Measuring and Modeling Concentrations of Defects in Metallic Samples Using Positron Annihilation Spectroscopy

by

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DEPARTMENT APPROVAL

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Positron Annihilation Spectroscopy is a non-invasive way to obtain defect concentration values in a given sample. Positron Annihilation Spectroscopy is based off of the Doppler broadening of the gamma ray spectrum created from the positron-electron annihilation. The low momentum portion section of the 511 keV curve produced can be represented by the $S$ parameter. This $S$ parameter is a linear combination of the $S$ parameter in bulk, $S_b$, and the $S$ parameter in a defect rich layer, $S_v$. Different copper samples were polished to introduce a layer of defects. $S_b$ is found to be constant for a given element, for copper $S_b = 0.509347$, and $S_v = 0.50666$. Using a well-known equation defect concentrations, $C_v$, can be measured with a given $S$ parameter. This method introduces errors due to the extrapolation of $S_v$. A different method can give better concentration values using the $b$ value, the percent positrons annihilated in a defect, of a sample. For example, a copper sample polished down to 32 μm gives a $b$ value of 0.4836 and a $C_v$ of $2.75 \times 10^{-6}$. 
To my parents, Andrew, Austin, Natalie, and Sarena
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I would like to thank the Physics Department at Brigham Young University – Idaho for the chance to work in their lab. I would like to thank all of my friends and family for their support through my years of studying what I love to do. I would especially like to thank Dr. Evan Hansen for his support and his excitement for physics. It was him who made this research so much fun and self-rewarding. Thank you for all of your time and your love for physics.
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Chapter 1

Background

1.1 Introduction

Positrons aren’t just a convenient theoretical “thing” that makes quantum mechanics work, but can be used in order to find defects in materials. The study of crystalline structures has been around for years. The crystalline structure of a sample is almost never perfect. In a given sample there are several types of defects in that sample. One type of particular interest is that of point defects: there is supposed to be an atom there but there is not. For years the scientific community has tried to come up with various ways of trying to figure out just how many point defects occupy a given sample. One example is trying to figure out the characteristics of X ray diffraction off of a defect compared to that of what should be noticed in a defect free sample [1]. Others have tried to look at the entropy of a point defect [2] and from their work the number of point defects could be extrapolated. Positron Annihilation Spectroscopy (PAS) is a non-invasive and a very useful way to find these point defects in a given sample. Exposing a sample to positrons will allow positrons to find defects in a sample and annihilate with electrons in that defect. An energy spectrum is created from the gamma rays which contains what is known as the 511 keV peak. Important details of this gamma ray spectrum can be extrapolated as the S parameter and W parameter.

In 1928, Paul Dirac found that there was a “duplexity” phenomenon in the theory of quantum mechanics when applied to a point charge in an atomic structure [3]. The result from this phenomenon was the proposal of the positron, the anti-matter counterpart of the electron.
This positive electron was then discovered in 1933 by Carl D. Anderson. Dr. Anderson was using a vertical cloud chamber, and while trying to observe cosmic rays he noticed that some particles were going in the positive direction when deflected in the magnetic field, but not with the mass of a proton [4]. From this result Dr. Anderson had discovered an anti-matter particle that is related to the electron; he then coined the term positron for this anti-matter counterpart.

Since the discovery of the positron, there has been an exponential growth on the research of this particle [5]. The scientific community has found out just how important this particle is, not just in the quantum mechanical model, but as well as the practical implications of positrons. Positrons have been used anywhere from the study of animals, from glucose metabolism to gene expression [6], and also to the study of crystalline structures. The study of crystalline structures comes from the unique interaction between the positron and electron, which can be shown by the Feynman diagram (figure 1.1); this interaction is known as positron-electron annihilation. This annihilation produces two gamma rays which can be picked up by detectors, and using PAS one can find out many different features about the structure of the sample in question, including how many defects are in a sample.

