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Study of Positron Annihilation in Metals

A Research

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By

Ali Mohammed Hashim Jalab
B.Sc.in physics
University of Mustansiriyah (2006)

Supervised by

Asst. Prof. Dr. Mohanad Hussein Oleiwi

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Supervisor Certification

I certify that this research entitled **" Study of Positron Annihilation in Metals"** was prepared by the student **(Ali Mohammed Hashim Jalab)** under my supervision at the College of Education for Pure Sciences, University of Babylon as partial fulfillment of the requirement for the Degree of Higher Diploma Education / Physics of Materials and its Applications.

Signature

Name: Dr. Mohanad H. Oleiwi

Title: Professor

(Supervisor)

Date: /12 / 2021

Head of the Department Certification

In view of the available recommendations, I forward this research for debate by the examining committee.

Signature

Name: Dr. Khalid H. Abass

Title: Professor

(Head of Physics Department)

Date: / 12 / 2021

Examining Committee Certification

We the examining committee, certify that we have read the research, "**Study of Positron Annihilation in Metals**" and examined the student (**Ali Mohammed Hashim Jalab)**in its contents. We found that it is adequate with as the research meets the standards for the Degree of Higher Diploma Education / Physics of Materials and its Applications.

Signature:

Name: Dr. Fouad A. Majeed

Title: Professor

Date: /12 /2021

Chairman

Signature:

Name: Dr. Rawaa M. Obaid

Title: Assistant Professor

Date: /12 /2021

Member

Signature:

Name: Dr. Ali O. Muhsen

Title: Assistant Professor

Date: /12 /2021

Member

Signature:

Name: Dr. Mohanad H. Oleiwi

Title: Professor

Date: /12 /2021

Supervisor

Approved by the Dean of the College of Education for Pure Science, University of Babylon

Signature:

Name: Dr. Bahaa Hussien Salih Rabee

Title: Professor

Date: /12 /2021

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This is certify that I have read this research, "**Study of Positron Annihilation in Metals**" and I found that this thesis is qualified for debate.

Signature:

Name: Dr. Khalid H. Abass

Title: Professor

Address: The College of Education for Pure Science, University of Babylon

Date: /12 /2021

Scientific Supervisor's Certification

This is certify that I have read this research, "**Study of Positron Annihilation in Metals**" and I found that this thesis is qualified for debate.

Signature:

Name: Fatema M. Hussein

Title: Assistant Professor

Address: The College of Education for Pure Science, University of Babylon

Date: / 12 /2021

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List of Abbreviations and Symbols

A	**Atomic mass**
C_d	Defect concentration
DB	Doppler Broadening
D_+	Positron diffusion
E_{B+}	Maximum Positron energy
E_g	Energy gap
E_{K+}	Positron kinetic energy
E_b	Binding energy
E_{cr}	Critical energy
E_i	Ionization energy
****	Fraction of annihilation positrons
(t)	Gaussian function
I	Intensity
K	Trapping rate
N(t)	total Number of count
$N_{b,d}$	Number of positrons in the bulk and deffect site respectively
$\bar{R}_+$	Mean implantation depth
T	Temperature (K^o)
U	Reduced energy parameters
****	Work function
a_{pc}	Bohr radius of Positronium
c	Speed of light in vacuum
d	Depth; Thickness
f	Fraction; Factor
g	Enhancement factor
k_B	Boltzmann constant
m	Magnetic quantum number
m_o	Electron(or positron) rest mass
n_-	Electron density
n_d	Fraction of positrons trapped
p	Momentum
p_T	Positron-electron pair transverse to the Photon emission direction
p_L	Positron-electron pair longiudinal to the Photon emission direction

Symbol	Definition
q	Screening parameter
$\mathbf{r_s}$	One electron radius
$\mathbf{r_o}$	Classical electron radius
s	Spin
$\mathbf{t_s}$	Slowing-down time
$\mathbf{t_{th}}$	Thermalization time
$\mathbf{t_D}$	Diffusion time
$\mathbf{t_z}$	Zero time
u_c	Specific trapping rate
x	Distance
$\boldsymbol{\alpha^+}$	Linear absorption coefficient of positron
A	atomic fine structure constant
Ψ	Wave function
β	Beta-rays
γ	Gamma-rays
τ	Lifetime
$\boldsymbol{\tau_1}$	Short-lived component
$\boldsymbol{\tau_2}$	Mid-lived component
$\boldsymbol{\tau_3}$	Long-lived component
$\boldsymbol{\bar{\tau}}$	Mean lifetime
λ	Annihilation rate
$\boldsymbol{\lambda_D}$	Mean free path
$\boldsymbol{\lambda_{p.o}}$	O-Ps pick-off annihilation rate
ρ	Mass density
σ	Standard deviation
Δ	Detrapping rate
$\bar{\upsilon}$	Antineutrino
$\mathbf{u^+}$	Positive muon
a. u	atomic unit
B	Random Coincidence (Background)
$\mathbf{r_s}$	electron radius
CFD	Constant-Fraction discriminator
FWHM	Full Width at Half Maximum
MCA	**Multichannel analyzer**

List of Abbreviations and Symbols

Symbol	Definition
ν_e	electron neutrino
$\bar{\nu}_\mu$	muon antineutrino
Z	nucleus atomic number
α	the atomic fine structure constant
Ps	positronium
Δf/f	frequency shift
v_L	longitudinal center of mass velocity
x	any atom, molecule, or ion

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Dedication

To ----------

my father -------

My mother--------

My wife --------

My supervisor

My heart throb, Iraq.

With all the love and appreciation

ALI

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Best praise is to Allah, God of all, most Merciful, leading me to achieve these results in my work.

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Ali

Abstract

This study, included simulating of positron interaction with the matter where the positron lifetime spectrum was generated by generating the time response function with decay function and convoluted with random coincidence (Background). The positron interaction simulation was performed with pure matter and defective matter, the effect of some parameter was studied on its lifetime spectrum, such as high and low resolution, short ($\tau_{1)}$, mid ($\tau_{2)}$ and long (τ_3) lived components.

Also Different values for one-Gaussian (lifetime response function) components were convoluted with constant values of positron lifetime for one, two and three components (τ_1, τ_2 and τ_3). All these components have been taken equal intensities to show the effect of resolution function on these components also the random coincidence (B) were fixed at 0.001% of the peak, where the resolution ranged from 500 - 1400ps.

It was concluded that the positron have been tended to annihilate in defects, and the background is completely disappeared at three components of lifetime spectrum, also as the resolution increase, the spectrum approach to Gaussian shape and as τ_1, τ_2, and τ_3 increase, the right hand side of spectrum approach to a linear shape, and it has been observed that the high resolution leads to distortion in lifetime spectral shape.

1.1 Introduction

In 1930 Dirac postulated positron, as the "negative" energy extension of his theory of electron energy levels [1].

The positron is the anti-particle of the electron, it has the same mass, the same spin, but has the opposite charge sign. Following the Anderson discovered the existence of positron in cosmic rays experimentally by using Wilson chamber , is a particle detector used for visualizing the passage of ionizing radiation. [2**]**.

The electron-positron system is unstable. It usually annihilates, emitting two gamma photons. The two-gamma annihilation process was discovered in 1937 when O. Klemperer showed by coincidence technique that annihilation photons with energy≈0.511 MeV are generated in opposite directions [3]. The angular correlation of gamma photons was measured for the first time in 1942 by Beringer and Montgomery. They found that the annihilating pair had a kinetic energy of order less than some keV [4].

Before annihilation, the positron and electron in some substances can form a bound state. The hypothesis of its existence was postulated by Mohorovicic in 1934 and named positronium by Ruark [5] in 1945 before its eventual confirmation by Deutsch in 1951 [6].

When a positron is surrounded by electrons, it may annihilate with one of them, and their masses are converted into gamma rays (photons), normally two or three photons. The converted energies and the emission of these photons can all be measured providing useful information about the material in which the positron annihilates [7].

In aconvential positron annihilation experiment, the positrons are injected into a solid with a mean energy of 200 keV. They slow down to thermal energies with in (1-10 ps) by ionization and excitation reaction in the solid [8]. During this time they penetrate a distance of (10-100)μm depending on the density of the solid.

The applications of positron annihilation to materials science is a kind of coupling with a nuclear technique represented by positron annihilation studied, such investigations require the combination with techniques electron microscopy and x-ray scattering for results comparison, but careful control of other effects is required.

1.2 Positron Sources

Positrons are usually produced from (i) β^+ decay, (ii) pair production, and (iii) μ^+ meson decay.

There are certain radioactive nuclides that decay by emitting positrons and neutrinos (υ) as follows

$$X(A,Z) \rightarrow Y(A,Z-1) + \beta^+ + \upsilon \qquad \text{....(1.1)}$$

parent daughter

There are more than 200 positron emitting nuclides in the table of isotopes of which, however only a few of them are suitable for practical purposes. ^{22}Na, ^{26}Al, ^{56}Co, and ^{58}Co are the most useful emitters of energetic positrons of several hundred keV. Among these, ^{22}Na is favorite mainly due to its convenient half-life (2.602 y), high fraction of decay into positrons (90.4%) and for its low production costs [9].

