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DIFRAC, single-crystal diffractometer output-conversion software.

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Abstract

Software is described that converts single-crystal diffractometer output files as produced by maufacturers' software into a standardized instrument-independent form consisting of a clear, complete, well documented record of the sample and the diffraction measurements performed upon it. Information not already available in the manufacturers' diffractometer files is obtained in an interactive question-and-answer session. The software is written in a modular way. Available modules can deal with Enraf–Nonius CAD-4, Philips PW1100 and Siemens $P2_1$ single-crystal diffractometers and produce output in CIF or SCFS format.

Introduction

Users of several models of four-circle single-crystal diffractometers may well have been struck by the diversity of form and content of the data files generated by diffractometer-manufacturers' software. The form of the file can create difficulties in its transfer to other computing equipment and further renders the corresponding computer programs specific to a certain type or types of diffractometer. The difficulties in the content of the files manifest themselves principally by the paucity of the available information necessitating additional input to the data-treatment software (*e.g.* type of radiation, wavelength of radiation, scan width, sense of rotation of angles on the single-crystal diffractometer *etc.*). The problem has become aggravated in recent times by the rapid development in electronic data exchange. It is now frequent to exchange files by computer networking and electronic mail rather than by the standard means of the recent past, the 1/2 in magnetic tape. The advent of machine-readable submission for publication and data-base and supplementary-material deposition further highlights the problem of missing data.

Our own motivation for producing this software arose from the work of the IUCr Subcommittee on Statistical Descriptors (Schwarzenbach, Abrahams *et al.*, 1989). We wished to be able to perform structure refinements on the directly observed quantities such as peak and background intensities (Schwarzenbach & Flack, 1991), crystal dimensions (Schwarzenbach, 1991; Blanc, Schwarzenbach & Flack, 1991) *etc.*, which should not be corrected for any systematic effects. In this project we also had to face the problem of producing refinement and data-treatment software that would function smoothly on data produced by three different types of single-crystal diffractometer. Furthermore, it became clear that with the advent of machine-readable submission of structural papers to journals and data bases it would be highly advantageous to obtain a clear, complete, instrument-independent record of the diffractometer measurements and conditions in the form of a data file at the earliest possible opportunity, *i.e.* while the crystal was still mounted on the instrument.

Storing raw intensities

Raw observed intensity data are output to the converted file. In the current version of the program we have dealt only with low-angle background – integrated peak – high-angle background counts, thus leaving the problem of the transfer of profile data to a later date. Conversion of raw counts to net intensities $P^{\rm obs}$ (*i.e.* with background subtracted and allowing for differences in effective scan speed) or to $|F^{\rm obs}|^2$ values (*i.e.* applying a Lorentz–polarization correction to the net intensity) is not undertaken by this software. As the raw data are conserved in the converted file, a more detailed modelling and refinement of background than that normally undertaken at present will be feasible, whilst retaining the possibility of a classic data reduction. As manufacturers' diffractometer-control software specifies and records its scan conditions (*i.e.* scan time, scan width, scan speed and number of scans) in many different forms, we have chosen to standardize this information into the four intensity-measurement coefficients c_p, c_b, c_l and c_h most convenient for least-squares calculations.

Let $Q^{\rm obs}$ be the observed integrated-intensity count measured by scanning over the reflection profile and let $L^{\rm obs}$ and $H^{\rm obs}$ be the observed low- and high-angle background counts respectively. The model relating the raw observations of a diffraction experiment to derived parameters may be written as $Q^{\rm calc} = c_p P^{\rm calc}(v_m) + c_b B^{\rm calc} \simeq Q^{\rm obs}$, $L^{\rm calc} = c_l B^{\rm calc} \simeq L^{\rm obs}$ and $H^{\rm calc} = c_h B^{\rm calc} \simeq H^{\rm obs}$. $P^{\rm calc}$ is the calculated net integrated intensity per unit inverse scan speed and is a function of v_m adjustable parameters describing the crystal structure, the scale factor, secondary extinction and possibly other physical quantities. $B^{\rm calc}$ is the calculated count rate per unit time of the mean background and is itself an adjustable parameter. One can see that, in general, c_p is equal to the time to count the peak divided by the scan width, *i.e.* the effective scan speed allowing for multiple scans over the same peak, c_b to the time to count the peak, c_l to the time to count the low-angle background and c_h to the time to count the high-angle background. It follows that the scan width is equal to c_b/c_p.

