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Evaluation of Mössbauer spectra linearization methods

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Abstract
Mössbauer spectra linearity is a critical parameter for Mössbauer spectrometer accuracy determination. This paper deals with comparison of various Mössbauer spectra linearizing methods. First method uses sine velocity waveform followed by linearization process. Next method introduces additional modulation based on the velocity error signal measured by laser vibrometer. Last evaluated method combines both. It uses the velocity error signal measured by laser vibrometer as linearization function. Custom Mössbauer spectrometer was constructed for the linearization evaluation. The spectrometer velocity driving system is based on the digital PID controller concept deployed in the FPGA chip of CompactRIO real-time hardware device. The obtained data demonstrate that all evaluated methods increases the linearity of spectra in a wider frequency and amplitude range of a drive signal in comparison with those measured using a traditional measurement method. Highest linearization effect has the method using sine velocity waveform, as generally harmonic movement is natural for used double loudspeaker type velocity transducers. Results show the possibility to use proposed linearization methods for higher velocity ranges using standard transducers and shows potential to be applied in the simple control of transducers without PID regulation or in piezoelectric transducer applications.

Keywords Mössbauer spectra · Velocity axis linearity · Linearization

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1 Introduction

Mössbauer spectra linearity is a critical parameter for Mössbauer spectrometer accuracy determination. In most studies so far, researchers focused on rising spectra linearity, for instance by using an improved PID regulator [1–4], modifying the velocity transducer [5] or velocity driving system [6]. Some other studies have been dedicated to a completely different approach, such as a time mode Mössbauer spectrometer [7, 8]. Our paper is focused on comparing three novel linearization methods and comparing them with a traditional method using triangular velocity signal with sinusoidal turnover points [2]. First method uses sine velocity waveform followed by linearization process [9]. Second method introduces additional modulation [10] based on the velocity error signal measured by laser vibrometer. Last evaluated method combines both and uses the velocity error signal measured by laser vibrometer as a linearization function.

2 Methods

First compared method uses sine velocity waveform followed by linearization process [9]. Mössbauer spectra are measured with sine waveform as a velocity reference signal. This results in spectra with sine velocity axis. After the spectra are measured, they are recalculated using the inverse function [9].

Second linearization method is based on the method proposed in [10]. A modification of this linearization procedure using a Keyence LK-G5000 laser vibrometer (see Fig. 1) is used. A laser vibrometer was used as it is not sensitive to electromagnetic interference like the coils moving in a magnetic field. This random electromagnetic interference can lead to an increase in spectral line width. Moreover, the laser system is not sensitive to inhomogeneities in the magnetic field of permanent magnets or coil windings, which results in velocity axis nonlinearity. The LK-G laser vibrometer was used to measure the transducer velocity. These velocity values were recorded and averaged. The measured velocity waveform was subtracted from the ideal velocity waveform (see Fig. 2a). Consequently, this difference was used to modulate the input signal. The modulated signal was recorded into the look-up table of the virtual speed generator (see Fig. 2b).

Fig. 1 Laser vibrometer and spectrometric bench (with back cover removed)

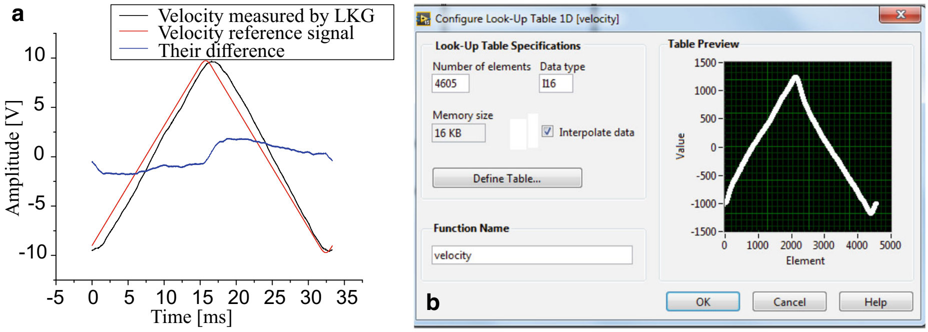

Fig. 2 The velocity signal measured by the LK-G5000, the ideal signal and their difference (**a**) and the reference signal modulated by this difference, recorded in the look-up table of the virtual speed generator (**b**). These signals were obtained at 30 Hz and ± 10 V input signal amplitude (corresponding to approximately ±120 mm / s) and at slightly mistuned PID parameters (for better recognition of the signals difference)

