A GRAPHICAL USER INTERFACE FOR POSITRON ANNIHILATION SPECTROSCOPY ANALYSIS USING COINCIDENCE DOPPLER BROADENING

by

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We present a new GUI application for the analysis of Coincidence Doppler Broadening (CDB) data. CDB is a technique used in Positron Annihilation Spectroscopy (PAS) to inspect the vacancy-type defects present in a metal sample. We used $^{22}\text{Na}$ as a positron source and placed two Germanium (Ge) detectors on either side of the experiment, which consists of two metal samples that sandwich the positron source. These samples should be nominally identical. CDB measurements help determine the relative defect concentration (i.e. produced by neutron damage), as well as chemical sensitivity to site where the positrons annihilate. The application uses the CDB data provided to create a number of analyses, including ratio curves and the sharpness and wing parameters. The strength of this application resides in the ability to quickly compare multiple data sets and to plot numerous data sets against each other.
to enhance the rapid analysis and elucidate trends. The preprocessing tech-
niques used, such as smoothing, are designed to be transparent, so the user
can tell what is being changed and maintain full control of those changes.
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Contents

Table of Contents vii

List of Figures viii

1 Introduction 1

2 The Experiment 3

3 Analysis Techniques 6
   3.1 Ratio Curves . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 6
   3.2 Sharpness and Wing Parameters . . . . . . . . . . . . . . . . . . . . 7

4 Description of Code 9
   4.1 Why Python/Tkinter . . . . . . . . . . . . . . . . . . . . . . . . . . . 10
   4.2 The Pre-Processing . . . . . . . . . . . . . . . . . . . . . . . . . . . 10
   4.3 Computing the S and W Parameters . . . . . . . . . . . . . . . . . . 12

5 Using the Application 14
   5.1 File Upload Form . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 14
   5.2 S and W Parameters . . . . . . . . . . . . . . . . . . . . . . . . . . . 16
   5.3 Ratio Curves . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 17
   5.4 SW tabs . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 18

6 Conclusion 20

Bibliography 21
List of Figures

2.1 Path of a positron in a material. An annihilation event occurs, releasing two photons traveling in opposing directions. Image courtesy of Chase Taylor ................................................................. 4

2.2 Experimental setup at Idaho National Laboratory. The horizontal, metallic detectors are used for coincidence Doppler broadening. The angled black detectors are for positron annihilation lifetime spectroscopy [1]. ............................................................................ 5

2.3 Two dimension plot of the energy of the photons collected by the Germanium detectors. Image created by the MATLAB script written by Xunxiang Hu ................................................................. 5

3.1 S and W parameters. The wing parameter also consists of an equivalent section on the left side of the graph. The vertical axis represents the number of photons detected by both detectors. Image courtesy of Chase Taylor. ................................................................. 7

3.2 Example S vs W Parameter Plot .................................................. 8

3.3 Example of S/Sref vs W/Wref Parameter plot .............................. 8

4.1 511 keV peak from the MATLAB script written by Xunxiang Hu. A normalized representation of the Photon counts are recorded on the y-axis, against energy (in keV) on the x-axis, with the peak at 511 keV. ................................................................. 11

4.2 First five lines in the output file of the raw data from the GUI. .... 11

4.3 An example of a ratio curve without folding. A rolling average of window size 3 was applied, as well as the shift peaks algorithm ................................................................. 13

4.4 The same data as Figure 4.3, but with the folding algorithm applied. Rolling average of window 3, and peak shifting algorithm applied ................................................................. 13

4.5 The two distinct slopes present here indicate distinct trap sites in the samples [2] ................................................................. 13

5.1 Loading tab for the CDB Analysis Tool. This is where the user adds and manages the datafiles ................................................................. 15

5.2 This tab is designed to allow the user quick access to the boundaries for the S and W parameters ................................................................. 16

