328-2503

ICDD Clinic on X-Ray Fluorescence Spectroscopy July 8-12, 1991 Fundamentals

July 15-19, 1991 Advanced Techniques

**Swarthmore College
Swarthmore, PA, USA**

Details and Contact: Same as ICDD Clinic on X-Ray Powder Diffraction (above).

American Crystallographic Association July 21-26, 1991

Toledo, Ohio, USA

Contact: Alan Pinkerton, Department of Chemistry, University of Toledo, OH 43606, USA.

PICXAM

Pacific-International Congress on X-Ray Analytical Methods

August 12-16, 1991

Honolulu, Hawaii, USA

The major thrust of this meeting will be the practical aspects involved in X-ray methods for materials analysis. The Congress will provide an international forum for discussion of the following methods: X-ray powder diffraction, X-ray fluorescence, X-ray aspects of surface analysis, X-ray emission, X-ray stress analysis, and thin film analysis by X-ray powder diffraction and X-ray fluorescence. Workshops will be offered at the University of Hawaii at Hilo on the island of Hawaii on August 7-9, the Wednesday through Friday preceding the Congress. Proceedings will be published as a volume of *Advances in X-Ray Analysis* with Paul Predecki as the Coordinating Editor.

Contact: Lynne Bonno, Conference Secretary, Department of Engineering, University of Denver, Denver, CO 80208, USA. Phone (303) 871-3515.

ECM-13, European Crystallographic Meeting

August 25-30, 1991

Ljubljana, Yugoslavia

Contact: Prof. L. Golic, ECM-13, Department of Chemistry and Chemical Technology, E. Kardelj University, POB 537, YU 41001 Ljubljana, Yugoslavia.

Satellite Meeting on Crystalline Structures and Defects in Ceramics

September 2-4, 1991

Ljubljana, Yugoslavia

Contact: same as for ECM-13.

International Centre for Diffraction Data

Fall Technical Meetings

October 23-24, 1991

Concordville, Pennsylvania, USA.

Contact: Ms. Josephine Felizzi, JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081, USA. Phone (215) 328-9403.

Fourth Beijing Conference and Exhibition on Instrumental Analysis

October 19-22, 1991 - Conference

October 18-24, 1991 - Exhibition

Symposia in the fields of electron microscopy, mass spectrometry, spectroscopy, chromatography, magnetic resonance and electroanalytical chemistry are scheduled.

Contact: The Secretariat of BCEIA, Room 5412, Building No. 4, XI YUAN Hotel, Er Li Gou, Beijing, 100046, P. R. China.

Materials Research Society Fall Meeting

December 2-7, 1991

Boston, Massachusetts, USA

Contact: M. Geil, Materials Research Society, 9800 McKnight Road, Suite 327, Pittsburgh, PA 15237, USA. Phone (412) 367-3003; FAX (412) 367-4373.

Report from the Commission on Powder Diffraction

Quotes from the Editorial by J. Ian Langford, Editor of Commission on Powder Diffraction (CPD) Newsletter No. 5

"One aim of the CPD Newsletter is to inform the powder diffraction community of various aspects of the subject which are of topical interest, for example, features on PD facilities, notes of particularly important developments in instrumentation or technique and so on. In this issue Drs Bob Cernik and Phil Pattison highlight the pioneering work of the powder diffraction group at the Science and Engineering Council's Daresbury Laboratory synchrotron radiation source. This is followed by reports on recent ventures organised, sponsored or supported by the CPD. 1990 has been a particularly busy year for the Commission. Two microsymbiosia and a discussion session were arranged by the CPD at the XVth IUCr Congress at Bordeaux in July. The Congress was preceded by the outstanding PD Satellite Meeting arranged by CPD at Toulouse, without a doubt a milestone in the annals of PD. During August the CPD sponsored a Rietveld Method Summer School for beginners at Cieszyn, Poland, another successful venture, which was over-subscribed by a factor of two. The Chairman and Secretary contributed substantially to the International School on Powder Diffraction held in Cairo in January, at which an excellent introductory lecture was given by Professor Mario Nardelli, then President of the IUCr. The Rietveld Refinement Round Robin is nearing completion – a preliminary report was presented at the Toulouse meeting by Dr Rod Hill – and the book on the method, based on the proceedings of the 1989 Petten workshop, should soon be with the publishers. The first issue of the Information Exchange Bank for PD programs, compiled by Professor Deane Smith, will be available shortly. An update on these projects will appear in the next Newsletter."