![Feynman diagram of electron-positron Annihilation](image)

**Figure 1.1** Feynman diagram of electron-positron Annihilation
1.2 511 keV curve

When positrons annihilate and the gamma rays are captured by detectors a 511keV peak is formed and from this peak we can obtain the concentration of defects in a given sample. To understand this so called 511keV peak the annihilation process has to be understood. First, why is it a 511keV peak and not some other energy? Well, if we look at Einstein’s equation from his theory of special relativity and solve it using the mass of a positron or an electron we see that:

\[ E = mc^2 = (9.109 \times 10^{-31} \text{ kg} ) \left( 2.99 \times 10^8 \text{ m/s} \right)^2 = 8.14 \times 10^{-14} J \approx 511 \text{ keV} \quad \text{Eq. 1} \]

Now that the energy is known, when the gamma rays are captured by a detector, the shape of the 511keV peak should be a sharp peak at that specific energy. This shape, as we will see later, is not quite right. The shape of the peak is actually rounded and resembles somewhat of a Gaussian distribution. This is because when an electron and positron annihilate they don’t give exactly 511keV, but some deviation from that value depending on the momentum of the electron that the positron annihilates with and the direction of the gamma rays produced. If the positron-electron annihilation produces two gamma rays 90° from the path of collision the two gamma rays produced will be very close to the expected 511 keV energy (there will be a small deviation of energy due to the small angle difference from the 180° expected from the annihilation) (figure 1.2a). However, if the positron-electron annihilation produces two gamma rays that are expelled in the same direction of collision, or close to it, there will be a large energy difference between the two (figure 1.2b). This conservation of momentum ends up broadening or narrowing the 511 keV peak depending on the path of gamma rays produced compared to the path of collision of the electron and positron—a phenomenon known as Doppler Broadening. It is from this Doppler Broadening that PAS is based off of to study the solid.
Figure 1.2 Doppler shift of electrons depending on path

(a) If the positron-electron annihilation produces two \( \gamma \) rays roughly 90° from the path of collision we will get roughly 511 keV for each gamma ray. (b) If the positron-electron annihilation produces two \( \gamma \) rays that are in the direction of the path from the electron and positron there will be a difference in energies. In both cases the momentum of the electron is greater than the positron.

Depending on the sample and how many defects are contained within it there will be a different shape to the 511keV peak. This is due to the difference of momentum explained in the previous paragraph. When there is a point defect there is a missing atom, which becomes replaced with a potential well from the valence electrons that are in the surrounding atoms. These valence electrons have a lower momentum then the core electrons. If you think of the orbit of an electron as that of the Bohr model, this is a simple thing to show. Think of the centripetal force of an electron in circular motion and the Coulomb force:

\[
\frac{m v^2}{r} = k \frac{e^2}{r^2}. \tag{2} 
\]

After doing some simple algebra it can be shown that,

\[
P = \sqrt{k e^2 m \frac{1}{r}}. \tag{3} 
\]
Since \( P \propto 1/\sqrt{r} \), the further out you are from the nucleus the lower your momentum is. This is why valence electrons have lower momentum than the core electrons of the atom. So, when a positron enters a defect it will annihilate with a low momentum valence electron and give off \( \sim 511 \) keV gamma rays. If the annihilation that occurs is with a core electron the positron annihilates with a high momentum electron. When data is collected, if a sample has no defects, then the 511keV peak will have mainly high momentum data. If a sample has several defects, then the 511keV peak will have more low momentum data. Depending on how much of this low/high momentum annihilations occur it will change the shape of the peak. As mentioned before the 511keV peak is roughly a Gaussian distribution. The peak of this distribution has to do with the low momentum annihilations while the outer regions of the peak have to do with the high momentum annihilations. This means that when we have only high momentum annihilations (no defects) the peak will be shallower and the curve broader. When the annihilations have a lot of low momentum annihilations (annihilations with defects) the peak will be taller and narrower.

