TEMPERATURE DEPENDENT DOPPLER BROADENING FOR POSITRON ANNIHILATION SPECTROSCOPY

by

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ABSTRACT

Positron Annihilation Spectroscopy (PAS) uses positrons to probe metals for information about material properties. This analysis is accomplished by studying the S-parameter, or energy distribution of the gamma-ray photons created from annihilation events. Using the free electron model and a wave picture for electrons and positrons, previous PAS results have been re-examined for deeper understanding of the S-parameter. Analysis of Doppler broadening using the Fermi velocity of aluminum predicts a maximum shift of 3.48 keV from expected photon energy. As the volume of a material changes with temperature, the Fermi energy shows a decrease of 1% in the maximum Doppler shift, resulting in a 0.74 % decrease to the S-parameter. Ongoing efforts to gain insight into the thermalization of positrons are presented.
Acknowledgments

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Introduction

When antimatter encounters matter, it annihilates. Annihilation is the process when the total energy of the two particles converts into electromagnetic radiation with wavelengths directly proportional to the initial energy of the two particles.

Positrons are a type of antimatter that have the similar properties to electrons, except the most notable being that the charge is positive. It is possible to study the inner atomic structures of solids through a method known as Positron Annihilation Spectroscopy (PAS). For the last four decades (Puska and Nieminen), research has been done to understand how positrons will behave in solids and to analyze the annihilation photons in order to probe beyond the surfaces of solids. Inconclusive work done to understand the thermalization process, or how positrons diffuse in a material, can be seen in appendix 1 and 2.

PAS is usually concerned with defects in a material. Information about defects is inferred from the distribution of the energies of the created photons. The rest masses of an electron and a positron are 511 keV/c². Therefore, annihilation of an electron with a positron in the center of mass frame would produce two gamma rays moving in opposite direction with each having an energy of 511 keV\(^1\). However, positron-electron annihilation in a material generally does not happen in the center of mass frame, and consequently the photon energies are not equal. When recorded, these shifts in photon energy are called the Doppler broadening (see figure 1). This broadening is the result of the initial velocity of the reacting particles. When

\[^1\text{This is important to conserve momentum for the annihilation event}\]
the net velocity has a component toward or away from the detector the lab frame observes a shift in the created photon energy. This reveals the integrity of the probed solid (see figure 2 on the following page).

![Figure 1: In the lab frame, the initial velocity of the positron and the electron creates a Doppler shift in the photon energy](faculty.sdmiramar.edu/fgarces/labmatters/instruments/aa/AAS_Instrument/AASInstruments.htm)

Measurements show that when more defects are present in a material, the energy distribution is narrower, while fewer defects result in a broader distribution (MacKenzie, Eady
and Gingerich). Keep in mind that the observed Doppler broadening is a result of many annihilation events.

![Image: Doppler broadening of gamma rays due to defects. Image from (Sprenkle)](image)

Figure 2: Doppler broadening of gamma rays due to defects. Image from (Sprenkle)

PAS experiments at Brigham Young University-Idaho use sodium-22 as a positron source in conjunction with a germanium detector and an incident detector. Past PAS experiments (Lafranceschina) have examined a wide variety of situations that range from temperature dependence (Sprenkle) to probing semiconductors (Hoiland).

One common assumption that often simplifies analysis is that positron annihilation events can be modeled through classical mechanics instead of quantum mechanics. However, this assumption leads to a loss of accuracy in the models as well as the conceptual
misunderstandings. The primary objective of this work is to construct a more accurate, quantum mechanical model for PAS.

