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RESEARCH ARTICLE

Simulation of Positron Lifetime Spectra in Aluminium: Influence of Time Response Function and Detector Configuration

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ABSTRACT

This study investigates the influence of various factors on the quality and analysis of positron lifetime spectra. Theoretical simulations were performed to examine how these factors affect the quality and analysis of the positron annihilation spectrum. An aluminium (Al) sample was used to assess the spectra quality. The factors studied in this simulation were: the thickness of the material, the gap between the sample and detectors, and the angle between the two detectors. The thickness of the material was varied as 0.5,1, 1.5, 2, 2.5, 3, 3.5 and 4 mm, and the gap was varied as: 1, 2, 3,4,5,6,7 and 8 n air, and the angle was varied as:180o,190o,200o and 210o. The positron annihilation spectra were analyzed using the PEPEPOSFIT program to obtain the values of the lifetime components and the resolution function (FWHM).

It was observed that as the thickness of the sample material and the gap between the sample-source sandwich and detectors increases, the spectra become distorted. Furthermore, with an increase in the angle between the two detectors, the spectra become highly distorted. The setup with two detectors in a collinear (180°) geometry yielded the optimal spectrum. The spectra deviated from this optimal shape as the angle increased. At an angle of 210°, the spectrum was completely distorted, where three peaks appeared. This is attributed to the effect of the non-collinearity function on the integrity of the positron lifetime spectrum.

Keywords: Positron, Lifetime spectrum, Annihilation, Time response function

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1. Introduction

Positron is the antiparticle of an electron, produced by the nuclear decay of neutron-deficient nuclides such as ^{22}Na, upon the injection of β^+ particle into a sample, it dissipates energy via inelastic collisions with its environment until achieving thermal equilibrium. Moderated positron experience spontaneous annihilation with a mediums electron occurs at a frequency depending upon the electron density of the medium, with lifetimes generally ranging from 100 to 500 picoseconds [1]. The positron is a member of the lepton group and follows to Fermi Dirac statistics[2].

PALS is the newest and most effective method used to measure microscopic size of defects in the molecular structure, Additionally, Positron Doppler Breading Annihilation Radiation (DBAR) is among the methods to obtain information about structural change [3]

The positron annihilation lifetime measurements produce a curve known as the positron lifetime spectrum [4]. Unique insights on math-material features may be obtained using the positron annihilation lifetime spectroscopy (PALS) approach, which employs the positron as a probe to detect the size of sub-nano-metric holes in amorphous solids or liquids [5]. In conventional PAT measurements, the positrons injected into the investigated material can penetrate a distance of 10 -1000 μm in solids before annihilation depending on the material density; hence, the positrons probe bulk material in such measurements[6].

The utility of positron annihilation spectroscopies (PAS) for the characterization of metals, ceramics, and polymers is undeniable, and its application to investigating flaws and pores in these materials is well-established. PAS encompasses several techniques that utilize positroniums (Ps) as probes of matter. Of them, positron annihilation lifetime spectroscopy (PALS) is the most well-liked because it uses the physicochemical features of the material to determine the relative intensities and lifetimes (τ) of positron states and how they interact with matter [7]. On an atomic scale, the positron is a probe particle; when it penetrates a substance, it exhibits a feature that makes PALS sensitive, During fast thermalization, positrons lose much of their initial kinetic energy due to collisions with electrons and, later, phonons. The positron is able to achieve thermal equilibrium with the material's lattice structure because to this energy dissipation [8].

When the temperature is just right, the positron may scan millions of sites in the crystal lattice all at once as it diffuses through it. When contrasted with the nearby undisturbed lattice structure, The positron repulsion and electron density are both reduced in materials with open volume defects, which include semiconductors, single-crystal metals, and vacancies, clusters of vacancies, dislocations, and grain boundaries [9].

In technical terms, the positron's lifetime may be determined by comparing the timestamps of the ^{22}Na and 1274keV gamma-rays that were released at its birth and those released upon its annihilation with an electron, respectively, and finding the time difference (511 keV). The gamma beam value, that comes with the start signal tothe1274 keV γ beam, is determined as the signal spectrum of the birth of positrons[10]. Utilizing scintillators allows for the conversion of gamma-rays into optical light. The photoelectrons generated from the photocathode by the scintillation light are amplified by coupling these scintillators with photomultiplier tubes (PMTs). An electrical signal with the crucial energy and temporal data is the end product of this amplification [4].

