

# Mosgraf-2009: The Mössbauer data processing suite of applications

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**Abstract.** This contribution gives general description of the Mössbauer data processing suite of applications Mosgraf-2009. The suite is designed to process data obtained in the energy domain. It contains many applications to generate off-line functionality files of the spectrometers and many applications to pre-process data or to plot results of the calculations. The suite is designed for the Microsoft Windows® systems and it is compatible with the MsAa-x spectrometers of the RENON family. It could be installed on the same computer as the spectrometer drivers provided a broadband Ethernet link is available for the computer in question. Applications are provided to accept data from other spectrometers as well. The suite contains a large collection of the applications to simulate or fit experimental data.

**Key words:** Mössbauer spectroscopy • energy domain • processing of data

## Introduction

The Mosgraf-2009 suite of applications is designed to process Mössbauer data obtained in the energy domain. There are already several such suites available commercially [3], but none of them is as complete as the Mosgraf-2009. Applications processing Mössbauer data obtained in the time domain are not enclosed in the Mosgraf-2009 as the responsibility to develop such applications rests with the few synchrotron laboratories worldwide offering facilities to perform experiments in the time domain. Such facilities are not freely accessible and the access is limited to handful of experimental groups worldwide. The range of resonant lines and sample environments is severely limited as well. The Mosgraf-2009 suite is designed for the most popular Microsoft Windows® (MW) systems and it could be operated either in the 32-bit or 64-bit environment. Some obsolete applications cannot be run in the 64-bit environment and they are installed mostly in the background for the sake of completeness. One can use all MW versions since Windows-98 second edition inclusive.

## General layout

All essential applications are accessible from the main panel. They are divided into four branches. The branch *File* is devoted to the basic maintenance and it contains useful general applications other than the numerical Fortran applications. Applications of this branch could be used in particular to customize the layout and to

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plot the various ASCII files, e.g. produced by other applications. The branch *Operations* contains applications used to generate off-line spectrometer functions, extract data from the spectrometer files (MsAa-x of the RENON family or other), pre-process data, and to post-process fitted/processed data. A set of applications to calibrate the velocity scale by means of the laser-based interferometer is enclosed in this branch. Applications to process  $\gamma$ -spectra with the appropriate windows are provided, too [1, 4]. This branch contains a sub-system *Offline* of the auxiliary applications as well. The branch *Applications* (not operable in Demo) contains a collection of fitting applications. All applications run in a mixed environment of the dialogue-menu character except some specialized applications of the branch *Operations* including *Offline* applications and applications of the branch *Applications*. The latter applications are based on the dialogue interface with all messages organized in such a way to avoid the time loss by the operator. The majority of these applications have provision to edit respective control file on-line – by default the *Notepad* is assigned for this task. The branch *Help* contains essential help files (PDF or TXT formats depending on the application) and some technical data including provision to check for upgrades over the Internet. Some branches contain sub-branches making trees in order to keep clarity of the layout. View of the main panel with the branch *Applications* opened is shown in Fig. 1.

The core of the suite is composed of the fitting applications grouped in the simple branch called *Applications*. Currently available fitting applications are able to process almost any kind of the Mössbauer spectrum in the transmission or CEMS arrangement except some rarely used arrangements. The run time depends on the complexity of the problem, but EXE files provided are highly optimized. The Mosgraf-2009 is especially useful, while using the most modern spectrometers of the highest quality with a large number of data channels. It is based on the experience gathered during the long time development of the Mössbauer data processing applications since the early applications written in the Fortran-77/Fortran-4 (MOSSLIB). Several transmission integral algorithms are adopted where necessary, i.e.,

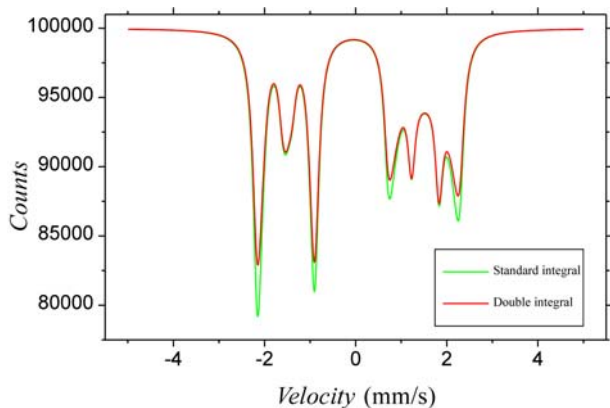


**Fig. 1.** View of the main panel with the *Applications* branch opened as the screen shot. Mössbauer data fitting applications are those with the names beginning as GM and AEFIT application.