Fermi Energy and Levels

Both positrons and electrons are fermions meaning they have half-integral spin. This is important to note because fermions obey the Pauli Exclusion Principle, which states that only one electron in a system can have a given set of quantum numbers. Electrons in a material will all try to occupy the lowest energy state; however, as only one particle can be in a given state there must be a gradient of increasing energies as new conduction electrons are introduced to the material. The energy state of the highest occupied level when temperature is at absolute zero is known as the Fermi energy (see figure 3b), and the velocity of the electron at the Fermi energy is called the Fermi velocity (Stokes, pg. 75-76). The Fermi energy is given by

$$ E_F = \left( \frac{\hbar^2}{2m} \right) \left( 3\pi^2 n \right)^{\frac{2}{3}} $$

where $n$ is the density of conduction electrons, $N/V$ (number per volume), and $m$ is the mass of an electron.
With this understanding of how conduction electrons behave, it is possible to show an additional observed Doppler broadening following an annihilation event.
Method

A shift in photon energies is shown by using the relativistic Doppler shift equation,

\[ f_{\text{observer}} = \sqrt{\frac{1 + \beta}{1 - \beta}} \cdot f_{\text{source}}, \]

where \( \beta = v/c \) (Serway, Moses and Moyer). In this case, the frequency of the source is the rest energy of the particle divided by Planck’s constant \( (m/h) \), and the observed frequency is found using the Fermi velocity\(^2\) for a valence electron in aluminum \( (2.03 \times 10^6 \text{ m/s}) \) (Ashcroft and Mermin). Multiplying the difference between the observed frequency and the source frequency by Planck’s constant produces the energy width that a detector would observe\(^3\). In this case, the difference is 3.48 keV, a difference large enough to show that, in order to understand the S-parameter the wave nature of atomic particles cannot be ignored.

This approach differs from previous methods because, rather than using a planetary model of atomic electron orbits (see figure 4), a quantum-wave model that utilizes an approach where Fermi energy electrons are exclusively preferred for annihilation.

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\(^2\) For this work, only Fermi energy level electrons are considered. Figure 3c shows that this is the highest density state. A more complete model would include the remaining states.

\(^3\) See Appendix 3 for Mathematica code
The above calculated Doppler broadening represents the maximum shifted value. This would be produced by an electron that had its momentum vector pointing directly towards or away from the detector when the annihilation event occurred, with the conservation of momentum causing one of the created photons to continue towards the detector. An electron with momentum in any other direction (see figure 5) would result in a smaller Doppler shift.
Figures 5: An electron with a momentum vector pointing in a direction other than the detector. Such electrons can be grouped according to a small difference in angle, dθ.

To calculate the adjusted Doppler broadening for electrons with any momentum vector we begin with a small range of momentum vectors that point in nearly the same direction. This generalized angle will be called θ. This is seen as a band on the surface of the sphere in figure 5. The area of this band will be $2\pi v_f^2 \sin \theta d\theta$, where $v_f$ is the Fermi velocity. This is then divided by $4\pi v_f^2$ to give,

$$\frac{\sin \theta d\theta}{2} = \frac{1}{2} \frac{\sqrt{v_f^2 - v_i^2}}{v_f},$$

which will be called here the percent angle, or the amount of photons reaching the detector per angle. Using the parallel part of the Fermi velocity,

$$v_\parallel = v_f \cos \theta,$$
leads to an adjusted relativistic Doppler shift energy. Figure 6 shows a parametric plot of the energy and the percent per angle, with the maxima corresponding to zero shift in the energy, and the x intercepts representing the maximum shift in the energy\(^4\). To find the percent of photons that have a given energy shift, integrate between the energy values in question.

The parallel component of the Fermi velocity can be expressed as

$$5) \quad v_\parallel = \frac{c \left( \frac{\hbar^2}{\hbar^2 f^2 - 1} \right)}{\left( \frac{\hbar^2}{\hbar^2 f^2 + 1} \right)}$$

which allows the percent angle to be plotted as a function of energy without using a parametric plot.

\(^4\) See Appendix 4 for Mathematic code
One final step in analyzing Doppler broadening is to convolve the percent angle by a Gaussian, because the detector used by BYU-I has a sigma value, or an uncertainty, of .6548 keV (Clark). An integration of this product spreads the endpoints of the distribution, as shown in figure 7. This figure represents the Doppler broadening in a defect-free material.

Figure 7: This plot shows how a detector would see a spectrum of positron annihilations within a material with no defects. The vertical lines indicate the S-parameter.
Temperature Dependence

In a previous work (Sprenkle) it was hypothesized that, as a material is heated, the thermal energy causes the lattice to vibrate and in time causes breaks and vacancies to form. This hypothesis was further solidified when, upon heating a sample of aluminum from 20° C to 350° C, there was a change of −1.2% in the S-parameter (see figure 8).

