INL/JOU-23-71315-Revision-0

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Prepared for the
U.S. Department of Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

SoftwareX 23 (2023) 101475

Contents lists available at ScienceDirect

SoftwareX

journal homepage: www.elsevier.com/locate/softx

Original software publication

CDB-AP: An application for coincidence Doppler broadening spectroscopy analysis

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ARTICLE INFO

Article history:
Received 12 April 2023
Received in revised form 20 June 2023
Accepted 10 July 2023

Keywords:
Positron Annihilation Spectroscopy
Coincidence Doppler Broadening
Data analysis software
Defect characterization

ABSTRACT

Coincidence Doppler Broadening (CDB) Positron Annihilation Spectroscopy (PAS) is a material analysis technique that can be used to non-destructively measure characteristics of structural defects in samples. Analyzing and comparing large datasets obtained using this technique, however, can be complicated and time intensive. The Coincidence Doppler Broadening Analysis Program (CDB-AP) is a graphical user interface that facilitates rapid analysis of many data files while using transparent processes. It is already used in three laboratories at Idaho National Laboratory and can be used in laboratories worldwide.

Code metadata

Current code version	v1.0
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-23-00218
Legal code license	GNU General Public License v2.0
Code versioning system used	Git
Software code languages, tools and services used	Python, GitHub
Compilation requirements, operating environments and dependencies	Python 3.8+, tkmacosx, Matplotlib, NumPy, Pandas, mplcursors, SciPy
If available, link to developer documentation/manual	https://github.com/IdahoLabResearch/CDB_Analysis_Program/blob/main/README.rst
Support email for questions	chase.taylor@inl.gov

1. Motivation and significance

Positron annihilation spectroscopy (PAS) is a non-destructive technique for characterizing vacancy-type defects in materials. In PAS, positrons emitted from a radioactive source (e.g., Na-22) enter a sample, rapidly thermalize, and then diffuse stochastically. If the positron encounters an atomic vacancy during this "random-walk", it may become trapped in the vacancy due to a lower electron density in the vacancy and the positive ionic repulsion of the void surface [1]. It also may form positronium. Regardless of whether the positron becomes trapped in a vacancy or forms positronium, the positron soon annihilates with an electron, converting their masses to energy by releasing two 511 keV photons. Several variations of PAS can be used to characterize this annihilation radiation. Positron annihilation lifetime spectroscopy (PALS) characterizes the time between positron birth and annihilation, the duration of which correlates to the average size of vacancies in the material. Doppler broadening spectroscopy (DBS), meanwhile, focuses on measuring the energy of one of the 511 keV photons generated by the annihilation. Specifically, DBS measures the subtle Doppler broadening that occurs in the photon's energy peak due to the non-zero kinetic energy of the electron in the annihilating positron–electron pair. Valence electrons have less kinetic energy than core electrons, so their contribution to the Doppler broadening is smaller than the contribution of core electrons. Furthermore, positrons are more likely to annihilate with a valence electron when the positron is trapped in a vacancy-type defect than when annihilation occurs within the bulk material. Thus, the relative defect concentration between samples, as well as some discernment of the elemental specificity of the annihilation sites, can be evaluated by comparing Doppler broadening spectra [2,3]. Angular correlation of annihilation radiation (ACAR) is another momentum-based PAS technique; however,

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https://doi.org/10.1016/j.softx.2023.101475

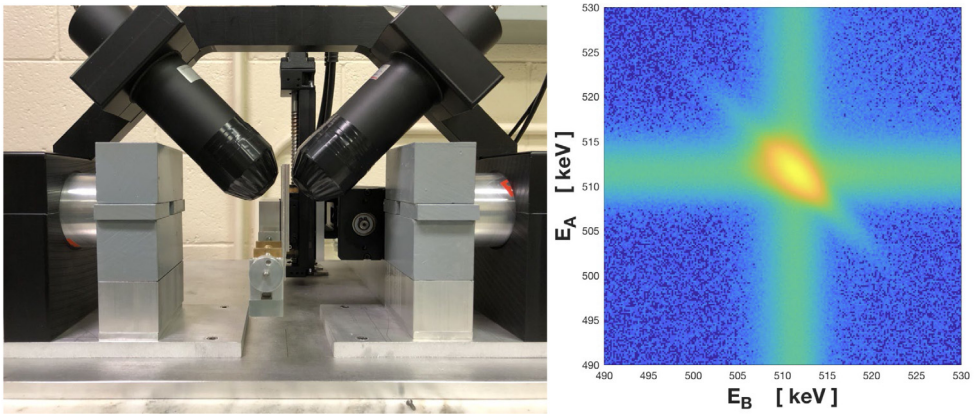

Fig. 1. (a) A typical benchtop PAS set up with PALS (performed using the black detectors) and CDB (performed using the silver detectors) [11]. (b) A typical two-dimensional CDB spectrum.

it measures the physical deviation from collinearity of the two annihilation photons instead of the Doppler broadening of the photons [4]. Though ACAR offers higher resolution than DBS, it is more complicated than DBS, requiring highly radioactive sources and intricate position-sensitive detectors. DBS grew more popular than ACAR when high energy resolution detectors became available. Coincidence Doppler Broadening (CDB), also called two-dimensional DBS, uses more advanced analysis and experimental systems than DBS to generate better results, as described in the next paragraph. Note that, even though it has much higher resolution than one-dimensional DBS, CDB still does not have as high of a resolution as ACAR. CDB is used worldwide in numerous applications, including analyzing semiconductors [5], relating load to defects in steel alloys [6], and studying neutron irradiated tungsten for fusion [7–9].

