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Science Engineering & Education Co.

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Using WMOSS to Calibrate the Velocity Scale of a Constant Acceleration Mössbauer Spectrometer

The working standard for calibrating the velocity scan of a Fe-57 Mössbauer Spectrometer is the spectrum of a high purity, natural Iron foil at the temperature 295 K. One supplier of such Iron foils is ESPI Metals (Ref. https://www.espimetals.com). Typically, the foil thickness is in the range of 0.006 mm to 0.025 mm. The spectrum of a 0.025 mm foil will exhibit some thickness broadening, but the distortion is small enough that a good velocity scan calibration can be achieved. The Iron metal spectrum line widths defines how much line broadening might be present from unwanted source motions. The ratio of the per cent dip of the resonant absorption peaks to the foil thickness reveals the efficiency of the spectrometer's gamma counting.

The WMOSS program has a procedure that analyzes the Iron foil spectrum and saves the resulting parameters to a disk file. The use of this "Iron Cal" procedure is described here.

The WMOSS menu structure and menu navigation keys are described in the WMOSS User Manual. The manual also has a tutorial and examples of the several theoretical models for simulation and fits. The manual can be downloaded at http://wmoss.org/Download1.html or www.seeco.us

Note: The WMOSS Iron Cal procedure can analyze spectra with velocity scan that span either all six lines of the sextet or that span just the inner four lines of the sextet. If your velocity scan only spans +/- 2 mm/s and only the two innermost lines are observed then you will have to manually fit the folded spectrum. This special case is discussed at the end of this document.

The goal of the Iron Cal procedure is to calculate the Doppler Shift Velocity for each channel (data point) in the Mössbauer spectrum. Given that each half of the velocity scan has constant acceleration, the velocity values will lie on a straight line. This line is defined by the channel value, named "C0", where the line crosses zero velocity and the line's slope, "dV". "dV" is also know as the "step" and has units of [mm/s/channel]. For i^{th} channel of the folded spectrum, the corresponding Doppler Shift Velocity can be calculated via Equation 1.

Eq 1. $V_i = dV (i – C0)$

Iron Cal Procedure steps:

Load the raw, unfolded data from disk via the WMOSS File/Data Load
You will need to choose the appropriate format for your data file. Enter the number of channels, e.g. 1024 for a file created by SEE Co Model W302, W3204 or W307 MCS.

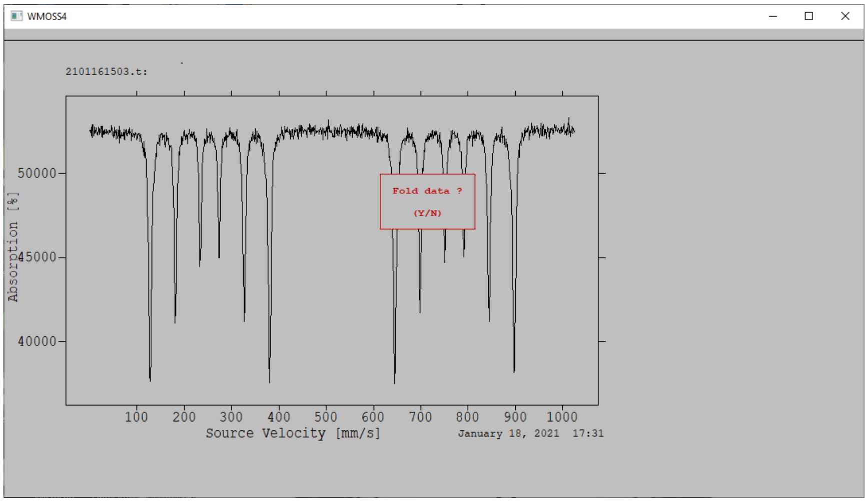


Fig. 1. Unfolded Iron Metal spectrum showing all six lines of the sextet.

To enter the Fold submenu, type “Y”.

WMOSS prompts “Interchange 1st & 2nd halves of spectrum?”.
If the spectrometer velocity scan is a triangular waveform with the first half having positive acceleration, the answer is “N”. Be careful. If you give the wrong answer the folded spectrum will be the mirror image of the proper spectrum.