for the linear and non-linear velocity scales either for the unpolarizing or polarizing medium. Applications of the general purpose are able to deal with the dipolar, quadrupolar or mixed transitions between excited and ground nuclear states having spins up to 9/2 each. Generally, the full diagonalization of the hyperfine Hamiltonians (Liouville operators, if required) is used except some specialized cases. There are two applications to process spectra obtained for the samples exhibiting the spin density wave. Relaxation and diffusion broadened spectra could be processed as well. The hyperfine field distributions could be evaluated within the modified Hesse-Rübartsch algorithm [5, 6] with the provision to use the transmission integral approximation – either for linear or for non-linear velocity scales. There are two data fitting applications of this kind – one of them uses standard transmission integral only, i.e., with the linear velocity scale. Corrections to the line intensities are evaluated either by using the irreducible texture tensors (unpolarizing medium) projected on the general spherical harmonics or by using directly the above tensors up to the fourth order [7, 9] and by direct integration over the unit sphere accounting for the polarizing properties of the medium. The latter approach is used in the applications devoted to the evaluation of the spectra obtained in the external magnetic field. One of them takes into account polarizing properties of the medium due to the broken inversion symmetry by the external field and finite thickness of the absorber. An application to fit simultaneously multiple spectra of any transition is provided. There are two applications to account for the impurity effect in the simple iron alloy and one of them is able to fit the order parameter. One application is devoted to the evaluation of the spectra of the fine particles moving in the ballistic limit within the viscous matrix. There are many more applications to deal with other specialized situations as well. The most critical applications are documented in detail in the branch *Help*. Many other features could be found in the help files with the references to the original literature – if required. Some auxiliary applications are provided within this branch or within the *Offline* sub-system of the branch *Operations*.

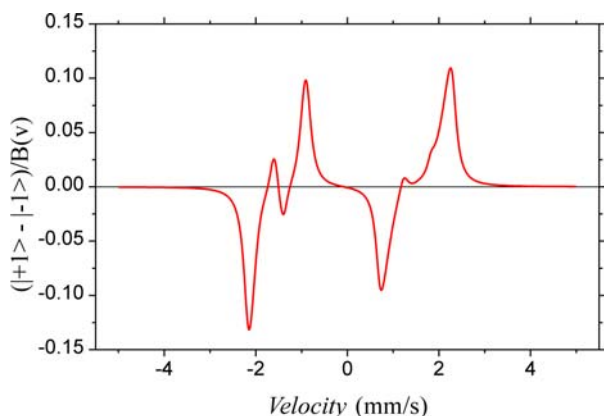
### Some highlights

Numerous things could be presented, as the suite is able to deal with many problems. We would like to concentrate on one particular problem described in some details. Namely, we are going to consider transmission of the narrow beam emitted from the resonantly thin, unpolarized and single line source emitting 14.41-keV resonant line connecting the excited and ground state in  $^{57}\text{Fe}$  (pure M1 transition). The beam is passed subsequently through the completely random (isotropic and with the isotropic recoilless fraction), flat and homogeneous absorber placed in the homogeneous external magnetic field oriented parallel to the wave vector of the radiation. The absorber temperature is sufficiently high to equalize the ground state hyperfine states. It is assumed that the field of 5 T acting on the  $^{57}\text{Fe}$  nucleus equals the applied field. A total shift between the source and absorber equals null. Intrinsic source and absorber line widths are the same and amount to 0.1 mm/s. The



**Fig. 2.** Comparison of the spectrum calculated without taking into account polarizing properties of the medium (green or thin line – Standard integral) with the spectrum calculated for each polarization mode separately (red or thick line – Double integral).

effective dimensionless thickness of the absorber equals 5.0, while the effective recoilless fraction of the source corrected for the background registered by the linear detector amounts to 0.56. The excited state of the  $^{57}\text{Fe}$  nucleus experiences an axial electric field gradient with the coupling constant  $A = [ecQV_eV_{zz}]/[4I_e(2I_e - 1)E_0] = +0.5$  mm/s. Here, the symbol  $e$  stands for the positive elementary charge. The symbol  $c$  denotes the speed of light in vacuum, while the symbol  $Q_e$  stands for the (positive) spectroscopic quadrupole moment of the first excited nuclear state in  $^{57}\text{Fe}$ . The symbol  $V_{zz}$  denotes the principal component of the electric field gradient tensor (the maximum component in the absolute terms), while the symbol  $I_e = 3/2$  stands for the nuclear spin of the above-mentioned state. Finally, the symbol  $E_0$  denotes resonant transition energy. It was assumed that the number of counts per data-channel far off the resonance is constant and amounts to  $10^5$ . It is assumed that the polarization of the passing beam is due solely to the resonant processes. The simulated spectra vs. applied source velocity against the absorber are shown in Fig. 2, while the relative beam polarization vs. velocity is shown in Fig. 3. The simulations were performed using GMFPILVD application belonging to the *Applications* branch.