Knowing these facts about Doppler Broadening, PAS is simpler to understand by extracting certain parameters from the areas of interest. PAS takes this 511 keV peak and quantifies it by describing it using the S parameter, or the sharpness of the peak, and the W parameter, or wing parameter (figure 1.3). These parameters are found by taking the area under the region of interest from the 511 keV peak and dividing it by the total area of the peak.

\[
S_{\text{parameter}} = \frac{S_{\text{region}}}{\tau} \quad \text{Eq. 4}
\]

The W parameter, or Wing parameter, takes the area under a portion of the outer ends of the peak, or wings of the peak, and divides those by the total area under the peak.
Because the W parameter has to do with the high momentum someone can do a ratio curve analysis and can actually find out if there are different atoms in a sample. Since the S parameter has to deal with the low momentum part of the peak, the S parameter can extrapolate data about the defects in a given sample and give us the concentration of defects.

\[
W_{\text{parameter}} = \frac{W_1 + W_2}{T} \tag{Eq. 5}
\]

The peak is split up into the separate regions. The \( S_{\text{region}} \) is the area under the central part of the peak, \( W_1 \) and \( W_2 \) are areas under the left and right wing, respectively, and \( T \) is the total area. The S parameter is given by the \( S_{\text{region}} \) divided by \( T \) and the W parameter is given by the sum of \( W_1 \) and \( W_2 \) divided by the total area, \( T \).

**Figure 1.3** Diagram of 511 keV peak
Chapter 2

Methods

2.1 Linear Relationship of \( S \) Parameter

Because the \( S \) parameter comes from the low momentum annihilations, the \( S \) parameter can be used in order to find the concentration of defects in a given sample. Before obtaining concentrations, the \( S \) parameter has to be better known. It is being researched, and shown by others [7,8], that the total \( S \) parameter of a sample is actually given by a linear combination of the \( S \) parameter of a defect free sample and a defect rich sample:

\[
S = aS_b + bS_v, \quad \text{Eq. 6}
\]

Where \( S_b \) is the \( S \) parameter for the bulk material, \( S_v \) is the \( S \) parameter for the defect material, and \( a \) and \( b \) are constants and are defined by \( a + b = 1 \) (figure 2.1). This means that \( a \), and in return \( b \), are the percentages of the \( S \) parameter of a defect free sample and a defect rich sample, respectively, and the equation can be re-written as,

\[
S = (1 - b)S_b + bS_v. \quad \text{Eq. 7}
\]

To test this experiment where defects were introduced, by polishing, was performed (for more details see experiment section). The results can express the \( S \) parameter of a given sample as a linear combination of the \( S \) parameter in the bulk and the \( S \) parameter in a defect. Through this same experiment we can see that \( S_b \) is constant for any sample made up of the same element, in this case copper. With this, we can also assume that the defect \( S \) parameter, \( S_v \), is also constant for any given sample of the same element.
The total S parameter of the above sample is made up of some percentage, \( b \), of \( S_v \) and some percentage, \( a \), of \( S_b \), where \( a + b = 1 \).

### 2.2 Equations for Concentration

A well-known equation gives the concentration of defects due to these three S parameters. Lynn’s equation is given by

\[
C_v = \frac{\lambda_b S - S_b}{\mu S_v - S}, \tag{Eq. 8}
\]

where \( \lambda_b \) is the inverse of the positron lifetime in a defect free sample, and \( \mu \) is the specific trapping rate. These two rates are found using Positron Annihilation Lifetime Spectroscopy (PALS). If we solve Eq. 7 for \( b \) we see that

\[
b = \frac{S - S_b}{S_v - S_b}, \tag{Eq. 9}
\]

It would be deceptive, and wrong, to assume that if we throw in a multiplication of \( \lambda_b/\mu \) in front of Eq. 9 we would get Eq. 8 and say that \( b \) is actually \( C_v \). There is a very slight difference in these two equations, excluding the \( \lambda_b/\mu \). In Eq. 9 the denominator is \( S_v - S_b \) while the
denominator in Eq. 8 is $S_v - S$. Because of this I went a different route and solved Eq. 8 for $S$ in terms of $S_b$ and $S_v$:

$$S = \frac{\lambda_b}{\lambda_b + C_v \mu} S_b + \frac{C_v \mu}{\lambda_b + C_v \mu} S_v. \quad \text{Eq. 10}$$