![Experimental aluminum lineshape](image)

To understand my temperature dependent change of the S-parameter, consider the thermal expansion of a material. The higher the temperature, the greater the volume a sample reaches (see figure 9). For aluminum the volume changes by $23.6 \frac{ppm}{°C}$, (parts per million per
degrees Celsius) (Agilent Technologies). Recall also that the Fermi energy is volume dependent, with the Fermi energy decreasing as the volume increases. Through a series of calculations, it can be shown that there is a 0.5% change in the Fermi energy from the volume increase for aluminum between 20 °C to 350 °C.

![Image of volume increase](image)

*Figure 9: Increasing the temperature of a material increases its volume but the number of electrons remains constant*

This temperature dependent change in the Fermi energy leads to an adjustment of the relativistic Doppler broadening. Originally 3.48 keV, the Doppler broadening decreases by 26.5 eV to 3.45 keV.  

By solving for the percent angle of a heated material, similar to what was explained above, it is possible to model a new energy distribution that results in a different S-parameter. Dividing this new, high temperature material S-parameter by the original S-parameter, shows a -0.74% change in the parameter.

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5 See Appendix 5 for Mathematica code  
6 See Appendix 6 for Mathematica code  
7 See Appendix 7 for Mathematica code
It was previously suggested that a -1.2% change to the S-parameter came from internal breaks to the lattice from thermal vibrations (Sprenkle). This present work indicates that roughly 60% of that change can be accounted for as relativistic Doppler broadening, leaving about 40% from thermal vibrations.

Conclusion

We have made progress in developing a quantum model of PAS. The concepts of Fermi energy and velocity lead to a deeper understanding of the Doppler broadening, which in turn, lead to an understanding of the temperature dependence of PAS. This expanded understanding could prove useful to future investigators as they further delve into other ways that PAS is affected by quantum mechanics.
Appendix 1

In an effort to further develop a quantum mechanical model for PAS, we simulate the thermalization of a positron as it interacts with an aluminum lattice. Thermalization is the physical interactions a particle undergoes to reach thermal equilibrium within the material in which it is implanted.

We developed a Matlab code to model how a positron, represented as a wave, would move, change in energy, reach an equilibrium state, and annihilate. Ultimately, the code provides information about the energy and position of a positron at the point of annihilation.

A one-dimensional lattice of 619 aluminum atoms, extends approximately 2500 Å, was selected as the probed material. The lattice makes a square finite potential well for the positron. This size corresponds to the penetration depth for near-certain annihilation of 3.1 keV positrons (Valkealahti and Nieminen). The potential boundaries that confine the positron are abrupt and the height is 4.08 eV, which is the work function, of aluminum in vacuum. To model the lattice itself, we estimated an atomic diameter of .44 Å, with a 1.8 Å spacing. The potential wells representing the atoms have a depth of $1.602 \times 10^{-19}$ C and the space between atoms have a potential of 0 eV. This creates a periodic lattice of finite square wells\(^8\) (see figure 10).

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\(^8\) See appendix 2 for the Matlab code in its entirety
Figure 10: A model of the Coulomb force from an aluminum lattice. The peaks correspond to atom location.

Next, the positron was modeled as a Gaussian wave packet, using a finite differential time development method (Cooper), and implementing the time dependent Schrödinger equation. To do this, we begin with the time dependent Schrödinger equation:

\[ 6) \quad i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + U(x,t)\psi(x,t) \]

Noting that \( \psi \) has real and imaginary parts, \( \psi_R \) and \( \psi_I \):

\[ 7) \quad \psi(x, t) = \psi_R(x, t) + i\psi_I(x, t) \]

\[ 8) \quad \psi^*(x, t) = \psi_R(x, t) - i\psi_I(x, t) \]
Making these substitutions, we can divide the Schrödinger equation into real and imaginary parts:

\[
9) \frac{\partial \psi_R(x,t)}{\partial t} = -\frac{\hbar}{2m} \frac{\partial^2 \psi_I(x,t)}{\partial x^2} + \frac{1}{\hbar} U(x,t) \psi_I(x,t)
\]

\[
10) \frac{\partial \psi_I(x,t)}{\partial t} = \frac{\hbar}{2m} \frac{\partial^2 \psi_R(x,t)}{\partial x^2} - \frac{1}{\hbar} U(x,t) \psi_R(x,t)
\]