A beam of monoenergetic slow positrons from eV to keV can be produced from higher-energy positrons emitted by a radioactive source that is thermalized and expelled from a moderator by the negative work function of the positron [10].

The other positron source is obtained in the pair production process. In this method, high energy electron beam from an accelerator is directed into a heavy target to produce bremsstrahlung with energies enough to produce the positron-electron pair. The energy of the electrons necessary to produce an intense beam of slow positrons by this process falls in the range (80-400) MeV. This method was first employed at the Lawrence Livermore National Lab in 1982 [11].

Bombarding nuclei by high-energy particles or photons (> 150 MeV) can evoke the emission of positive or negative π-mesons from the target nuclei. The π^+ meson decays with a mean lifetime of 20.03 ns into a positive muon (μ^+) which in turn decays into a positron with a longer mean lifetime of 2.2μs according to[12]:

$$\mu^+ \rightarrow \beta^+ + \nu_e + \bar{\nu}_\mu \qquad \text{..... (1.2)}$$

where ν_e and $\bar{\nu}_\mu$ are the electron neutrino and the muon antineutrino respectively.

The positron is emitted with a high probability in the direction of the spin of μ^+ [13].

1.3 The Annihilation Process

The annihilation of a positron with an electron is a unique feature of positron interaction in the matter. The electron-positron annihilation process occurs as a result of an overlap between the electron and positron wave functions.

The particles rest mass are converted into electromagnetic energy of $2m_oc^2$ (or 1.022 MeV) where m_o is the electron (or positron) rest mass, and c is the speed of light in vacuum. Positrons may annihilate either in a free state or in a bound state. Selection rules governing the annihilation process lead to [15]:

1. Annihilation with the emission of 0 or 1 photon is forbidden for an isolated electron-positron system. In the presence of a medium, this result is relaxed.
2. Annihilation of electron-positron pairs occurs within an initial distance of the order of Compton wavelength ($\approx 4\times 10^{-13}$ m).
3. Symmetry under charge conjugation requires that the singlet state (total spin s=0 and magnetic quantum number m=0) decays into an even number of photons and that the triplet state (s=0,m=0,$\overline{+}$1) decays into an odd number of photons. The probability of the process decreases rapidly with the number of emitted photons. Thus, only two and three-photon annihilation occur in practice.

In the free annihilation process, three modes of annihilation are considered, single, two, and three-gamma emission modes and their Feynman diagrams are shown in Figure (1.1).

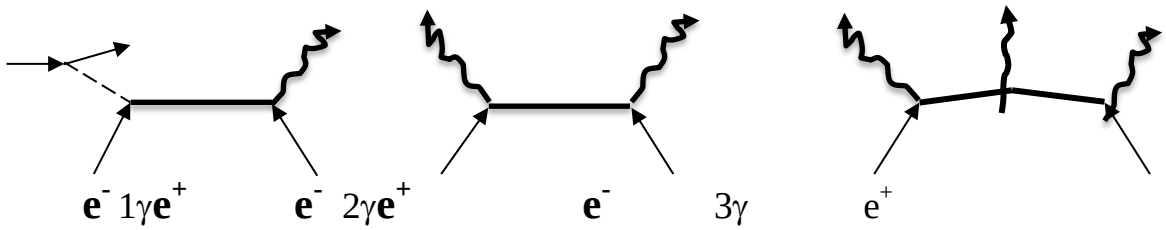

Fig. 1.1: Feynman diagrams for different annihilation modes. Courtesy of [16]

Single-gamma annihilation is possible only in the presence of a third body absorbing the recoil momentum (nucleus or electron). The cross section for this process free space is given by [16]:

$$\sigma_{1\gamma}=\frac{4\pi r_{\circ}^{2}\alpha^{4}Z^{5}}{(\gamma^{2}-1)^{1/2}(\gamma+1)^{2}}\left(\gamma^{2}-\frac{1}{3}\gamma+\frac{4}{3}\right) \qquad \text{..... (1.3)}$$

where r_o is the classical electron radius (2.82 fm), α is the atomic fine structure constant ($\frac{1}{137}$), $\gamma = (1-\frac{v2}{c2})^{-1/2}$, v is the velocity of positron, and Z is the nucleus atomic number. At a nonrelativistic limit, one obtains:

$$\sigma_{1\gamma} = \frac{4}{3}\pi\, r_\circ^2 \alpha^4 Z^5 \frac{c}{v} \quad \text{.... (1.4)}$$

The very strong Z dependence implies that this process is considerable only for the heaviest element, but in practice, the relative probability of this mode is negligible [15].

The predominant mode of annihilation is the two-gamma emission in which two photons of equal energy (0.511MeV) are emitted at 180^o to one another. The Dirac cross section for this mode (in case of free positron annihilates with stationary electron) is [14]:

$$\sigma_{2\gamma}=\frac{\pi r_\circ^2}{\gamma+1}\left\{\frac{\gamma^2+4\gamma+1}{\gamma^2-1}1n[\gamma+\sqrt{\gamma^2-1}]-\frac{\gamma+3}{\sqrt{\gamma^2-1}}\right\} \quad \text{..... (1.5)}$$

At the nonrelativistic limit, $\sigma_{2\gamma}$ is inversely proportional to the positron velocity (v)as [14]:

$$\sigma_{2\gamma} = \pi r_\circ^2 \frac{c}{v} \quad \text{.... (1.6)}$$

The annihilation rate (i.e annihilation probability per unit time) is [14]:

$$\lambda_{2\gamma} = \sigma_{2\gamma} v\, n_- = \pi r_\circ^2 c n_- \quad \text{.....(1.7)}$$

where $n_-$is the electron density at the positron site (r_+), or $|\psi_-(\overrightarrow{r_+})|^2$

In the three-gamma annihilation mode, three photons are emitted approximately 120^o apart with cross section [14]:

$$\sigma_{3\gamma} = \frac{4}{3}(\pi^2-9) r_\circ^2\, \alpha \frac{c}{v} = \frac{4}{3\pi}(\pi^2-9)\alpha\, \sigma_{2\gamma} \quad \text{..... (1.8)}$$

and thus: $\lambda_{3\gamma} = \sigma_{3\gamma} v n_- \simeq \frac{\lambda_{2\gamma}}{372}$ …. (1.9)

The positron lifetime is the inverse of its annihilation rate. Free positrons usually have some kinetic energy (few eV) when they annihilate. In their center-of mass system, the photon energy in the normal mode (two-gamma emission) is exactly $m_o c^2$ =0.511 MeV and the photons are moving strictly into opposite directions. In the laboratory system, the non-zero momentum of the pair causes small deviation from π radians (normally few milliradians). As illustrated in Figure (1.2), the momentum conservation yields a result:

$$\theta \simeq \frac{p_T}{m_o c} \qquad \text{.... (1.10)}$$

where $(\pi - \theta)$ is the angle between the two photons in the laboratory frame, and p_T is the momentum component of the positron-electron pair transverse to the photon emission direction.

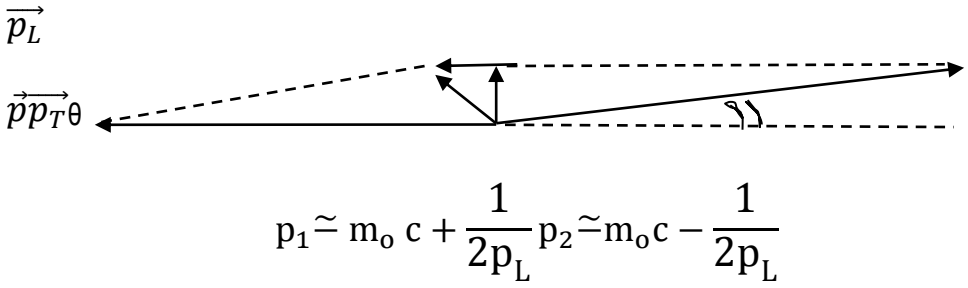

Fig. 1.2: Vector diagram of the momentum conservation in the two-gamma annihilation process. P_L and P_T are the momentum longitudinal and transverse components of the annihilating pair. Courtesy of [16]

A shift of few keV in the energy of annihilation photons is induced by Doppler effect if the pair is not at rest.The frequency shift is $\Delta f/f = v_L/c$, where $v_L$represents the longitudinal center of mass velocity and $v_L = p_L/m_o$. Doppler shift at the energy $m_o c^2$ is [17]:

$$\Delta E = \left(\frac{v_L}{c}\right) E = \frac{1}{2} c\, p_L \qquad \text{.... (1.11)}$$

An overall quantum mechanical treatment of the positron-electron interactions was presented by Arponen and Pajanne [18].

1.4 Positronium; Formation and Annihilation

In some substances, and as a final stage before the positron gets annihilated, a slowing down process may take place in a complicated way. A certain number of positrons from a bound state of a positron and an electron, referred to as positronium.