The purpose of this study is to simulate the annihilation of positron in aluminium theoretically by programing calculations of decay function and response function to determine the effects of configuration of instrumental response function such as configuration of detectors, where different angle (θ) between detector (D1) and detector (D2) are taken into accounts, i.e the deviated angle from co-linear configuration (180°), these angles has been determine by the percentage of photons that detected by detectors, in other word, the intensity of counted photons, also the effect of voids in the aluminium on positron lifetime spectrum has been determine and the different thickness (x) of sample are taken into accounts to show its effect on behavior and analysis of positron lifetime spectrum. Second part of this study is the analysis of obtained spectra to determine the values of one and second components of positron lifetime spectrum $(\tau_1$ and $\tau_2)$, respectively, also determine resolution function (R) quantity, or the FWHM (full width at half maximum).

2. Method and Theory

A material's electrical structure can affect the positron's behavior. The electron-density distribution in the host material may be inferred from the positron lifetime τ, which also gives valuable insights on metal and material flaws**.**

The simulation method was concerned on the of the configuration of the practical instrumental function such as detectors adjustment, sample thickness and the distance between positron source-sample sandwich (figure1) using the following theory:

One way to characterize the positron implantation profile inside a sample is by [11]:

$$P(x) = e^{-\alpha_+ x} \qquad (1)$$

where x is the thickness of sample and α_+ is positron absoption coefficient which given by:

$$\alpha_+ = \lim_{x \to 0}\left(\frac{-d(P(x))}{dx}\right) \qquad (2)$$

One can define a practical mean positron implantation range ($R_+ = \alpha_+^{-1}$), which depends on the sample-mass density $\rho(g/cm^3)$ and the maximum energy E_m^n (MeV) of the positron spectum as [11].

$$\alpha_+ = R^{-1} = \frac{c_+ \rho}{E_m^n} \quad \left(\frac{cm^{-1}}{MeV}\right) \qquad (3)$$

where ρ is the mass density of the target of atomic number (Z) and E_m represents the positron maximum energy. n is constant correlated to the forbiddenness and allowed of β^+ transitions.

According to the practical parameter cosidrations[3], $c_+ = 16 \ \left(\frac{cm^2}{g}\right)$ and $n = 1.4$ independed of the atomic number of the sample.

As fraction (f) of positron absorbed in a target of thickness (x) equals $(1 - \exp(\alpha_+ x))$, the transmission range (R) of positron can then be easily determined from [3]:

$$R\left({}^{g}/_{cm^2}\right) = \frac{\ln\left(\frac{1}{1-f}\right)}{\alpha_+} \qquad (4)$$

Each of the many possible states of a positron has its own unique lifespan, denoted as $\tau_i = 1/\lambda_i$.This means that the positron lifespan spectrum, which is the likelihood of annihilation at time t, is the product of the components of exponential decay [5]:

$$-\frac{dN(t)}{dt} = \sum_i I_i \lambda_i e^{(-\lambda_i t)} \qquad (5)$$

$$\sum_i I_i = 1$$

Where I_i is intensity

by integrating eq.(5) one gets $N(t) = \sum_i I_i e^{-\lambda_i t}$

subjected to relative intensities Ii. In this case, N(t) is the likelihood that a positron will still be alive at time t following its emission.

The lifetime spectrum can be characterized by a continuous decay function [12]:

$$N(t) = \int_0^\infty I(\tau) e^{-\frac{t}{\tau}} d\tau \qquad \text{where } \int I(\tau) = 1 \qquad (6)$$

The response function may be described as a sum of Gaussians [13]:

$$G(t) = \sum_{i=1}^{m} w_i G_i(t) \qquad (7)$$

where w_i represents the weight of the i^{th} Gaussian, such that $\sum_{i=1}^{m} w_i = 1$

$$G_i(t) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{((t-t_z)-\Delta t_i)^2}{2\sigma^2}} \qquad (8)$$

The variables σ and FWHM/2.356 reflect the standard deviation and statistical volatility of the prompts, respectively.

Δt_i is the shift in the centroid position and t_z: time zero channel number.

That is, asymmetrical resolution curves are possible by shifting their centroids relative to one another.

The correct choice number of Gaussian components is necessary for accurate description of the time response function

The positron lifetime spectrum is the convolution of resolution function and decay function and superimpose with random coincidence. The problem is to convolve the time response function with decay function to give lifetime spectrum.