CDB, like DBS, focuses on precisely measuring the Doppler-broadening of the gamma rays emitted by positron annihilation. A typical benchtop CDB measurement is set up using two high purity germanium (HPGe) detectors placed on either side of a sample, colinear with the sample and oriented 180 degrees from each other (see Fig. 1.a). The sample generally consists of a pair of nominally identical samples with the positron source sandwiched between them. CDB reduces background noise by several orders of magnitude compared to DBS [10]. CDB does this through two methods: first, by only accepting counts when gamma rays are measured in both detectors approximately in coincidence; and second, by only analyzing data where the sum of the energies of the detected photons is approximately 1022 keV. The annihilating positron contributes its thermal rest energy of 511 keV to the total energy of the gamma rays, and the annihilating core or valence electron contributes its rest energy of 511 keV minus the energy binding the electron to the matrix. Therefore, the total energy released by the generated pair of photons is $E_A + E_B \approx 1022$ keV, where E_A is the energy of the count measured in detector A and E_B is the energy of the count measured in detector B. Data where E_A and/or E_B are far away from 511 keV (e.g., >50 keV) is often also discarded as part of processing. The collected data is often displayed as 2-dimensional spectrum where $E_A + E_B \approx 1022$ keV appears as a diagonal line [3] (see Fig. 1b).

Analyzing CDB data is more computationally difficult than analyzing DBS data due to the complexity of extracting the diagonal and analyzing data files that contain tens of millions of data points (e.g., 8192^2). Individual labs and researchers typically write scripts to process the data, although a few publicly available programs are available (such as those in Refs. [12,13]). These analysis methods are time-intensive, do not provide an easy method for rapidly comparing and manipulating large datasets, or do not provide the necessary options and transparency in data analysis to ensure that artifacts are not introduced due to hard-coded data reduction algorithms.

The CDB Analysis Program (CDB-AP) was developed at Idaho National Laboratory (INL) to address these issues by providing rapid data reduction and analysis of many data files while remaining transparent to the user regarding data processing methods. As the user uploads data files to CDB-AP, CDB-AP processes them and populates several graphs with analyzed data (see Section 2). Once loaded into CDB-AP, datasets can easily be compared to each other within CDB-AP using counts vs. energy and S parameter vs. W parameter graphs, with the option to normalize the datasets to a reference dataset. The user can then quickly and easily adjust parameters such as smoothing, shifting peaks, and reference dataset. These features dramatically streamline the data analysis process while mitigating human error, allowing for a more thorough, dynamic analysis of large quantities of data files, and thus enhancing scientific understanding of the material system being studied.

2. Software description

CDB-AP is a graphical user interface (GUI) that facilitates the rapid analysis of multiple CDB datasets. Its functionality is divided among the five tabs described briefly below:

- The “Load” tab: Facilitates the processing, loading, and saving of data.
- The “S and W Parameters” tab: Facilitates specifying the numerical values used to calculate S and W parameters from the counts vs. energy curves.
- The “Ratio Curves” tab: Facilitates the comparison of counts vs. energy curves against each other using a reference curve.
- The “S vs. W” tab: Displays an S parameter vs. W parameter plot containing a data point for each loaded dataset.
- The “S vs. W (Ref.)” tab: Displays an S parameter vs. W parameter plot containing a data point for each loaded dataset normalized to a reference data point.

2.1. Software architecture

CDB-AP’s GUI was built using the Python package `tkinter`. The GUI is divided into tabs according to functionality. The program enters a loop in `main.py`, which then calls the file `application.py` from within the folder `source_code`. The file `application.py` then builds the GUI using other files contained within `source_code`. Specifically, `file_upload_form.py` is used