For a classical treatment, the net intensity $P^{\rm obs}$ may be calculated from the raw counts by using $P^{\rm obs} = [Q^{\rm obs} - 0.5c_b(L^{\rm obs}/c_l + H^{\rm obs}/c_h)]/c_p$.

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Table 1. *Content of the converted output file*

Compound, measurement and experimenter identification

- General descriptive title
- Compound/measurement identification code
- Date and method of creation of the converted output file
- General experimental technique and special details
- Name and postal, e-mail, telephone and telefax addresses of the experimenter

Instrument specification

- Type of single-crystal diffractometer
- Specification of software used to control the instrument
- Detector dead time and e.s.d.

Radiation description

- Type of radiation (*i.e.* neutrons, electrons, X-rays)
- Mean wavelength
- Wavelengths and intensity weights of radiation components
- Polarization ratio and e.s.d.
- Angle between the normals to the diffraction planes of the monochromator and sample
- Incident-beam spatial half-width at the crystal

Filter and attenuator information

- Wavelength of β-filter absorption edge
- For each attenuator filter: its reciprocal transmission factor with e.s.d. and index

Environmental conditions

- Temperature with e.s.d.
- Pressure with e.s.d.

Compound and crystal specification

- Measured density with e.s.d. and temperature
- Melting point
- Colour and description of the crystal
- Source
- Common chemical and mineral names
- Measured formula mass with e.s.d.
- Chemical formula
- Chemical analysis in mass %
- Number of formula units per cell

Cell dimension and its determination

- Cell dimensions with e.s.d.s
- Cell volume with e.s.d.
- Temperature
- Specification of radiation used
- Minimum and maximum 2θ of reflections
- Number of reflections
- h, k, l, 2θ and wavelength code of each reflection

Crystal-shape description; either (*a*), (*b*) or (*c*)

- (*a*) h, k and l of each face and its distance with e.s.d. from centre
- (*b*) Radius with e.s.d. of a spherical crystal
- (*c*) Radius and length with e.s.d.s of a cylindrical crystal

Intensity measurement procedure

- Minimum and maximum $(\sin\theta)/\lambda$
- Total number of reflections measured
- Minimum and maximum values of h, k and l

Reference-reflection description

- Time interval between measurement of reference reflections
- Number of reference reflections measured
- For each reference reflection: its h, k and l Miller indices and reference code

Table 1. (*cont.*)

Reflection-specific information

- Miller indices h, k and l
- Peak count and low- and high-angle background counts (Q^{obs}, L^{obs} and H^{obs})
- Intensity-measurement coefficients: c_p, c_b; c_l and c_h (defined in text)
- Crystal-based azimuthal angle
- Elapsed time of measurement
- Attenuator-filter index
- Scale-factor index
- Reference-reflection index
- Background scanning mode
- Scan type
- Total horizontal and vertical detector aperture

System design

Table 1 presents the list of items that we considered essential to include in the converted single-crystal diffractometer output file. This information is intended to be complete and independent of the particular instrument used. It serves for the calculations of structure determination and refinement and contains the items considered necessary for machine submission of documents for publication or data bases. Some of the items we have chosen to include or exclude from our output list require special comment:

(*a*) The chemical formula has been included in the converted output file although in some cases this might have to be revised as a result of the crystal structure analysis. The formula is useful in identifying the compound and the element names and composition are necessary for running structure-solution and refinement software. Moreover, the subroutine (see below) which undertakes the interpretation of the chemical formula was already available to us.

(*b*) On the other hand, the space group of the crystal has not been included. For a crystal of unknown structure, the exact space group will not be determined reliably until after structure refinement. Furthermore, it was thought that flexible software to test the integrity of the input of space-group information in any form (*e.g.* a symbol, generators or individual symmetry operations) would have greatly lengthened the time necessary to produce this version of *DIFRAC*.

(*c*) The crystal orientation matrix (or matrices in the case of resetting) for the diffractometer (often called the **UB** matrix) and the diffractometer setting angles (ω, 2θ, χ, φ or κ) for each reflection have not been included in the converted output file. All orientation information has been condensed into a crystal-based azimuthal angle ψ for each reflection measurement. This ψ is independent of the instrument geometry and axial definitions of the instrument. Full details are to be found in Schwarzenbach & Flack (1989, 1992).

