Calibration of ^{57}Fe Mössbauer Spectrometer for Hyperfine Interaction Analysis

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Introduction to Mössbauer Lattices

The Bohr model is used to describe atomic resonance fluorescence, in which an excited atom emits a photon. This photon can give a ground-level atom of the same type enough energy to transition to the same excited state, producing a photon in the visible range. Nuclear resonance fluorescence was predicted to be the same. However, it was quickly shown that nuclear resonant scattering did not behave similarly to atomic fluorescent resonance due to the conservation of momentum. When a γ-ray is emitted by a free atom, the atom experiences a recoil in the opposite direction of the emitted γ-ray. The recoil takes away energy from the γ-ray, so the γ-ray cannot be absorbed by a similar atom to the same excited state. Mössbauer discovered that when an atom is bound in a crystal lattice the recoil will be absorbed into the atom's surrounding bonds. Recoil is minimized when the recoil energy is smaller than the energy of the chemical bonds keeping the atom bonded to other atoms.

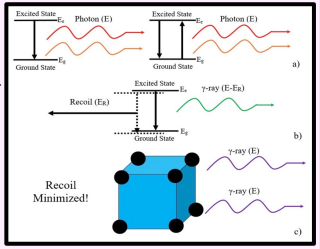


Figure 1: Depiction of a free atom going through a) atomic resonance fluorescence, b) nuclear resonant scattering, and c) bound in a crystal lattice.

Introduction to Hyperfine Interactions

The three hyperfine interactions Mössbauer spectroscopy can study are electric monopole interactions, electric quadrupole interactions, and magnetic dipole interactions .An isomer shift is the shifting of the entire resonance spectrum and is caused by the electric monopole interactions. The electron density around a nucleus causes a shift in excited and ground state levels. The difference in energy levels is the isomer shift. Electric quadrupole interactions are due to asymmetric electric fields around the nucleus which causes splitting of spectral lines. If an atom has a spin quantum number greater than 1/2 its electron configuration is an asymmetric electric field. In electric quadrupole splitting we see a degeneracy in the magnetic spin number. This occurs because the energy levels are too close to each other. When a magnetic field is applied to the magnetic moment of the nucleus the degeneracy becomes apparent. This effect is called Zeeman splitting.

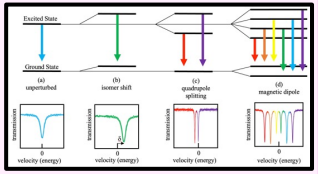


Figure 2: Mössbauer spectrum of ^{57}Fe showing various hyperfine interactions. Image from "Mössbauer Spectroscopy." Mineral Physics, 17 Dec. 2022.

Data Collection

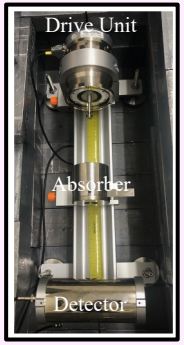


Figure 3:Mössbauer Spectrometer.

To collect the absorption spectrum of ^{57}Fe we connected the ^{57}Co source with a nominal power of 25 mCi to the Wissel Mössbauer Drive System-360. The drive unit was set to have a maximum velocity of 12.026+/-0.002 mm/s and a triangular function was used to drive the velocity unit. We collected data using 4 different absorbers, an α-Fe, Fe_2O_3, $^{57}FeC_2O_4{\bullet}2H_2O$, and $K_2Mg^{57}Fe(CN)_6$. The data collection lasted 1 and 3 hours respectively for each of the absorbers. The absorbers were placed in a holder and remained stationary. All data was collected using the Wissoft 2003 software. We made sure that we collected data only for the 14.4 keV line using a discriminator threshold internal to the Multi Channel analyzer. The distance between the absorber and drive unit was 20.6 mm and the distance between the absorber and the detector was 16.5 mm.

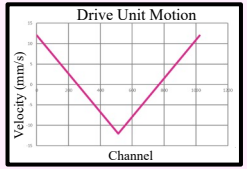


Figure 4: Drive unit velocity for every channel for the triangle drive shaping.

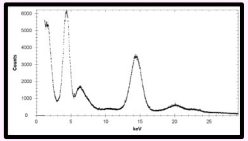
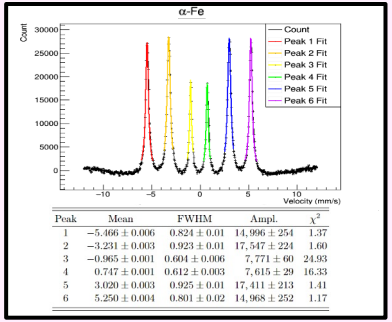