The above equation gives us a linear combination of the S parameters with their weights being a ratio of the rates. The term in front of $S_b$ is a ratio of the rate of a positron in the bulk divided by the total rate, and the term in front of $S_v$ is the ratio of the rate of a positron in the defect divided by the total rate. The fact that this is a linear combination of $S_b$ and $S_v$ Eq. 10 resembles Eq. 7. Since we are interested with what percentage of $S_v$ there is we can set the two terms, from the two equations, in front of $S_v$ equal to each other. Doing this we get Eq. 11.

$$C_v = \frac{\lambda_b}{\mu} \frac{b}{1 - b}. \quad \text{Eq. 11}$$

Now $C_v$ can be found from the $b$-value instead of the S parameter.
Chapter 3

Experiment

3.1 Experimental Setup

The S parameter can be obtained by using a gamma ray detector, a positron source, some sort of gamma acquisition software for the detector, and then, by some means, obtaining the S parameter by using Eq. 4. The positron source that I used for this experiment was a $^{22}\text{Na}$ source. This source has a decay of, $^{22}\text{Na} \rightarrow ^{22}\text{Ne}^{*} + e^+ + \nu$, and then the Neon in the excited state comes down by releasing a $\gamma$ ray with an energy of 1.27 MeV. The fact that a $\gamma$ ray with a specific energy is very useful when using PALS. PALS will find the time between the 1.27 MeV and the 511 keV; when these times are measured you can find the lifetime of a positron in a given sample. Other samples can be used, such as $^{68}\text{Ge}$, but the $^{22}\text{Na}$ source is readily available because of how cheap it is, and its lifetime is much longer than that of the $^{68}\text{Ge}$ source.

In the experiment I had 10 copper pieces that would be paired to become a single sample. In order to sandwich the positron source between the two copper pieces (see figure 3.1). Each size of the copper pieces is 0.208cm $\times$ 0.952cm $\times$ 1.4cm. All of the samples were annealed at 500°C in the presence of argon gas. 500°C is not necessarily the ideal temperature because we can see that if we anneal at 700°C a lower S parameter can be reached, meaning less defects [9]. In this experiment we made the assumption that 500°C is close enough to say that annealing at this temperature will rid all defects in the copper samples. After every sample was annealed, the S parameter was measured and, as seen in figure 3.2, it is very close to a single value. The small
deviations could come from the fact that the temperature used to anneal the samples was not high enough. Because of this consistency in the S parameter we can easily assume that the S parameter for a fully annealed copper sample is the same for any copper sample.

In order to collect the gamma rays that were coming from the annihilation sites a high purity Germanium (HpGe) detector was used as well as an Osprey NaI scintillation detector that was set up collinearly with the HpGe detector. The detectors were hooked up to a Lynx Digital Signal Analyzer which was then connected to the computer. Gamma acquisition software, Genie 2000, was used in order to analyze and display the gamma radiation that was detected. The two detectors were set up collinearly so that coincidence could be used. Coincidence mode only allows data to be collected when two gamma rays reach both of the detectors within a certain time window allowing background gamma rays to be filtered out. Essentially, the NaI detector is a gate that allows, when a γ ray enters it, gamma rays to enter the hpGe detector and be collected in Genie, for a certain amount of time. After data was collected for each sample the S parameter has to be extracted somehow. Positron Annihilation Spectroscopy Data Analysis (PASDA) software allows a user to input a file from a collection of different gamma acquisition software, in my case Genie 2000, and input the data.