Third linearization method uses averaged error signal for later "offline" spectrum recalculation. The spectrum is recorded in very high channel resolution mode and the average error signal (the difference between the actual velocity waveform and the ideal velocity waveform) is also recorded. Mössbauer spectrum is recalculated using the inverse function of the average error waveform after its collection. The algorithm works the same way as sine linearization algorithm [9]. It is divided into small intervals that are not the same length, but they have the same velocity range. The algorithm deletes individual points from the spectrum, so the intervals of same velocity are the same length. Furthermore, the spectrum is summed up to 1024 points and folded (if required). This method is also similar to the "time mode" Mössbauer spectrometer [6, 7], the main difference is that this method is done offline, after the spectra recording.

3 Experiment

Customized Mössbauer spectrometer setup [11] (including the digital PID controller [4, 5], the double loudspeaker-type transducer [5] and the gamma-ray detector [12]) was used for the measurements. Used Mössbauer spectrometer was modified to record data in very high channel resolution of hundred thousand or even millions of channels [9]. The spectra quality was described with the full-width at half minimum parameter (FWHM) of the fifth spectral line and nonlinearity of the spectrum velocity scale, calculated as in [7]. Mössbauer spectra of the $^{57}Fe_2O_3$ (enriched by ^{57}Fe) hematite were measured for the linearization process evaluation. Several spectra were measured while using different frequencies and amplitudes. The spectra parameters were compared for frequencies of 30 Hz and 100 Hz. The velocity signal amplitudes were 1 V and 10 V (those voltage values approximately correspond to ±12 mm·s^{-1} and ± 120 mm·s^{-1} in the presented spectrometer configuration). As the spectra measured in different velocity ranges are not comparable, the error signal amplitude was used for linearization methods comparison.

4 Results and discussion

Figure 3a shows the dependence of the spectrum velocity axis nonlinearity on the reference spectra using different linearization methods. The appropriate spectral line FWHM parameters

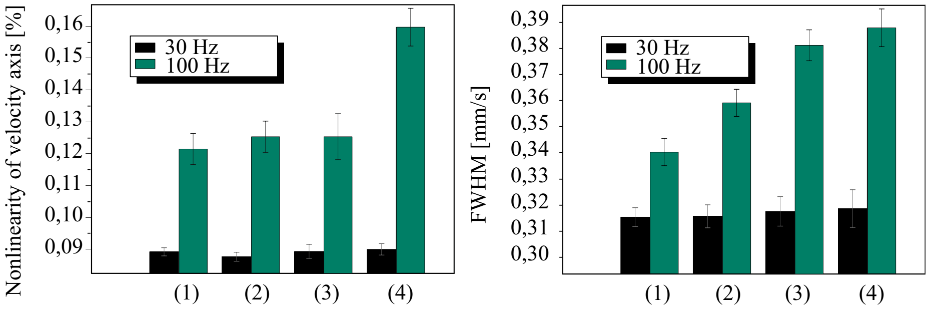

Fig. 3 Comparison of spectrum velocity axis nonlinearity (**a**) and spectral line widths (**b**) of the enriched sample $^{57}Fe_2O_3$ while using different linearization methods - sine velocity waveform followed by linearization process (1), velocity signal reference modulation by error signal (2), and offline spectrum recalculation using error signal (3) with traditional method using triangle with sinusoidal turnover points (4). Black bars are values for spectra measured at 30 Hz and green bars are values at 100 Hz

are shown in Fig. 3b. Black bars are values for spectra measured at 30 Hz and green bars correspond to values at 100 Hz. Figure 3a shows that the Mössbauer spectra have a higher velocity axis nonlinearity at a higher frequency of transducer motion. However, this increase in nonlinearity is lower when using additional linearization methods. All three methods compared have approximately the same effect on reducing the non-linearity of the velocity axis. On the other hand, the comparison of the spectral line FWHM parameters shows that the sine linearization method achieves the best values, followed by the reference signal modulation method. The offline linearization method by error signal does not reduce the spectral line width so much. Figure 4 shows a dependence of the error signal amplitude and the input signal amplitude for various linearization methods. Sine linearization method has the lowest error