WMOSS prompts “Use previous calibration?”
For a normal sample, the answer would be “Y”. If you are using the newly loaded spectrum as a calibration spectrum, the answer is “N”.

WMOSS prompts “Remove parabolilc or linear baseline?”
The answer is “N” except for unusual cases.

Now WMOSS presents the “Fold” sub-menu. Use the down arrow to highlight “Iron Cal” and press ENTER.

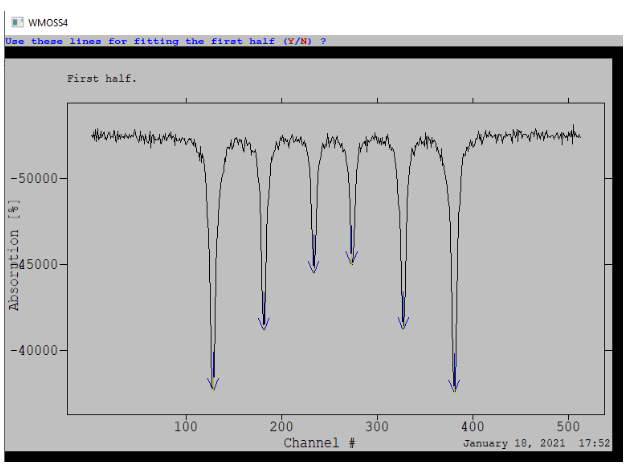


Fig. 2. The first half of the data is plotted with arrows at estimated peak positions.

If the spectrum has reasonable signal to noise then the estimated peak positions are mostly likely good enough to start the fit. If not, the starting peak positions can be set manually using the PC mouse.

Now WMOSS prompts "Add Mask to this half?"
If there are no portions of the data that you wish the fit to ignore then press "N". Then WMOSS loads a parameter file for performing a Least Squares Fit to the data using a model with six Lorenztian lines with independent positions, widths and areas. The results are presented in the "Post-Fit" plot. The

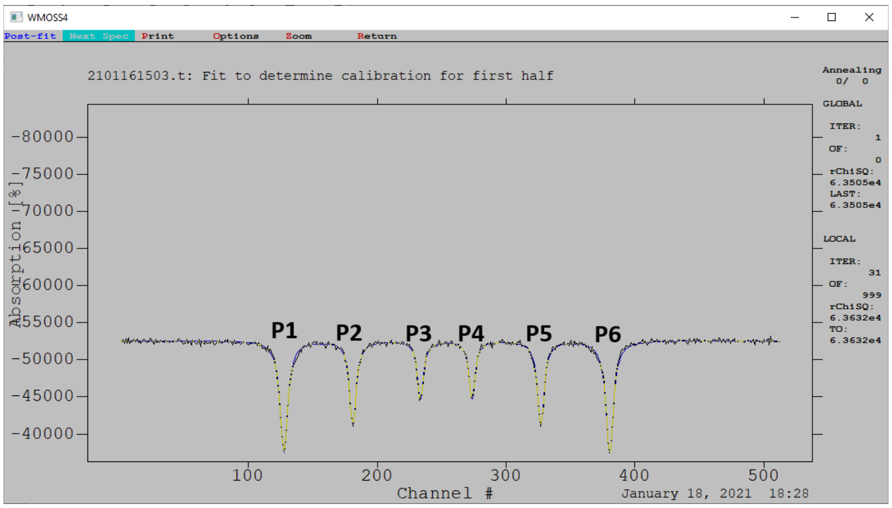
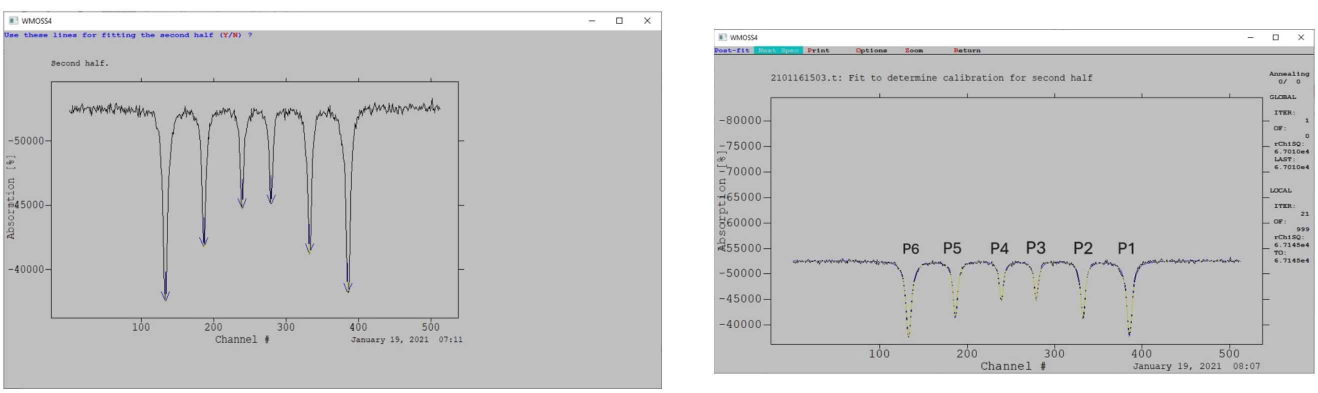


