Positron Annihilation in Single Crystal Zinc at 250 Degrees Centigrade

Jon Wayne Swanson
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POSITRON ANNIHILATION
IN SINGLE CRYSTAL ZINC
AT 250 DEGREES CENTIGRADE

by

Jon W. Swanson

A Thesis
Submitted to the
Faculty of the School of Graduate Studies in partial fulfillment of the
Degree of Master of Arts

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Jon W. Swanson
CHAPTER I

INTRODUCTION

In recent years an increasing amount of research has been conducted using the technique of angular correlation of positron annihilation radiation to furnish information about the electronic properties of metals. A good review of this technique can be found in (1).

It has been shown, for many metals studied, that the angular correlation of positron annihilation radiation is temperature dependent. The correlation curves become narrower as the temperature of the specimen is increased, as indicated in Figure VII, Chapter IV of this work. This effect of temperature on the angular correlation is much larger than can be explained by the increase in specimen volume with temperature. At present the reason for this change in the angular correlation curves is not known with certainty.

A possible explanation for the change in angular correlation curves is that the observed temperature effect might be connected with the anisotropic properties of the metal crystal structure being investigated. Since a polycrystalline metal sample gives an average over all possible crystallographic directions, one might expect that if the lattice is playing a significant role in producing changes in the angular correlation with temperature, that observable deviations from the average change might be seen.
in experiments on oriented single crystals.

Zinc was chosen to be studied in this work because a large effect on the angular correlation curve is observed with a change in temperature (2).

For these reasons the method of angular correlation of gamma ray pairs produced by positron annihilation was used to study polycrystalline zinc and single crystal zinc oriented in the (0001) and (1120) directions at room temperature and at 250 degrees centigrade.
CHAPTER II

POSITRON ANNIHILATION IN METALS

A Brief History

In 1930, Dirac predicted the existence of positrons while working on his relativistic theory of quantum mechanics (3). It was not until 1933 that they were observed by Anderson with the use of a Wilson cloud chamber (4). Later that same year the phenomenon of positron annihilation was discovered separately by Joliet (5) and Thibaud (6). Then, in 1942, Beringer and Montgomery measured the angular distribution of photons produced by two quantum positron annihilation in copper and lead (7). Seven years later, in 1949, S. DeBenedetti (8), (9) showed that the gamma rays produced by an annihilation are not exactly anticollinear and that the angle between their paths is determined by the motion of the electrons in the solid matter where the annihilations take place. Since 1949 extensive experimental and theoretical work has been conducted by various workers using the technique of angular correlation of positron annihilation radiation to study the electronic properties of many different solids and liquids.
The Annihilation Process

In the annihilation process at least two other particles or quanta besides the positron and electron must be involved so that the law of conservation of momentum is not violated. From the conservation laws and symmetry considerations it can be shown that if the positron and electron have their spins aligned, in the so-called triplet state, that this state cannot undergo two quantum decay. It can decay only with the emission of three or a larger odd number of quanta, whereas the singlet state, which exists when the direction of the spins of the electron and positron are opposite each other, can decay by two quantum emission.

This work involved the study of two photon annihilation so this process will be elaborated on somewhat.

Upon entering a solid metal, the positrons are slowed down rapidly because of collisions with the lattice and with electrons. Usually after approximately $10^{-10}$ seconds the positron annihilates with an electron, where usually the mode of decay is by two gamma ray emission (10). If the momentum of the center of mass of the annihilating positron and electron were zero at the time of annihilation then the gamma rays would be emitted in directions 180 degrees from each other. If the momentum of the center of mass were not zero then the gamma rays would go off in directions other than 180 degrees from each other.
The Angular Correlation Technique

The angular correlation of positron annihilation radiation is measured by counting gamma ray pairs which are coincident in time, at various angles of the detector as indicated in Figure I.

In this arrangement the angle \( \theta \) is changed by moving the detector and slit combination on the right of the diagram along the arc of a circle with the sample at the center and the detector at the left remaining fixed. The detectors and their collimating slits are long compared to the sample length and aligned perpendicular to the plane of the drawing.

Figure II is a momentum diagram for the gamma rays produced by an annihilation. The x component of momentum is essentially integrated over because the long collimating slits in the geometrical arrangement of the apparatus are parallel to the x direction. The y component of momentum of the gamma rays is perpendicular to the detector collimating slits and causes a Doppler shift of, at most, a few electron volts. The detection electronics is set to accept gamma rays having energies in a range of several KeV so the y component of momentum is integrated over also. Therefore it is the relative number of gamma ray pairs with a given z component of momentum that is measured in the angular correlation experiment. \( \vec{P}_{yz} \) in Figure II is the projection of the momentum of the center of mass of the annihilating pair on the yz plane. \( \phi \) is the angle \( \vec{P}_{yz} \) makes with the y-axis.
Figure I Detector Arrangement

Figure II Momentum Diagram
Assuming the two coincident gamma rays have a total momentum $\mathbf{P}$, it has been shown (11) that the component of momentum $P_z$ is approximately equal to $mc\theta$. Since $\theta$ is directly proportional to $P_z$, information about the distribution of electron momenta in a metal can be obtained by measuring the coincidence counting rate as a function of $\theta$.