5.3 Ratio Curve tab in the CDB Analysis Program .................................................. 18
5.4 S vs W plot from the CDB Analysis Program ................. 19
5.5 S vs W Reference plot from the CDB Analysis Program ....... 19
Chapter 1

Introduction

Fusion, a nuclear reaction in which two nuclei are combined, is a promising source for clean sustainable energy [3]. The most efficient fusion reaction found on Earth thus far is the deuterium-tritium reaction [4]. These are both isotopes of hydrogen, where deuterium has one neutron and tritium has two. Deuterium is found abundantly in ocean water, as well as other sources, so it is easily procured [4]. Tritium, on the other hand, is radioactive with a half-life of about 12 years [4]. Thus, it must be artificially produced by other nuclear reactions.

One major approach to fusion is through magnetic confinement [4]. This consists of a large machine that uses toroidal magnetic fields to contain a super-hot plasma. Inside this plasma is where fusion occurs. The plasma consists of neutrons, protons, electrons, and other light nuclei. The byproducts of D-T fusion include $^4\text{He}$ and fast neutrons. These fast neutrons escape the confinement of the magnetic field since they are electrically neutral and induce reactions in the walls of the machine. This causes defects to form, potentially compromising the integrity of the wall [5]. To identify and categorize these defects we can use techniques such as positron annihilation lifetime spectroscopy (PAS) and coincidence Doppler broadening (CDB) [6]. The latter is the
focus of my project.

Positron annihilation spectroscopy is a technique used to probe the inside of materials [7]. Since there are no fusion relevant neutron sources readily available in the world at the time of this study, the neutron irradiated samples used were damaged by fission neutrons, as a surrogate for fusion neutrons. The ultimate objective is to determine how long Tungsten will last as a material for the reactor walls.

One configuration for a magnetic confinement reactor is a Tokamak\(^1\). Our technique is not limited to Tokamaks, but is directed towards the walls of any plasma confining device.

\(^1\)Tokamak is derived from Russian and means toroidal chamber with magnetic coils
Chapter 2

The Experiment

The goal of this experiment is to use coincidence Doppler broadening positron annihilation spectroscopy to analyze various metal samples for their defect content. Since the width and shape of the annihilation peak is independent of the annihilation source [8], we use radioactive Sodium ($^{22}$Na) as the standard to produce positrons. This is sandwiched between two Tungsten samples, each of which have been exposed to high temperature neutron irradiation. The emitted positrons enter into the material where they bounce around until they annihilate with an electron [9]. Alternatively, they could get trapped in a vacancy (missing atom) and then annihilate (see Figure 2.1). The photons from these annihilation events have energies centered around 511 keV, the rest energy of an electron. The actual energy of the photon pair is offset by the momentum $p$ of the positron and electron before the annihilation, so each photon carries a momentum of $511 \text{ keV}/c \pm p$, where $p$ varies depending on the binding energy of the electron with which the positron annihilates. [10] (see Figure 2.1 for the path of a positron in a material). Two Germanium detectors are placed in coincidence around the samples (one on either side). This allows us to detect both photons as they arrive at the Ge detectors.
By having two Ge detectors we are able to restrict the data recorded to only those events that occur simultaneously. The event of a photon reaching the detector is recorded as a count, and is placed into a bin corresponding to the photon’s energy. This data is saved in a file, which we then load into the MATLAB script in preparation for analysis by the application. The Germanium detectors are the horizontal, metallic detectors in Figure 2.2.

The 2D plot in Figure 2.3 is generated from the energy of the detected photons, with the x-axis containing the energy of the photon recorded by one detector, and the y-axis defined similarly for the second photon, so that $E_1 + E_2 = 2 \times 511$ keV. The diagonal is where the sum of the two photon energies is 1022 keV, and when $E_1 + E_2 \neq 1022$ keV the behavior is irrelevant. These situations are non-coincident.