![Figure 3.1](image_url) 

**Figure 3.1** A $^{22}Na$ source (black) sandwiched between two copper plates (grey).
Defects were introduced at different levels for each sample through polishing. Four samples received a polish with four different grit sizes: 120 grit, 400 grit, 800 grit, 2674 grit. A grit size conversion table was used in order to figure out how deep defects would be introduced. The different depths, for each grit, are 212 \( \mu m \), 64 \( \mu m \), 32 \( \mu m \), and 9.5 \( \mu m \), respectively. The fifth sample was left alone at the annealed stage which corresponds to a 0 \( \mu m \) depth of defects introduced. Depending on the depth of the introduced defects, only so many positrons will stay in the defects while the other percentage continues on to penetrate further into the bulk material. These percentages can be found using a formula for stopping profiles:

\[
\begin{align*}
S_{\text{parameter}} &= 0.505 \quad \text{for} \quad 0 \mu m \\
S_{\text{parameter}} &= 0.51 \quad \text{for} \quad 1 \mu m \\
S_{\text{parameter}} &= 0.515 \quad \text{for} \quad 2 \mu m \\
S_{\text{parameter}} &= 0.52 \quad \text{for} \quad 3 \mu m \\
S_{\text{parameter}} &= 0.525 \quad \text{for} \quad 4 \mu m \\
S_{\text{parameter}} &= 0.53 \quad \text{for} \quad 5 \mu m \\
S_{\text{parameter}} &= 0.535 \quad \text{for} \quad 6 \mu m \\
S_{\text{parameter}} &= 0.54 \quad \text{for} \quad 7 \mu m 
\end{align*}
\]

![Figure 3.2 S parameters of each sample after the annealing process.](image)

**Figure 3.2** S parameters of each sample after the annealing process.
\[ P(x) = \alpha e^{-\alpha x}, \]
\[ \text{Eq. 12} \]

where \( \alpha \) is the positron linear absorption coefficient, given by
\[ \alpha = \frac{2.8 \cdot \rho \cdot Z^{0.15}}{E_{\text{avg}}^{1.19}}, \]
\[ \text{Eq. 13} \]

where \( \rho \) is the density of the material, \( E_{\text{avg}} \) is the average energy of the positron emitted by the \(^{22}\text{Na}\) source, and \( Z \) is the atomic number of the element [10]. The density of copper is 8.96 g/cm\(^3\), the average energy of the positron emitted by the source is \( \sim 0.26 \) MeV [10], and the atomic number is 29. Using these values and plugging them into Eq. 13 we get \( \alpha = 206.54 \) [cm]\(^{-1}\). When using this linear absorption coefficient, \( \alpha \), we get a probability curve like that of figure 3.3.

Knowing this probability curve will allow us to know what percentage of positrons that will get down to certain depths. For this experiment we are interested in not necessarily knowing what percentage of positrons that go down to that depth, but the positrons that are left behind. When looking at the positron profile curve (figure 3.3) the five red vertical lines show each of the polished depths. When we introduce the defects through polishing, the defects only go down to a certain depth while the rest of the sample is left defect free, and since a certain percentage of positrons reach that depth there is a specific percent that is left behind (i.e. 100\% minus the percent reaching that depth). Since the defects are within this region, we want the percentage of the ones left behind because this is the percent of positrons that are in the defects (figure 3.4).
Figure 3.3 Probability curve produced from Eq. 12 and Eq. 13.

The five red vertical lines are the defect depths from polishing (x axis) to the probability curve, thus getting percent positrons at that depth (y axis).

Figure 3.4 Positrons penetrating to a depth $z$ with probability $P(z)$

Since some percentage of positrons, $P(z)$, reach a depth of $z$ there are $100\% - P(z)$ left behind in the defect rich area. For example: if a sample was polished down to a depth $z$, where 25% of the positrons
Chapter 4