The positronium (Ps) is a two-body system with properties similar to that of the hydrogen atom, except for quantum electrodynamic details. In case of Ps composed of particles of the same mass, i.e. $m_{e-} = m_{e+} = m_o$,the Ps reduced mass is $\frac{m_o}{2}$ and the Bohr radius is twice that in a hydrogen atom. The binding energy of Ps is numerically equal to 6.8eV. The Ps exists in two states, the singlet $^1s_0$ state or Para-Ps with antiparallel spins of positron and electron, and a triplet $^3s_1$ state or Ortho-Ps with parallel spins of the pair. As the size of Ps is twice that of a hydrogen atom, Ps formation occurs mainly in molecular media which have relatively open structures. This process can be expressed as [17]:

$$e^+ + x \rightarrow Ps + x^+ \quad \text{.... (1.12)}$$

where x may be any atom, molecule, or ion.

Two models have been proposed for the mechanism of Ps formation in condensed matter; the Ore model [19] and the Spur model [20]. The Ore model states that Ps formation is most probable when the positron energy during its slowing down, lies within a gap, such that the kinetic energy of the positron (E_k^+) required to capture an electron from molecule of the medium with ionization energy (E_i), must be greater than E_i-E_b^{Ps}, where (E_b^{Ps}) is the Ps binding energy.

For $E_k^+ > E_i$, the Ps atom is formed with a kinetic energy greater than its binding energy and a rapid break up into a positron and an excited electron occurs during the collision [19].

Inelastic collisions will compete with Ps formation until the positron kinetic energy is less than the lowest electronic excitation energy (E_{exc}). Hence, the formation process is most probable with the energy gap [19]:

$$E_i - E_b^{ps} < E_k^+ < E_{exc} \quad \text{……. (1.13)}$$

Which represents the Ore gap. Its width indicates the fraction of positrons which have formed Ps.

Ps negative ion (Ps^-) may be produced in a medium. It has one bound singlet state which is stable against break up into Ps + e^- by 0. 3267eV [21].

1.5 Positron Lifetime in Different Materials

1.5.1 The Lifetime Method

The lifetime of the positron in a certain material, depends mainly on the electron density distribution around the positron. Usually, positron lifetimes are in the range of (100ps – 142ns), such short lifetimes can be accurately measured with the fast timing technique employed in nuclear spectroscopy.

The positron lifetime (or annihilation rate) is measured in a direct way using the coincidence system by recording the time elapsed between two-gamma photons signaling the birth and death of the positron. The birth signal is a gamma photon emitted simultaneously with the positron from the source nucleus 1.275MeV for the commonly used ^{22}Na isotope) and the death signal is the 0.511MeV annihilation photon. The three-photon annihilation rates can be measured using the triplet coincidence system, but its rate is less than that the two-photon coincidence by a factor of 372. The triplet system is, thus, not frequently used, and only 3-4 counts/s or μci were detected using one of the most improved systems.

The positron lifetime spectrum in a free state has a form of a simple exponential. In any material, positrons may exist in other states, and Ps may also be formed, thus the lifetime spectrum has a finite number of discrete components (states), each is characterized by a lifetime (τ) and relative intensity (I). The lifetime is associated with the effective electron density in the corresponding positron state. The intensity(I) provides a measure of relative positron population [22].

1.5.2 Positron Annihilation in Metals

In metals, the positron interacts strongly with the conduction electrons and forms a many-body system, with the electrons forming a characteristic screening cloud around the positron. Core electrons are tightly bound to the relative nucleus; thus, they are expected to the less perturbed by the presence of the positron than will be the conduction or valance electrons, which are to a large extent free.

The theory of positron annihilation in metals was first developed by Kahan [23], then modified by B randt and Reinheimer [24], and Arponen and Pajanne [25,26]. Starting from the classical expression of Dirac (Eq. 1.7) which does not take into account the fact that thermalizatied positron attracts valence electrons which in turn screen its positive charge, these theories suggest that, the electron density increases near the positron. Resulting in an increase in the annihilation rate.The positron interaction with valance electron or conduction electron may be described by the screened Coulomb potential of the form $\frac{-e^2}{r\exp(-qr)}$ where q is a screeing parameter.

According to Held and Kahana [27] calculations, the Ps bound state formation occurs for $r_s \geq 8.5$. This is not fulfilled by metals and thus, Ps formation is not possible.

The positron can also be annihilated with core electrons which are, in general, much more numerous than the conduction electrons. But the positron is kept away from the core because of the Coulomb repulsion exerted on it by the nucleus. This repulsion, reduces the overlap between the positron and a core electron wave functions and consequently their contributions to the annihilation rate is reduced.

Measurements on positron lifetimes in metals were performed many times during the last two decades. However, different results were obtained. This can be attributed mainly to the uncertainties in data analysis in addition to the methods of sample preparation and to the performance of the timing system used. Only single-lifetime component was observed for perfect (defect-free) metals in all of the previous works.

1.6 Literature Survey

V.P. Shantarovich *et al.* in 2006[28], studied the formation of positronium in solids they found that the large size of defects yields long positronium lifetime.

G.Dulbek *et al.* in 2007[29], developed a new routine (LT 9.0) to examine the defects in material with varying the parameters pressure- volume- temperature, they conclude that the change of pressure- volume- temperature give change in the size of defects in material.

N.Djourelov *et al.* in 2007[30], studied the annihilation lifetime of positron in polymer using positron annihilation spectroscopy technique, they found that the lifetime component increase in large defects of polymer.

C.J.Edwardson in 2013[31], studied the annihilation of positron in thin films and semiconductor variable energy positron annihilation spectroscopy (VEPAS) was used as a problem of oxide film. VEPAS has been found to be useful in studying the more exotic types of material.

D.G. Green *et al.* in 2013[32], used diagrammatic many body theory to calculate the scattering phase shifts, normalized annihilation for positron collisions with the hydrogen like ions, they found that their results for positron annihilation in hydrogen ions provided insights the problem of positron annihilations with core electrons in condensed matter.

E.Boroński, in 2013[33], developed calculations of electron-positron momentum densities in solids, their calculations of annihilation spectra yield lower values for greater momentum.

I.Makkonen *et al.* in 2013[34], developed a computational first principle study of positron trapping at vacancies defects in metals and semiconductor, they found that in the case of metal vacancy, the positron induced ion relaxation has a noticeable effects on the calculated positron lifetime.

S.Pan *et al.* in 2014[35], employed the positron annihilation technique to study the defect recovery in 40 MeV alpha irradiation undopedInSb, they concluded that the increase in the line shape parameter along with defect specific parameter in the temperature reign 75^0C to 150^0C & 200^0C to 300^0C indicate the migration of vacancies and the formation of vacancy clusters, and the defects start disappearing between 300^0C and 400^0C.

K.V.A.Kumar *et al.* in 2015[36], exposed the Bakelite polymer detector material to 8MeV of electron beam, the microstructure changes on electron beam irradiation have beam studied using positron annihilation lifetime spectroscopy, The positron lifetime spectroscopy and its intensity show chain scission at lower doses due to radical reaction.

C.Y. Lee in 2016[37], explained that the coincidence Doppler broadening and positron lifetime methods in positron annihilation spectroscopy (PAS) has been used to analyze defect structure in metal, semiconductor and polymer, he indicate that scanning electron microscope (SEM) image and PAS it is more effected by the defect.

E.V. Ahmanova *et al*. in 2017[38], studied the results and possibilities of the samples surfaces research by the Doppler methods of (PAS) for monochromatic beam of the positron at the LEPTA facility.

Mohanad H. Oleiwi and Teeba M. Talib in 2017 [39], studied the positron interaction with matter and the effects of low resolution on positron lifetime spectrum ; they found that the positron tend to annihilate in voids .

2.1 Introduction

The lifetime of positron in certain medium is extremely sensitive to changes in the electron density in the annihilation site. Hence the positron annihilation lifetime technique (PAT) has become a valuable tool to study the microstructure changes of materials and thereby several applications in physics [40].

All information about the material, such that defects, electron density have been obtained by analysis of positron lifetime spectrum, so that to study the impurity of material by positron annihilation technique, must study the positron lifetime spectrum. This spectrum can be produced theoretically, by produce the time response function and decay function of positron, then convoluted and superimpose with background, then can be studied the parameters that affected the spectrum theoretically.

In this chapter, we explain the theoretical basis of decay function, time response function and convolution by using some imperical equations.

2.2 Dynamics and Annihilation of Positrons in Matter

When a fast positron penetrates a medium, it undergoes several collisions losing its excess kinetic energy until it becomes thermalized and subsequently annihilates with an electron from the surrounding medium into γ-photons. Positron through interaction with matter is slowing down to energy of 10 eV with in 10^{-11} sec, which is shorter than the reciprocal of the annihilation rate (10^{-9} sec^{-1}), which reflects that the annihilation during slowind down is unlikley for most system [8]. The slowing down for a fast positron is similar to that for a fast electron, but a fast positron is distinguished from a fast electron in its interaction with matter because of its positive charge[5].