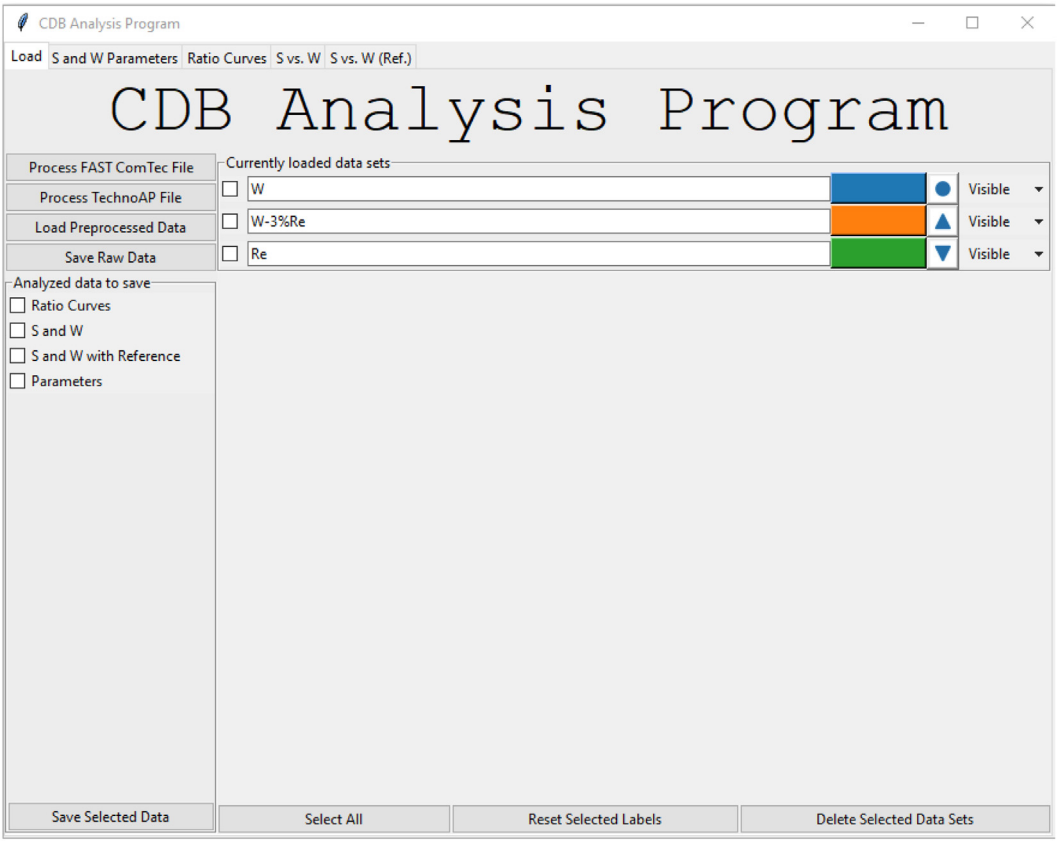

Fig. 2. The "Load" tab facilitates processing, loading, and saving data. On display are processed datasets corresponding to a pair of 99.99% pure tungsten samples, a pair of 99.98% pure rhenium samples, and a pair of W-3%Re samples [7]. This data was previously analyzed in Ref. [7].

to build the "Load" tab, `SW_parameter_form.py` is used to build the "S and W Parameters" tab, `ratio_curves_plot.py` is used to build the "Ratio Curves" tab, `S_vs_W_plot.py` is used to build the "S vs. W" tab, `SvsW_ref_plot.py` is used to build the "S vs. W (Ref.)" tab, `math_module.py` is used throughout CDB-AP to facilitate mathematical calculations, and `plot_module.py` is used throughout CDB-AP to facilitate plotting. The classes within CDB-AP frequently inherit the properties and methods of other classes. The folder `images` contains twenty-four PNG files used as markers within CDB-AP.

2.2. Software functionalities: The "Load" tab

The "Load" tab facilitates the processing of data, the loading of preprocessed data, and the saving of data (see Fig. 2). The tab currently accepts data files in two separate formats for processing. This accounts for the two different sets of hardware/software used at INL for CDB analysis. The FAST ComTec [14] hardware and software described in Appendix A.1 produce MPA data files. These MPA data files can be processed via the **Process FAST ComTec File** button and are described in Appendix A.1. The TechnoAP [15] hardware and software described in Appendix A.2 produce CSV data files. These CSV data files can be processed via the **Process TechnoAP File** button and are described in Appendix A.2. When processing data, only one data file can be selected for processing at a time.

The procedures for processing the two file formats are nearly identical. Raw data is generally measured in counts per channel, so CDB-AP begins by obtaining the conversions from counts per channel to counts per keV for each detector, i.e., the energy calibration of each detector. For FAST ComTec's MPA data files, CDB-AP obtains the energy calibration from the file's header (see Appendix A.1). For TechnoAP's CSV data files, after reformatting the data to mimic the format of the dual parameter spectrum in the MPA data file, CDB-AP asks the user for the energy calibration of each detector by asking for a and b in the equation $E = ac + b$ for each detector, where E is the energy and c is the channel. CDB-AP then uses that calibration to trim the data down to a 100 keV by 100 keV square centered around the 511 keV peak (from 461 keV to 561 keV). It does this using linear interpolation to create a grid of data points spaced every 0.15 keV, where the x-coordinate corresponds to the energy value detected in detector A, the y-coordinate corresponds to the energy value detected in detector B, and each data point corresponds to the number of counts detected at those coordinates. The peak is found by locating the coordinates with the most counts. The $E_A + E_B \approx 1022$ keV diagonal is then extracted by discarding data for which the sum of the coordinates is more than approximately 2 keV away from the sum of the peak's coordinates (from 2 keV below the sum to 2.15 keV above the sum, asymmetric to mitigate a ringing artifact that appears when extracting the diagonal). The extracted diagonal is then saved to a CSV file that can be loaded in the future via the **Load Preprocessed Data** button, no processing required. Note that the user chooses the name and location of this CSV file and any other saved CSV files that are created as part of this application. After being saved, the diagonal is normalized and loaded into CDB-AP. The user can click the **Save Raw Data** button to save the extracted diagonals of all currently loaded datasets into a single CSV file. Loading this single CSV file via the **Load Preprocessed Data** button is the equivalent of loading all the preprocessed data files individually.

