

Journal of
**Applied
Crystallography**

ISSN 0021-8898

Editor: **Gernot Kosterz**

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Elisabeth Rossmannith

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The Fortran90 source of the program *PSILAM*

Elisabeth Rossmannith

Received 1 December 2006
Accepted 21 December 2006

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

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The Fortran90 source code of the program *PSILAM* has been deposited with the IUCr.

1. Introduction

To facilitate further developments and improvements of analysis in the field of kinematical multiple diffraction, the Fortran90 source code of the program *UMWEG* (Ro-03b, Ro-06a)¹ was given in succeeding papers (Ro-06b, Ro-06c and Ro-07). This paper presents the central program units of the program *PSILAM* (Ro-03a), which is a derivative of *UMWEG*, and the corresponding PostScript-plot software routines that have been deposited as supplementary material.² The corresponding 'true crystallographic' subroutines of *PSILAM* are identical to those of *UMWEG* (see Ro-07-§3) and can therefore be obtained from the above-mentioned papers.

2. The central program units of *PSILAM*

The Fortran90 sources of the central subroutine *PSILAM* are available, for non-commercial use only, from the deposited material (file *psilam.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 *PSILAM* is included. Also deposited is the input description (file *input_help.txt*).

3. The PostScript-plot subroutines

Using a collection of PostScript-plot software subroutines, the graphical output of the program *PSILAM* is generated and saved as a PostScript file. These routines can be downloaded, for non-commercial use only, from the deposited material (file *psilam_plot.f90*).

4. Concluding remarks

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

The unpublished expressions used in *UMWEG* and *PSILAM* for the correction of absorption effects, primary extinction and mosaicity of the crystal, represent very first attempts, capable of improvement (see Ro-07-Appendix A). They have to be reconsidered and replaced by more sophisticated approaches.

References

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¹ Most of the expressions and figures discussed in this paper were derived or presented in previous papers of the author. These expressions, figures, Appendices, etc., will be referenced in the following by the abbreviation Ro-*xy*-(*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 equation, figure, Appendix, etc., under consideration.

² Available from the IUCr electronic archives (Reference: FE5017). Services for accessing these data are described at the back of the journal.