Figure 3. Iron Cal Procedure: Fit of six Lorentzians to first half of unfolded Iron foil spectrum.

Press "R" to Return to the Iron Cal procedure. Next, the second half of the unfolded spectrum is fit in the same way as the first half was.



A B

Figure 4. Second half of unfolded spectrum A) estimated peak position marked and B) with fit using six Lorentzian peaks.

Next the Iron Cal procedure calculates C0 and dV for both halves of the spectrum. The published splittings of the Iron metal are:

S16 = 10.66 mm/s

S25 = 6.17 mm/s

S34 = 1.68 mm/s

Given the lines positions in channels from the results above, C0 is set equal to the area weighted average of all the line positions. C0 is the center of the room temperature Iron Metal spectrum and is the zero of the conventional Mossbauer Doppler Shift velocity scale.

The three doublets are centered on C0. The six line positions is [mm/s] are given by

V1 = - 5.33 mm/s
V2 = - 3.085 mm/s
V3 = - 0.84 mm/s
V4 = +0.84 mm/s
V5 = +3.085 mm/s
V6 = +5.33 mm/s

A plot of six (P, V) points with Channels on the horizontal axis and Velocity [mm/s] on the vertical axis is fitted with straight line. The slope of that line is the value of dV.

The residuals from this fit are plotted as shown in Figure 5.

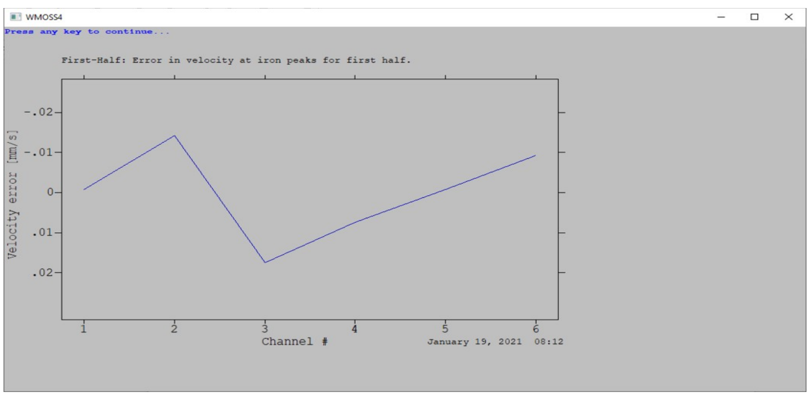


Figure 5. Residuals of Linear Regression to Iron metal peak positions in first half of unfolded spectrum.

Pressing any key will display the similar fit to the peak positions of the second half of the unfolded data.