The probability that a pair of photons with momentum $\mathbf{p} = \hbar \mathbf{k}$ will be produced by the annihilation of a positron with the wave function $\psi_+(\mathbf{r})$ and an electron with the wave function $\psi_-(\mathbf{r})$ is given in (12) to be proportional to $\Pi(\mathbf{r}) = \int \psi_+(\mathbf{r}) \psi_-(\mathbf{r}) e^{-i \mathbf{r} \cdot \mathbf{r}} \, d^3 \mathbf{r}$.

By considering the case of annihilation in a free electron gas it has been shown (13) that the angular correlation curve is an inverted parabola which is symmetrical about $\theta$ equals zero and which goes to zero at plus and minus $\theta_F$, the angle corresponding to the Fermi momentum. The equation of the parabola is $y = A \left( 1 - \theta^2 / \theta_F^2 \right)$. 

http://example.com
CHAPTER III

EXPERIMENTAL APPARATUS AND PROCEDURES

Geometrical Arrangement

Figure III is a simplified diagram of the geometrical arrangement of the positron source, the sample, the gamma ray detectors and the steel frame upon which these are mounted. The five millicurie sodium twenty-two source and the sample are surrounded by two-inch thick lead bricks in the shape of an eight by eight by eight inch cube. The source is suspended vertically on a threaded steel rod which allows it to be moved toward or away from the sample as desired. The sample rests on the top of a copper cylinder which also serves as the core for the sample heating element. The base of the copper cylinder is threaded so it can also be moved up or down depending on the sample size. This allows adjustment of the top surface of the sample to the height of the center of the one quarter inch beveled slits in the collimating lead bricks as indicated in Figure III.

Twelve inches from either side of the lead cube are two-inch thick lead bricks with horizontal slits, 3/8 of an inch by four inches, cut through the center to provide collimation of the beams. On both ends of the steel frame, directly in front
Figure III Geometrical Apparatus

1. Linear Amplifier
2. Rough Collimating Bricks
3. Source Chamber
4. Source
5. Sample
6. Drive Motor
7. Detector Housing

50"

50"
of each of the detectors, are located a pair of lead bricks to provide more collimation. These bricks are each three inches thick, two and one half inches high, and twelve inches long. They are placed one above the other, and separated by 0.05 inches. These openings are adjustable by means of an adjusting bolt on the top brick which raises or lowers it to the desired opening. To assure alignment of these slits with the source chamber slits, three large bolts positioned at the vertices of a triangle are used to adjust the tilt of the platforms upon which the detectors sit. Behind the collimation bricks, at a distance of fifty inches from the positron source, the detectors are located. This gives the apparatus a geometrical angular resolution of one milliradian. The detectors are two inch diameter, six inch long thallium activated sodium iodide scintillators. These detectors are surrounded by two-inch thick lead bricks, with the exception of the side where the detectors are coupled to the Hamner NB-12 preamplifiers. In this arrangement, as was previously mentioned, the source, sample and one of the detectors remain stationary while the other detector pivots, in steps of one milliradian, through the arc of a circle. This pivoting is accomplished by employing a 1/20 horsepower, 115 V.D.C. Bodine Motor, which through the use of a worm gear rotates a threaded steel shaft which raises and lowers the detector platform upon receiving a signal from the control unit.
The Control Unit

The purpose of the control unit is to provide automatic operation of the entire angular correlation experiment. This allows data to be taken twenty four hours a day.

The unit employs a series of relays, microswitches and a Microflex HZ40 timer. The timer can be set to allow counting for intervals of time of ten seconds to intervals of 66 minutes and 10 seconds.

Assuming the detector platform is in its extreme lower position the sequence of operation of the control unit is as follows:

After the timer has been set for the desired count time at each position of the detector, the control unit is energized and the scaler will begin counting coincident pulses. After the preset time elapses a relay engages and prevents the scaler from counting any more pulses. The number from the scaler is then printed out on the printer and the scaler is reset to zero. At this time 115 V.D.C. is applied to the 1/20 horsepower Bodine motor causing it to rotate the threaded steel rod 360 degrees which causes the movable detector platform to rise to its next position. In doing this the detector has swept an arc of one milliradian. Once the rod has rotated 360 degrees a protruding steel peg activates a normally closed microswitch which removes the power from the motor and allows the scaler to begin counting again for the preset time. Once the entire
desired arc has been swept in this manner, the detector plat-
form engages another microswitch which causes the motor to
reverse direction and lower the detector platform to its lowest
position, at which time the sequence of events is repeated.
The control unit is designed so that it can be operated manually
also.