The user can modify how a loaded dataset is displayed on other tabs. Specifically, the user can change the labels, colors, and markers corresponding to the datasets. Clicking the **Reset**

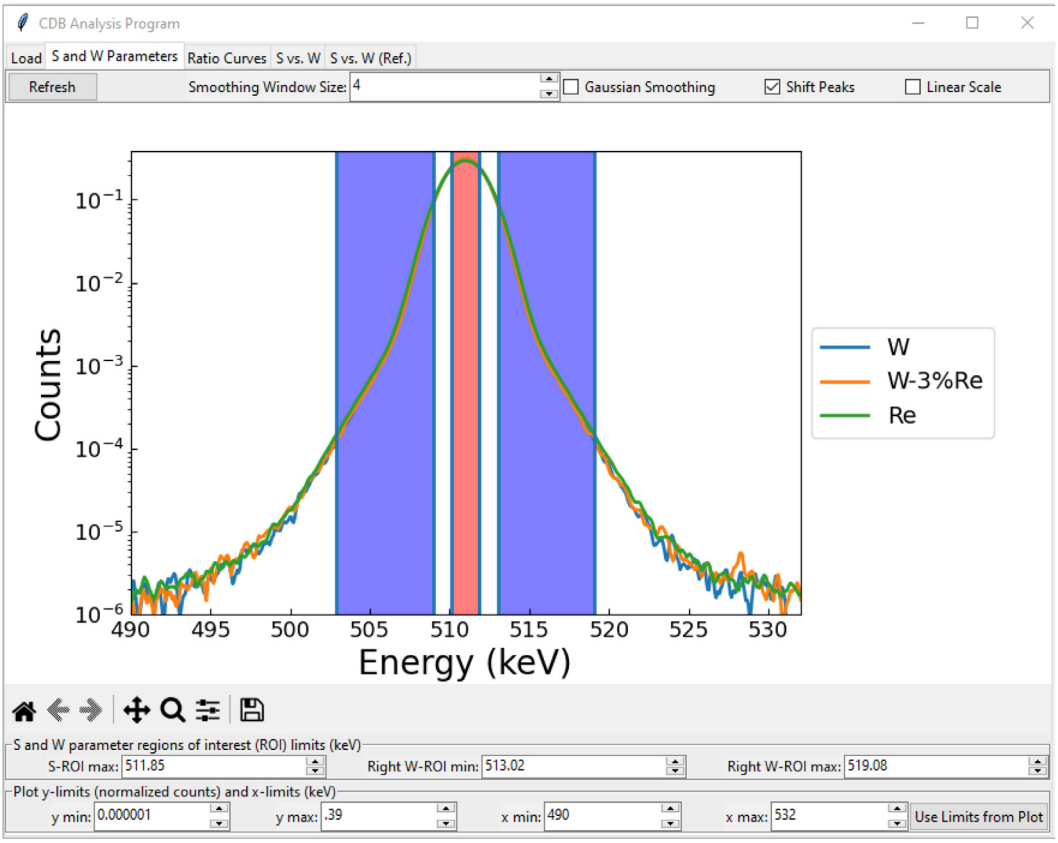

Fig. 3. The "S and W Parameters" tab allows for selecting S and W parameter values. The red band shows the selected region of interest (ROI) defining the S parameter, and the blue bands show the symmetric ROI defining the W parameter. On display are normalized count vs. energy curves obtained using the same W, W-3%Re, and Re datasets discussed in Fig. 2. The curves have been shifted so that each curve's peak is at 511 keV, and the datasets were smoothed using a rolling average with a window size of four data points. The counts were normalized such that the integration of counts over the energy equals one.

Selected Labels button sets the labels of selected datasets back to their default form. Alternatively, the user can remove any selected datasets from the application using the **Delete Selected Datasets** button. The user can select datasets individually via the toggles next to each dataset or click the **Select All** button to select every loaded dataset. Changes to loaded datasets do not change the data file from which the dataset was obtained. Datasets can also be toggled between "Visible" and "Hidden", which toggles whether that dataset can be seen on other tabs.

Once the datasets have been analyzed via each of the other tabs (see Sections 2.3–2.6), returning to the "Load" tab allows the user to save the results. To do so, the user selects from the following types of analyzed data: "Ratio Curves" (see Section 2.4), "S and W" (see Section 2.5), "S and W with Reference" (see Section 2.6), and "Parameters" (see Section 2.3). Next, the user clicks **Save Selected Data** to create a CSV file for each selected type of data.