(*d*) An index or code is included to identify the reference reflections. In our view, it is not possible to identify a reference reflection correctly from its Miller indices alone. The inclusion of an index eases the work and programming of data-treatment and refinement software analysing the variations in the reference reflections.

(*e*) The file includes a fairly detailed description of the incident-beam characteristics. This has been done to allow

the calculation of polarization and beam-inhomogeneity corrections (Harkema, Dam, van Hummel & Reuvers, 1980; Markov, Fetisov & Zhukov, 1990).

A choice had to be made concerning the format of the converted output file. The necessity of being able to transmit the file over networks or by electronic mail imposes a clear-text (ASCII) form with no more than 80 characters per line. Additionally, we required that the content and format of the file be clearly defined and relatively compact. Both the SCFS-90 – Standard Crystallographic File Structure-90 (Brown, 1988) – and the more recent CIF – Crystallographic Information File (Hall, Allen & Brown, 1991) – are available for just this purpose and we have adopted both of them.

The information to be included in the converted output file is obtained from the following sources: (*a*) fixed geometrical details of the single-crystal diffractometer, (*b*) information in the diffractometer parameter file, (*c*) information in the diffractometer data file and (*d*) interactive questions and answers. An underlying design principle in this arrangement is that information from the diffractometer files should be used, if available, otherwise a question will be asked once only. This is most important to avoid confusion and frustration on the part of the user. It further explains our preference for installing the executable programs on the computer controlling the diffractometer so that each installation may be customized for its instrument and have access to those files which are not specific to the user.

DIFRAC

This is a set of free-standing programs written in Fortran77 and consisting of modules having precisely defined functions described below. Entry points to each module and cross-reference calling and linking information are given in Table 2. Each program is diffractometer and output specific and is generated from the general module (*GN.FOR*), from one of the diffractometer modules (*C4V4.FOR*, *C4V5.FOR*, *NIV411.FOR*, *PW.FOR*), from one of the output modules (*CF.FOR*, *SF.FOR*) and the included file of COMMON definitions (*COMMON.TLB*). Due to the modular construction of *DIFRAC*, it is easy to produce additional programs for other types of single-crystal diffractometer and output styles by writing diffractometer-specific or output-specific modules having the same entry points and functionality as the existing modules. The salient features of the modules and individual implementations are given below.

General module

This contains the main controlling section of the program and the interactive free-format question-and-answer subroutine. *DIFRAC* uses a file ADDRESS.LST containing the names, addresses, telephone numbers, telefax numbers and e-mail addresses of the users on the local installation. The subroutine *CHFORM* for the conversion and verification of chemical formulae is adapted from the program *CASTOR* (Brett, Miebach, Boese & Eyl, 1990) with the authors' permission.

Diffractometer modules

Currently, modules are provided for Philips PW1100, Enraf–Nonius CAD-4 (versions 4.*x* and 5.0) and Syntex/

Table 2. *DIFRAC construction*

General module (GN.FOR)

Subroutine	Called by	Use
DIFRAC		Main program
BLOCKD		Block data constants and initializations
CHFORM	*QUESAN*	Conversion of chemical formula into components
COMPNM	*DIFRAC*	Ask for compound name
FREAD	Many	Free-format interactive read
QUESAN	*DIFRAC*	Interactive question and answer
TRIM	Many	Trim non-significant blanks from strings

Output modules

File name	Output type
CF.FOR	CIF – Crystallographic Information File
SF.FOR	SCFS-90 – Standard Crystallographic File Structure – 90

Subroutine	Called by	Use
BASOUT	*DIFRAC*	Output all other information
CONOUT	*INITLZ*	Output for changed conditions
DTFLND	*DIFRAC*	Finish off converted output file
HEDOUT	*DIFRAC*	Output starting section
REFOUT	*REFRD*	Output reflection information
SET	*DIFRAC*	Set up output style
VALOUT	*BASOUT*	Convert value and e.s.d. into string

Diffractometer modules

File name	Diffractometer type
C4V4.FOR	Enraf–Nonius CAD-4 (version 4.*x*)
C4V5.FOR	Enraf–Nonius CAD-4 (version 5.0)
NIV411.FOR	Nicolet $P2_1$ (version 4.11 and earlier)
PW.FOR	Philips PW1100