With the five millicurie sodium twenty-two source it is
possible to count about twenty-thousand annihilations in two
days at the position where the detectors are 180 degrees apart.
Instead of counting for eighty minutes at each position and
sweeping the arc once, it was decided to count at each of thirty
six positions for ten minutes and sweep the arc eight times
which means the apparatus returns to, and is counting at, the
same position every six hours. This method is used to minimize
the effects of long-term electronic drift.

The Sample

The polycrystalline zinc sample, Figure IV, is produced by
melting a piece of 99.999% pure zinc and pouring it into a
cylindrical mold which is slightly tapered to make removal of
the sample from the mold easier. The surface of the sample is
then made flat by machining.

The single crystals are shaped in the form of a \( \frac{1}{2} \) inch
high and \( \frac{1}{4} \) inch in diameter cylinder. These are at least
99.99% pure and are available from Semi Elements Corporation
of Saxonburg, Pennsylvania.
Sample Heating Arrangement

The heating of the sample is accomplished with the use of a Nichrome V wire, which is inside a cylindrical Inconel sheath, six inches long and 0.045 inches in diameter, and packed with magnesium oxide powder. The sheath is looped around a solid copper cylinder in which grooves were milled to fit the sheath. The element is available from the Aero Research Instrument Department of the American Standard Corporation. High melting point solder was used to insure good thermal contact of the element to the copper cylinder. Power is supplied to the heating element by a Variac which receives its power from a 115 V.A.C. regulated power supply.

Temperature Monitoring of Sample

To monitor the temperature near the surface of the sample a 0.046 inch diameter hole is drilled horizontally to the center of the sample as near to the surface as possible, Figure IV. In this hole is inserted a GB41J1 Fenwal Thermistor, whose leads are coated with Wantz teflon repair fluid to insure against electrical shorting of the leads. The thermistor is calibrated by placing it in an oven at various temperatures and measuring its resistance at each temperature. By knowing the resistance of the thermistor at the desired temperature, a resistor of that resistance can be placed in parallel with a Varian G-11 chart recorder, Figure V, and the Heathkit EUW 30
Figure IV Sample (Side View)

Figure V Temperature Monitoring Circuit
decade resistance box adjusted so that the chart recorder will read midscale. Then the resistor which was placed in parallel with the chart recorder can be replaced by the Fenwal thermistor. Once the sample has reached the desired temperature the chart recorder will again read center scale. At 250 degrees centigrade a change of 1.2 degrees in the sample temperature will be indicated by a movement of one scale division off center on the chart recorder. If the movement of the chart recorder off center occurs, the Variac mentioned in the heating arrangement can be adjusted to compensate for this. The experiment was carried out with the chart recorder always within ±1 scale division of center scale which corresponds to ±1.2 degrees variation in temperature of the sample.

It was thought that possibly after drilling the hole for temperature monitoring that the surface of the sample would no longer be a single crystal. For this reason, once the angular correlation of positron annihilation radiation measurements had been taken the samples were inverted and the experiments repeated at room temperature and at 250 degrees centigrade. The same results were obtained with the inverted crystals as were obtained with the crystals in the upright position. The crystals were then etched in dilute HCl and it was observed that a slight damage had occurred in the vicinity of the hole. This damage covered an area of only about 0.5% of the total surface area of the crystal. Because positron annihilation can occur over the total surface area of the crystal, the
small percentage of damage that did occur to the crystal was negligible.

Electronics

Figure VI is a block diagram of the electronic equipment used in the experiment. The gamma rays are detected by two Harshaw Type SMFA24/2A thallium activated sodium iodide crystal detectors which are two inches in diameter and six inches long. These detectors are sealed in aluminum containers and optically coupled to two inch diameter RCA6342-A multiplier phototubes. The pulses from each channel are then fed to separate Hamner NB-12 preamplifiers which are followed by Hamner NA-12 double delay line amplifiers. The pulses then go into Hamner NC-14 low jitter pulse height analyzers. The outputs of the pulse height analyzers are monitored by Hamner NR-10 linear ratemeters and also fed into a Hamner NL-16 fast ramp coincidence module. If two of the pulses are coincident in time they are assumed to have resulted from the same annihilation and a pulse will be fed into the scaler. After the preset counting time elapses the Computer Measurements Corporation 400-C digital printer records the number of annihilations indicated on the scaler. A Hamner NV-13 high voltage power supply is used to supply the necessary high voltage to the photomultiplier tubes. All other necessary voltages required by the Hamner equipment are supplied by a Hamner NH-84A power supply. A Sorensen 2000-S line voltage regulator is also used to insure a constant voltage
Figure VI
Block Diagram of Electronics
source for all equipment.