2.3. Software functionalities: The "S and W Parameters" tab

The "S and W Parameters" tab facilitates the extraction of the S and W parameters from loaded CDB data (see Fig. 3). It displays the extracted counts (normalized number of counts in the energy bin) vs. energy (keV) curve. The S parameter is defined as the number of counts in a region of interest (ROI) symmetrically centered around 511 keV divided by the total counts under the Doppler-broadened 511 keV peak. Such analysis provides insight on the relative defect concentration between samples, where samples with a higher defect concentration have a higher S parameter. The precise energy limits for the ROI are subjective but are typically chosen so that $S \approx 0.5$ for an approximately defect-free sample, where S is the S parameter of the sample. Alternatively, the limits of the ROI might be chosen as the intersection of two Doppler-shifted 511 keV spectra, which produces the highest sensitivity for defect-induced changes between two samples [16]. The user can freely adjust the maximum energy of the ROI, and CDB-AP then mirrors the maximum energy across 511 keV to deduce the minimum energy of the ROI. Similarly, the user can freely set the minimum and maximum energies of the right-hand side of the ROI defining the W parameter, and CDB-AP mirrors those energies across 511 keV to deduce the left-hand side of the ROI defining the W parameter. The W parameter, like the S parameter, is defined as the number of counts in an ROI divided by the total counts under the Doppler-broadened 511 keV peak. Unlike the S parameter, though, the W parameter's ROI is made up of the "wing" regions on either side of the peak, as shown in Fig. 3.

The user can then control further data processing via a toolbar at the top of this tab. The **Smoothing Window Size** Spinbox widget sets the number of data points over which CDB-AP averages when processing data. At the time of this publication, even-numbered smoothing sizes are recommended to avoid a subtle ringing artifact created while extracting the diagonal due to the discrete nature of the data. By default, all points are evenly weighted in the centered rolling average CDB-AP performs. However, the user can toggle **Gaussian Smoothing** to use the following weights instead: $w(n) = \exp\left(-(1/2)(n/\sigma)^2\right)$, where $w(n)$ is the weight of the nth data point in the rolling window. The **Shift Peaks** toggle fits a Gaussian peak to the experimental data to find the peak center. In some cases, especially

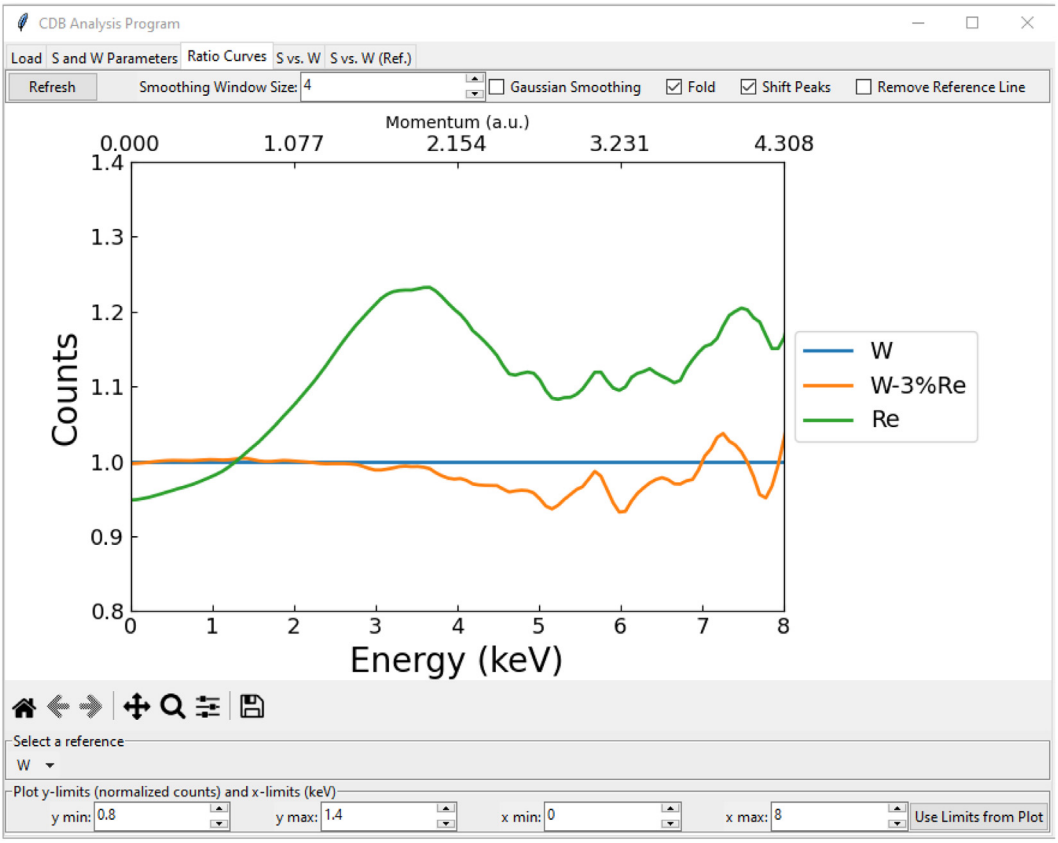

Fig. 4. The "Ratio Curves" tab facilitates comparison of counts vs. energy curves. On display are normalized count vs. energy curves obtained using the same W, W-3%Re, and Re datasets discussed in Fig. 2. The datasets have been normalized to the tungsten sample. As with Fig. 3, curves have been shifted so that each curve's peak is at 511 keV, and the datasets were smoothed using a rolling average with a window size of four data points. The datasets have also been folded, approximately doubling the available counts for analysis.

if the measured counts are relatively low, the fitted peak is not precisely at 511 keV. The **Shift Peaks** option uses the Gaussian fit to linearly shift all spectra so their peaks align at 511 keV. By default, CDB-AP uses a log scale to display the data, but the user can turn log-scale off via the **Linear Scale** toggle. After updating these settings, clicking **Refresh** updates the graph. Navigating to a tab with a plot or hitting the **Return** key within a Spinbox widget also updates the graph.