Subroutine	Called by	Use
CHOOS	*DIFRAC*	Set up diffractometer type options
DTFLRD	*DIFRAC*	Read diffractometer data file
INITLZ	*DTFLRD*	Interpret non-intensity data
JUNPAK	*PRFLRD*	Packing function for CAD-4
PRFLRD	*DIFRAC,FREAD*	Read diffractometer parameter file
PSIC	*REFRD,INITLZ*	Crystal-based azimuth calculation
REFRD	*DTFLRD*	Interpret diffractometer intensity datum

Include module (COMMON.TLB)

Include file of COMMONs used by all modules

Linking information

Program	Modules needed
CAD4V4CF	*GN, C4V4, CF*
CAD4V4SF	*GN, C4V4, SF*
CAD4V5CF	*GN, C4V5, CF*
CAD4V5SF	*GN, C4V5, SF*
NICOCF	*GN, NIV411, CF*
NICOSF	*GN, NIV411, SF*
PW11CF	*GN, PW, CF*
PW11SF	*GN, PW, SF*

Nicolet/Siemens $P2_1$ (versions 4.11 or lower) single-crystal diffractometers.

*PW*1100 *Philips*. This is a modified system, similar to others described in the literature (Grigg & Barnea, 1990; van Hummel & Graafsma, 1989) which no longer uses the original paper tape, magnetic tape or Teletype output. The Teletype has been replaced by an IBM-compatible PC running KERMIT which captures all of the output into a data file of name ⟨compid⟩.DAT (or ⟨compid⟩01.DAT, ⟨compid⟩02.DAT, ..., ⟨compid⟩*nn*.DAT for a sequence of *nn* data files on the same compound). The .DAT file should start with the output of the PW1100 instruction PAR followed by the intensity collection itself. A parameter file called ⟨compid⟩.TTH may also be prepared containing the results of the accurate centring of reflections intended for cell-dimension determination. For compatibility with other software, this file should start with one line which may contain anything, followed by one line containing an integer code defining the default wavelength of the centred reflections, followed by lines containing h, k, l, $+\omega$, $-\omega$ in degrees (the latter being the ω values of the centring of the reflection at positive and negative 2θ) and the wavelength code of the measurement. The wavelength codes are defined as follows: 0 or blank indicates a default value, 1 means α_1 line, 2 means α_2 line and any other value indicates the mean α value. At present, the *DIFRAC* software has been installed on a DEC VAX 8700/VMS. We have not yet attempted to install it on the IBM-compatible PC serving as an interface to the diffractometer.

CAD-4 Delft Instruments (*Enraf–Nonius*). Modules for versions 4.*x* and 5.0 of the manufacturer's software are available. The module for version 4.*x* reads only a crystal data file ⟨compid⟩.DAT, whereas that for version 5.0 can read the goniometer constant file GONCA0.PAR, the crystal parameter file ⟨compid⟩.CRY and the crystal data file ⟨compid⟩.DAT (or ⟨compid⟩01.DAT, ⟨compid⟩02.-DAT,..., ⟨compid⟩*nn*.DAT for a sequence of *nn* data files on the same compound). The *DIFRAC* software has been installed on the DEC MicroVAX 3100/VMS controlling the diffractometer running version 5.0 of the control software.

$P2_1$ *Siemens* (*previously Syntex–Nicolet*). This module was written for a machine running version 4.11 of the control software but takes account of the specifications of version 4.12 and higher, up to but not including version 5.1. *DIFRAC* can read the crystal parameter file ⟨compid⟩_PAR.DCF, the crystal data file ⟨compid⟩_REF.DCF and has been installed on the MicroVAX II controlling the diffractometer. There are a few known restrictions in the code. The $P\bar{1}$ version of the Syntex machine had the monochromator oriented at 90° to the current arrangement and this condition is not tested for by the software. (It would need to be set manually by the variable FMNHED in the *CHOOS* subroutine). Furthermore, the current software does not treat data measured with Wyckoff scans.

Output modules

In the current version of *DIFRAC*, modules are provided for CIF (Hall, Allen & Brown, 1991) and SCFS-90 output (Brown, 1988). Both the Fortran source code of the CIF output module and the CIF output files it produces have been checked for conformity with the CIF definitions contained in the CIF Dictionary (core version 1991) as contained in the electronic file cifdic.c91 by using the checking program *CYCLOPS* of Hall (1991). The only non-standard names are _diffrn_refln_fbcoeff_peak_z, _ diffrn_refln_fbcoeff_bg_peak_z, _diffrn_refln_bg_1_z and _diffrn_refln_fbcoeff_bg_2_z for the intensity-measurement coefficients c_p, c_b, c_l and c_h defined above and _cell_measurement_refln_wl_id_z giving the wavelength code of each reflection centred for cell-dimension measurement.