The time required for a positron to slow down and become thermalized in a medium at temperrature T is given as [15]:

$$t_{th}(ps) = \frac{186.5}{r_s^2} \quad , \text{for } \frac{3}{2}U \leq \frac{T}{T_\circ}$$

$$= \frac{560}{U^2 r_s^2}\left[\left(\frac{8}{3}U\right)^{1/2}\left(\frac{T}{T_\circ}\right)^{1/2} - 1\right] , \text{for } \frac{3}{2}U > \frac{T}{T_\circ} \qquad ....(2.1)$$

where r_s is the electron radius, U is the reduced energy parameter given by $\frac{E_{cr}}{k_B T_\circ}$, where E_{cr} is the critical epithermal positron energy, k_B is Boltzman constant, $T_\circ$= 316 K chosen to achives $k_B T_\circ = 3\times10^{-11}$ a.u (a.u is the energy in atomic units) and T is the medium temperature.

The positron in an inelastic collision with a nucleus can lose its energy by emitting bremsstrahlung, creation of a phonon or through atomic displacements [12].

The stopping power of a medium due to phonon excitations exceeds electronic stopping in many materials at particle energies below E_{cr} (critical positron energy), i.e. the phonon-positron interactions dictate the final thermalization process [15].

Fast positrons ($\approx$ 1MeV) possess sufficient momentum to displace atoms from their normal lattice sites directly through nearly head-on collisions.The probability of this process increases with positron energy and target atomic number [41].

The positron implantation profiles [41,42] provide information about the thermalization and diffusion processes which may strongly be influenced by the internal structure of the medium [43]

Multiple scattering of the positrons of energy E during the slowing down process in solids produces an implantation profile of the form [41]:

$$A(d,E_{\beta+}) = \exp (- \alpha_{+} (E_{\beta+}) d) \quad ....(2.2)$$

With a mean implantation depth

$$\overline{R}_{+} = \alpha_{+}^{-1} = b\, E^{n} \quad ....(2.3)$$

where α_{+} is the linear absorption coefficient of positrons, b is constant and d is the depth. This formula is valid for both continuous energies (from radioactive sources) and monoenergetic positron beams. The exponent n range between 1.4 to 1.6 [15].

According to the implantation profile of positrons which was suggested by Brandt and Paulin [42] for a radioactive source of maximum positron energy $E_{\beta+}$, α_{+} in a wide variety of materials is given by :

$$\alpha_{+} (cm^{-1}) \simeq \frac{16\ \rho\ (g/cm^3)}{E_{\beta+}^{1.4}\ (MeV)} \quad ....(2.4)$$

where ρ is the mass density.

Hence the implantation range in solids may be of the order of a millimeter. The mass absorption coefficient (α_{+}/ρ) is found to rise with the material atomic number (z) through the following empirical formula [44]:

$$\frac{\alpha_{+}}{\rho}(cm^{-1}/g) = 2.8\ \frac{z^{0.15}}{<\beta_{+}>^{1.19}} \quad \text{for } ^{22}Na \text{ source} \quad ....(2.5)$$

$$= 1.1\frac{z^{0.25}}{<\beta_{+}>^{1.58}} \quad \text{for } ^{64}Cu \text{ source} \quad ....(2.6)$$

where $< \beta_{+} >$ is the mean positron energy in MeV.

The slowing-down time (t_s) of a fast positron of initial energy E_i to about 100 eV (which represents the lower limit of energy of the electronic excitations in a medium) can be estimated [15] as:

$$t_s(ps) \simeq 7.7\ \rho^{-1}\left(\frac{E_i}{0.511}\right)^{1.2} \quad \text{....(2.7)}$$

Where the initial energy E_i is given in MeV. For practical positron sources of a few hundred KeV, t_s is $\leq$1 ps in all materials. Thus, positrons slow down to epithermal energies in very short times if compared with their lifetimes (normally longer than 100ps).

The thermalized positron as scattered by phonons, diffuses until it annihilates finally. The diffusion process is described as a random walk of a point particle characterized by a mean free path λ_D and a collision frequency t_D^{-1} (reciprocal diffusion time). The diffusion constant D_+ is related to λ_D and t_D by [46]:

$$D_+ = \frac{\lambda_D^2}{3\ t_D} \quad \text{.....(2.8)}$$

Positrons after thermalization diffuse over distances of about $(4D_+\tau)^{1/2}$, where τ is the positron lifetime in the bulk. During the time τ, thermal positrons diffuse over a volume of about $(100\ nm)^3$ [45]. For small α_+ values, fraction of these positrons of about $\alpha_+ = (2D_+\tau)^{1/2}$ can diffuse back to the surface [46]. Figure (2.1) Show the path and annihilation of a beam of positrons in the matter.

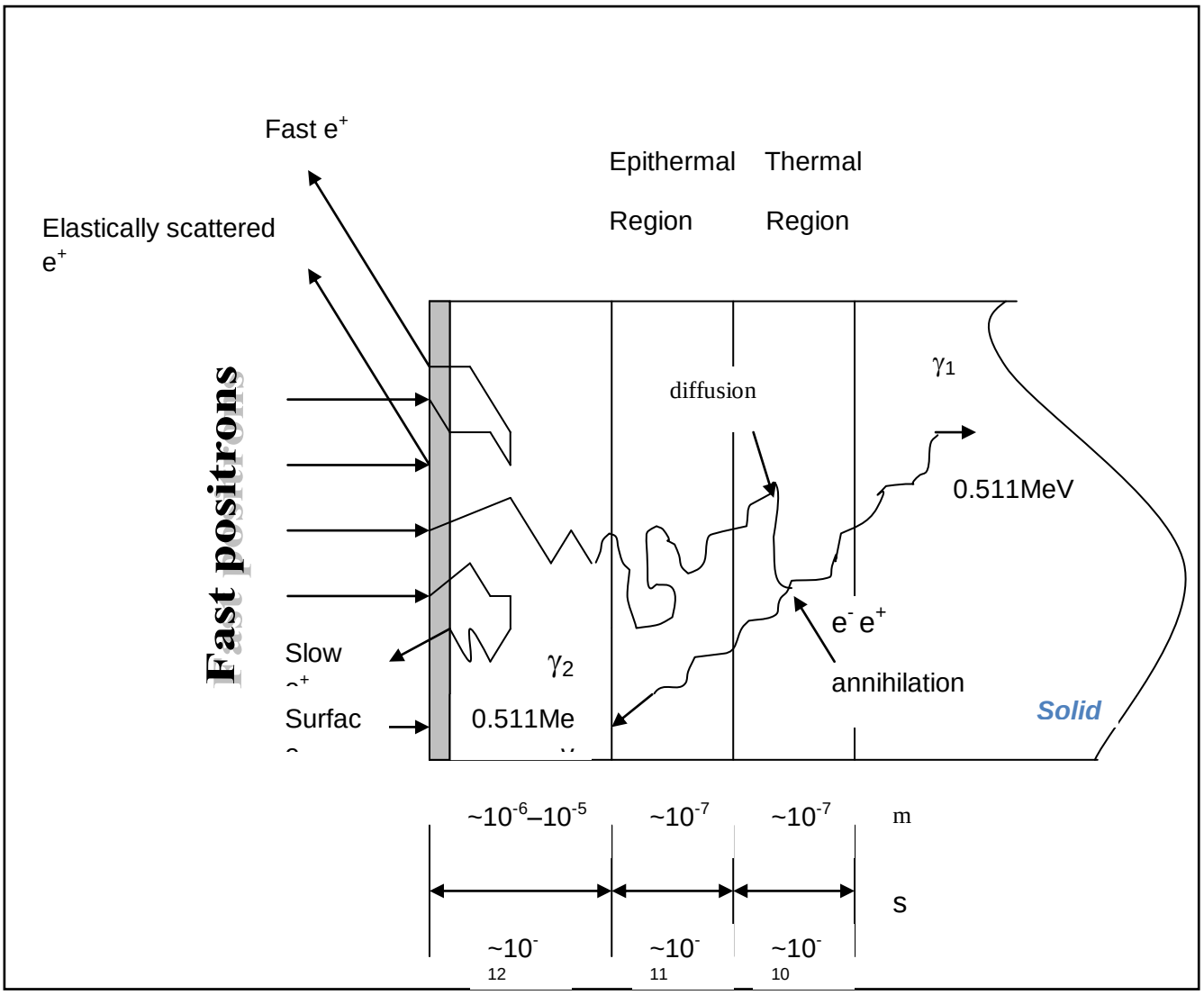

Fig.(2.1) Schematic positron paths in a solid. Courtesy of [16]

2.3 The Trapping Model

Brandt [47], Bergersonand Stott [48], and Connersand West [49], have developed simple models which were used to distinguish between annihilation of positron in the perfect lattice and annihilation of positrons trapped in (or at) a defect. This two-state trapping phenomenon is described by the rate equations,

$$\frac{dN_b}{dt} = -\lambda_b N_b - KN_b \quad \text{... (2.9)}$$

$$\frac{dN_d}{dt} = -\lambda_d N_d - KN_d \quad \text{... (2.10)}$$

Where N_b,N_d are the number of positrons, existing in the defect- free bulk and at defect- trapped states at time t, respectively. λ_b and λ_d are the annihilation rates from these states.

