

its parameters FWHM and the 'shape factor'. Their e.s.d.s can be set to zero if not available. Other input data required are Miller indices and angular positions of reflections.

If more than two reflections are available, the program calculates values by means of a weighted least-squares linear fit. The parameters calculated by the 'double-Voigt' method include r.m.s.s. averaged over different characteristic distances, both surface- and volume-weighted domain sizes, and some auxiliary parameters. The first 50 Fourier coefficients are generated. The simplified integral-breadth methods (Cauchy–Cauchy, Cauchy–Gauss and Gauss–Gauss approximations) yield volume-weighted domain sizes and an 'upper limit' of strains from the same data set.

The program creates output files in the ASCII format. As well as the main output file of results, other files are created to aid the plotting of data. They contain size coefficients, strain (distortion) coefficients, r.m.s.s. and both surface- and volume-weighted column-length distribution functions, all as functions of the averaging distance.

Software and hardware environments: This program runs on an X86 IBM PC and clones with a mathematical coprocessor under MS-DOS 3.3 and higher versions.

Program specification: The program is written in Microsoft Fortran 5.1, that is, Fortran 77 with some Microsoft-specific extensions. It has about 2000 lines of source code.

Documentation and availability: Both ASCII and Wordperfect 5.2 documentation with the executable program file and sample input and output files are available from the author by either e-mail (by sending a request to dbalzar@olimp.irb.hr) or by supplying a 3.5 in diskette.

Keywords: Diffraction line broadening, integral-breadth methods, profile fitting, Voigt function, Warren–Averbach method.

References

- Balzar, D. (1993). *J. Res. Natl Inst. Stand. Technol.* **98**, 321–353.
 Balzar, D. & Ledbetter, H. (1993). *J. Appl. Cryst.* **26**, 97–103.
 Klug, H. P. & Alexander, L. E. (1974). *X-ray Diffraction Procedures*, 2nd ed. New York: John Wiley.
 Warren, B. E. & Averbach, B. L. (1952). *J. Appl. Phys.* **23**, 497.

Crystallographers

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to The Executive Secretary, 2 Abbey Square, Chester CH1 2HU, England.

J. Appl. Cryst. (1995). **28**, 245–246

Raymond Pepinsky 1912–1993

Raymond Pepinsky, Professor of Physics and Metallurgical and Materials Engineering at the University of Florida, died at the age of 81 on 7 May 1993, following his slow recovery from Guillain–Barré syndrome. His wife Louise died only a few months later, in December 1993. She will be remembered fondly by Ray's students and many visiting scientists for her kindness and gracious hospitality. Two sons, Peter and David, survive.

Ray began his career in crystallography as a graduate student of W. H. Zachariasen at the University of Chicago, where he received his PhD in 1940. He worked for the US Rubber Company, and then in 1941 joined the Physics Department at the Alabama Polytechnic Institute, now known as Auburn University. During World War II he worked on wartime radar at the MIT Radiation Laboratory, returning to Auburn in 1945. He moved to Pennsylvania State University in 1949, to Florida Atlantic University in 1963 and Nova University in Florida in 1965, and ultimately to the University of Florida in 1968. Some older crystallographers will remember a contentious side of Ray's personality, which made problems for him throughout his career. He was, however always notable for his generous and devoted giving of effort, time and insight to his students and colleagues, and highly respected for his scientific capabilities and accomplishments.

Reading over his papers today, one is struck by the quality and range of his work. Probably best known is XRAC, the large electronic analog computer for rapid summing and display of Fourier and Patterson series, which was built at Auburn and moved to Penn State; there it helped solve many crystal structures in the 1950s and early 1960s, and would doubtless have given rise to successors at other laboratories had not the digital computer arrived soon thereafter. This was only one of Ray's contributions to structure-solving methods, however. In 1955, with Y. Okaya and Y. Saito, he wrote what is probably the earliest paper on phase determination by anomalous dispersion, and with the same authors in 1957 gave an improved method for the use of anomalous dispersion in determining absolute config-

