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Fortran90 sources of the subroutines of *UMWEG*. III. The *UMWEG*-specific subroutines

Elisabeth Rossmanith

Mineralogisch-Petrographisches Institut der Universität Hamburg, Grindelallee 48, D-20146 Hamburg, Germany.
Correspondence e-mail: rossmanith@mineralogie.uni-hamburg.de

The Fortran90 sources of the *UMWEG*-specific subroutines of the program *UMWEG* are presented and deposited, together with the PostScript-plot software subroutines and the simple and short main program of the command-line version of the program *UMWEG*.

1. Introduction

In order to enable and simplify further developments and improvements in analysis in the field of kinematical multiple diffraction, the Fortran90 sources of the program *UMWEG* (Ro-03,[1] Ro-06*a*) are given in succeeding papers. In Ro-06*b* the subroutine *UPFORM* for the determination of dispersion corrections and scattering factors for free atoms and ions is discussed. In Ro-06*c* the Fortran90 sources providing the crystallographic data necessary for intensity calculations are presented and deposited. These subroutines can be called by any crystallographic program (for non-commercial use only) needing the data given in the DATA statements. It is also possible to extract the DATA statements for programs having other purposes. These subroutines were therefore given separately.

In the present paper, the *UMWEG*-specific subroutines will be presented and deposited, together with the PostScript-plot software subroutines and the simple and short main program of the command-line version of the program *UMWEG*. One of the intentions of this paper is to refer to the crystallographic expressions published by the author and made use of in the program *UMWEG* and to point out possible or necessary further developments and improvements (Appendices *A* and *B*).

In the last paper of this series, the windows version of *UMWEG* will be presented and deposited. Also given will be the 'thesaurus', *i.e.* the input files for many examples.

2. The PostScript-plot subroutines

By means of the collection of the PostScript-plot software subroutines *UPLOT*, *PLOTS*, *PLOT*, *SYMBOL*, *NUMBER*, *NEWPEN*, *FRAME*, *LINE*, *LINE1*, *LINE2*, *AXIS*, *SYMBO1*, *DASH*, *FONTS*, *TRANSL* and *SYMBOL_HKL*, which imitate the routines of the *CALCOMP* software, the graphical output of the program *UMWEG* is generated and saved as a PostScript file. These routines can be downloaded (for non-commercial use only) from the deposited material (file `plot.f90`). After appropriate adjustment, these subroutines can be used in any non-commercial program for generating PostScript figures.

[1] Most of the expressions and figures discussed in this paper were derived or presented in previous papers by the author. These expressions, figures, appendices *etc.* will be referenced in the following by the abbreviation Ro-*xxy*-(*z*), where *xx* represents the two last digits of the year of publication, *y* stands for *a*, *b*, *c etc.* if more than one paper in the respective year is referenced and *z* represents the number of the expression, figure, appendix *etc.* in consideration.

3. The true crystallographic subroutines

The Fortran90 sources of the subroutines *BRAVAIS*, *CHUK*, *CHUK1*, *FCALC1*, *FCALC1_N*, *MUE_N*, *POLFA*, *UPSI*, *CAD4*, *HASYL4* and *NEUTRON* can be downloaded (for non-commercial use only) from the deposited material (files `subr_1.f90`, `subr_2.f90` and `subr_3.f90`).

3.1. The file `subr_1.f90`

This file contains the subroutines necessary for intensity calculation:

BRAVAIS. The subroutine provides symmetry information depending on the Bravais type of the lattice.

CHUK and *CHUK1*. The two subroutines provide the primary extinction correction for a particular mosaic block radius and Bragg angle calculated according to Chukhovskii *et al.* (1998). Because of the shortcomings of this correction discussed in Ro-00*b*-§2.3.2 and Ro-00*b*-§2.3.3, the primary extinction correction provided by these two subroutines is used with restrictions for single diffraction only (Ro-00*b*-§3).

FCALC1. This subroutine is a derivative of the various widespread programs for X-ray structure-factor calculation written by pioneers of crystallographic programming (unfortunately the particular names are unknown to the author). It returns the phase and modulus of the complex structure factor [Ro-03-(4)] multiplied by the temperature factor [Ro-03-(5)].

