Fit;o) - A Mössbauer Spectrum Fitting Program

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Introduction

Fit;o) is a program for fitting and analyzing transmission and scattering geometry ^{57}Fe Mössbauer spectra. This program package provides a powerful tool for rapid fitting of complex Mössbauer spectra. When fitting it is possible to control all model parameters.

Fit;o)'s main features

- Microsoft Windows 2000/XP compatible.
- Easy and safe installation, no external dependencies.
- Created with Object Oriented Technology (OOT).
- Working with several spectra (MDI[1])at a time is possible.
- Complete point-and-click graphical user interface.
- Easy saving and loading of fit models.
- Export of data for other programs such as for example Origin, OpenOffice.org Calc or MS Excel.
- Export fit reports as plain text or LaTeX files.
- Most program parameters are customizable.
- Multilingual support in next version.
- To be released as open source (GPL) in near future.
- Completely free.

Fitting windows

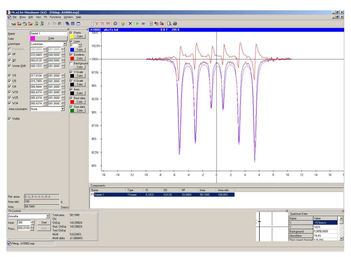

Figure 1: *The fitting window before a fitting run.*

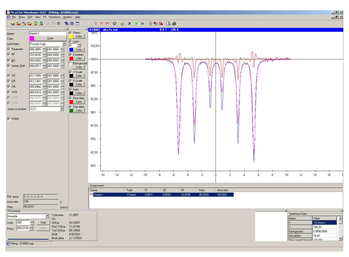

Figure 2: *The fitting window after the fitting run.*

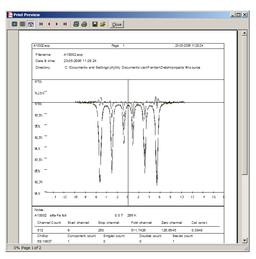

Figure 3: *Print preview of a fitted transmission Mössbauer spectrum.*

Fitting objects

Components

- Singlet
- Doublet
- Sextet.

Line profiles

- Gaussian, Lorentzian
- Pseudo-Voigt, Pseudo-Lorentz, Pearson-VII
- Split-Lorentzian

Screen shots

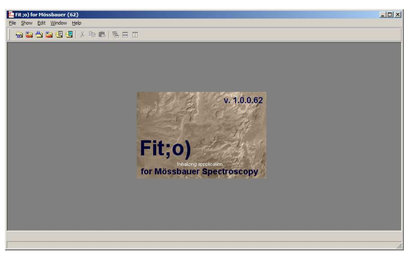

Figure 4: *The main window, which acts as base for all other windows.*

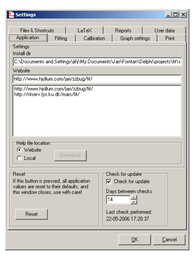

Figure 5: *The settings window.*

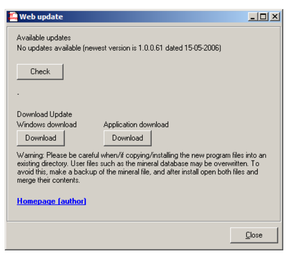

Figure 6: *The web update option keeps the software updated.*

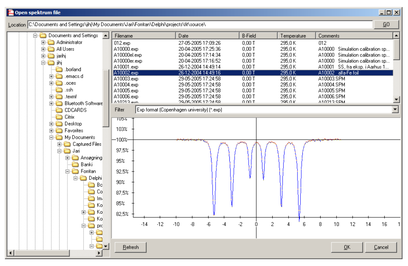

Figure 7: *The common open file dialog window, from which all spectrum files are opened.*

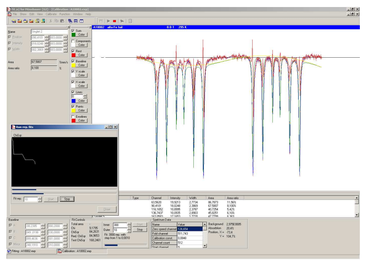

Figure 8: *The calibration window, which is used for finding calibration data.*

OOT

Advantages:

- Inheritance is used to create child classes, which inherit most of the properties and methods, but introduce some new.
- Isolation makes it easy to correct errors or undesirable behavior, without affecting other parts of the program, thereby minimizing program errors.

Disadvantages:

- Processing speed will in most cases be lower than that of a procedural program due to larger overhead.
- The implementation process will be longer and the source code will be larger, since similar behavior is implemented multiple times to maintain isolation.

Data views

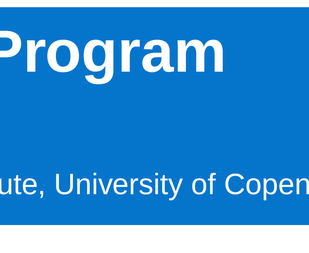

Figure 9: *1 Fit results can be viewed as reports and saved as both plain text ...*

Figure 10: *2 ... and in customizable LaTeX-format.*

Figure 11: *3 Calibration report.*

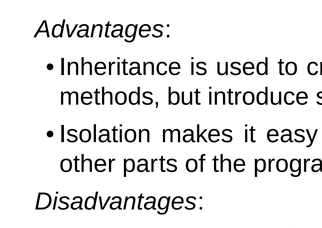

Figure 12: *4 The data format of the exported data files can be customized.*

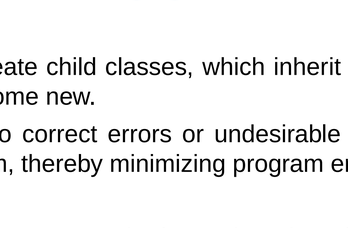

Figure 13: *5 The export data can be viewed in grid and text layout.*

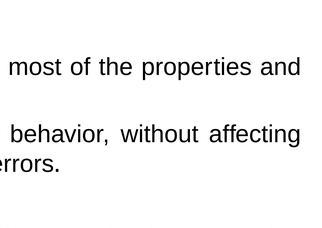

Figure 14: *6 A precompiled customizable list of the Mössbauer data of many common iron compounds.*

Conclusion

With Fit;o) we have created a solid tool for the analysis and fitting of Mössbauer spectra. With Fit;o) even an inexperienced user can analyze and fit relatively complex Mössbauer spectra of mineralogical samples quickly without programming knowledge.
Fit;o) is intended as a base onto which more modules can be added. The strictly object oriented architecture provides safety, and invites to additions and new modules, so contributors are welcome.

Future

Fit;o)will be maintained and new versions released on a regular basis in the future, and released as open source in the near future.

Contact

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References

[1] J. í Hjøllum, *Fit;o) - A Mössbauer spectrum fitting program*, In preparation, 2006.

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[3] W. H. Press and S. A. Teukolsky and W. T. Vetterling and B. P. Flannery, *Numerical Recipes in Fortran 77*, Cambridge University Press,1996.

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Keywords: Mössbauer, Analysis, Software, Fitting, Instruments, OOT
PACS: 33.45.+x , 82.80.Ej , 61.18.Fs

[1]Multi Document Interface