The quantity K is the positron trapping rate, or the probability per unit time that a positron will become trapped in a defect, and is proportional to the defect concentration (C_d) as:

$$K = u_d C_d \quad \text{... (2.11)}$$

Where u_d is the specific positron trapping rate at these defects?

Using the boundary condition that no positron are trapped at t=0, i.e. $N_d(t=0)$, the probability that the positron annihilates at time t is given by [29]:

$$N(t) = \frac{1}{\lambda_b - \lambda_d + K} \left[(\lambda_b - \lambda_d)(\lambda_b + K) \exp(-(\lambda_b + K)t) + K\lambda_d \exp(-\lambda_d t) \right] \quad \text{...(2.12)}$$

Considering the intensities I_b and I_d as the probabilities of positron annihilation in the bulk and in a defect state respectively, the intensity ratio is:

$$\frac{I_d}{I_b} = \frac{K}{\lambda_b} \quad \text{... (2.13)}$$

In a lifetime experiment, it is suitable to derive the ratio between the intensities I_1 and I_2 of the two lifetime components in Eq. 2.12 when they are extrapolated back to t=0. Thus

$$\frac{I_2}{I_1} = \frac{k}{\lambda_b - \lambda_d} \quad \text{.... (2.14)}$$

where $I_1 + I_2 = 1$.

The following lifetime spectrum parameters can deduced from Eq. 2.12,

$$\tau_1 = \lambda_1^{-1} = (\lambda_b + k)^{-1} \quad \text{.... (2.15)}$$

$$\tau_2 = \tau_d = \lambda_d^{-1} \quad \text{.....(2.16)}$$

$$I_1 = \frac{(\lambda_b - \lambda_2)}{(\lambda_1 - \lambda_2)} \quad \text{.... (2.17)}$$

$$I_2 = \frac{(\lambda_1 - \lambda_b)}{(\lambda_1 - \lambda_2)} = \frac{k}{(\lambda_1 - \lambda_2)} \quad \text{.... (2.18)}$$

Using Eqs. 2.14 and 2.15, 2.16, the bulk lifetime τ_b can be calculated using τ_1 and τ_2 with their corresponding intensities I_1 and I_2 as:

$$\tau_b = \lambda_b^{-1} = \left(\frac{I_1}{\tau_1} + \frac{I_2}{\tau_2}\right)^{-1} \quad \text{.... (2.19)}$$

The mean lifetime $\bar{\tau} = I_1 \tau_1 + I_2 \tau_2$ .... (2.20)

The trapping rate K can be estimated either from the decomposed lifetime parameters (Eq. 2.14), or from the mean lifetime, using:

$$K = \lambda_d \frac{\bar{\tau} - \tau_b}{\tau_d - \bar{\tau}} \quad \text{.... (2.21)}$$

In this treatment, detrapping of positrons from the localized state is assumed to be negligible. However, this two-state trapping model (shown schematically in Fig. 2.4) has served as the primary description of the behavior of the positron in metals containing vacancies or dislocations which act as positron trapping centers [50, 51].

This model was extended to include more than one kind of defects [52], thermal detrapping [53], and pre-thermalization trapping [54, 55].
Considering two kinds of defects with concentrations C_{d1} and C_{d2}, the corresponding trapping rates are [15].

$$K_1 = u_{d1}C_{d1}, \qquad K_2 = u_{d2}C_{d2}$$

and the measured lifetime curve contains three exponential components with the following parameters [15]:

$$\tau_1 = (\lambda_b + k_1 + k_2)^{-1} \quad \ldots.(2.22)$$

$$\tau_2 = \tau_{d1} = \lambda_{d2}^{-1} \quad \ldots.(2.23)$$

$$\tau_3 = \tau_{d2} = \lambda_{d2}^{-1} \quad \ldots.(2.24)$$

$$I_1 = 1\text{-}I_2\text{-}I_3 \quad \ldots.(2.25)$$

$$I_2 = \frac{k_1}{(\lambda_b - \lambda_{d1} + k_1 + k_2)} \quad \ldots.(2.26)$$

$$I_3 = \frac{k_2}{\lambda_b - \lambda_{d2} + k_1 + k_2)} \quad \ldots.(2.27)$$

$$\bar{\tau} = I_1\tau_1 + I_2\tau_2 + I_3\tau_3 \quad \ldots.(2.28)$$

and $$\tau_b = \left(\frac{I_1}{\tau_1} + \frac{I_2}{\tau_2} + \frac{I_3}{\tau_3}\right)^{-1} \quad \ldots.(2.29)$$

The common situation in the presence of two different positron traps is that the longest component (τ_b) is observed originating from a positron trapped at a vacancy, cluster or void.

The three-state trapping model is shown schematically in Fig. 2.2b. General treatment for n-number of states is presented [17].

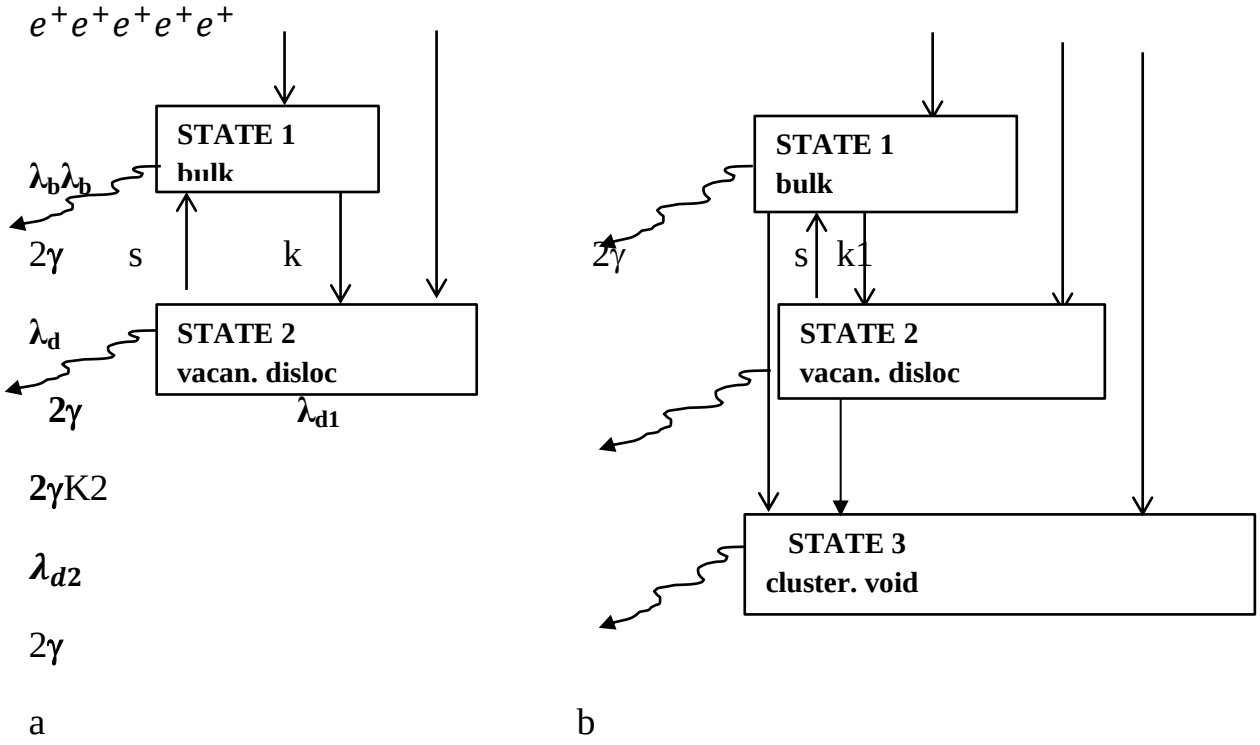

Fig. 2.2: The trapping model in the presence of (a) one type of defects, (b) two types of defects. Trapping and possible detrapping transitions are illustrated. Courtesy of [16]

In the detrapping process, the positron is released from the trap. The energy needed for this process is normally provided by thermal fluctuations.

Considering this process, the rate equations 2.9 and 2.10 will include an additional term $+\delta N_d$,$-\delta N_d$ respectively, where δ denotes the detrapping rate Generally, the lattice vibrations seem to decrease thermal detrapping, where as an harmonic lattice expansion increases it [15].

The thermodynamics of the detrapping process has been considered by Mannien and Nieminen [56]. Warburton and Shulman [54], and Brandt and Arista [55] proposed in their models, that not all positrons can reach thermal equilibrium before being trapped. According to this pre-thermalization effect, Eq. 2.16 is only correct if there is no direct trapping for the time t=0, and if thermal detrapping does not occur. Otherwise, if n_d^0, the fraction of positrons trapped in defects at t=0 does not equal to zero, Eq. 2.19 becomes:

$$\tau_b^{-1} = \lambda_b = \lambda_b' - (\lambda_b' - \lambda_2) n_d^0 \quad \text{....(2.30)}$$

Here, $\lambda_b$denotes the annihilation rate for the untrapped positrons as obtained from the application of the two-state trapping model to the experimental data, whereas λ_b' would be the "true “value.