Results

4.1 Simulating Linear Combination of S

Using Eq. 12 and Eq. 13 with each of the depths that were polished we get a percentage of positrons that reach this depth and a percent of positrons that are left behind in the defects (table 1 columns 2 and 3). After collecting the coincidence data, the data was read into PASDA in order to take off some background and compute the S parameter for each of the samples (table 1 column 4). Knowing the percent of positrons in defects, from the stopping profile the b-value can be plotted with respect to its S parameter figure 4.1. The result is linear, just as it was predicted! Since the theoretical model works out, I created a computational model to see if a similar result will come about. The computational model reads in the PASDA report file and will fit up to six convolved Gaussian’s; the fit with the lowest reduced chi-square value is chosen. This is done for both the annealed sample and the sample with the most defects (figure 4.2). I then used a form of Eq. 7, where instead of the S parameters I used a sum of the two functions, the annealed and defect rich functions, to create a “total function”:

\[ f(x) = (1 - b)A(x) + b D(x) \]  \hspace{1cm} \text{Eq. 14}

At each iteration, the S parameter was calculated for \( f(x) \). When the S parameter for \( f(x) \) was plotted versus the b-value it turns out that it too is linear (figure 4.3). This seems obvious at first, because we set up the equation to be linear, but when you add two Gaussian functions together you do not get a Gaussian; the fact that we still get a line confirms the theory and matches empirical data.
<table>
<thead>
<tr>
<th>Polished depth (μm)</th>
<th>% positrons to depth</th>
<th>% positrons in defects</th>
<th>S-parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>100.00%</td>
<td>0.00%</td>
<td>0.509347</td>
</tr>
<tr>
<td>9.5</td>
<td>82.18%</td>
<td>17.82%</td>
<td>0.512238</td>
</tr>
<tr>
<td>32</td>
<td>51.64%</td>
<td>48.36%</td>
<td>0.522286</td>
</tr>
<tr>
<td>64</td>
<td>26.66%</td>
<td>73.34%</td>
<td>0.524651</td>
</tr>
<tr>
<td>212</td>
<td>1.25%</td>
<td>98.75%</td>
<td>0.530399</td>
</tr>
</tbody>
</table>

Table 1  b values and S parameters for copper samples

Figure 4.1 Plot of the S parameters with respect to the percent of positrons in the defects.
Figure 4.2 Annealed (a) and non-annealed (b) data with fitted convolved Gaussians
(a) The 511 keV peak (black diamonds) for the annealed sample with a double Gaussian fit (yellow line). (b) The 511 keV peak (black diamonds) for the defect rich sample (the sample polished down to 212 μm) fit with a sextuplet Gaussian fit (black line).
4.2 Concentration Values

Since the total S parameter is shown to be a linear combination of the S parameter of the bulk material and the S parameter for the defect part of the material I can continue to find the concentration of defects. There has been a ratio that I have left out that is in Eq. 8 and Eq. 11, the ratio between $\lambda_b$ and $\mu$. Since $\lambda_b$ is the inverse lifetime of a positron in a given sample it can be found using PALS. The value that is used in my calculations is $\tau_b \approx 100$ ps, so $\lambda_b \approx 0.01\, ps^{-1}$ [11]. The value for the specific trapping rate for copper, $\mu$, is found using empirical data. This value is found to be $\mu = (4.25 \times 0.8) \times 10^{14}\, sec^{-1}$ [12]. Using the ratio of these two numbers I can now calculate the defect concentrations of my copper samples. To have a control value for the concentration of defects, I first calculated the concentrations using an equation that is widely used, Eq. 8. Now that we know what we should expect for concentrations, with the parameters obtained, the b-value equation (Eq. 11) was used in order to find the concentrations of defects.
These values can be seen in table 2. The $S_v$ value used for Eq. 8 can be found by solving Eq. 9 for $S_v$ and plugging in the other values; this $S_v$ value turns out to be 0.530666. The reason for the different values is simple, we had to extrapolate $S_v$ which brings in more uncertainty into using Eq. 8, and instead of having some parameter, $S_v$, explain the concentrations, something physical, $b$, is explaining the concentrations in a sample. It can be taken even further and absolute number of defects can be given for the sample. This is easily found if you multiply the concentrations by how many atoms there are in a defect free sample using the density of the sample.