The lifetime spectra are generally assumed to be well approximation by a sum of decaying exponentials convoluted with the resolution function of the system and superimposed with random coincidence (background). The starting point for the generation of lifetime spectra is the convolution integral describing the content of the kth channel of a lifetime spectrum, F_k[14]:

$$F_k = \int_{t=t_k}^{t_{k+1}} dt \int_{t=-\infty}^{+\infty} dt\, G\,(t - \Delta t - t_z) \sum_i I_i \lambda_i e^{(-\lambda_i t)} + B \tag{9}$$

G(t) is the resolution function of the measuring system (normalized to one). t_z , the time-zero point of the system, is regarded as a constant, B means the constant background in the lifetime spectrum.

In Eq.(9), the function $N(t)$ represents the decay curve consisting of n exponential terms:

$$\begin{aligned} N(t) &= \sum_{i=1}^{n} I_i \quad e^{(-\lambda_i\, t)} \qquad \text{For } t \geq 0 \\ &= 0 \qquad \text{For } t < 0 \end{aligned} \tag{10}$$

If one writes for the variables of the integrations in Eq.(9)

$$t_k = k * \Delta \ (k=0,\pm1,\pm2,\ldots) \tag{11a}$$

$$t_j \ = j \ * \ \Delta\,/2 \quad (j = 0, \pm1, \pm2, \ldots.) \tag{11b}$$

where Δ is the channel width of spectra to be generated (time calibration), and defines the abbreviation

$$h(t) = G(t - \Delta t - t_z) * \ N(t) \tag{12}$$

the t-integration in Eq.(9) can be replaced by a sum of $h(t)$ values by using Simpson's integration formula:

$$F_k - B = \int_{t=t_k}^{t_{k+1}} dt \frac{\Delta}{3}\{\ldots + h_{(t-3)} + 2h_{(t_{-2})} + h_{(t_{-1})} + 2h_{(t_0)} + h_{(t_1)} + 2h_{(t_2)} + h_{(t_3)} \ + \ldots\ldots.\} \tag{13}$$

Where $h(t)$ is the convolution of response function with decay function

This leads to the expression

$$F_k - B = \frac{\Delta}{3} \sum_{j=-\infty}^{\infty} \{2N(t_{2j}) \int_{\tau=t_k-t_{2j}}^{t_{k+1}-t_{2j}} d\tau\, G(\tau - t_z) + N(t_{2j+1}) \int_{T=t_k-t_{2j+1}}^{t_{k+1}-t_{2j+1}} d\tau\, G(\tau - t_z)\} \tag{14}$$

and by using Eqs.(11a) and (11b) one gets[14]

$$\begin{aligned} F_k - B = \frac{\Delta}{3} \sum_{j=-\infty}^{\infty} \{ &2N(\Delta j) * [\int_{\Delta(2k-2j)/2}^{\Delta(2k-2j+1/2} d\tau\, G(\tau - t_z) + \int_{\Delta(2k-2j+1)/2}^{\Delta(2k-2j+2)} d\tau\, G(\tau - t_z)] + N(\Delta(2J \\ &+ 1/2) * \ [\int_{\Delta(2k-2j-1)/2}^{\Delta(2K-2j)/2} d\tau\, G(\tau - t_z) + \int_{\Delta(2k-2j)/2}^{\Delta(2k-2j+1)/2} d\tau\, G(\tau - t_z)]\} \end{aligned} \tag{15}$$

Eq.(15) contains only integrals of the resolution function over the channel width Δ/2:

$$p_l = \int_{\Delta 1/2}^{\Delta(1+1)/2} d\tau\, G(\tau - t_z). \tag{16}$$

If one defines P_l' as the l^{th} count number of a measured prompt spectrum (channel width Δ/2); background (B). The expression for the normalized l^{th} channel reads[14]

$$P_l = \frac{P'_l - B}{\sum_{l_1}(P'_{l_1} - B)} \tag{17}$$

If Eqs.(10) and (16) are used in Eq.(15), one gets after some simple transformations

$$F_k - B = \frac{\Delta}{3}\sum_{i=1}^{n} I_i\{2p_{2k+1} + \sum_{j=0}^{\infty} \exp\,(-\lambda_i \Delta j[2 + \exp\left(-\frac{\lambda_i \Delta}{2}\right) p_{2k-2j} + \exp\,(-\lambda_i \Delta\big(2 + \exp(+\lambda_i \Delta/2)\, p_{2k-2j-1}\big]\} \tag{18}$$

This equation contains the resolution function no longer as an analytical function but in the form of discrete values. Eq(18) enables to generate lifetime spectra with n component, lifetimes τ_i ($^1/_{\lambda_i}$), and intensities I_i.

