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New Graphical Interface to the MOSGRAF Suite

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A contribution is devoted to the recent development of the MOSGRAF suite used to process Mössbauer data and to generate reference functions for the modern spectrometers of the MsAa-x ($x = 1, 2, 3, 4$) family. Newly developed interface is designed for the Microsoft Windows-XP® or higher system of this class. However one can use some older system of this class as well provided some plug-ins are installed additionally. The lowest useable system is Microsoft Windows-98® — 32-bit edition. The new version of the MOSGRAF suite is compatible with 32-bit and 64-bit systems. MOSGRAF is fully compatible with MsAa-x spectrometers, however a powerful tool to convert ASCII data files from other spectrometers is provided. Data processing programs are compiled by the high efficiency Fortran-90 Lahey-Fujitsu® compiler. One of the most important new features is the ability to process velocity calibration data obtained by the new method based on the measurement of the time lapse between fringes of the Michelson–Morley interferometer.

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1. Introduction

MOSGRAF suite has been developed basing on the original Mössbauer data processing system MOSSLIB developed by Ruebenbauer and Birchall [1]. The first graphical interface was designed for DOS by Terlecki and Ruebenbauer and based upon HALO Professional Graphics Library® for Fortran (version 1.0) designed by Media Cybernetics Inc. The present version is based upon this previous suite. Basically one can distinguish the following layers within MOSGRAF: (1) data pre-processing system, (2) reference function generators, (3) post-processing data handling, (4) main processing programs, and (5) integrated auxiliary programs. Some diagnostic programs concerned with the spectrometer operation are enclosed as well. Some additional tools are provided within the sub-system (4), too.

The most important features of the sub-system (1) are as follows: (a) ability to process γ-ray spectra in order to estimate background under the resonant line, and (b) programs used to calibrate the velocity scale and fold data. Three independent calibration methods are implemented. The first one is based traditionally on the spectrum of α-iron, while remaining two methods employ Michelson–Morley interferometer equipped (preferably) with the He-Ne laser. One can use traditional fringe counting method [2, 3] or to use newly developed method based on the measurement of the time lapse between subsequent fringes. The sub-system (4) is able to process almost any Mössbauer spectrum. Exact diagonalization of the Hamiltonians is employed together with the *ab initio* calculation of the line intensities. Various versions of the transmission integral algorithm are available as well. Texture effects and/or local anisotropy of the recoilless fraction could be treated up to the fourth order including all relevant components of the respective irreducible tensor [4, 5]. Simple program is added within sub-system (5) to transform crystallographic anisotropy tensors into respective Goldanskii–Karyagin coefficients for any transition encountered in the Mössbauer spectroscopy.

The MOSGRAF suite has been used already for very long time. Hence, the present contribution is focused on the new features, i.e., on the new methods employed. Details of the new interface implementation seem less relevant and therefore we would like to concentrate on the new calibration method by means of the interferometer.

2. Time lapse method for the velocity calibration

A signal $S(t)$ from the photo-diode takes on the following form for the Michelson–Morley interferometer equipped with the monochromatic beam laser and for standard setup without recognition of the velocity sign [2]:

$$S(t) = A + B \sin\Big(\Big(\frac{4\pi n\nu}{c}\Big) \int_0^t dt' v(t') + \Phi\Big). \qquad (1)$$

Here the symbol $t \geq 0$ denotes current laboratory time with the origin at the beginning of the spectrometer cycle. The symbol $A > 0$ stands for the "constant" component varying very slowly with time, while

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the symbol $0 < B < A$ stands for the modulation depth. The modulation depth varies very slowly with time as well. The symbol $n \geq 1$ denotes refractive index of the transparent medium surrounding prism mounted on the transducer. The refractive index is close to unity and its variation with time is almost negligible. It varies with time very slowly, too. The symbol $\nu >> 0$ stands for the frequency of the almost monochromatic laser beam. The symbol $c = 2.99792458 \times 10^{11}$ mm/s denotes speed of light in vacuum. Function $v(t)$ describes velocity of the transducer projected on the laser beam. It is a periodic function without constant component. The extreme velocities are small compared to the speed of light in vacuum. The phase angle $0 \leq \Phi < 2\pi$ is generally unknown and it varies very slowly with time as well. One can assume that the phase angle stays constant during single spectrometer cycle. A spectrometer period $T > 0$ should be long enough to cover many distances of the order $c/(2n\nu)$. One can define derived function $y(t)$ having the following form:

$$y(t) = S(t) - A = B \sin\Big(\Big(\frac{4\pi n\nu}{c}\Big) \int_0^t dt' v(t') + \Phi\Big). \quad (2)$$

The function (2) is suitable to seek for subsequent zeros versus time. Zeros could be relatively easy recognized against synchronized, calibrated and stable high frequency clock and slight vertical offset of the zero-detector is not detrimental. Hence, the exact subtraction of the "constant" component is not required. Times of zeros do not depend practically on the values of the parameter B as well. One can assume that the phase angle remains constant within single period. Let us assume that all zeros of the function (2) have been detected for particular cycle at subsequent times $0 \leq t_1 < t_2 < \ldots < t_m < \ldots < t_N \leq T$, where $N >> 1$. One can calculate corresponding velocities in this cycle (absolute values) by using the following algorithm:

$$|v(t_k)| = \frac{\Delta x}{t_{m+1} - t_m}, \quad k = 1, 2, \ldots, N-1,$$
$$m = 1, 2, \ldots, N-1, \quad t_k = \frac{1}{2}(t_m + t_{m+1}). \quad (3)$$

