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PROFVAL: functions to calculate powder-pattern peak profiles with axial-divergence asymmetry

L. W. FINGER

Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany, and Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road, NW, Washington, DC 20015–1305, USA.
E-mail: finger@gl.ciw.edu

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The crystallographic problem: In a powder diffractometer, the curvature of the Debye—Scherrer rings causes an asymmetry in the peak profiles as the Bragg angle approaches either 0 or 180°. For accurate Rietveld refinement, this asymmetry, which is known as axial divergence, must be modeled correctly. Traditionally, empirical *ad hoc* functions such as a split-Pearson-VII function or multiple overlapping Gaussian peaks have been employed. Finger *et al.* (1994) extended the method of van Laar & Yellon (1984) for convolution of the ring shape with an intrinsic peak profile – a procedure that describes extremely asymmetric profiles and involves only physically meaningful parameters. To date, however, only the program *GSAS* (Larson & von Dreele, 1990) has incorporated this method. This contribution makes available tested code for the convolution of the asymmetry function with the intrinsic line function in the hope that more Rietveld codes will incorporate this method.

Method of solution: As described by Finger *et al.* (1994), the convolution is performed using a Gauss–Legendre quadrature procedure, with the weights and abscissae generated with routine *GAULEG* of Press *et al.* (1992). For speed, these values have been previously calculated and are stored in large initialization statements in the Fortran and C versions of the code. In the present versions, the overall profile is evaluated as a convolution of the asymmetry function with a pseudo-Voigt function; however, this choice is arbitrary, and any other functional shape can be substituted. Although this method is computationally intensive for very asymmetric peaks, the amount of extra computation drops rapidly as the Bragg angle of the peak deviates from 0 or 180°. Experience has shown that the calculation of an entire profile with this algorithm is as fast, or faster, than using the multiple-Gaussian method. The routines provide not only the value of the convolved function, but also analytical partial derivatives of each of the parameters, so that the routines may be used for least-squares minimization.

Software environment: The code consists of functions written in Fortran, C and Pascal that implement the calculation; a user may select their language of choice. Each of the functions includes a test driver showing the method of calling the routine. The routines are written in generic dialects of these languages and should compile and run under any software environment. They were written and tested on a PC running Windows 95 using Microsoft PowerStation Fortran V4.0, Microsoft C V5.1 and Borland Turbo Pascal V6.0.

Hardware environment: These routines will run on any computer that has any of the three languages implemented.

Documentation: The source codes for the convolution function are heavily commented, with each section referring to the appropriate equation in Finger *et al.* (1994). In addition, an output file of the results for each language is included with the software distribution.

Availability: The source code for these routines is available by anonymous ftp from cryst.ciw.edu in directory anonymous.profile as files profile.for, profile.c and profile.pas. The output files are named o_for.out, o_c.out and o_pas.out.

Keywords: Rietveld refinement, axial divergence, peak asymmetry.

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Powder Diffraction File

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, the 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, fully automatically and unambiguously, to 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/I_c values, concentration of components in identified solid solutions, all degrees of preferred orientation in a specimen, the crystallite size and strain 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 the 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. The ICDD expects the combination database to contain:

Total number of entries:	~115 000
Number of organic compounds:	~20 000
Number of inorganic compounds:	~95 000
Total number of entries with I/I_c:	~50 000
Number of unique entries with I/I_c:	~37 000

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

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

International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA (e-mail: information@icdd.com)

Books Received

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.

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Applied superconductivity 1997, Institute of Physics Conference Series, No. 158, Vols. 1 & 2. Edited by H. ROGALLA and D. H. A. BLANK. Pp. xl + 1712. Bristol and Philadelphia: Institute of Physics Publishing, 1997. Price £300.00, US $495.00. ISBN 0 75 030487 1. This volume contains 422 (after review) of the 431 invited and contributed papers presented at the third biennial European conference on the title topic, held in Veldhoven, The Netherlands, 30 June–3 July 1997.