In addition to the normal navigation toolbar provided by `Matplotlib`, the user can set the visual boundaries of the graph using the **y min**, **y max**, **x min**, and **x max** Spinbox widgets. Alternatively, the **Use Limits from Plot** button fills in those boundaries with the x and y values for the current window display, allowing the user to manipulate the visual boundaries using `Matplotlib's` tools then set them with **Use Limits from Plot**. Setting the boundaries mitigates the need to reset boundaries after refreshing the graph.

Saving "Parameter" data on the "Load" tab generates a CSV file that contains the following information/parameters for each dataset: name of the source data file, label, color, marker, S parameter, W parameter, S parameter normalized to a reference dataset (see Section 2.6), W parameter normalized to a referenced dataset (See Section 2.6), uncertainty in the S parameter, uncertainty in the W parameter, whether the peak has been shifted, whether the curve has been folded (see Section 2.4), the smoothing window size, whether the smoothing is Gaussian, the reference dataset's label (see Section 2.4), the maximum and minimum energies for the ROI defining the S parameter, and the maximum and minimum energies for both ROIs defining the W parameter.

2.4. Software functionalities: The "Ratio Curves" tab

The "Ratio Curves" tab lets the user better compare the counts vs. energy curves by normalizing them to a reference curve (see Fig. 4). Along the top of the graph, there is also the momentum in atomic units. Ratio curves can provide chemical specificity of the annihilation site [10]. The top toolbar includes the same **Refresh** button, **Smoothing Window Size** Spinbox widget, **Gaussian Smoothing** toggle, and **Shift Peaks** toggle as the "S and W Parameters" tab. Due to the theoretical symmetry of the ratio curve, the data to the left and right of the peak's center can be summed together, or "folded". Folding the data allows for improved statistics since the CDB spectra are nearly symmetric around the 511 keV peak and the folded data contain approximately double the counts as just one side. The **Fold** toggle performs this function but requires the **Shift Peaks** toggle to have been selected first. The **Remove Reference Line** toggle stops the curve corresponding to the reference dataset from being displayed.

At the bottom of this tab, the user can adjust the plot boundaries and use `Matplotlib's` navigation toolbar, like on the "S and W Parameters" tab. There is also an option to select the reference dataset. Saving "Ratio Curves" data on the "Load" tab generates a CSV file from which this plot can be replicated, with the first column of the file being the x-axis, then subsequent columns being the normalized counts of each dataset's curve. Note that saving "Ratio Curves" data saves the datasets that have been smoothed, shifted, and/or folded (per the user's selections), as opposed to the raw datasets.