By combining Eqs. 2.19 and 2.30, one can estimate n_d^ovalues experimentally, such that:

$$n_d^0 = [\lambda_b' - (\lambda_1 I_1 + \lambda_2 I_2)] (\lambda_b' - \lambda_2)^{-1} \quad \text{....(2.31)}$$

3.1 Introduction

In this chapter, the results and discussions have been illustrated, the effects of some parameters that effected on positron lifetime spectrum such as low and high resolution (R), short, mid, and long lived components (τ_1, τ_2 and τ_3); where τ_1 represent the lifetime of positron in pure lattice of matter, τ_2 represent the life time of positron in defect (missing of one atom) and τ_3 represent the lifetime of positron in the voids, all lived component are taken with constants values of intensity to show the effect of three components of lifetime (τ_1, τ_2 and τ_3),so that when low resolution notice the positron spectrum when increase the resolution (R) the right hand side approach to Gaussian shape then, the decomposition become difficult, but when high resolution the right hand side of spectrum when increase (R) approach to linear shape then the decomposition become better and random coincidence (B) is completely disappear, the random coincidence (B) are taken as constant value (0.001% of peak), it has been studied the effects of lifetime components (τ_1, τ_2 and τ_3) on positron decay function the increasing in values τ make the right hand side of spectrum approach to linear shape and (B) disappear. The program used is visual basic and all the theoretical spectra are normalize to one.

3.2 Decay Function with Three Lifetime Components

In order to investigate the effect of long lived component (τ_3), different values ofτ_3 are taken ranged between 330ps to 480ps, where τ_1 and τ_2 were fixed at 100ps and 250ps respectively as shown in Fig.(3.1). It is clear that from Fig.(3.1) the increasing in τ_3 make the decay function approach to linear shape, and the background is completely disappear where the long lived component (τ_3) make the background values linked with positron decay function.

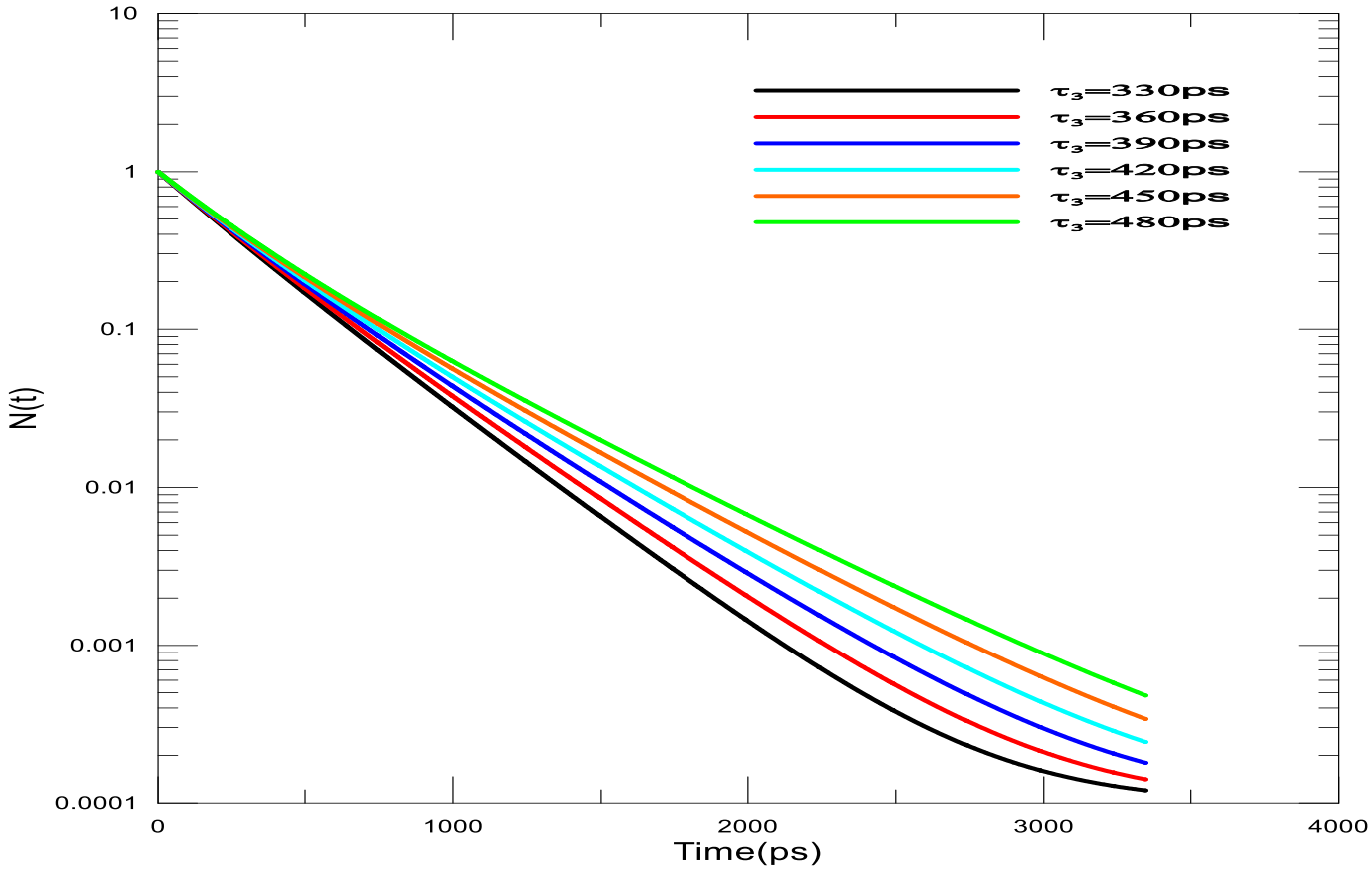

Fig. (3.1) Three components positron decay function (τ_1,τ_2,τ_3)shape

3.3 The Effect of Low Resolution on One Lifetime Component

In order to investigate the influence of system low resolution (R) on short lived components, different values of resolution (R) values ranging between 50ps to 400ps were considered, were the short lived lifetime component was fixed at (τ_1=100ps). Fig. (3.2) shows a convolution of single-Gaussian response function of low resolution (R) with single decay function (τ_1=100ps). It is obvious that as resolution (R)increase, the short lived component disappear and the spectrum tends to have a Gaussian shape.

As shown in Fig. (3.2), the right hand side of spectrum be linear at R=50ps and R=100ps, but at R= (200,300,400) ps the right hand side of spectrum be curved. The decreasing (improvement) in resolution (R) lead to better decomposition. The higher values of resolution make the decay function linked with time response function, so that the lifetime spectrum approach to response function shape.

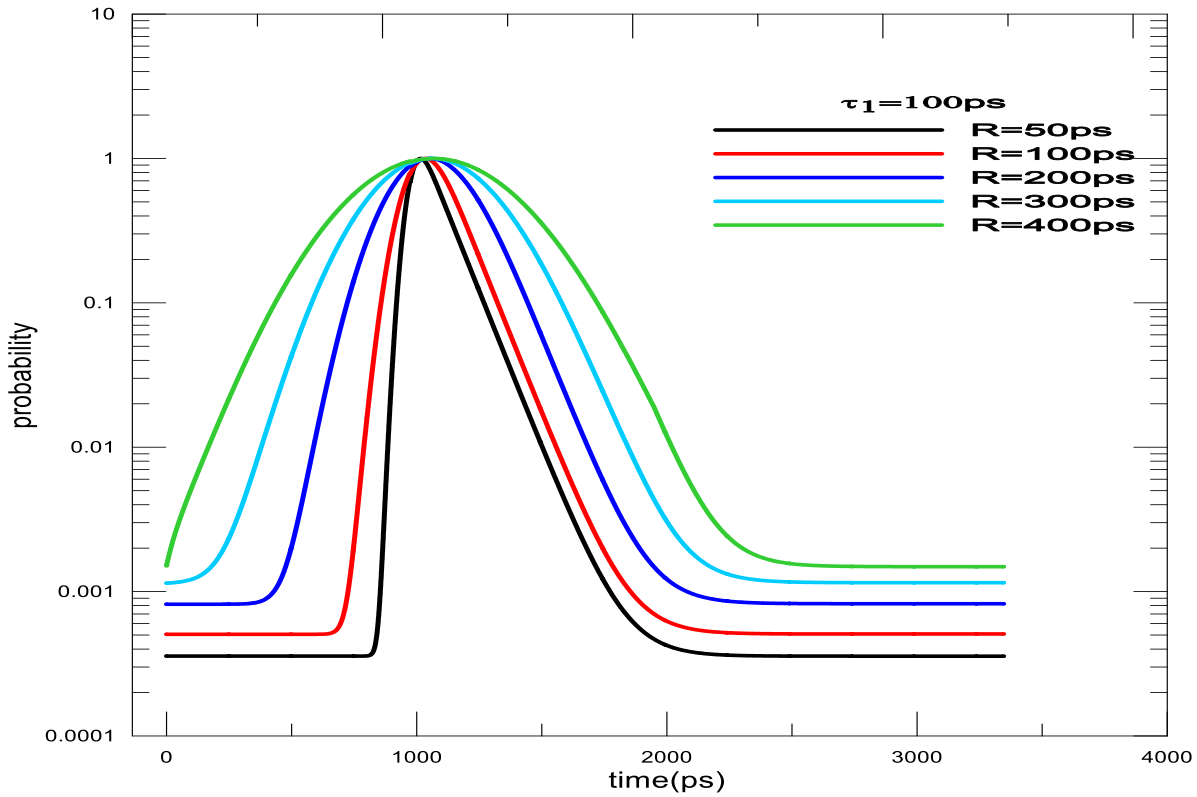

Fig. (3.2) lustrate the effect of resolution (R) on one positron lifetime component

3.4 The Effect of Low Resolution on Two Lifetime components

In order to study the effect of low resolution (R) on the spectrum of two lifetime components, different values of resolution (R) ranging between 50ps to 400ps were convoluted with short and mid lived components where τ_1 and τ_2 are fixed at 100ps and 250ps respectively. As shown in Fig. (3.3).