We then use a finite differential approximation for the derivations.

\[
11) \frac{\partial \psi(x,t)}{\partial t} = \frac{\partial (\psi(x,t+\Delta t) - \psi(x,t))}{\Delta t}
\]

\[
12) \frac{\partial^2 \psi(x,t)}{\partial x^2} = \frac{\psi(x+\Delta x,t) - 2\psi(x,t) + \psi(x-\Delta x,t)}{\Delta x^2}
\]

The resulting real and imaginary Schrödinger equation then read

\[
13) \psi_R(x,t) = \psi_R(x,t) - C1(\psi_I(x+1,t+1) - 2\psi_I(x,t) + \psi_I(x-1,t-1)) + C2(U(x,t)\psi_I(x,t))
\]

\[
14) \psi_I(x,t) = \psi_I(x,t) + C1(\psi_R(x+1,t+1) - 2\psi_R(x,t) + \psi_R(x-1,t-1)) - C2(U(x,t)\psi_R(x,t))
\]

where

\[
15) C1 = \frac{\Delta t \hbar}{2m \Delta x^2}
\]

and

\[
16) C2 = \frac{\Delta t}{\hbar}
\]

The initial Gaussian wave packet is expressed as
17) \( \psi_R = \exp\left(-0.5 \left(\frac{x-x_c}{s}\right)^2\right) \cos\left(\frac{2\pi(x-x_c)}{\lambda}\right) \)

18) \( \psi_I = \exp\left(-0.5 \left(\frac{x-x_c}{s}\right)^2\right) \sin\left(\frac{2\pi(x-x_c)}{\lambda}\right) \)

where \( \lambda \) the wavelength, \( s \) is the envelope width, and \( x_c \) is the center of the wave packet.

Normalization requires:

19) \( \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = \int_{0}^{L} (\psi_R^2 + \psi_I^2)dx = 1. \)

The kinetic energy operators are expressed as

20) \( \hat{T} = -\frac{\hbar^2}{2m} \nabla^2 \)

21) \( \langle \hat{T} \rangle = \int_{-\infty}^{\infty} \psi^*\hat{T}\psi dx = C3 \int_{-\infty}^{\infty} (\psi_R(x) - i\psi_I(x))(\psi_R(x+1) - 2\psi_R(x) + \psi_R(x-1) + i[\psi_I(x+1) - 2\psi_I(x) + \psi_I(x-1)])dx \)

where

22) \( C3 = -\frac{\hbar^2}{2m\Delta x^2} \).

The potential energy operator is similarly expressed.

23) \( \langle \hat{U} \rangle = \int_{-\infty}^{\infty} \psi^*U\psi dx \)

which becomes

24) \( \langle \hat{U} \rangle = \int_{-\infty}^{\infty} U(x)(\psi_R(x)^2 + \psi_I(x)^2)dx \)

due to the commutitive properties of the potential \( U \) as a constant.
The kinetic and potential energy added together to find the total energy of the positron.

This energy is needed to evaluate the annihilation cross section of the positron:

\[ \sigma = \frac{4\pi \alpha^2}{3s} \left(1 + \frac{4m^2}{s} + \frac{4m^4}{s^2}\right), \]

where \( \alpha \sim \frac{1}{137} \) and \( s = 2mE_{\text{total}} \), where \( E_{\text{total}} \) is the lab frame energy.

The validity of this code, in its present state, is questionable. Errors are likely originating with the Gaussian wave packet, and propagate throughout the code.

One would expect the positron wavefunction to be sharply peaked at the edge of the material, and then shrink in height and grow in width as the wavefunction moves forward in time. However, this code results in a peak that grows from zero before the expected behaviors occur.

Additional evidence for propagated error is found in the kinetic energy of the positron. The expectation value is calculated every step and includes a non-negligible imaginary term and kinetic energy should be real. This, in turn, results in inaccurate values for the total energy and for the annihilation cross section.