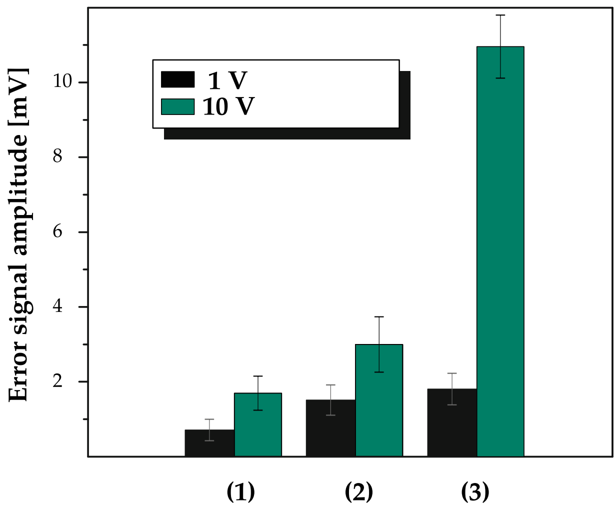

Fig. 4 Comparison of error signal amplitude for different linearization methods - sine velocity waveform followed by linearization process (1), velocity signal reference modulation by error signal (2), with traditional method using triangle with sinusoidal turnover points (3). Black bars characterize 1 V amplitude (corresponding to approx. 12 mm / s) and green bars describe 10 V amplitude (corresponding to approx. 120 mm / s)

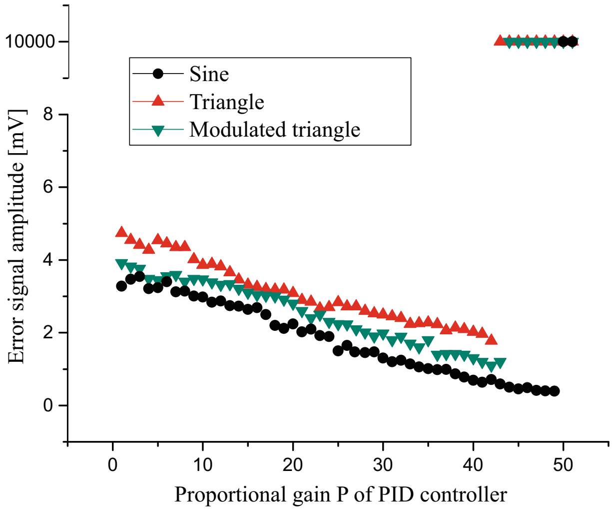

Fig. 5 Error signal amplitude for different spectrometer modes depending on proportional gain setting of PID controller

signal, followed by error signal modulation. The third method using error signal for offline linearization has no effect as the linearization process is completed after the measurement.

Figure 5 shows error signal amplitude for different spectrometer modes for different proportional gain settings of the PID controller. The proportional gain was chosen, because it has the greatest influence on the PID control quality. Parameters I and D have been fixed at 0. Figure 5 shows that the error signal amplitude differs same as saturation onset. This saturation is state where the PID controller is not able to control the transducer. Instead of the PID regulation, it switches between the maximum and minimum AD (analog-digital) converter values (in this case ±10 V). This condition is easily recognizable as the transducer begins to emit a high frequency tone (transducer begins to move at higher frequencies). Figure 4 shows that the smallest amplitude of the error signal can be achieved by using a sine velocity reference signal. In this case, the error signal amplitude is below 1 mV. When using sine reference signal, saturation occurs when P is set to 47 or more. If the reference signal is modulated triangle, the error signal amplitude is higher (below 2 mV) and saturation occurs when P is set to about 44. For an ordinary triangle (with sinusoidal turnover points [2]) saturation occurs when P is set to more than 42. In this case, the error signal amplitude slightly higher than 2 mV. However, this amplitude is mainly caused due to error signal peaks that occur at the point of the velocity turning, where the spectrum is not measured. The amplitude of the error signal is lower in the areas, where the spectrum is not measured [13].

5 Conclusion

The obtained data demonstrate that all evaluated methods increases the spectra linearity in a wider frequency and amplitude range of a drive signal. Method using sine velocity waveform has the highest linearization effect, as generally harmonic movement is natural for used double loudspeaker type velocity transducers. Results show the possibility to use proposed linearization methods for wider velocity ranges using standard transducers. It also shows potential to be applied in the simple control of transducers without PID regulation or in piezoelectric transducer applications.

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