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1The low energy bands with $E_1, E_2 < 511$ keV are caused by one detector recording a photon in

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Figure 2.1 Path of a positron in a material. An annihilation event occurs, releasing two photons traveling in opposing directions. Image courtesy of Chase Taylor
Figure 2.2 Experimental setup at Idaho National Laboratory. The horizontal, metallic detectors are used for coincidence Doppler broadening. The angled black detectors are for positron annihilation lifetime spectroscopy [1].

Figure 2.3 Two dimension plot of the energy of the photons collected by the Germanium detectors. Image created by the MATLAB script written by Xunxiang Hu.

behaviour. The best feature of CDB is that the background is reduced by 4 orders of magnitude, which then allows for elemental sensitivity of the annihilation site.

photopeak (or the normal range), and the other detector reporting a lower energy due to incomplete charge collection. The phenomenon of incomplete charge collection occurs when a photon scatters on the detector imparting only a part of its energy, resulting in a detector measuring a signal lower than expected [11]. The high energy bands $E_1, E_2 > 511$ keV are due to one detector recording a single photon near 511 keV, with the other detector recording a piled up event, or more than one photon arriving at one time [10].
Chapter 3

Analysis Techniques

The following techniques described can be calculated in many ways. Most labs currently use spreadsheets or other manual software, such as Microsoft Excel [12]. These have the advantage that the user maintains complete control of everything that processes the data, with the expense of the time to enter the parameters every time. In this section we describe ratio curves and the sharpness and wing parameters, and how they are produced.

3.1 Ratio Curves

Ratio curves exploit the chemical sensitivity of the annihilation site. They are created by taking the annihilation energy spectrum from one sample and dividing it by the spectrum of another sample. This can be seen in Figures 4.3 and 4.4. It is common to divide the spectrum around 511 keV and fold (i.e. mirror across the line $x = 511$) the data across the 511 keV line and then average before computing the ratio. This is allowable because of the symmetry of the situation. The photons produced through the annihilation events are sent out in random directions, and thus have no preference
3.2 Sharpness and Wing Parameters

Figure 3.1 S and W parameters. The wing parameter also consists of an equivalent section on the left side of the graph. The vertical axis represents the number of photons detected by both detectors. Image courtesy of Chase Taylor.

toward either Germanium detector. Thus, the numbers of counts of photons with an energy greater than 511 keV will be about the same as the number of counts less than 511 keV in both detectors.

3.2 Sharpness and Wing Parameters

These two parameters are based on arbitrarily chosen energy bounds, but using the same bounds across several samples allows for valuable comparison.

The “sharpness” (S) parameter is calculated by computing the area under the curve (where the y values are the counts, see Figure 5.2) between two bounds, and then dividing by the total area under the curve [8]. These bounds isolate the peak of the curve, and commonly are defined to be where several curves intersect, if we
are plotting multiple curves at once. The exact boundaries are arbitrary, and they only need to be the same across multiple samples in order to make comparisons. This gives us a value in a fixed central momentum window. This value is sensitive to annihilation with low momentum valence electrons, and thus a high S parameter indicates a defect rich material.

The “wing” (W) parameter is calculated in a similar manner, using two sections to the right and to the left of the peak, or the wings of the spectrum. This parameter is more sensitive to annihilation with high momentum core electrons, and thus a higher W parameter indicates a more defect free material. This plot can be seen in Figure 3.2.

The S and W parameters from a given sample can be compared to those of a reference sample. This is done by dividing S or W of the material of interest by the S or W parameter of the reference sample (See Figure 5.5). Two slopes present in the plot indicates two types of defects present such as mono vacancies vs large vacancy clusters.

![Figure 3.2 Example S vs W Parameter Plot](image1.png)

![Figure 3.3 Example of S/Sref vs W/Wref Parameter plot](image2.png)
Chapter 4

Description of Code

A MATLAB script written by Xungxiang Hu is used to reduce the exceptionally large 2D CDB data of the experiment to a 1D plot along the diagonal where \( E_1 + E_2 = 1022 \) keV. Our own graphical user interface (GUI) application will maintain transparency in this processing by allowing the user to control everything that has the potential to change the data. The main processing that will occur will be smoothing with a moving average with an option to weight the data, and shifting energy axis so the peak occurs at 511 keV. This smoothing can be changed through a widget in the sections of the application that show data plots.