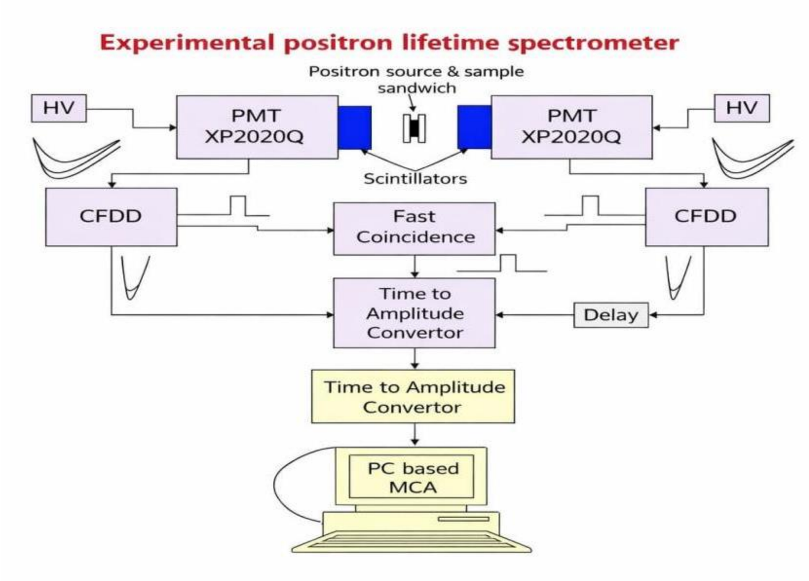

Figure 1. A schematic diagram of the positron annihilation lifetime spectroscpy system.

3. Results and dicussion

3.1. Influence of Instrumental Response Function

To know the effect of configuration of time response function, different distances between sample-source sandwich and detectors are taken. The gaps in between sample of 1mm in thickness are varied as: 4,5,6,7mm both in the left and right. As shown in figure2, the left-hand side be more distortion as the gap increases, where the increasing of gap negatively affects the spectra quality. The analysis of these spectra gives the increasing in full width at half maximum (R) as gap increase. FWHM obtained correspond to the gaps values as obtained by PEPOSFIT program [15] are: when the gap 4mm, the obtained FWHM was 200ps, gap with value 5mm, the obtained FWHM was 300ps, gap with 6mm, the obtained FWHM was 400ps and when the gap was 7mm, the FWHM was 500ps.

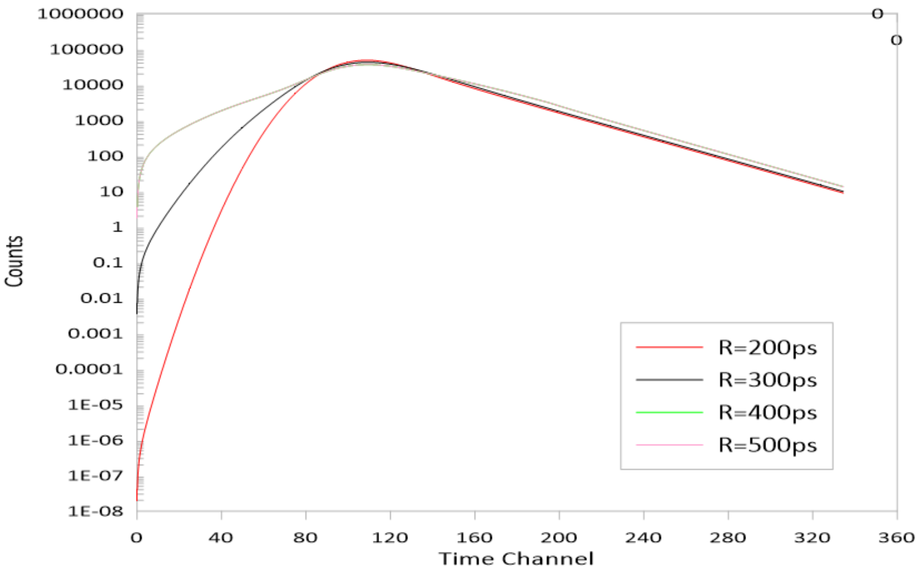

Figure 2. Shows the effect of time resolution on behavior of positron lifetime spectra according to gap variation.

3.2. Influence of Material Thickness

In the first part of this section, we examine how the variation in the thickness of the sample affects the positron lifetime spectrum. This includes four different thickness variants are considered: (0.5,1,1.5, and 2) mm. As the thickness of the sample increases, the lifetime spectrum tends to shift towards the right-hand side, as shown in figure3.