uration. In the early 1950s, he wrote papers on direct methods with C. H. MacGillavry and J. Goedkoop, and with V. Vand, and organized and edited the proceedings of an important conference at Penn State on 'Computing Methods and the Phase Problem in X-ray Analysis', with a later conference and volume (with J. M. Robertson and J. C. Speakman) on the same subject in 1961. The Penn State period was also the period in which Pepinsky created a major school of research in ferroelectricity. This program would provide benchmark structural data on representative members of almost all of the ferroelectric systems that were known up to 1963. One of us (BCF) has described this work in more detail in an obituary for Ray in *Ferroelectricity*. Finally, in the late 1960s and early 1970s, the range of his interests was shown in papers on ultra high speed printing devices, on documentation theory and a national information network, on phase information from multiple-beam scattering, and on the non-uniqueness of the solutions of Patterson functions in non-periodic non-centrosymmetric cases.

In his general life as a scientist, Ray was a member of numerous major panels and committees, was invited to travel and lecture in numerous countries, was a Fellow of the American Physical Society and the AAAS, and in 1965 was the recipient of an honorary doctorate from the Justus Liebig University in Giessen, Germany. His great avocation lay in his extraordinary collection of many thousands of records of classical, especially vocal, music, and in his program *The Art of Song*, which from 1977 was heard every week on the Public Radio station of the University of Florida.

DAVID SAYRE
B. CHALMERS FRAZER

Professor **Frank C. Hawthorne**, Professor of Crystallography and Mineralogy at the University of Manitoba, Canada, was the 1994 recipient of the Hawley Medal of the Mineralogical Association of Canada. The medal is awarded for the work judged to be the most significant in the previous year's volume of the journal of the Association; the work used a variety of crystallographic and spectroscopic techniques to unravel the crystal structure and crystal chemistry of the important metamorphic mineral staurolite.

Nobel Laureate Dr **Jerome Karle**, Chief Scientist of the Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, DC, USA, is a co-recipient of the 1992 Ettore Majorana – Erice – Science for Peace Prize from the Ettore Majorana Centre for Scientific Culture in Erice, Italy. The

award recognized Dr Karle for his discoveries relative to the structure of materials with diffractive methods and for his engagement to promote international scientific collaboration above any ideological-political-racial barrier.

Professor **Clifford G. Shull**, Emeritus Professor at MIT, Cambridge, MA, USA, and Professor **Bertram N. Brockhouse**, Emeritus Professor of Physics at McMaster University, Hamilton, Ontario, Canada, have jointly been awarded the 1994 Nobel Prize in Physics for their pioneering contributions to the development of neutron scattering techniques for studies of condensed matter.

Professor **M. Vijayan**, Professor of the Molecular Biophysics Unit and Chairman of the Division of Biological Sciences, Indian Institute of Science, Bangalore, India, was awarded the Professor G. N. Ramachandran 60th Birthday Commemoration Medal of the Indian National Science Academy in December 1994 for his outstanding contributions to biological crystallography

New Commercial Products

Announcements of new commercial products are published by the Journal of Applied Crystallography free of charge. The descriptions, up to 300 words or the equivalent if a figure is included, should give the price and the manufacturer's full address. Full or partial inclusion is subject to the Editor's approval and to the space available. All correspondence should be sent to the Editor, Dr A. M. Glazer, Editor Journal of Applied Crystallography, Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, England. The International Union of Crystallography can assume no responsibility for the accuracy of the claims made. A copy of the version sent to the printer is sent to the company concerned.

J. Appl. Cryst. (1995). **28**, 246

Domestic Source for β -Barium Borate (BBO)

After three years of development, INRAD has begun full scale production of **single-crystal β -barium borate (BBO)**. This important nonlinear crystal offers several advantages such as a broad phase-matchable range, a large effective nonlinear coefficient and high damage threshold.

This fortunate combination of features makes BBO the optimum choice for doubling of near-infrared high average power lasers. These low UV absorption crystals make harmonic generation possible down to 197 nm. An important application for the defense community and environmental monitoring is optical parametric oscillators for the ultraviolet and near-infrared.