FCALC1_N. This subroutine is a derivative of *FCALC1* adjusted for neutrons.

MUE_N. The subroutine returns the density of the structure in the neutron case.

3.2. The file `subr_2.f90`

POLFA. The expressions for the various electric vectors, polarization factors and corresponding angles underlying this subroutine are defined in Ro-04-(1)–(6) and Ro-04-Appendix *B*.

UPSI. This subroutine returns the angle ψ_D defined in Ro-99-Fig. 5, *i.e.* the relation between the zero point of the azimuthal angle calculated by *UMWEG* and that of the diffractometer.

3.3. The file `subr_3.f90`

This file contains the subroutines necessary for the input of measured scans and scale-factor evaluation.

CAD4. This subroutine reads the rough data of the ψ scan and reference reflections according to the manual of the Enraf–Nonius

CAD-4 diffractometer. It returns the measured scan with its maximum and minimum intensity values after corrections for background. If reference reflections are given in the measured file, the variable einint defined in the program unit *UMWEG* (see §4) is replaced by the scale factor skal/iskal (see glossary of variables, Appendix *A*).

HASYL4. This subroutine reads the rough data of the ψ scan and reference reflections according to the manual of the HUBER four-circle diffractometer at HASYLAB/DESY beamline D3 (version 1991–2000). It returns the measured scan with its maximum and minimum intensity values after corrections for background. If reference reflections are given in the measured file, the variable einint defined in the program unit *UMWEG* (see §4) is replaced by the scale factor skal/iskal (see glossary of variables, Appendix *A*).

NEUTRON. This subroutine is a derivative of *HASYL4* adjusted for neutrons.

4. The central program units

The Fortran90 sources of the central subroutine *UMWEG* can be downloaded (for non-commercial use only) from the deposited material (file `UMWEG.f90`). The file also contains the module *INTENSITY DATA*. At the end of the file the short main program of the command-line version of the program *UMWEG* is included. Also deposited is the input description (file `input-help.txt`).

UMWEG. This subroutine is the central unit of the program. Some relevant variables developed or discussed in publications by the author are listed in Appendix *A*.

5. Concluding remarks

Kinematical single and multiple diffraction takes place inside perfect crystallites. The theory underlying the program *UMWEG* was therefore developed and published for non-absorbing extinction-free ideal perfect spherical crystals.

The unpublished expressions used in *UMWEG* for the correction of absorption effects, primary extinction and mosaicity of the crystal represent very first attempts, capable of improvement. They should be reconsidered and replaced by more sophisticated approaches.

APPENDIX *A*
Glossary of some relevant variables defined or discussed in the author's papers

aint(i). The scan intensity is defined in Ro-06*a*-(13).

aintau. The definition of the *Aufhellung* intensity for double diffraction integrated over θ and ψ can easily be understood by the expressions Ro-98-(7), Ro-00*c*-(9) and Ro-04-Appendix *B*. There are four provisional terms involved: the absorption corrections abso and abs02 and the extinction-corrected beam path lengths t02 and tpo. These terms are capable of improvement.

ainth1 $\equiv I_0 q R_h^{ext} n_{mosaic} A$, where I_0 is the incident intensity, q is the cross section of the irradiated crystal volume normal to the incident beam, R_h^{ext} is defined in Ro-98-(4) or Ro-00*b*-(4), n_{mosaic} is the number of consecutive mosaic blocks being in diffraction position for a particular incident ray (Appendix *B*), and A is the absorption correction.

aintum. The definition of the *Umweganregung* intensity for double diffraction integrated over θ and ψ can easily be understood by the expressions Ro-98-(6), Ro-00*c*-(8) and Ro-04-Appendix *B*. There are two provisional terms involved: the absorption correction abs12 and the extinction-corrected beam path length t12. These terms are capable of improvement.

anpr. This variable is equal to 1 for perfect crystals. For mosaic crystals the variable corresponds to n_{mosaic}, the number of consecutive mosaic blocks being in diffraction position for a particular incident ray (Appendix *B*).