In another part of this section, the thickness of the sample more than 2 mm has been studied. Four samples with different thicknesses varying from 2.5 to 4 mm, separated by 0.5 mm increments, are considered. As shown in figure4, the positron lifetime spectra tend to shift towards the right-hand side, it has the same of the thickness considered in the first part, but the spectra rise to the right-hand side sharply and become more divergent.

3.3. Analysis of Spectra

The analysis of the spectra of figure3 gives a one-component lifetime spectrum (τ_1). Each spectrum has a τ_1 value related to the thickness of the sample. When the thickness was (0.5, 1, 1.5, 2) mm, τ_1 values were (50, 60, 70, 80) ps, respectively, as obtained from the analysis program (PEPOSFIT). This indicates that as the thickness increases, the positron lifetime inside the material also increases, meaning that the positron takes more time inside the material before annihilation. The occurrence of one component of lifetime, which analyzed from the spectra in figure.3, indicates that there are no defects in the studied sample. There are two components obtained by analysis of the spectra in figure.4 (τ_1, τ_2). In each spectrum, τ_1 was 50 ps, and τ_2 varied as (200, 220,240,260) ps. The occurrence of two components indicates that the there are voids in the sample, where some of the positrons annihilate in these voids. The values of τ_2 correspond to the variation in the thickness of the sample used. Thus, τ_2 = (260) ps corresponds to thickness = (2.5, 3, 3.5, 4) mm. This leads to that, as the thickness of the material increases, the second lifetime component (τ_2) increases, where the material becomes more defective with thickness increasing.

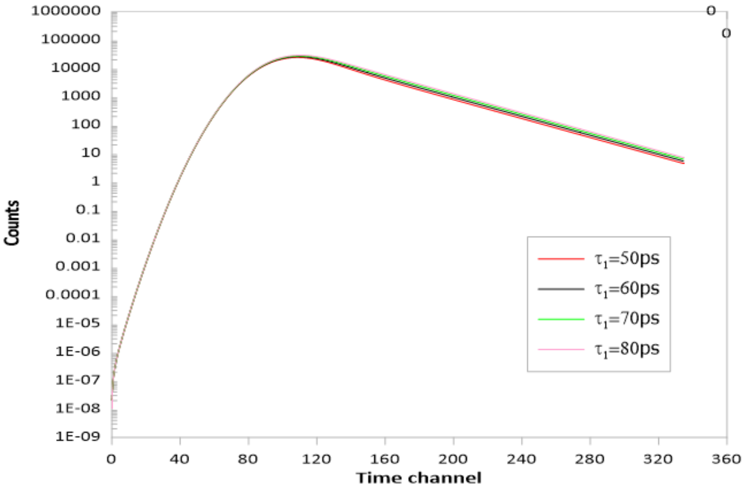

Figure 3. The shows the effect of thickness variation (0.5,1,1.5,2) mm on the PALS.

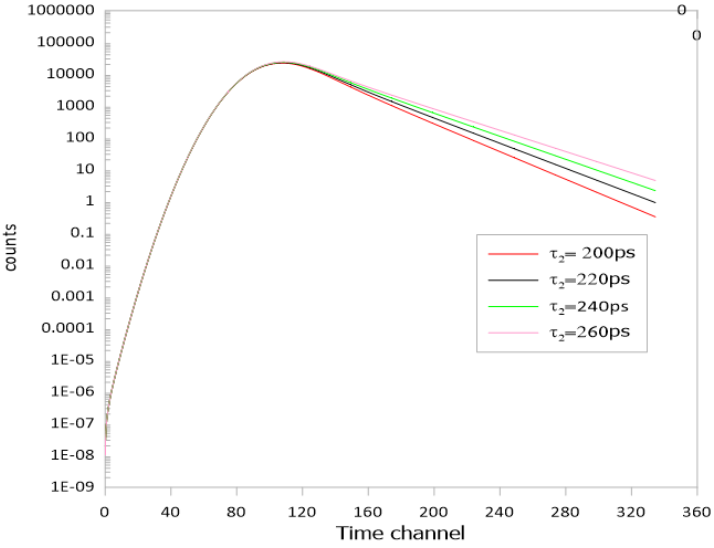

Figure 4. The shows the effect of thickness variation (2.5,3,3.5,4) mm on the PALS.