On a positive note, once formed the Gaussian does behave as expected. In addition, if the plot of the wavefunction is zoomed in on far from the main wave packet, we find a minuscule probability of the positron being found at those positions, and it would have a
possibility of annihilating at a location far from the center of the wave packet (figure 11).

Figure 11: With lattice position on the x-axis and probability on the y, this plot shows a possibility of the particle existing far from the centralized wave packet.
Appendix 2

%Finite Difference Time Dependent Method

clear;
close all;

%%%%%%%%%%%%%%%%%%%
%initial conditions%
%%%%%%%%%%%%%%%%%%%
dx = .1*10^(-10); %meters
E0 = 4.96675 * 10^(-16); %J or 3100ev
m = 9.10938356*10^(-31); %kg positron mass
e = 1.60217662*10^(-19); %C positron charge
hbar = 1.054571726e-34; %J*S see also (e-14) plank's constant
dt = .1*10^(-19); % time step
C1 = (dt*hbar)/(2*m*(dx^2)); % Schrodinger constant
C2 = (dt)/hbar; % Schrodinger constant
L = 2499*10^(-10); %meters size of box
Img = 1i; % Changing the imaginary variable so I can use i as an iterator
% I believe that the next to commented out conditions would be more accurate
% if a computer had enough memory to run it
spaceN = (2500)-1; %loop iterations and # of angstroms * 10
x = linspace(0,L,spaceN);%linspace(0,spaceN/10,spaceN);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Positron pulse as a Gaussian%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%initializing and normalizing the wave function
phiReal = zeros(1,spaceN);
phiI = zeros(1,spaceN);
phiReal(1) = 0;
phiI(1) = 0;
phiReal(spaceN) = 0;
phiI(spaceN) = 0;

center = round(spaceN/15); % pulse center (close to the left edge)
width = L*100; % pulse width
wL = (2*pi*hbar) / sqrt(2*m*E0); % wave length
\begin{verbatim}
for i = 1:spaceN
    phiReal(i) = exp(-.5*((x(spaceN)-x(center))/width)^2)*cos(2*pi*(x(spaceN)-x(center))/wL);
    phiI(i) = exp(-.5*((x(spaceN)-x(center))/width)^2)*sin(2*pi*(x(spaceN)-x(center))/wL);
end

%initializing
phi = phiReal.^2 + phiI.^2;
area = simpson1d(phi,0,L);
phiReal = phiReal./sqrt(area);
phiI = phiI./sqrt(area);

i = 0; %clear my loop iteration variable

%Creating the potential lattice
for i = 0:spaceN-1
    [V] = getLattice(i); %Need to fix the ratio to achieve proper stepsize
    potential(i+1) = V; %while keeping physical correctness
    i = i + 1;
    potential(i+1) = 0;
end

i = 0; %clear my loop iteration variable

%Initializing Kinetic Energy

%Kinetic Energy Operator: T = -(hbar^2)*partial^2/2m
for i = 2:spaceN-1
    expectationKE(i) = (-hbar^2 / (2 * m* (dx^2))) * ...
\end{verbatim}
(\phi_{\text{Real}}(i) - \text{Img} * \phi_{\text{Im}}(i)) * (\phi_{\text{Real}}(i+1) - 2 * \\
\phi_{\text{Real}}(i) + ... \\
\phi_{\text{Real}}(i-1) + \text{Img}*(\phi_{\text{Im}}(i+1) - 2*\phi_{\text{Im}}(i) + \phi_{\text{Im}}(i-1))); \\
i = i + 1;
end

avgKE = simpson1d(expectationKE,2,spaceN-1);
i = 0; %clear my loop iteration variable

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%
%Initializing Potential Energy%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
for i = 2:spaceN-1
    expectationPE(i) = potential(i) * (phi_{\text{Real}}(i).^2 + \\
phi_{\text{Im}}(i).^2);
    i = i + 1;
end

avgPE = simpson1d(expectationPE,2,spaceN-1);
i = 0; %clear my loop iteration variable