The Hamner linear ratemeters which monitor the count rate of each channel are useful in checking the operation of the electronic equipment and also in checking the geometrical alignment and positioning of the source, sample, and detector slits.

The resolving time of the Hamner NL-16 fast ramp coincidence module can be adjusted from $5 \times 10^{-9}$ seconds to $1.5 \times 10^{-7}$ seconds, but was set at $1.5 \times 10^{-7}$ seconds for this experiment. By knowing the resolving time of the electronics the chance coincidence rate was calculated using the equation, $N_c = 2TN_1N_2$, where $N_1$ and $N_2$ are the individual count rates of each channel and $2T$ is the resolving time of the electronics. The chance coincidence rate was calculated to be typically 3.6 counts per 10 minutes. At the tails of the angular correlation curve about 40 counts per 10 minute time interval were observed, which meant that about 10% of the counts result from chance coincidences. At the peak of the curve, approximately 2000 counts were observed in a 10 minute time interval so only about 0.2% of the counts were chance coincidence counts.
CHAPTER IV

ANALYSIS OF THE DATA

The arc that is swept out by the detector can be varied by adjusting limiting microswitches on the equipment. These switches are adjusted so that the lowest position of the detector is approximately one degree below the horizontal and the highest position is one degree above the horizontal. It is not necessary to sweep an arc greater than this because beyond these limits virtually no annihilations can be observed, only chance coincidence counts.

The raw data, which is the number of counts at each angle of the detector, is in the form of \( n \) sets of numbers, where \( n \) is the number of detector positions. Each set of \( n \) numbers has \( m \) members where \( m \) is the number of times counted at each position. To get the total number of counts at a given angle a sum must be carried out over the \( m \) members of all \( n \) sets. The angular correlation curve is a plot of these values versus the angle at which they were obtained. The raw data is listed in Appendix A of this paper. Simpson's rule is used to approximate the area under the angular correlation curve. The area is then normalized to \( 10^5 \) so that a comparison can be made when other experiments are carried out. Figures VII, VIII, and IX are the normalized angular correlation curves for polycrystalline zinc, single crystal zinc oriented...
Counting rate in arbitrary units

Zinc - Polycrystal

Figure VII

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Figure VIII

ZINC - (0001)

COUNTING RATE IN ARBITRARY UNITS

ANGLE IN MILLIRADIANS

25°C

250°C

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Figure IX

ZINC - (11\(\overline{2}0\))
in the (0001) direction and single crystal zinc oriented in the 
(1120) direction respectively.

It has been suggested by G. Lang and S. DeBenedetti (13) that the tails of the angular correlation curves can be approximated by a Gaussian and the center by an inverted parabola. This suggestion is employed in this work in the analysis of the data.

Defining \( Y \) to be the number of counts and \( \theta \) to be the angle from the horizontal at which these counts were taken, a least squares fit is calculated using the values on the tails of the angular correlation curve for the Gaussian and the central values of the angular correlation curve minus the corresponding central values of the fitted Gaussian for the parabola. Points in between those used in the Gaussian calculation and those used in the parabola calculation are omitted.

Fitting The Gaussian

The equation for the Gaussian is \( y = B \exp(-\theta^2/2\sigma^2) \), where \( \sigma \) is the half width of the angular correlation curve at six tenths maximum. Letting \( c = 1/2\sigma^2 \) and \( x = \theta^2/\sigma^2 \) yields \( y = B \exp(-cx) \).

Assuming no uncertainty in \( Y \), the normalized values of the angular correlation curve, the least squares fit is accomplished by minimizing \( S = \sum w_i R_{yi}^2 \) where \( w_i = 1/Y_i \) and \( R_{yi} = Y_i - y_i \). Therefore \( S = \sum (Y_i - B \exp(-cx_i))^2/Y_i \). Taking the partial derivatives of \( S \) with respect to \( B \) and \( c \) yields the following two equations:
Setting these two equations equal to zero and equating, yields the following transcendental equation:

\[
\begin{align*}
\frac{\partial S}{\partial B} &= \sum_i \left[ -2e^{-c\chi_i} + \frac{2Be^{-ac\chi_i}}{Y_i} \right] \\
\frac{\partial S}{\partial c} &= \sum_i \left[ +2B\chi_i e^{-c\chi_i} - \frac{2B^2\chi_i e^{-ac\chi_i}}{Y_i} \right]
\end{align*}
\]