In the *XTAL* 3.0 system (Hall & Stewart, 1990) the SCFS-90 file is read by the program *REFM*90 (Flack, 1990) to form an *XTAL* bdf which may then be processed by *STARTX* in update mode. Following *STARTX*, the treatment of the intensity measurements is undertaken by *REFCAL* (Flack, 1992). This arrangement has been functioning in the Geneva laboratory to our thorough satisfaction for about 1 year with the PW1100 and CAD-4 diffractometers. For the input of a CIF file into *XTAL*, the same type of arrangement will use the program *CIFIO* (Hall, 1990). At the present time, the reading of the CIF file is much less reliable than the mature SCFS-file-reading software.

Concluding remarks

It must be emphasized that the program modules described in this paper are no more than a stop-gap solution on the way to standarized, complete, documented and easily transmissible single-crystal diffractometer output files. There can be no substitute for the diffractometer-control software itself being upgraded to produce such data files. Nevertheless, the conversion of diffractometer output by way of *DIFRAC* is a useful step in the right direction. Program packages for structure solution, refinement and publication can thus be updated to become instrument independent with all information on the experiment coming from the data file itself. The user interaction with his favourite software can thus be reduced entirely to the task of specifying the calculations to be undertaken rather than being a mixture of data and operational commands.

The current paper is the prime source of documentation concerning *DIFRAC*. A computer file of ancillary material contains updates and corrections to this paper. The source code and ancillary material of *DIFRAC* are available from flack@sc2a.unige.ch or flack@cgeuge52.bitnet by e-mail.

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*LS*1 – a computer program for simultaneous refinement of material structure and microstructure.

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Abstract

A computer program has been written to introduce profile analysis into the Rietveld method. The devised algorithm simultaneously refines both structural and microstructural parameters, also accounting for anisotropy in crystallite size and microstrain. Instead of using phenomenological relations to describe the trend of profile width and shape as a function of diffraction angle, a model based on the Warren–Averbach approach has been developed that permits extraction of more information from data, also achieving faster convergence.

Introduction

In the last decade the Rietveld (1967, 1969) method has been increasingly employed for structure refinement from neutron and X-ray diffraction (XRD) powder data (Albinati & Willis, 1982; Cheetham & Taylor, 1977; Taylor, 1985), and several computer programs have been written, such as *DBWS* (Wiles & Young, 1981) or *GSAS* (Larson & Von Dreele, 1988) and fully tested. It has also been recognized that the method is suitable for quantitative analysis of polycrystalline mixtures, without the need of standards (Hill & Howard, 1987; Bish & Howard, 1988). It has been shown recently (Lutterotti & Scardi, 1990; Scardi, Lutterotti, Di Maggio & Maistrelli, 1991; Scardi, Lutterotti & Di Maggio, 1992) that more information can be obtained on the microstructure of samples by introducing line-broadening analysis into the refinement routine. Existing programs, following the original procedure indicated by Rietveld (1967, 1969), use the Caglioti, Paoletti & Ricci (1958) formula to model the change of profile full width at half-maximum (FWHM) as a function of 2θ and a further expression for profile-shape parameters [*i.e.* η for a pseudo-Voigt function and m for Pearson VII function (Young & Wiles, 1982)]. Five or more fitting parameters are usually necessary for these relations, which do not add useful information and cannot reproduce all possible broadening effects (Scardi, Lutterotti, Di Maggio & Maistrelli, 1991). For this reason a model has been developed to connect profile width and shape directly to crystallite size (column length) and microstrain, along the various crystallographic directions, using conditions on cosine Fourier coefficients and their derivatives (Lutterotti & Scardi, 1990; Scardi, Lutterotti, Di Maggio & Maistrelli, 1991). In this way, relationships can be derived for profile parameters which are based on reliable line-broadening theory, achieving convergence using less fitting parameters and adding useful microstructural information. The program can also be used for microstructural characterization, including quantitative phase analysis, of material whose structure is known (or can be refined).

In the present paper an outline of the main features of the program is given, with references to the authors' previous works for theoretical details and comparison with standard structure-refinement routines (Lutterotti & Scardi, 1990; Scardi, Lutterotti, Di Maggio & Maistrelli, 1991; Scardi, Lutterotti & Di Maggio, 1992). The typical output of the program is also described along with some practical

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