As we notice in Fig. (3.3), the right hand side of spectra is linear shape at R=(50,100,200,300)ps, then be curvature at R=400ps that is mean the short and mid lived components (τ_1,τ_2) are clear at R=(50,100,200,300)ps and this lead to better decomposition and not clear at R=400ps, where at R=400ps the decay function linked with time response function, then the decomposition become difficult, therefore, the resolution between R=50ps to 300ps are influenced by short and mid lived components.

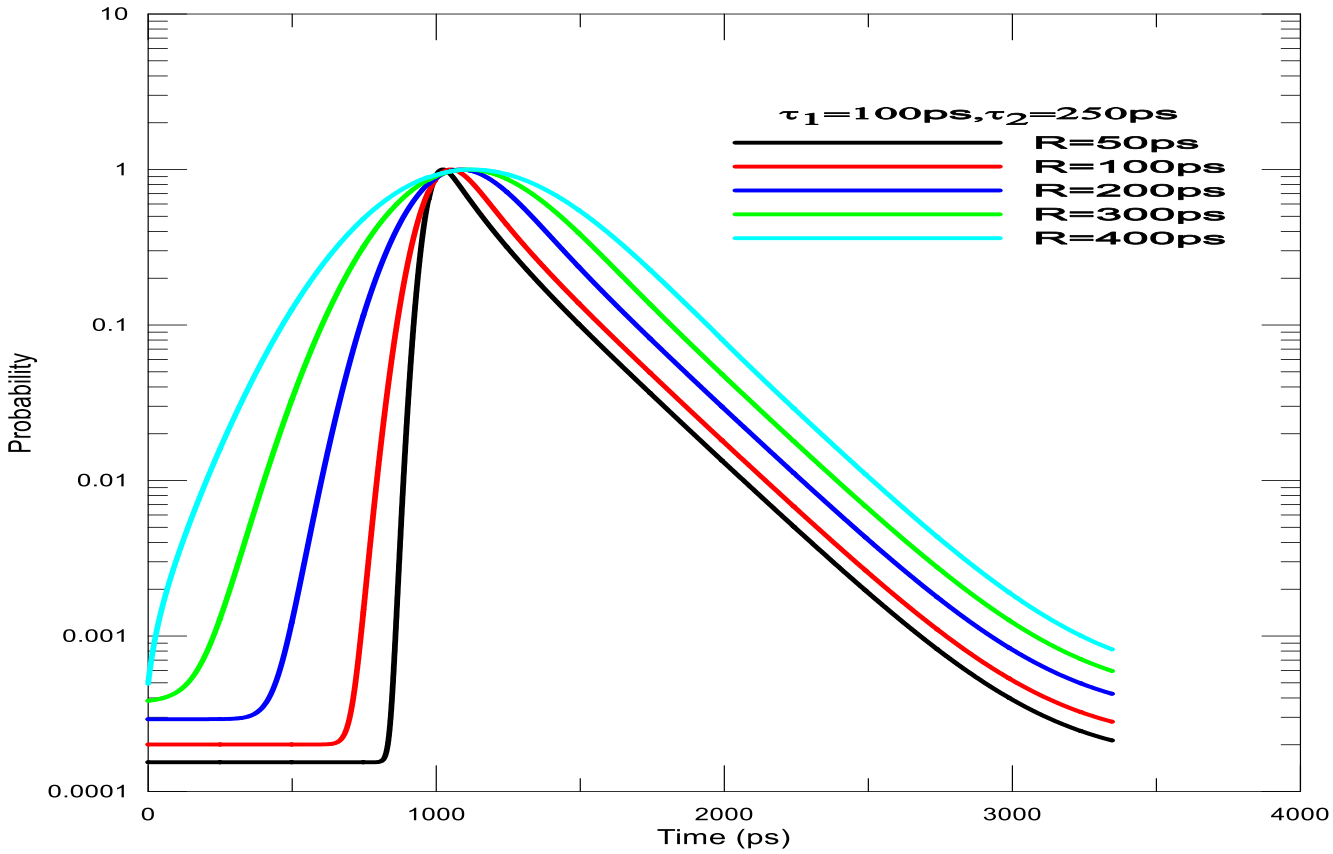

Fig. (3.3) lustrate the effect of resolution (R) on two positron lifetime components

3.5 The Effect of Low Resolution on Three Lifetime Components

Fig. (3.4) explain the effect of R on the positron lifetime spectrum, in this case τ_1, τ_2 and τ_3 are fixed at 100ps, 250ps and 400ps respectively, and the resolution are varied from 50ps to 400ps, as we notice from Fig. (3.4) as the resolution increase the right hand side approach to linear shape and the random coincidence (Background) is completely disappear.

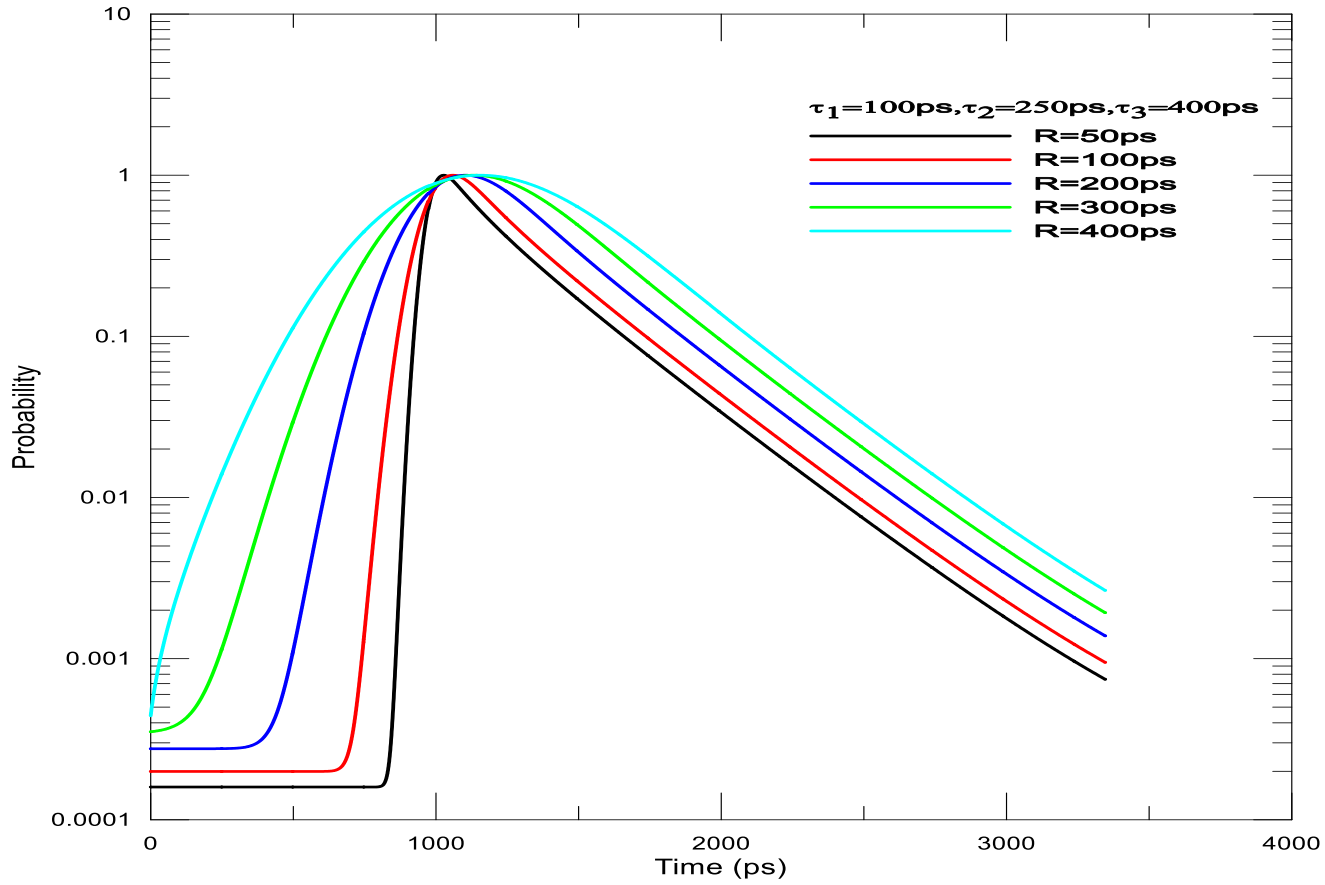

Fig. (3.4) The effect of different resolution(R) on the spectral shape of three positron lifetime components

3.6 The Effect of High Resolution on One Lifetime Component

In order to study the high resolution on short lived component (τ_1) different high value of resolution (R) ranged between 800ps to 1400ps are convoluted with decay function of positron for one lifetime component (τ_1=100ps) as shown in Fig. (3.4). It is clear that, from Fig. (3.4), the increase in resolution causes a significant distortion in lifetime spectral shape, and the right hand side of spectra be exponential shape, and this lead to difficult in decomposition.