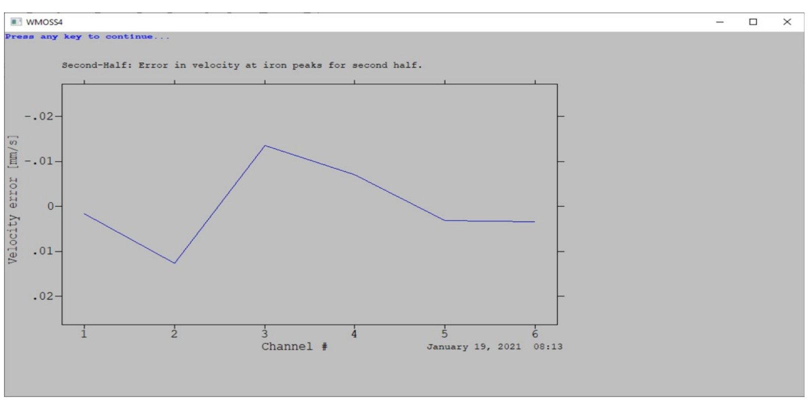


Figure 6. Residuals of Linear Regression to Iron metal peak positions in second half of unfolded spectrum.

Prompt: Save as?

Type any convenient two-letter label.

Results are saved in the two ASCII text files CAL.LOG and CAL.HST. The entries in the two files for the results of one Iron Cal fit are:

CAL.LOG

210119 2101161503.t 10 253.89 0.04224 512.49

127.718 181.183 233.580 273.591 326.934 380.285

644.957 698.365 750.895 790.821 844.210 897.363

CAL.HST

210119 2101161503.t 10 253.89 0.04224 512.49

The first line lists the data, data file name, two letter label entered by WMOSS user, V = 0 channel for folded spectrum, velocity step [mm/s / channel] for the folded spectrum, fold channel.

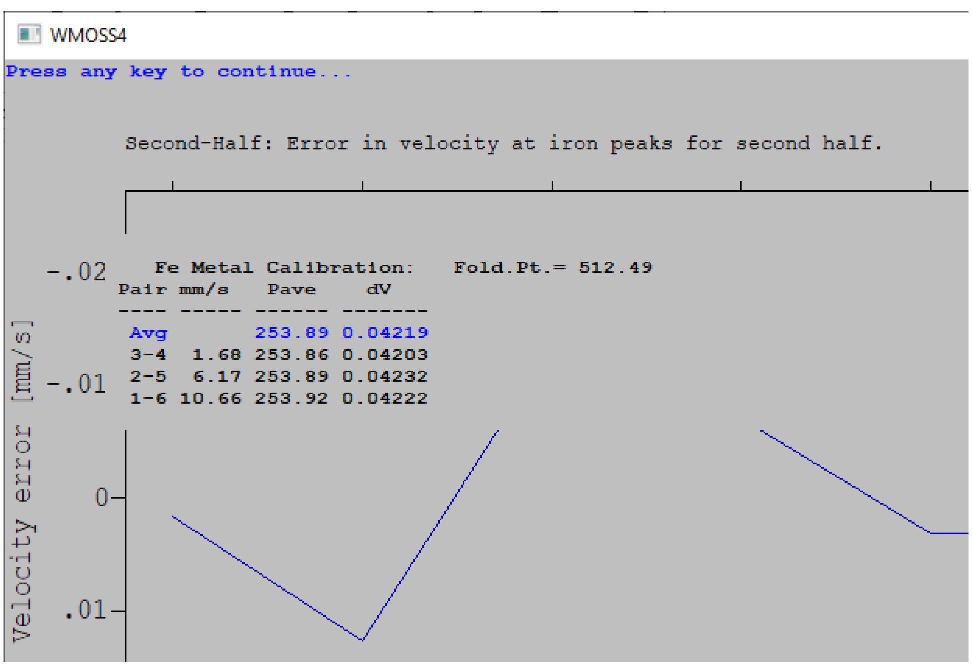


Figure 7. Calibration parameters for folded spectrum.

Linearity of the Velocity Scan

The Integral Non-Linearity (INL) of the velocity scan is defined by the magnitude of the residuals divided by the velocity span of the Iron Metal spectrum. In the example above, for the largest residual was 0.02 mm/s. The data span 10.66 mm/s. That give a INL equal to 0.02 / 10.66 = 0.0019 = 0.19%.

The nominal specification is usually INL <= 0.1%.

Another way to estimate the INL of the velocity scan is to compare the linewidths observed in the unfolded data with those of the folded data. If no significant broadening is seen in the folded data then any non-linearity of the velocity scan is insignificant.