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%
%Finite Difference Time Dependent Solution to Schrodinger Equation%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
for i = 1:spaceN
    %Storing the previous values of phiReal and PhiI allow the new values 
    %to be calculated without any discrepancy on which time step is being %looped
    phiRealStored = phiReal; 
    phiIStored = phiI;

    for j = 2:spaceN-1
        phiReal(j) = phiRealStored(j) - C1*(phiIStored(j+1) - \\
2*... \\
phiIStored(j)+phiIStored(j-1)) + 
        C2*potential(j)*phiIStored(j); 
        j = j + 1;
end

for k = 2:spaceN-1
    phiI(k) = phiIStored(k) + C1*phiRealStored(k+1) - 2*phiRealStored(k) - phiRealStored(k-1) - C2*potential(k)*phiRealStored(k);
k = k + 1;
end

phi = phiReal.^2 + phiI.^2;
area = simpson1d(phi,0,L);
phiReal = phiReal./sqrt(area);
phiI = phiI./sqrt(area);

psi = phiReal.^2 + phiI.^2;

% Kinetic Energy %

for n = 2:spaceN-1
    expectationKE(n) = (-hbar^2 / (2 * m* (dx^2))) * ...
                       (phiReal(n) - Img * phiI(n)) * (phiReal(n+1) - 2 * phiReal(n) + phiReal(n-1)));
    n = n + 1;
end

avgKE = simpson1d(expectationKE,0,spaceN);

% Potential Energy %

expectationPE(i) = potential(i) * (phiReal(i).^2 + phiI(i).^2);
avgPE = simpson1d(expectationPE,0,spaceN);

ETotal = avgKE + avgPE;

% Calculating an Annihilation %
\[
\text{alpha} = 1/137;
\text{s} = 2\times m\times E_{\text{Total}}; \quad %\text{lab frame of reference}
\text{sigma} =
(4\times \pi \times \alpha^2 / (3\times s)) \times (1 + (4\times m^2) / s) + (4\times m^4) / (s^2));
\]

% Plotting
plot (x, psi)
axis([0, L, 0, 2.5e9])
title('Wave Interpretation of a Positron in a Lattice')
xlabel('Meters')
ylabel('Probability')
drawnow

subplot(2,1,2)
plot(x, potential)
title('Electric Potential From An Atomic Aluminum Lattice')
xlabel('Meters')
ylabel('Potential(C)')
drawnow

i = i + 1;
end
Appendix 3

ClearAll["Global`*"]
c=2.99*10^8;
v=2.03*10^6;
\(\beta = \frac{v}{c}\);
h=4.135*10^{-15};
fs=511000/h; (*Frequency of the source*)
fo=\(\sqrt{\frac{1-\beta}{1+\beta}}\)fs; (*frequency of the observer*)
(fo-fs)h (*The resulting shift in the energies that would be detected*)
=3481.19 (*ev*)
Appendix 4

ClearAll["Global`*"];
c=2.99*10^8;
vfermi=2.03*10^6;
dθ=0.0872665; (*5 degrees*)
percentAngle=(Sin[θ]dθ)/2;
vpar=vfermi*Cos[θ];
β=vpar/c;
h=4.135*10^-15;
fs=511000/h;
fo=Sqrt((1+β)/(1-β))*fs;
Enew=(fo)h;
percentAngle=(Sin[θ]dθ)/2;
ParametricPlot[{Enew/100000,percentAngle},{θ,0,π}]}
ClearAll["Global`*"];

expansion=23.6/1000000; (*ppm/C*)
dTemp=350-20;
ΔVolume=expansion*dTemp;
n=1.79388*10^29(*1.32*10^29*1.359*);
V=1;
NewVolume=V+V*ΔVolume;
n2=n*V/NewVolume;
ℏ=1.0546*10^-34; (*Js*)
m=9.11*10^-31; (*Kg*)

FermiEnergy=\( \frac{\hbar^2}{2m} \left( \frac{3\pi^2 n}{2} \right) \right)^{2/3} / (1.602*10^{-19});
NewFermiEnergy=\( \frac{\hbar^2}{2m} \left( \frac{3\pi^2 n2}{2} \right) \right)^{2/3} / (1.602*10^{-19});
FermiEnergy-NewFermiEnergy;
ΔEnergy=(1−(NewFermiEnergy/FermiEnergy))*100