I was able to create the GUI using the Tkinter library inside of Python. The goal is to let the user know exactly what is being done to the data, so check buttons have been included at the top of each plotting window that allow the user to turn data processing features on and off. By default, the data are imported without any processing from the input source. The main buttons control the smoothing window size for a moving average, an option to use a weighted average using a Gaussian function to perform the weighting, and the choice to center all spectra precisely to 511 keV by shifting the peaks.
4.1 Why Python/Tkinter

Python is an open source programming language, and can quickly produce a working product. Python includes several convenient libraries such as Matplotlib [13] and Numpy [14], which provide excellent graphic and numerical tools. Tkinter was chosen to build the GUI application because it is included in base Python, which meant additional separate packages wouldn’t be required to install. Ultimately the goal was to produce an application with as few dependencies as possible, and also keep the code intelligible for future developers.

4.2 The Pre-Processing

The data loaded into the application (see Figure 4.1) is the 511 keV peak that was reduced from the 2D plot (see Figure 2.3) using the Matlab script. This data comprises the diagonal slice of the 2D plot where \( E_1 + E_2 = 1022 \text{ keV} \pm 2 \text{ keV} \). The first column (x-axis) represents an energy bin of the Germanium detector. The second column (y-axis) lists the number of photons that were grouped into the bin, i.e. a count of photons with an energy within the bin (see Figure 4.2). This data is noisy, and it can be difficult to interpret in the plot. This becomes a problem when we try to calculate the ratio curves, since the noise will be enhanced by the division. To fix...
4.2 The Pre-Processing

Figure 4.1 511 keV peak from the MATLAB script written by Xunxiang Hu. A normalized representation of the Photon counts are recorded on the y-axis, against energy (in keV) on the x-axis, with the peak at 511 keV.

This we need to smooth the data, which is done using the rolling average function from the Pandas Library [15]. Several plots were made comparing various parameters for this function with the data from MATLAB to ensure that no significant information was lost.

The next change is to shift the peaks to line up with 511 keV. In the smaller data sets that we tested, the peaks did not all line up with 511 keV and will cause issues with the ratio curve calculations if not corrected. This variance in the peak from 511 keV was not seen in the MATLAB analysis when using data sets which had collected data for a much longer time. To shift the data, the program fits the data...
4.3 Computing the S and W Parameters

Once the data has been appropriately processed, the calculation of the ratio curves is simple. The photons counts of a given sample are divided by the corresponding counts of a reference sample, which the user can select with a drop down box.

The user can specify the upper bounds for the S and W parameters, which are then
4.3 Computing the $S$ and $W$ Parameters

Figure 4.3 An example of a ratio curve without folding. A rolling average of window size 3 was applied, as well as the shift peaks algorithm.

Figure 4.4 The same data as Figure 4.3, but with the folding algorithm applied. Rolling average of window 3, and peak shifting algorithm applied.

used to calculate the parameters. The $S$ parameter is calculated using the trapezoid method, with the NumPy function $np.trapz$. This same function is used for the wing parameter.

The calculation for the $S$ and $W$ parameters with the reference data is created by taking the $S$ or $W$ parameter for a sample and normalizing/dividing it by the $S$ or $W$ parameter of the reference sample. This reference is again provided by a drop down box made available to the user.

Figure 4.5 The two distinct slopes present here indicate distinct trap sites in the samples [2]
Chapter 5

Using the Application

The following sections describe the layout and functions of the five major “tabs” of the application.