This equation is solved by first inserting a value for \(c\) which is obtained by measuring \(\Gamma\), the half width of the angular correlation curve at 0.6 maximum, solving the equation \(c = 1/2\Gamma^2\), and then iterating to obtain the correct value of \(c\). The correct value of \(c\) is that which makes the difference between the two sides of the transcendental equation a minimum. This is accomplished using the IBM 1620 Computer and the program listed in Appendix B of this paper. The computer program is designed such that a value for \(c\) can be inserted into the equation by a typewriter. Then the difference between the two sides of the resulting equation is typed out. By looking at whether this difference is negative or positive, one can determine \(c\) to 12 decimal places in about 15 iterations. Table I lists the values obtained for \(c\) in the various experiments.

Once \(c\) has been found it is inserted into the equation for the Gaussian and the \(y\) values are calculated.
<table>
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<th>K</th>
<th>B</th>
<th>$\theta_F$</th>
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<td>Polycrystal Zn at Room Temperature</td>
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<td>6.64</td>
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*Table I*
The values calculated for the central portion of the Gaussian are then subtracted from the corresponding central values of the original normalized angular correlation curve. The resulting values are then used in fitting the parabola.

Fitting the Parabola

The equation for the parabolic portion of the curve is

\[ y = A \left(1 - \frac{\theta^2}{\Theta^2} \right) \]

where \( \Theta_p = \sqrt{A/K} \) is the angle at which the parabola intersects the \( \theta \) axis. The least squares fit to the parabola is accomplished by minimizing \( S = \sum \frac{w_i R_{yi}^2}{\sum w_i} \) where \( w_i \) is the weighting factor equal to \( 1/ (Y_i + \bar{Y}_i) \) where the \( \bar{Y}_i \) are defined to be the calculated Gaussian values.

Taking partial derivatives of \( S \) with respect to \( A \) and \( K \) and setting these equations equal to zero yields the following two equations:

\[
A \left( \sum w_i \Theta_i^2 \right) - K \left( \sum w_i \Theta_i \right) = \sum w_i Y_i \\
A \left( \sum w_i \Theta_i \right) - K \left( \sum w_i \Theta_i^2 \right) = \sum w_i Y_i \Theta_i
\]

Once these equations are obtained, \( A \) and \( K \) can be solved for by using determinants. This is also done using the IBM 1620 Computer, and the program listed in Appendix C of this paper. The results of these calculations can be found in Table I. Because the annihilation of positrons with core electrons is the main cause for the Gaussian it was desired to know what fraction of the total area of the fitted angular correlation curve was included in the Gaussian. The area under the Gaussian was also
calculated using the equation: \[ \text{Area} = B \int_{-\infty}^{\infty} \exp(-cx^2)dx = B\sqrt{\pi}/\sqrt{c}. \]

The area of the parabola was calculated with the use of the equation: \[ \text{Area} = \int_{-\infty}^{\infty} (A-K\theta^2)d\theta = 2A\theta_p - (2/3)K\theta_p^3. \]

\[ \chi_g^2 = \frac{1}{Q} \sum \frac{(Y_i - B e^{-cx_i})^2}{Y_i} \]

was calculated for the fitted Gaussian and \[ \chi_p^2 = \frac{1}{Q} \sum \frac{(Y_i - Y_i)^2}{Y_i} \]

was calculated for the fitted parabola by the computer to check for goodness of fit. In the equations for \( \chi_g^2 \) and \( \chi_p^2 \), the \( Y_i \) values are the normalized \( Y \) values of the angular correlation curve and \( Q \) is the normalizing factor which is equal to \( 10^5 \) divided by the area of the angular correlation curve. In a reasonably good fit, \( \chi_g^2 \) and \( \chi_p^2 \) should be of the same order as the number of degrees of freedom used in the fit. The number of degrees of freedom is equal to the number of data points used in making the fit minus the number of free parameters used in the fit.

Once \( \chi_g^2 \) and \( \chi_p^2 \) are calculated, each of their parameters are varied separately, first by increasing them by a small amount and then by decreasing them by a small amount, and then \( \chi_g^2 \) and \( \chi_p^2 \) are calculated each time with these varied parameters as a check to see that the originally calculated parameters really did produce a minimum \( \chi^2 \).