Due to the differential character of the Eq. (3) the unknown phase shift is almost removed from the estimation of the velocity (absolute value). A distance travelled by the transducer between subsequent zeros of the signal amounts to $\Delta x = c/(4n\nu)$. The latter algorithm applies to the smooth regions of the reference function (absolute value) with significant slope, and hence regions around velocity turning points and zero-velocity points are to be excluded from the data analysis. The phase angle does not enter time points t_k as they are based on the clock readouts. The same properties have time markers described by Eq. (3). The latter statements are valid for the phase angle being constant over the full spectrometer cycle. Therefore the variation of the phase angle has to be very slow and very smooth. However small variation of the phase angle is not detrimental as all data points are based on the actual clock readout and the phase angle is unlikely to change significantly between two adjacent zero points.

A time scale could be readily transformed into the data channel scale provided the number of data channels and spectrometer period are known. It is assumed that the dwell time of the data channel is the same for all data channels. Namely, one has the following channel address for a particular time $x_k = (t_k/T)(N_c - 1) + 1$. Here the channel scale runs from unity till the number of channels $N_c >> 0$.

Simulation has been performed for the double ramp triangular mode of the spectrometer operation. The number of the data channels per full cycle was adopted as $N_c = 4096$. The extreme velocity is defined as $v_0 > 0$ (maximum velocity). The phase angle was chosen at random from its range. Essential parameters are listed in Table I.

TABLE I
Essential parameters used in simulation.

n	ν [Hz]	v_0 [mm/s]	T [s]
1.0	4.736×10^{14}	0.005	5.0

Figure 1 shows simulation results, while numerical results are gathered in Table II. It is obvious that the proposed method works even for such extreme low velocity range. There are enough useful data points in each quarter of the cycle to fit reliably straight line by means of the linear regression.

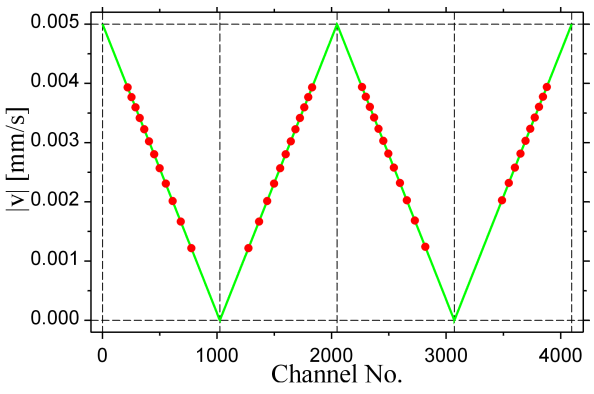

Fig. 1. (Color online) Calibration results obtained by the time-lapse method.

These are very good results for such extremely low velocity range. There is no better method for the absolute calibration of the Mössbauer spectrometer at such low velocity range. It has to be stressed that this method is extremely fast as the calibration is performed for single

TABLE II

Results of the velocity calibration. The symbol VBGN stands for the velocity in the first channel of the folded data. Exact values are derived from the applied reference function.

Parameter	Exact value	Calibration
Left ZERO [channel]	1024.5	1024.8 (+.3)
Right ZERO [channel]	3072.5	3072.3 (-.2)
Folding point [channel]	2048.5	2048.5 (.0)
First channel velocity [mm/s]	4.998×10^{-3}	4.998×10^{-3} (.0)
No of folded channels	2048	2048
VBGN [mm/s]	-4.998×10^{-3}	-4.998×10^{-3} (.0)
Velocity increment per channel [mm/s]	4.883×10^{-6}	4.883×10^{-6} (.0)

spectrometer cycle. There is no need to use phase shifter even for very low velocity range.

Sign of the velocity does not need to be recognized by the calibration system as it is fixed by the hardware setup and reference function.

In order to perform calibration one has to know the constant $\Delta x = c/(4n\nu)$, the spectrometer period T, number of data channels per spectrometer cycle N_c and to derive from hardware the number of zeros N and table of times $0 \leq t_1 < t_2 < \ldots < t_m < \ldots < t_N \leq T$. The calibration could be performed for each cycle separately. Hence, one can control spectrometer stability in precise way.

For the double ramp triangular mode one can estimate the number of all time markers per full spectrometer cycle as $N = (2n\nu v_0 T)/c$. Corresponding maximum deviation from the equilibrium position of the transducer equals $x_0 = \frac{1}{8} v_0 T$. Hence, one can estimate the number of time markers per cycle as $N = (16n\nu x_0)/c$. For $x_0 = 3$ mm (usually higher deviations are not used) one obtains about $N = 75828$ for the parameters of Table I. This value is close to the upper limit encountered for the velocity range of the order of $v_0 = 1000$ mm/s, and it could be handled still by the modern hardware. Therefore the proposed method has dynamic range of the order of 200000 at least. It covers all velocity ranges encountered in the Mössbauer spectroscopy. It is particularly useful for very low velocity range, where all other methods fail.

Conclusions

MOSGRAF suite was implemented within the modern systems like Microsoft Windows-XP®, Microsoft Vista® and Microsoft Windows-7® all of them either 32-bit or 64-bit. Some obsolete functions have been removed, while some new features were added. A time lapse method seems the most important new feature as far as functions concerned with data pre-processing are considered. MsAa-4 spectrometers have capability to use this new method of the velocity calibration.

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