**Fig. 3.** Relative difference between spectra due to  $|+1\rangle$  and  $|-1\rangle$  orthonormal polarization modes vs. velocity. The symbol  $B(v)$  stands for the constant baseline, i.e., for the number of counts per data-channel far off the resonance. This is a beam polarization far away beyond the absorber.

It is obvious that the lack of the inversion centre (definite orientation of the axial vector of the applied field) leads to the significant polarization of the initially unpolarized beam provided the absorber is rather thick. The complex character of the spectrum is due to the varying orientation between the magnetic field and the  $V_{zz}$  component of the electric field gradient tensor. One has to be very careful while evaluating total (isomer) shift from such spectra. The shift equals null as stated above. However, the average calculated in the unpolarizing medium approximation amounts to  $+0.057$  mm/s, while upon properly taking into account the polarizing properties of the medium equals  $+0.087$  mm/s. The shift of the  $|+1\rangle$  spectrum is  $-0.426$  mm/s, while the corresponding shift of the  $|-1\rangle$  spectrum amounts to  $+0.597$  mm/s. The real shift could be, of course, evaluated provided the double transmission integral algorithm is used as the asymmetric shape of the spectrum is accounted for. Otherwise serious errors could be introduced (particularly in the thin absorber approximation) leading to some unphysical conclusions especially while looking for the (usually small) second order Doppler shift (SOD). The shift remains unaffected by the non-scalar hyperfine interactions, as this part of the Hamiltonians is traceless, however the finite thickness of the absorber introduces some shift provided terms higher than linear in the exponent expansion are significant and the spectrum has no mirror symmetry around the central shift. This problem is quite common for the complex spectra fitted to some heuristic ill-defined models, and hence SOD obtained this way is completely meaningless for evaluation of the local atomic dynamics leading to some large, albeit completely unphysical variation of the lattice hardness vs. some chosen parameter like the impurity concentration.

## Conclusions

The Mosgraf-2009 suite is a collection of the various Mössbauer data processing applications and generators of the spectrometer functions. Almost any kind of the spectrum could be either simulated or processed by means of this suite – with some exceptions. The fitting applications could simulate spectra, simulate and compare with the experimental data or to fit the data to the predefined set of the parameters by means of the  $\chi^2$  method. There is a provision to set linear relationships between various parameters in order to make the algorithm faster convergent or in order to comply with the physical symmetries. The suite is designed in such a way to be run on the personal computers including laptops. The earlier stage of the suite has been reported in [2] with references to the older underlying work.

**Acknowledgments.** Mosgraf-2009 is based on the earlier versions. Numerous people contributed to the earlier versions. T. Birchall, K. Ruebenbauer and G. Dénès developed original version of the GMFP application. Fitting subroutines have been supplied by H. D. Grundy and developed by A. J. Stone. G. Czjzek and W. Berger devised early algorithms for expansion of the hyperfine structure distributions into central moments. A transmission integral procedure

is based upon the method devised by T. E. Cranshaw and refined by G. K. Shenoy. The inclusion of corrections for the source resonant finite thickness is based upon the work of J. G. Mullen. Some integration algorithms come from the McMaster University Computing Center. Cyfronet in Kraków developed some algorithms for the random-number generation. Quantum mechanical complex operators are processed by EISPACK/LAPACK (B. T. Smith, J. M. Boyle, B. S. Garbow, Y. Ikebe, V. C. Klema and C. B. Møler). Complex matrix inversion subroutines are adopted from the CERN library (G. A. Erskine) and some other numerical subroutines come from the ANL library. Some basic concepts of the general layout for GMFP have been developed independently by E. Görlich and K. Tomala. B. Miczko, K. Ruebenbauer and B. Sepiol developed early calibration applications. Early links to the operational systems have been based upon the work of J. Rafa and M. Kwater. T. Terlecki developed first graphical interface. It was based on either original or modified graphical drivers developed by Media Cybernetics®. R. Batchelor contributed to the development of the early versions of the final results plotting software. An independent development of the applications dealing with the MsAa-1 spectrometers is due to R. Górnicki (RENON-Company), M. Kwater, M. Pochroń, K. Ruebenbauer, T. Terlecki and U. D. Wdowik. R. Górnicki developed drivers for the subsequent MsAa-x spectrometers. Older versions of the suite contain some free-ware tools documented within respective version. The work of A. Marszałek on the early stages of the Mosgraf-2009 is acknowledged. J. Cieślak and P. Bonville developed independently (of each other) and previously applications dealing with the spin density wave. J. Żukrowski developed independently a similar application to treat spectra affected by the spin density wave. Applications able to fit simultaneously multiple spectra have been developed independently by several groups including application by J. Cieślak. Many other people contributed by giving important comments and remarks. Some ideas employed here were pursued independently by other groups.