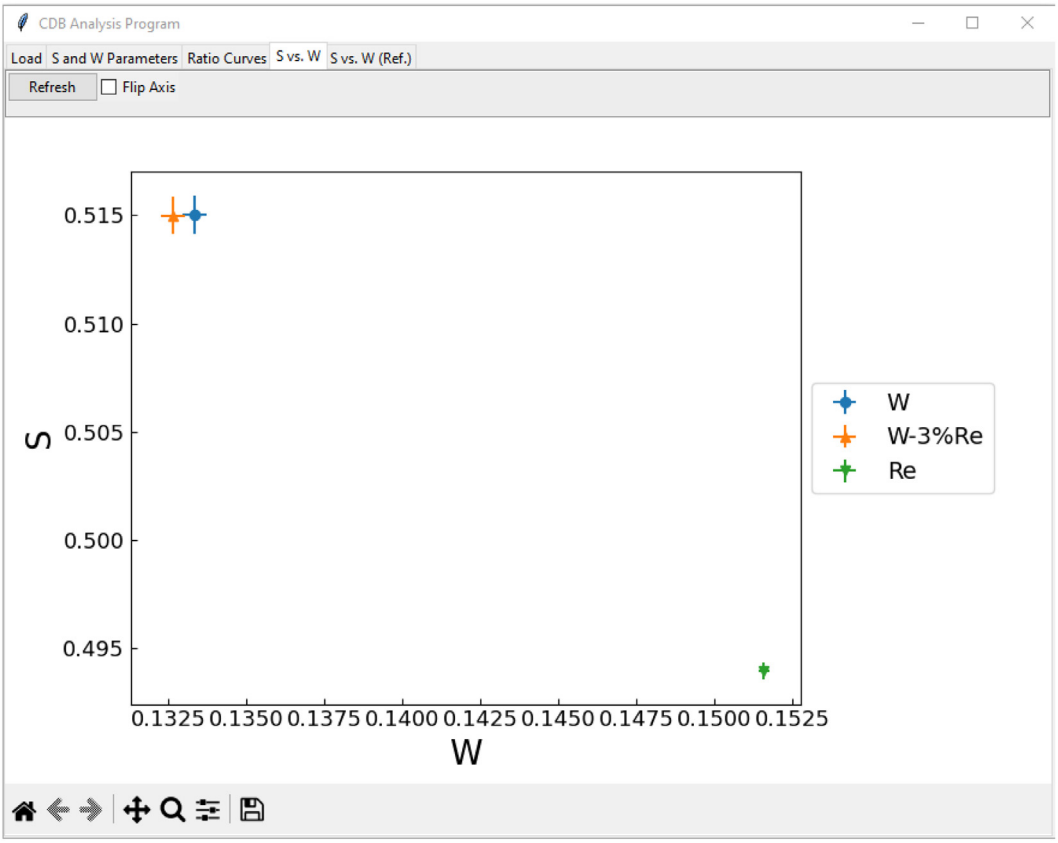

Fig. 5. The "S vs. W" tab facilitates visualizing and obtaining the relative defect concentrations of the loaded datasets and the correlation between the S and W parameters of those datasets. On display are the S and W parameters obtained using the settings and datasets displayed in Fig. 3.

2.5. Software functionalities: The "S vs. W" tab

Using the "S vs. W" tab requires the "S and W Parameters" tab to have been previously loaded. The "S vs. W" tab displays the S and W parameters of all loaded datasets using what is called an *S*–*W* plot (see Fig. 5). *S*–*W* correlation plots can be used to compare relative defect concentration and analyze the nature of positron-trapping defects [7,17]. Note that the calculated S and W parameters are affected by the smoothing and shifting of count vs. energy curves that occurs on the "S and W parameters" tab. Error bars are included and are generated using standard error analysis by assuming the uncertainty in counts to be the square root of the counts then propagating the uncertainty accordingly [18]. The *x*-axis and *y*-axis can be flipped by clicking the **Flip Axis** toggle then clicking the **Refresh** button. Hovering over data points shows a label with their coordinates and the uncertainty in those coordinates. This graph has `Matplotlib's` standard navigation toolbar. Saving "S and W" data on the "Load" tab saves the S and W parameters and their uncertainties from each dataset to a CSV file.

2.6. Software functionalities: The "S vs. W (Ref.)" tab

The "S vs. W (Ref.)" tab mimics the "S vs. W" tab except that data points are normalized to a reference dataset (see Fig. 6). The reference dataset can be chosen using the drop-down menu in this tab's bottom left corner. Labels and error bars are included and are identical to the error bars displayed on the "S vs. W" tab (although they may appear different due to scaling). Saving "S and W with Reference" data on the "Load" tab saves the S and W parameters and their uncertainties from each dataset to a CSV file after normalizing them to the reference dataset.

3. Impact

CDB-AP greatly enhances productivity by reducing hours of data analysis time to minutes while reducing human error and using transparent processes. It does this by performing full data reduction and analysis in a single application, facilitating rapid comparison of results, and producing a file that includes full traceability of processing steps taken during the data's reduction and analysis. Three laboratories at INL already use CDB-AP, and CDB-AP is applicable to many laboratories and universities outside of INL. In addition, CDB-AP being open source makes it easily accessible to institutions worldwide.

A recent study used CDB-AP to analyze a large number of neutron irradiated tungsten samples [7]. The data included spectra from seventeen sample pairs. Results of the *S*–*W* plot and multiple ratio curves produced by CDB-AP were included in the publication. Being able to dynamically analyze and adjust parameters on all datasets simultaneously was enabled by CDB-AP. The resulting conclusions provided insights that may have not been otherwise found due the laborious nature of traditional manual analysis.

4. Conclusions

CDB-AP was developed to facilitate rapid and dynamic analysis of large quantities of CDB data. It does so while offering transparency and control throughout the data reduction and analysis. CDB-AP has already been tested and used in a research publication [7]. Overall, CDB-AP, as a free, open-source application, can be used in laboratories worldwide to optimize their CDB data analysis process.