Values for \( \theta_p, \chi_g^2, \chi_p^2 \), the fractional area of the parabola, denoted \( A_p/(A_p+A_g) \), the fractional area of the Gaussian, denoted \( A_g/(A_p+A_g) \), and the number of degrees of freedom can be found in Table II. Figures X and XI show two fits obtained by the above calculations. The symbols used in Figures X and XI are, \( \Delta \) = normalized angular correlation curve, \( - - - \) = fitted Gaussian, \( \circ \) = central part of Gaussian minus central part of normalized angular correlation curve, \( \bullet \) = fitted parabola.
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**Table II**
Polycrystalline Zinc at 25° C

Figure X
Polycrystalline Zinc at 250° C

Figure XI
CHAPTER V

CONCLUSION

With an angular resolution of one milliradian, no difference was observed in angular correlation curves for polycrystalline zinc and single crystal zinc at room temperature and at 250 degrees centigrade. It is possible that there may be some difference, which might be observed if the experimental apparatus had a better angular resolution, but the temperature effect is clearly observable at one milliradian resolution so this should have been adequate in determining if lattice orientation does affect the angular correlation curves at high temperatures. This seems to indicate that lattice structure has little to do with the change in the angular correlation of positron annihilation radiation curves, due to temperature changes.

By looking at Figure X and XI, one can see that the room temperature angular correlation curves do seem to fit the Gaussian and the parabola as suggested in (13), but at 250 degrees centigrade the curves do not fit the parabola very well.

The method of calculation for determining that the angular correlation curve was a parabola, assumed that the annihilating electrons had a free electron wave function. Because the fit of the angular correlation curves to a parabola at sample temperature...
of 250 degrees centigrade is poor, it appears that the free electron model is not sufficient in determining the angular correlation curves at sample temperatures of 250 degrees centigrade.

The Fermi angle \( \Theta_p \), calculated from the analysis, seems to be slightly larger, for both the room temperature and the 250 degree centigrade experiments, than that calculated for zinc in (14) by using the free electron model. A probable reason for the difference is that the effects of angular resolution of the apparatus were not removed from the experimental data.

Recently it has been shown (15) that plastically deformed metals produce changes in the angular correlation curves similar to those caused by increased temperatures. A phenomenon common to plastically deforming and heating a metal is the production of vacancies. A vacancy is a lattice site in the metal which is missing an ion.

Heating a metal will create vacancies at some lattice sites, which causes a decrease in the electron density at these sites. Because of the lack of a positive ion at a vacancy site, a positron will be more attracted to the site than to lattice sites at which there are no vacancies. Therefore positrons are more likely to annihilate at vacancy sites, causing more annihilations to take place with conduction electrons at sample temperatures of 250 degrees centigrade than at room temperature.

Because the Fermi angle decreases with a decrease in electron density, and because the creation of vacancies decreases the density of electrons of lattice sites, the Fermi angle, \( \Theta_p \), will decrease
in the angular correlation curves of positron annihilation radiation. The values of $\theta_p$ in Table I, Chapter IV, do not seem to be following the pattern of decreasing with increasing temperature. The reason that $\theta_p$ does not decrease when the temperature is increased to 250 degrees centigrade, could be, because the fit of the angular correlation curve to a parabola is poor at 250 degrees centigrade, and it is the values obtained from the fit that are used to calculate $\theta_p$.

There is no reason to believe that vacancies will not be produced in a single crystal just as well as in a polycrystal so the results of this work are consistent with the interpretation that vacancies are responsible for the changes in angular correlation of positron annihilation curves at sample temperatures of 250 degrees centigrade.
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(O0001) Zinc at 250 Degrees Centigrade

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APPENDIX B

Calculation of $c$ Using
The IBM Computer 1620
In Fortran II Language.
DIMENSION X(40), Y(40)

READ 31, J

FORMAT(I2)

READ 3,(X(I), Y(I), I=1, J)

FORMAT(F6.3, F5.0)

READ 49, N, L, K

FORMAT(I2, I2, I2, I2)

ACCEPT 975, C

FORMAT(F14.12)

ES = 0

FS = 0

QS = 0

PS = 0

L = 0

F = 0

P = 0

Q = 0

QP = 0

DO 20 I = 1, N

E = E + EXP(-C*X(I))

F = F + EXP(-2*C*X(I))/Y(I)

Q = Q + X(I)*EXP(-C*X(I))

P = P + (X(I)*EXP(-2*C*X(I)))/Y(I)

CONTINUE

DO 21 I = M + J

ES = ES + EXP(-C*X(I))
FS = FS + EXP(-2.0*C*X(I))/Y(I)
QS = QS + X(I)*EXP(-C*X(I))
PS = PS + (X(I)*EXP(-2.0*C*X(I)))/Y(I)