<table>
<thead>
<tr>
<th>Polished depth (µm)</th>
<th>$C_v$ using Eq. 8</th>
<th>$C_v$ using Eq. 11</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>9.5</td>
<td>4.61405E-07</td>
<td>6.37611E-07</td>
</tr>
<tr>
<td>32</td>
<td>4.54107E-06</td>
<td>2.7547E-06</td>
</tr>
<tr>
<td>64</td>
<td>7.48277E-06</td>
<td>8.08945E-06</td>
</tr>
<tr>
<td>212</td>
<td>0.000231567</td>
<td>0.000231567</td>
</tr>
</tbody>
</table>

Table 2 Concentration Values

4.3 Computer Simulation for Concentrations

Are these concentrations what we would expect to see? Looking at the two equations (Eq. 8 and Eq. 11) they are both nonlinear: Eq. 8 will diverge to infinity when $S = S_v$ and Eq. 11 diverges to infinity when $b = 1$. This can be seen by looking at $b$ in terms of percentage. If $b = 1$ that means that one hundred percent positrons were captured in a defect, which is highly improbable. The majority will be captured by a defect and stay there to annihilate (because of quantum mechanics there is still a non-negligible probability that the positron will annihilate with a core electron outside a vacancy). This non-linear relationship can be seen by plotting the $S$
parameter (which is related to the concentration of defects) versus the depth of defects introduced through polishing (see figure 4.4).

![Figure 4.4 S parameter with respect to the polishing depth.](image)

Since defect depth has to do with amount of defects, the polished depth is proportional to $C_v$, so here we can conclude that the relationship between the S parameter and $C_v$ is non-linear.

To verify this non-linear relationship a simplified computer model was created in order to see if I would get this non-linear relationship between $b$ and $C_v$. I created a stochastic simulation to model a positron diffusing in a sample. Before going into the simulation there were several assumptions that were made that need mention before going forward.

1. Thermalization has already occurred, allowing the simulation to only depict the diffusion of the positron through the sample.

2. This simulated copper sample is a simple cubic (sc) crystalline structure, not a faced centered cubic (fcc) lattice.
3. One positron is in the lattice at one time, and another one won’t enter until the previous one annihilates.

4. The positron has no preference towards a defect or an atom.

5. The total simulation is a classical one. There are no quantum wave functions that have probabilities checking different places besides nearest neighbors.

6. When a positron enters into a defect it is “trapped” and annihilates there.

With the six assumptions that were made a copper sample was set up as an $11 \times 11 \times 11$ simple cubic lattice. The simulation starts by placing one defect in a random position in the simple cubic lattice and has a positron do a random walk throughout the sample until it has either annihilated or has reached its lifetime expectancy. The number of steps that the positron takes was found by taking the diffusion length of positrons in copper, $\sim 100$nm [13], and divided it by the length of atoms in copper, $3.61\,\text{Å}$. In the simulation, 100,000 positrons go through the sample, per run, and counts how many times a positron annihilates with a defect or an atom. This process is then repeated ten times and an average is taken to get a percentage of positrons annihilating with the single defect. The number of defects then increases one by one until the entire sample is filled with defects. As you can see from Figure 4.5 the shape is exactly what we would expect. To double check how well this simulation works, a function was fit to the simulated data with the equation. This fitted function is Eq. 11 solved for $b$.

$$b = \frac{C_p}{\alpha + C_p}, \quad \text{Eq. 15}$$

where $\alpha$ is a parameter corresponding to $\lambda_b/\mu$. With this fitted function we ended up with a reduced chi-square value of 52.389. This large reduced chi-square value is due to some of the assumptions (e.g. no quantum effects). The actual $\lambda_b/\mu = 2.94 \times 10^{-6}$, but the parameter in Eq.
15 is $6.99 \times 10^{-3}$. These values differ by a factor of one thousand because of the lattice size of my simulation, along with the assumptions made.

Using the fitted function we already know what the percent of positrons should be in defects from our empirical data; setting Eq. 15 equal to these values we can then solve for $C_v$. Unfortunately, the concentrations will be off by at least a factor of $10^4$. The number of lattice sites, the atoms of the sample, for the $11 \times 11 \times 11$ lattice is 1,331 atoms. If one defect is in the simulation then the defect concentration is on the order of $10^{-4}$. On the other hand, the samples used in the experiment have around $5.89 \times 10^{21}$, so if a single defect is in the sample we have a defect concentration on the order of $10^{-22}$. This is a discrepancy on the order of $10^{18}$. My simulation could never simulate so many lattice points with the equipment available, so the $C_v$ values for my simulation are not very realistic compared to even our small samples.