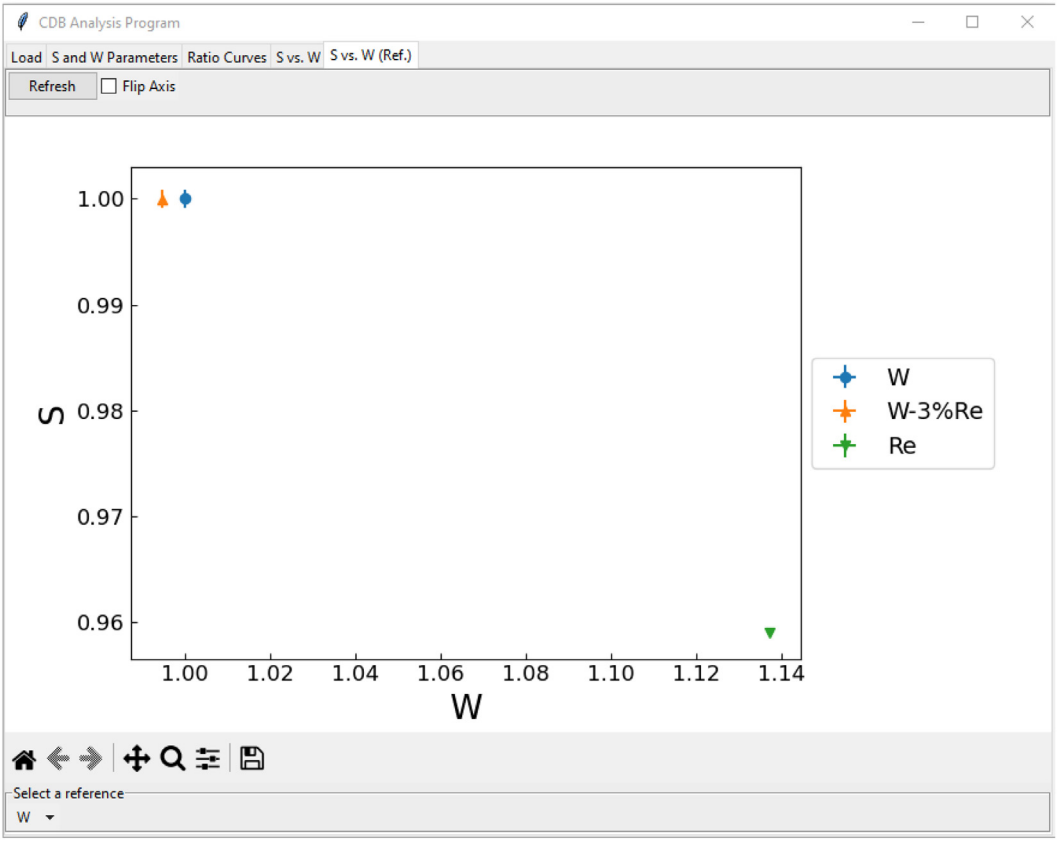

Fig. 6. The "S vs. W (Ref.)" tab facilitates visualizing and obtaining the relative defect concentrations of the loaded datasets and the correlation between the S and W parameters of those datasets. On display are the S and W parameters obtained using the settings and datasets displayed in Fig. 3 after the S and W parameters were normalized to the tungsten sample.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgments

We acknowledge the INL Laboratory Directed Research and Development (LDRD) program that sponsored this research under award 21A1050-054FP. This work was performed by Battelle Energy Alliance, LLC, for the United States Department of Energy under contract DE-AC07-05ID14517.

Appendix A. Hardware, software, and data file format

This appendix describes the hardware and software used to produce data files and the produced data files. Appendix A.1 describes the FAST ComTec hardware and software used in the production of CDB-AP and the MPA data files the hardware/software produce. Appendix A.2 describes the TechnoAP hardware and software used in production of CDB-AP and the CSV data files the hardware/software produce. In each experimental setup, high purity germanium detectors were arranged in standard positions for CDB.

A.1. FAST ComTec hardware, software, and MPA data files

For experimental setup, one laboratory at INL uses FAST ComTec's MPA4, 8 Channel Multiparameter Data Acquisition System [14]. FAST ComTec also provided the MPANT software with the system.

The MPA data files begin with an ASCII header containing the system's settings and information required for obtaining the energy calibration of each detector, followed by the spectrum of the first detector and the spectrum of the second detector, each spectrum preceded by a header. Finally, there is a dual parameter spectrum, with length equal to the lengths of the first two spectra multiplied together. In the tests for CDB-AP, the individual spectra were 8192 rows long, meaning the dual parameter spectrum was 67,108,864 rows long. This leads to MPA files that were hundreds of megabytes. The process of obtaining the energy calibration and reading data from these data files is carefully tuned to the format of this header.

A.2. TechnoAP hardware, software, and CSV data files

For an experimental setup, two laboratories at INL use a measurement system composed of the following hardware from TechnoAP [15]:

- Model APV8002 Digital Signal Processor for gamma ray spectrum measurement,
- Model APV3304 High voltage power supply,
- Model APV4004 Pre-amp power supply.

TechnoAP also supplied an application, "Positron Annihilation", to facilitate use of their hardware.

Using the above experimental setup and software, CSV data files produced from CDB measurements are organized into two sections as follows: The first section is "[Header]". It contains information such as the duration of the experiment, total counts measured, and the range of channels within which data was recorded. The second section is "[Data]". CDB-AP ignores all rows up to and including the row containing the title "[Data]". The next row of the CSV data file is made up of three cells containing the text "CH1(ch)", "CH2(ch)", and "Counts", respectively. The text in these cells is used as the column names in data processing. The first column describes which channel in detector 1's data is being referenced, the second column describes which channel in detector 2's data is being referenced, and the third column describes how many counts were found at those coordinates. If no counts were found at a given set of coordinates, those coordinates are not recorded in the CSV data file.

Appendix B. Additional notes on CDB-AP use

- Note that CDB-AP may malfunction if the user attempts to save analyzed data before loading all five tabs. Furthermore, the user must refresh the graphs after making any changes in the data analysis (such as smoothing or folding the data, as described in Sections 2.3–2.4) before saving any analyzed data. Otherwise, the changes may not be saved.
- To remove a label on the "S vs. W" and "S vs. W (Ref.)" tabs, right click the label.
- At the time of publication, the reference line must not be hidden when saving "Ratio Curves" data.
- When saving files, the user must change or removing the asterisk that appears by default in the names before saving the file.
- The **Use Limits from Plot** button only registers position data to five decimal places, so the graph may move upon refresh after using this feature.

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