21 CONTINUE
E = E + ES
F = F + FS
Q = Q + QS
P = P + PS
QP = (E/F) = (Q/P)

TYPE 921, QP
921 FORMAT (3HQP=, F20.8)
GO TO 974
END
APPENDIX C

Fitting The Gaussian And Parabola Using The IBM 1620 Computer in Fortan II Language.
**ZZFORX**

*FANDK1404*

```
DIMENSION X(40), Y(40), YY(40), YY(40), T(40), U(40), N(40), XX(40)

DIMENSION ZZ(40), R(40), TD(40)

DIMENSION X(40), XZ(40), YZ(40)
```

301  B = 0

```
AA = 0
BB = 0
CC = 0
CD = 0
DD = 0
EE = 0
FF = 0
SU1 = 0
SUN = 0
SUP = 0
SUR = 0
SUS = 0
SUT = 0
SUV = 0
SW = 0
SUX = 0
SUY = 0
PA = 0
PA = 0
PA = 0
PAE = 0
```

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READ 31, J
31 FORMAT(I2)

READ 3, (X(I), Y(I), I=1, J)
3 FORMAT(F6.3, F5.0)

READ 49, N, L, K, M
49 FORMAT(I2, I2, I2, I2)

974 ACCEPT 975, C
975 FORMAT(F14.12)

ES = 0
FS = 0
QS = 0
PS = 0
E = 0
F = 0
P = 0
Q = 0

23 DO 20 I = 1, N

E = E + EXP(-C*X(I))
F = F + EXP(-2*C*X(I))/Y(I)
Q = Q + X(I)*EXP(-C*X(I))
P = P + (X(I)*EXP(-2*C*X(I)))/Y(I)
20 CONTINUE

DO 21 I = M, J

ES = ES + EXP(-C*X(I))
FS = FS + EXP(-2*C*X(I))/Y(I)
QS = QS + X(I)*EXP(-C*X(I))
PS = PS + (X(I)*EXP(-2*C*X(I)))/Y(I)
21 CONTINUE

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CONTINUE

E = E + ES
F = F + FS
Q = Q + QS
P = P + PS
GP = (E/F) - (Q/P)
S = E/F

DO 18 I = 1, J

YY(I) = B * EXP(-C * X(I))
TD(I) = Y(I) - YY(I)
T(I) = Y(I) + YY(I)
W(I) = 1 / T(I)

CONTINUE

DO 45 I = L - K

AA = AA + W(I) * TD(I)
BB = BB + W(I) * X(I)
DD = DD + W(I) * TD(I) * X(I)
EE = EE + W(I) * (X(I) ** 2)

CONTINUE

FE = (BB + BB)

A = ((-AA + EE) + (C * CB)) / ((-C * CB) + FF)
WW = (DD - CD + AA * BB) / (1 - (DD * EE) + FF)

DO 10 I = L - K

XX(I) = A - WW * X(I)
ZZ(I) = XX(I) - TD(I)
PAA = PAA + W(I) * (TD(I) - XX(I)) ** 2

CONTINUE

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\[ XY(I) = CR - wW\cdot X(I) \]
\[ PAB = PAB + w(I) \cdot (TD(I) - XY(I)) \cdot **2 \]
\[ CS = A+1 \]
\[ XZ(I) = CS - wW\cdot X(I) \]
\[ PAC = PAC + w(I) \cdot (TD(I) - XZ(I)) \cdot **2 \]
\[ CT = WW - 1 \]
\[ YX(I) = A - CT \cdot X(I) \]
\[ PAD = PAD + w(I) \cdot (TD(I) - YX(I)) \cdot **2 \]
\[ CU = WW + 1 \]
\[ YZ(I) = A - CU \cdot X(I) \]
\[ PAE = PAE + w(I) \cdot (TD(I) - YZ(I)) \cdot **2 \]
\[ 10 \text{ CONTINUE} \]
\[ DO 920 1 = 1, N \]
\[ SUM = SUM + (Y(I) - \sigma \cdot EXP(-C\cdot X(I))) \cdot **2) / Y(I) \]
\[ AB = B + 1 \]
\[ SUN = SUN + (Y(I) - AB \cdot EXP(-C\cdot X(I))) \cdot **2) / Y(I) \]
\[ AC = B - 1 \]
\[ SUP = SUP + (Y(I) - AC \cdot EXP(-C\cdot X(I))) \cdot **2) / Y(I) \]
\[ CL = C \cdot 60000001 \]
\[ SUR = SUR + (Y(I) - \sigma \cdot EXP(-CL \cdot X(I))) \cdot **2) / Y(I) \]
\[ CM = C \cdot 60000001 \]
\[ SUS = SUS + (Y(I) - \sigma \cdot EXP(-CM \cdot X(I))) \cdot **2) / Y(I) \]
\[ 920 \text{ CONTINUE} \]
\[ DO 930 1 = M \cdot J \]
\[ SUT = SUT + (Y(I) - \sigma \cdot EXP(-C\cdot X(I))) \cdot **2) / Y(I) \]
\[ AB = B + 1 \]
\[ SUV = SUV + (Y(I) - AB \cdot EXP(-C\cdot X(I))) \cdot **2) / Y(I) \]
\[ AC = B - 1 \]
\[
\text{SU}_n = \text{SU}_n + \frac{C + \exp(-C \cdot \text{x}(I)) \cdot \text{x}(I) \cdot \text{X}(I)}{Y(I)}
\]