INRAD offers custom cuts over a wide range of sizes, even wafers as thin as 0.1 mm. Crystals can be AR coated and can be supplied in a variety of mounts. Technical staff can help in the selection of the most appropriate cut and configuration to suit customer requirements.

INRAD manufactures crystals, laser components, optical coatings, laser systems and instruments for scientific, defense, aerospace and industrial markets.

INRAD, 181 Legrand Avenue, Northvale, NJ 07647, USA.

J. Appl. Cryst. (1995). **28**, 246

New Temperature-Controlled Harmonic Generator

INRAD introduces the **Heated Crystal Cell and Temperature Control System, Model 5-200**, which is a microprocessor-based unit designed specifically for controlling the temperature of small crystals. The system may be used for maintaining a preset temperature for crystals such as KTP and LiNbO₃ or for temperature tuning with LBO and KNbO₃. Temperatures can be controlled over a range from 30°C above ambient to 190°C with an accuracy of 0.1°C.

The controller uses a sophisticated algorithm to control the crystal temperature. The power required to maintain the cell at the setpoint temperature is based on a proportional, integral and derivative (PID) servo loop. The system can be configured by the customer to operate over a specified temperature range with an appropriate maximum heating rate for the housed crystal. A bidirectional RS-232 interface is available for direct computer control.

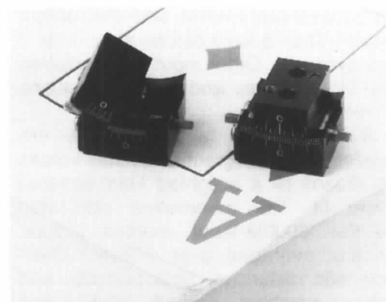
INRAD, 181 Legrand Avenue, Northvale, NJ 07647, USA.

J. Appl. Cryst. (1995). **28**, 246

Tiny Arcs Simplify Positioning

A new line of tiny goniometric arcs that can be mounted in tight spaces to provide angular adjustability for the fine-tune positioning of lasers and other instruments is being introduced by Charles Supper Company, Inc. of Natick, Massachusetts, USA.

Supper UltraMicro Arcs measure only 0.500 (W) × 0.440 (H) × 0.750'' (L) (including drive screw) to fit into tight spaces for making final adjustments using an external drive key. Machined from aluminium, black anodized and stamped with white vernier scales, these tiny arcs incorporate either dry or permanently lubricated nonmagnetic stainless steel drive screws and can be used in any orientation.



Supper UltraMicro Arcs

Available with two distinct arc radius verniers, one of the Supper UltraMicro Arcs provides $\pm 15^\circ$ travel with 0.406'' radius and the other has $\pm 15^\circ$ travel with a 0.844'' radius. Both are drilled and tapped for 1–72 cap screws and can be individually mounted or concentrically stacked, achieving a common center.

Supper UltraMicro Arcs sell for US \$410 (list) each and can be supplied stacked for US \$795. Literature is available on request.

Charles Supper Company, Inc., Donald E. Goodwin, Product Manager, 15 Tech Circle, Natick, MA 01760, USA.

Books Received

J. Appl. Cryst. (1995). **28**, 246

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Modern crystallography, Vol. 1, Fundamentals of crystals. Symmetry, and methods of structural crystallography. (Second enlarged edition.) By *Boris K. Vainshtein*. Pp. xxii + 480. Berlin: Springer-Verlag, 1994. Price DM 119. ISBN 3-540-56558-2. A review of this book, by Douglas L. Dorset, has been published in the March 1995 issue of *Acta Crystallographica Section A*, pages 234–235.

Crystallographic computing 6. A window on modern crystallography. (IUCr Crystallographic Symposia No. 6.) Edited by *H. D. Flack, L. Párkányi* and *K. Simon*. Pp. x + 130. Oxford: IUCr/Oxford University Press, 1994. Price £40.00. ISBN 0-19-855788-4. A review of this book, by Edward Prince, has been published in the March 1995 issue of *Acta Crystallographica Section A*, page 235.