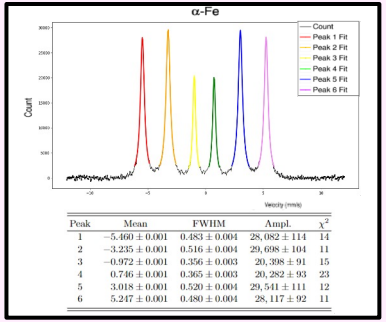
Figure 5: 14.4 keV Spectrum for ^{57}Co

Analysis



Peak	Mean	FWHM	Ampl.	χ^2
1	−5.466 ± 0.006	0.824 ± 0.01	14,996 ± 254	1.37
2	−3.231 ± 0.003	0.923 ± 0.01	17,547 ± 224	1.60
3	−0.965 ± 0.001	0.604 ± 0.006	7,771 ± 60	24.93
4	0.747 ± 0.001	0.612 ± 0.003	7,615 ± 29	16.33
5	3.020 ± 0.003	0.925 ± 0.01	17,411 ± 213	1.41
6	5.250 ± 0.004	0.801 ± 0.02	14,968 ± 252	1.17

Figure 6: ROOT analysis of an α-Fe absorber run for three hours.



Peak	Mean	FWHM	Ampl.	χ^2
1	−5.460 ± 0.001	0.483 ± 0.004	28,082 ± 114	14
2	−3.235 ± 0.001	0.516 ± 0.004	29,698 ± 104	11
3	−0.972 ± 0.001	0.356 ± 0.003	20,398 ± 91	15
4	0.746 ± 0.001	0.365 ± 0.003	20,282 ± 93	23
5	3.018 ± 0.001	0.520 ± 0.004	29,541 ± 111	12
6	5.247 ± 0.001	0.480 ± 0.004	28,117 ± 92	11

Figure 7: Python analysis of an α-Fe absorber run for three hours.

We fit each peak to a Lorentzian probability density function to find the peak positions and FWHM, for each peak in the absorption spectrum. We repeat the fit using an algorithm developed for both Python and ROOT. In the case of the python fit we assumed just a Lorentzian p.d.f. while using ROOT we use both a Gaussian and a Lorentzian. In Python the Lorentzian function was applied to each peak with orthogonal distance regression (ODR) using SciPy's ODR package. In ROOT we graphed the data using the TGraph package and made a TFit variable for each peak in a given graph. In both cases we fit the amplitude, the FWHM, and the mean peak positions for each peak in the absorption spectrum.

Results

Absorbers		g_0 [meV]	g_1 [meV]	ϵ [mm/s]	δ [mm/s]
α-Fe	Python	1.92 ± 0.01	1.08 ± 0.01	$(-1.21 \pm 0.08) \times 10^{-2}$	-0.109 ± 0.004
	ROOT	1.92 ± 0.01	1.08 ± 0.01	$(-8.07 \pm 2) \times 10^{-3}$	-0.104 ± 0.004
	Theo.				$[-0.1090 \pm 0.0001]$
Fe_2O_3	Python	2.96 ± 0.02	1.67 ± 0.02	-0.105 ± 0.070	0.284 ± 0.004
	ROOT	2.96 ± 0.02	1.67 ± 0.02	(-0.106 ± 0.007)	0.252 ± 0.004
	Theo.			$[-0.1000 \pm 0.0005]$	$[0.24 \pm 0.04]$
$^{57}FeC_2O_4{\cdot}2H_2O$	Python			0.881 ± 0.001	1.11 ± 0.004
	ROOT			(0.887 ± 0.001)	1.11 ± 0.004
	Theo.			$[1.72 \pm 0.84]$	$[1.19 \pm 0.07]$
$K_2Mg^{57}Fe(CN)_6$	Python				-0.216 ± 0.004
	ROOT				-0.201 ± 0.004
	Theo.				$[-0.10 \pm 0.12]$

Figure 8: Error in known values of quadrupole splitting (ϵ) and the isomeric shift (δ) in mm/s for all the absorbers, acquisition times is 3 hours for all absorbers, fit performed using Python and ROOT and expected theoretical values.

We found that Python had a δ (isomer shift) within 0.1% of the expected value in α-Fe, outperforming ROOT. However, ROOT had a maximum δ error of 12.1% in Fe_2O_3, which was more accurate than Python for the same absorber. $^{57}FeC_2O_4H_2O$ and $K_2Mg^{57}Fe(CN)_6$ had roughly similar values for both fitting procedures. $K_2Mg^{57}Fe(CN)_6$ in particular had a very large error for both programs. We posit that this is due to the single peak, which means that we cannot take multiple measurements to find the weighted average. ϵ (quadrupole splitting) errors were roughly the same for both fitting procedures, and the data does not definitively suggest that one program is more accurate than the other.

Conclusion

When the Zeeman effect is present in the absorber spectrum, we found that ROOT consistently had a better goodness of fit for peaks 1,2,5, and 6, but Python fit the inner peaks, peaks 3 and 4, with a better goodness of fit. Despite that, peaks 3 and 4 still had the largest reduced $\chi2$ with respect to any of the other peaks. We believe the inner peaks consistently had the largest reduced $\chi2$ because they are a superposition of both Gaussian and Lorentzian distributions. When no Zeeman effects were present we found that Python had a better goodness of fit. We compared Mössbauer spectrum parameters to known values and found no significant discrepancies between ROOT and Python's analyses.

Acknowledgements

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