\[
\text{CL} = C + \exp(-C \cdot \text{x}(I)) \cdot \text{x}(I) \cdot \text{X}(I)
\]

\[
\text{SU}_x = \text{SU}_x + \frac{(Y(I) - \exp(-\text{CL} \cdot \text{x}(I)) \cdot \text{x}(I) \cdot \text{X}(I)) \cdot \text{x}(I)}{Y(I)}
\]

\[
\text{CH} = C + \exp(-\text{CL} \cdot \text{x}(I)) \cdot \text{x}(I) \cdot \text{X}(I)
\]

\[
\text{SU}_y = \text{SU}_y + \frac{(Y(I) - \exp(-\text{CH} \cdot \text{x}(I)) \cdot \text{x}(I) \cdot \text{X}(I)) \cdot \text{x}(I)}{Y(I)}
\]

\[
\text{CONTINUE}
\]

\[
\text{SU}_x = \text{SU}_x + \text{SU}_y
\]

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\text{SU}_n = \text{SU}_n + \text{SU}_y
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\text{SU}_n = \text{SU}_n + \text{SU}_y
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\text{SU}_n = \text{SU}_n + \text{SU}_y
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\text{SU}_n = \text{SU}_n + \text{SU}_y
\]

\[
\text{SU}_n = \text{SU}_n + \text{SU}_y
\]

\[
\text{PUNCH 500, B}
\]

\[
\text{509 FORMAT(2Hd=, F10.4)}
\]

\[
\text{PUNCH 42, (I, X(I), I, Y(I), I, YY(I), I=I+1,J)}
\]

\[
\text{FORMAT \(2 \pi X(12, 2H) = F_6 \cdot 3, ZmY(12, 2H) = F_10 \cdot 4, 3mYY(12, 2H) = F_10 \cdot 4\)}
\]

\[
\text{PUNCH 101, (I, T(I), I, I(I), I=I+1,K)}
\]

\[
\text{FORMAT \(2 \pi T(12, 2H) = F_15 \cdot 8, 2mW(12, 2H) = F_15 \cdot 8\)}
\]

\[
\text{PUNCH 107, (I, T(I), I=I+1,K)}
\]

\[
\text{FORMAT \(3HTS(12, 2H) = F_15 \cdot 8\)}
\]

\[
\text{PUNCH 200, C}
\]

\[
\text{FORMAT \(2HC=, F_20 \cdot 12\)}
\]

\[
\text{PUNCH56, (I, XX(I), I, ZZ(I), I=I+1,K)}
\]

\[
\text{FORMAT \(3HXX(I2, 2H) = F_15 \cdot 8, 3mZZ(I2, 2H) = F_15 \cdot 8\)}
\]

\[
\text{PUNCH 700, A, WW}
\]

\[
\text{FORMAT \(2H=, F_25 \cdot 8, 3HVV=, F_25 \cdot 8\)}
\]

\[
\text{PUNCH 911, PAA}
\]

\[
\text{FORMAT \(4HPAA=, F_20 \cdot 8\)}
\]

\[
\text{PUNCH 102, SUN, B, SUN, A}
\]

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PUNCH 103, SUP, AC

102 FORMAT ( 4H$UM=, F15.8, 2$AB=, F10.4, 4H$UN=, F15.8, 3$AB=, F10.4)

103 FORMAT ( 4H$UP=, F15.8, 3$AC=, F10.4)

PUNCH 104, SUR, CL, SUS, CM

104 FORMAT ( 4H$UR=, F15.8, 3$CL=, F10.4, 4H$US=, F15.8, 3$CM=, F10.4)

PUNCH 800, PAB, PAC

800 FORMAT ( 4H$AB=, F20.8, 4$PAC=, F20.8)

PUNCH 801, PAD, PAE

801 FORMAT ( 4H$AD=, F20.8, 4$PAE=, F20.8)

PUNCH 921, UP

921 FORMAT ( 3H$P=, F20.8)

100 CONTINUE

GO TO 301

END
BIBLIOGRAPHY