3.4. Influence of detectors configuration

In order to investigate the detectors configuration effect, different two-detectors configuration has been simulated. In this part, the thickness of material fixed at 1 mm and the vertical size of the gap with air fixed at 1 mm on each side of the detectors. Different angles between the two detectors are considered (180°, 190°, 200° and 210°)

As shown in figure.5 the distortion in the spectrum increase as the angle increase (>180°). The optimal spectrum is obtained when the angle equal to 180°. At this angle all photons resulted from positrons annihilation are detected and recorded in the instrumental function. The positron lifetime spectrum deviated from optimal spectrum when the angle increases more than 180°, where three peaks appear at angle 120° .

Distortion is clear at the left-hand side of the spectra. As we notice in the figure, there are three peaks that appear when the angle is 210°.

This indicates that the instrumental system produces three Gaussian convolutions with the decay function of positron annihilation. This is due to the fact that some of the photons resulting from positron generation and annihilation (start and stop) cannot be detected by the detectors.

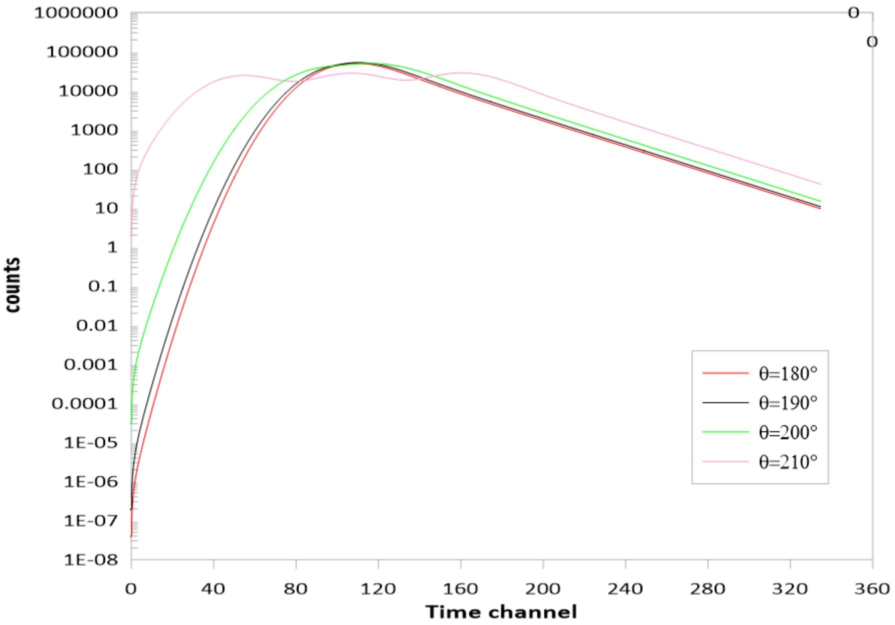

Figure 5. Effect of angle variation between the two detectors on the PALS.

4. Conclusions

The findings of this study clearly demonstrate that the quality of the positron lifetime spectrum is strongly influenced by several experimental parameters, particularly the thickness of the aluminium, the separation distance between the detectors, and the overall geometric configuration of the detection system. A systematic study found that the positron lifetime spectra become noticeably less clear and accurate when the thickness of the aluminum and the space between detectors are increased. The interpretation of the positron annihilation properties becomes more ambiguous due to this deterioration, which directly impacts the capacity to analyze the lifetime spectra.

Plus, the research proved that the degree of spectrum distortion is highly dependent on the detectors' angular layout. The likelihood of losing annihilation photons rises, leading to distorted lifetime spectra, when the detection angle surpasses ideal circumstances (> 180°). Severe spectrum distortion occurs at angles 210°, when this effect is most noticeable. It is vital to create a valid lifetime spectrum, however there is a reduced possibility that detectors detected all photons resulting from the annihilation process, which is the fundamental source of this distortion.

The system, on the other hand, performs much better when the detectors are arranged in a co-linear fashion (180°). The photons produced by positron annihilation are more likely to be detected at this angle, leading to less spectrum distortion and more accurate results. Better dependability is supported by this ideal alignment. extraction of lifetime components and contributes to a more accurate understanding of the microstructural characteristics of the studied material.

In order to get high-quality positron lifetime spectra, the study highlights the significance of adjusting material thickness, detector spacing, and angular arrangement. To improve spectral resolution, decrease measurement errors, and guarantee robust and accurate analysis in PALS applications, these parameters must be carefully controlled. These findings show how experimental settings affect the technique's performance and point the way toward future research that aims to make lifespan assessments more reliable and easier to understand.

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