5.1 File Upload Form

The opening tab in this application is designed to simplify loading and reloading the sample data. The button “Select a cdb peak file” as seen in Figure 5.1 will let the user add data one file at a time. The user may then rename the samples by clicking in the “Current loaded files” area and adjusting the name as they wish. (The default name includes the full file path.) Once the user is finished changing any names, they need to click “Update filenames” to save those name changes to the data.

To reduce the need to repeat this process every time the app is opened, the user may click “Save raw data” to create a csv file containing the data with the names that were selected. Then, when they are ready to resume analysis, the user may click “Load a previous configuration,” which will prompt the user to select a file that they have saved using the previously described feature. The first column of the csv file
5.1 File Upload Form

Figure 5.1 Loading tab for the CDB Analysis Tool. This is where the user adds and manages the datafiles.

contains the x-axis or energy levels, and then each subsequent column contains the numbers of photon counts. This data will be the original data that was loaded, where the only change was to align the energy axis.

When the user has finished their analysis, they may wish to export their results to be edited by another program, such as a data plotting application. The “Processed data to save” section will allow the user to produce a csv file containing ratio curves, the S and W parameters (with or without the reference applied), and the processing that was applied to the data. This allows the user to keep a record of all the processing that happened, so that the data is reproducible. These options may be selected, and then exported to the csv by clicking “Save selected data.” These saved files have a different format than those loaded into the application, and thus cannot be reused in
the application.

5.2 S and W Parameters

This section is not where we calculate the Sharpness and Wing parameters, but where the user may adjust the bounds for the S and W parameters. The bounds are symmetrical, therefore if the user enters the boundary for the opposite side of the graph, the correct value is calculated by mirroring the entry across the 511 keV line.

![Figure 5.2](image)

**Figure 5.2** This tab is designed to allow the user quick access to the boundaries for the S and W parameters.

The processing options available are shown at the top of the page. The “Smoothing window size” determines the window size for a moving average. This is calculated by using the rolling mean method in the Pandas library. The window size specifies the number of data points the will be averaged together, and then the mean is placed in the central index of the window. To reduce the amount of data lost, min_period is set to 1, meaning the window size is allowed to be smaller than specified at the endpoints.
As is visible in Figure 5.2, the endpoints are quite noisy, so this will simply keep the photon counts closer to where they started. The “Gaussian Smoothing” check-button will toggle a Gaussian window type for the rolling mean, which will apply a weighted average with a spread of a Gaussian distribution.

The shift peaks option is very important for the reliability of the ratio curves. As described in section 4, this will fit the data to a Gaussian to find the correct location of the peak, and then adds the needed amount to the energy axis to allow the peak to line up with 511 keV. Any time the user changes a parameter or loads into a new tab, they will need click the “refresh” button to see the new changes.

5.3 Ratio Curves

There are only a couple unique features to this tab, the first of which is folding. This is a check-button the user can select, which will take the data and mirror it across the 511 keV line, averaging the photon counts together. The user may use the drop-down box at the bottom of the window to select the sample they wish to use as a reference file.
5.4 SW tabs

The SW and SW ref tabs are very similar, as can be seen in Figures 5.4 and 5.5. The “Flip Axis” button will swap the x- and y-axes. The reference file may be selected from this tab as well, not restricting the user to evaluating the ratio curves first. The calculation here is produced using the data from the SW Params tab, which will not have been folded.

Figure 5.3 Ratio Curve tab in the CDB Analysis Program.
Figure 5.4 S vs W plot from the CDB Analysis Program

Figure 5.5 S vs W Reference plot from the CDB Analysis Program
Chapter 6

Conclusion

A graphical user interface has been created for the purpose of analyzing data from a coincidence Doppler broadening experiment using positron annihilation spectroscopy. The data collected is used to create ratio curves and calculate the sharpness and wing parameters based on the preferences of the user. The primary goal was to maintain transparency, or to make it obvious to the user what changes are being made to the data and provide as many options as possible with regard to data processing.
Bibliography