![Figure 4.5](image.png)

**Figure 4.5** Positron simulation results with best fit curve (Eq. 15)
Chapter 5

Conclusion

5.1 Summary

The $S$ parameter can be represented by a linear combination of the $S$ parameter of the bulk and the $S$ parameter of the defects. This linear relationship can be seen empirically and computationally which agrees with the theory. Both Eq. 8 and Eq. 11 show a non-linear relationship between the concentrations and the $S$ parameter and $b$-value. This non-linear relationship is seen in both computational models and the plot of the $S$ parameters versus the depth of defects from empirical data. This relationship of linearity and non-linearity are represented by figure 5.1. Concentration values can be obtained from Eq. 11 by a factor of $b/(1 - b)$ which is the ratio of the percent positrons that annihilate in defects and percent positrons that annihilated in the bulk material. These concentration values match up with those from Eq. 8 which is what the scientific community uses to find concentrations. The difference between Eq. 8 and Eq. 11 is that Eq. 8 deals with some mathematical parameter from the 511 keV peak where Eq. 11 uses a physical value from the experiment (yes, the $b$-value comes from the mathematical parameter, but $b$ is still something physical compared to the $S$ parameter, which is a ratio of areas of a curve).
5.2 Future Work

This experiment was done specifically with close to pure copper, an extension to different metals and finding their defects wouldn’t be much of a stretch, but if we can get all important parameters for different types of pure metals \((S_v, S_b, \lambda_b, \mu)\) then a database can be created so we can obtain the \(S\) parameter for some known metal and a concentration and absolute number of defects can be given. The biggest assumption throughout this entire experiment was that positrons only annihilate in monovacancy point defects. This assumption is of course false; there are divacancies, dislocations, and point defects with an extra atom or different type of atom. In order to figure out where positrons are annihilating and in what different types of defects they are annihilating with, PALS needs to be used: which I cannot do here because we do not have the equipment for it.

Background is can be an issue with PAS when trying to calculate very precise numbers. Coincidence is a good method to rid some of the background, but there is still a better way—true coincidence. Coincidence only matches the times that the gamma rays enter each of the collinear detectors. True coincidence will not only match the time, but the energies as well; doing this will filter out more of the background from \(\gamma\) rays produced from other sources entering from the
sample, resulting in extra gamma ray energies being added. This true coincidence, although is a
good technique, as of right now it is still out of reach for this experiment until the coding to get
this data is more efficient. Another way to obtain less background is to have two hpGe detectors
set up collinearly a significant amount of background in the peak is reduced almost to zero. Since
I do not have two hpGe detectors, a method called High Momentum Analysis (HMA), created by
Dr. Haaks, Dr. Staab, and Dr. Maier from the Helmholtz institution in Bonn, Germany [14], can
do the trick. This computational analysis only requires one hpGe detector and can obtain the
same data as two hpGe detectors set up collinearly for coincidence. The only downfall is that a
$^{68}$Ge source is needed to do this, which I do not have.

In the positron simulation the assumption was made that time, and in respect the number
of steps it took for the positron to travel, is proportional to the distance traveled ($N \propto r$). It is
well known though that it is actually $N \propto \langle r^2 \rangle$ [15]. If we used the correct proportionality we
could possibly see better $\chi^2$ values for the fitted curve and better concentration values. In the
same positron simulation, as mentioned before, the number of steps was found by taking the
diffusion length of a positron in copper and dividing it by the distance of atoms in copper, but a
second method could possibly be used. This second method would be using the simple $d = vt$
equation. This allows for step values depending on the velocity of the positron through the
lattice, which could bring more accurate values for $b$. 
Bibliography