0.515854

The change in Fermi energy of the heated sample is increased by 0.5% from the increased volume. This is using an expansion coefficient for pure Al.
ClearAll["Global`*"]
expansion=23.6/1000000; (*ppm/C*)
dTemp=350-20;
ΔVolume=expansion*dTemp;
n=1.79388*10^29(*1.32*10^29*1.359*);
V=1;
NewVolume=V+V*ΔVolume;
n2=n*V/NewVolume;
ℏ=1.0546*10^-34; (*Js*)
m=9.11*10^-31;
NewFermiEnergy=(ℏ^2/(2m))(3π^2 n^2 n2)^(2/3);
ExcitedFermiVelocity=Sqrt((2/m)NewFermiEnergy);
c=2.99*10^8;
v=2.03*10^6;
h=6.62607*10^-34;
β=ExcitedFermiVelocity/c;
fs=511000/h;
fo= Sqrt((1+β)/(1-β))*fs;
(fo-fs)h (*The resulting shift in the energies that would be detected*)

=3454.65
Appendix 7

ClearAll["Global`*"]

expansion = 23.6/1000000; (*ppm/C*)

dTemp = 350 - 20;

\[\Delta Volume = \text{expansion} \times \text{dT}\]

n = 1.79388 \times 10^{29} (*1.32 \times 10^{29} \times 1.359*);

V = 1;

NewVolume = V + V \times \Delta Volume;

n2 = n \times V / \text{NewVolume};

\[\hbar = 1.0546 \times 10^{-34}; (*\text{Js}*)\]

m = 9.11 \times 10^{-31};

FermiVelocity = 2.03 \times 10^6;

NewFermiEnergy = \left(\frac{\hbar^2}{2m}\right) \left(3n^2 \times n2\right)^{2/3};

\text{ExcitedFermiVelocity} = \sqrt{\left(\frac{2}{m}\right) \text{NewFermiEnergy}};

FermiVelocity = 2.03 \times 10^6;

\sigma = .6548 \times 1000;

d\theta = 0.0872665; (* 5 degrees*)

c = 2.99 \times 10^8;

h = 4.135 \times 10^{-15};

f = 511000/\hbar;

Vparallel = (c(\text{Energy}^2/(h^2 \times f^2) - 1))/ (\text{Energy}^2/(h^2 \times f^2) + 1);

\text{percentAngleLowTemp} = \left(\frac{1}{2}\right) \sqrt{\text{FermiVelocity}^2 - Vparallel^2}/\text{FermiVelocity} \, d\theta;
percentAngleHighTemp=(1/2) Sqrt(FermiVelocity^2-Vparallel^2)/ExcitedFermiVelocity dθ;

(* This shows finding the S-Parameter for the two. A good S-parameter comes out to 50% of the total curve.


(NIntegrate[NIntegrate[percentAngleHighTemp*1/Sqrt[2π σ^2]*e^(-(Energy-EnergyInt)^2/(2σ^2)),{Energy,507569,514454.5}],{EnergyInt,509576,512424}])/(NIntegrate[NIntegrate[percentAngleHighTemp*1/Sqrt[2π σ^2]*e^(-(Energy-EnergyInt)^2/(2σ^2)),{Energy,507569,514454.5}],{EnergyInt,505000,517000}])

This is the end of the comment*)

(1-(NIntegrate[NIntegrate[percentAngleHighTemp*1/\sqrt{2π σ^2} \times e^{-\frac{(Energy-EnergyInt)^2}{2σ^2}} \}, {Energy,507569,514454.5}], {EnergyInt,509576,512424}))/(NIntegrate[NIntegrate[percentAngleLowTemp*1/\sqrt{2π σ^2} \times e^{-\frac{(Energy-EnergyInt)^2}{2σ^2}} \}, {Energy,507542.5,514481}], {EnergyInt,509566,512434}]) \times 100

= 0.73
References


faculty.sdmiramar.edu/fgarces/labmatters/instruments/aa/AAS_Instrument/AASInstruments.htm. n.d.