## References

1. Błachowski A, Ruebenbauer K, Żukrowski J, Górnicki R (2008) Early design stage of the MsAa-4 Mössbauer spectrometer. *Acta Phys Pol A* 114:1707–1713
2. Duraj Ł, Ruebenbauer K (2011) New graphical interface to the MOSGRAF suite. *Acta Phys Pol A* 119:75–77
3. For availability of the software see: [www.mossbauer.org/instruments.html](http://www.mossbauer.org/instruments.html)
4. Górnicki R, Błachowski A, Ruebenbauer K (2007) Mössbauer spectrometer MsAa-3. *Nukleonika* 52;Suppl 1:S7–S12
5. Hesse J, Rübartsch A (1974) Model independent evaluation of overlapped Mössbauer spectra. *J Phys E: Sci Instrum* 7:526–532
6. Le Caër G, Dubois JM (1979) Evaluation of hyperfine parameter distributions from overlapped Mössbauer spectra of amorphous alloys. *J Phys E: Sci Instrum* 12:1083–1090
7. Ruebenbauer K (1991) Goldanskii-Karyagin effect in the absence of inversion centres. *Physica B* 172:346–354
8. Ruebenbauer K, Duraj Ł (2009) [www.elektron.up.krakow.pl/mosgraf-2009](http://www.elektron.up.krakow.pl/mosgraf-2009)
9. Ruebenbauer K, Wdowik UD, Kwater M (1996) Expansion of the Lamb-Mössbauer factor into semi-invariants. *Physica B* 229:49–54

## Appendix

A free .NET Framework® 3.5 or higher (.NET) environment designed by Microsoft has to be implemented prior to installation of the suite. The .NET environment (3.5 or higher) is already preinstalled in the full versions of MW-XP (since the Second Service Pack inclusive) and higher systems. Registered users of the Mosgraf-2009 could download .NET from the official page of this suite [8]. The full version has to be implemented for all systems till the MW-Me inclusive, while the short version has to be installed since the MW-2000 inclusive (note that some OEM versions of MW-XP do not have .NET environment – implement the full version). In the absence of the suitable .NET environment it is recommended to install proper version downloaded from the official page of the suite with the broadband connection to the Internet being active during installation. The main application of the suite calling other applications relies on the following libraries (DLL files): LOG4NET, MAGIC-LIBRARY and ZEDGRAPH. They are included in the installations. Some other tools are useful as well. It is desirable to have Microsoft Office® 97 (or higher), some PDF format reader (version 5.0 at least), and some plain text editor supplied usually with the system (since the MW-XP inclusive the Notepad is sufficient for all purposes). Some file manipulation software like, e.g. Windows Commander® is very useful, too. The numerical layer of the suite is written under Fortran-90 and all source-files are supplied. They are compiled under the Lahey-Fujitsu Fortran-90® version 4.00 (IMSL library has to be acquired, too). A Demo version is available free as well as all essential documents [8]. Registered users may download the older version (MOSGRAF) as the ZIP file. Some libraries of the MOSGRAF are used in the current version and they are included in the proper installations. Some other commercial applications/suites are of course necessary to produce publishable results or to exploit to the full extent the older version – MOSGRAF. The hardware requirements are relatively modest. One needs Intel-486 or higher processor with the mathematical co-processor, 128 MB RAM at least, and several GB of the free disk space. A standard mouse and keyboard are essential to run the applications. The graphical card has to have 800 × 600 resolution at least with not less than 256 color levels. A broadband connection to the Internet is required while installing .NET and checking for upgrades of this suite or downloading them not to mention data and results transfers. Results are printed into files and hence, one can use any suitable printer to make hardcopies – if required. Some other hardware components are used by the applications being currently obsolete and installed only for the purpose of the completeness. The suite is constantly developed and hence one has to check regularly for upgrades – see [8]. The current version could be delivered as the image of the official page recorded on the CD-ROM. The installation applications (Demo or the full version) build the proper trees at the destination shown by the user (c:\ as default). The first execution under the MW-Vista (or other MW systems installed in some non-standard way) has to be performed from the administrator level. This statement applies to the switching between Demo and full version and *vice versa* provided both of them are installed.