cosint. The interference term is defined in Ro-06*a*-(7). The provisional usage of the variable anpr in the interference term, which is irrelevant (= 1) in the case of perfect crystals, should be reconsidered.

ddlam. The wavelength spread $\Delta\lambda/\lambda$ of the synchrotron radiation caused by the perfection of the monochromator crystals was discussed in Ro-93*a*-p.85 and in more detail in Ro-02-§4.2. The expression for this wavelength spread used in *UMWEG* was found to be appropriate for the double-crystal monochromator system with small offset from parallelism at the HASYLAB/DESY beamline D3 during the experiments of the author (1987–2000). Especially for synchrotron radiation equipment with very small divergence, ddlam should be adjusted according to the considerations discussed in Ro-02.

dlam1. For the case of synchrotron radiation, this variable is discussed in Ro-93*a*, Ro-93*b* and Ro-02.

einint. The incident intensity I_0 is defined, for example, in Ro-00*a*-(1) and used, for example, in Ro-00*a*-(14). The value given in the lines 66–212 of the program unit *UMWEG* for the particular experimental condition is a rough estimate, which is replaced by the value skal/iskal obtained from the analysis of the reference reflections in the subroutines *CAD4*, *HASYL4* and *NEUTRON*.

peakb. The concept for the calculation of the peak widths was first introduced in Ro-92. The expressions used in the actual version of *UMWEG* were developed in 1995 (unpublished). They will be discussed in Ro-07 together with the actual expressions for the Lorentz factors.

psilor. The Lorentz factor was first defined in Ro-92-(19*a*). The definition of the variable psilor used in the downloadable version of *UMWEG* was developed in 1995 (unpublished). It will be discussed in Ro-07 together with the actual expressions for the peak widths.

$$\text{skal/iskal} \equiv \left\{ \sum_{\text{iskal}} I_{\text{measured}}^{\text{abscor}} / \left(q R_h^{ext} n_{mosaic} \right) \right\} / \text{iskal},$$

where $I_{\text{measured}}^{\text{abscor}}$ is the absorption-corrected measured integrated intensity, q is the cross section of the irradiated crystal volume normal to the incident beam, R_h^{ext} is defined in Ro-98-(4) or Ro-00*b*-(4), and n_{mosaic} is the number of consecutive mosaic blocks being in diffraction position for a particular incident ray (Appendix *B*).

thelor. The Lorentz factor was first defined in Ro-92-(10*c*). It was also discussed in Ro-00*a*-§2.2.

APPENDIX *B*
Provisional rough estimate of n_{mosaic}

The total intensity reflected by an ideal mosaic crystal will depend on the number and magnitude of mosaic blocks being in diffraction position and the reduction of the primary intensity during its path through the crystal. For a small spherical perfect mosaic block the 'integrated intensity' is defined, for example, in Ro-00*a*-(14). For a large perfect block, the primary extinction correction has to be taken into account according to Ro-00*b*-(5). If n_{mosaic} is defined as the number of consecutive mosaic blocks being in diffraction position for a particular incident ray, for a perfect crystal $n_{mosaic} = 1$. For an ideal mosaic crystal, on the other hand, n_{mosaic} will be much larger than 1.

It will be assumed that the spherical mosaic crystal with radius R is composed of spherical mosaic blocks all having the same radius r,

with $R \gg r$. For the estimation of the mean number of $n_{\rm mosaic}$, the crystal sphere is replaced by a cylinder with thickness $4R/3$ and cross section $R^2\pi$. The mean value of $n_{\rm mosaic}$ is then given by $4R/3$ divided by $2r$, *i.e.*

$$n_{\rm mosaic}^{\eta=0} = (2R)/(3r).$$

The number of consecutive mosaic blocks being in reflection position will be reduced in the case of a non-zero mosaic spread, η. To account for this effect, in a very first attempt in *UMWEG*, $n_{\rm mosaic}$ is estimated by

$$n_{\rm mosaic} = n_{\rm mosaic}^{\eta=0}\{(3\lambda/4r)/[(3\lambda/4r) + \eta]\},$$

an expression capable of improvement.

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