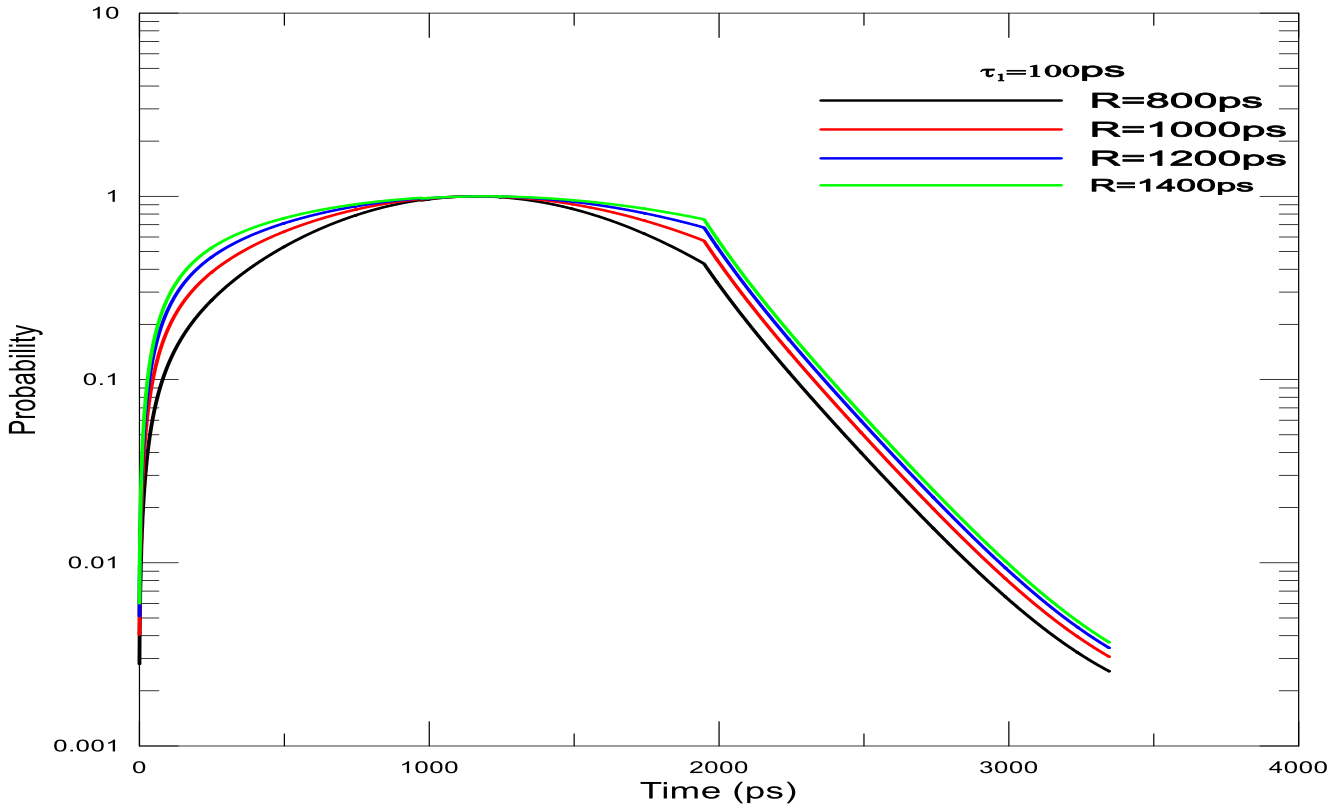

Fig. (3.5) Illustrate the effect of high resolution(R) on one positron lifetime component

3.7 The Effect of High Resolution on Two Lifetime Components

Figure (3.6) illustrates the effects of resolution (R) for two components lifetime spectrum (τ_1 and τ_2), different values of resolution (800,1000,1200,1400)ps are convoluted with two component (τ_1=100psand τ_2=250ps), as we notice from fig.(3.6), the spectrum become linear shape in the right hand side.

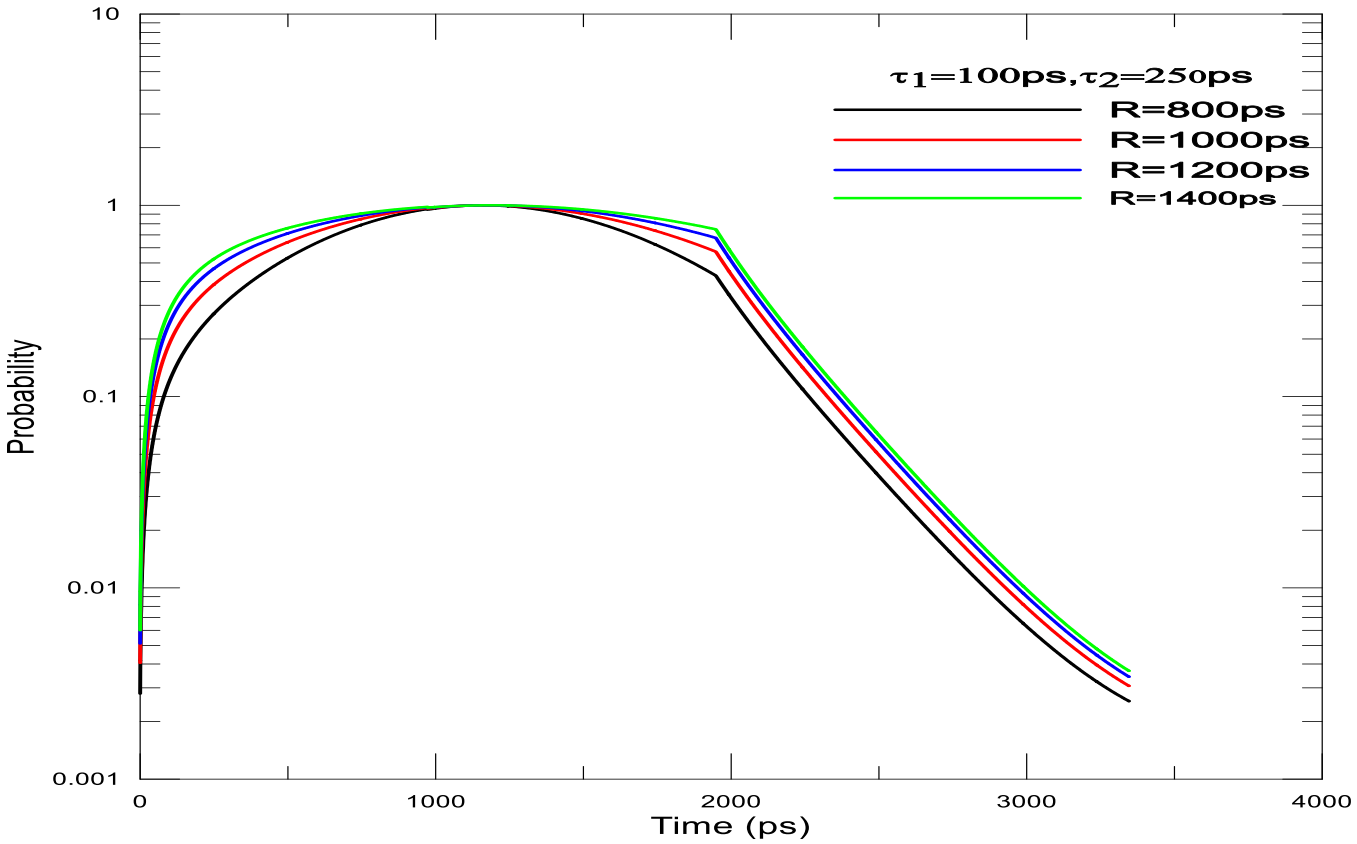

Fig. (3.6) Illustrate the effect of high resolution(R) on two positron lifetime components

3.8 The Effect of High Resolution on Three Lifetime Components

Different values of resolution (800,1000,1200,1400)ps are studied with constants values of three lifetime components (τ_1=100psand τ_2=250ps and τ_3=350ps),as shown in fig.(3.7) these three positron values of lifetime components in matter (τ_1 and τ_2 and τ_3) makes the right hand side of positron spectrum becomes linear.

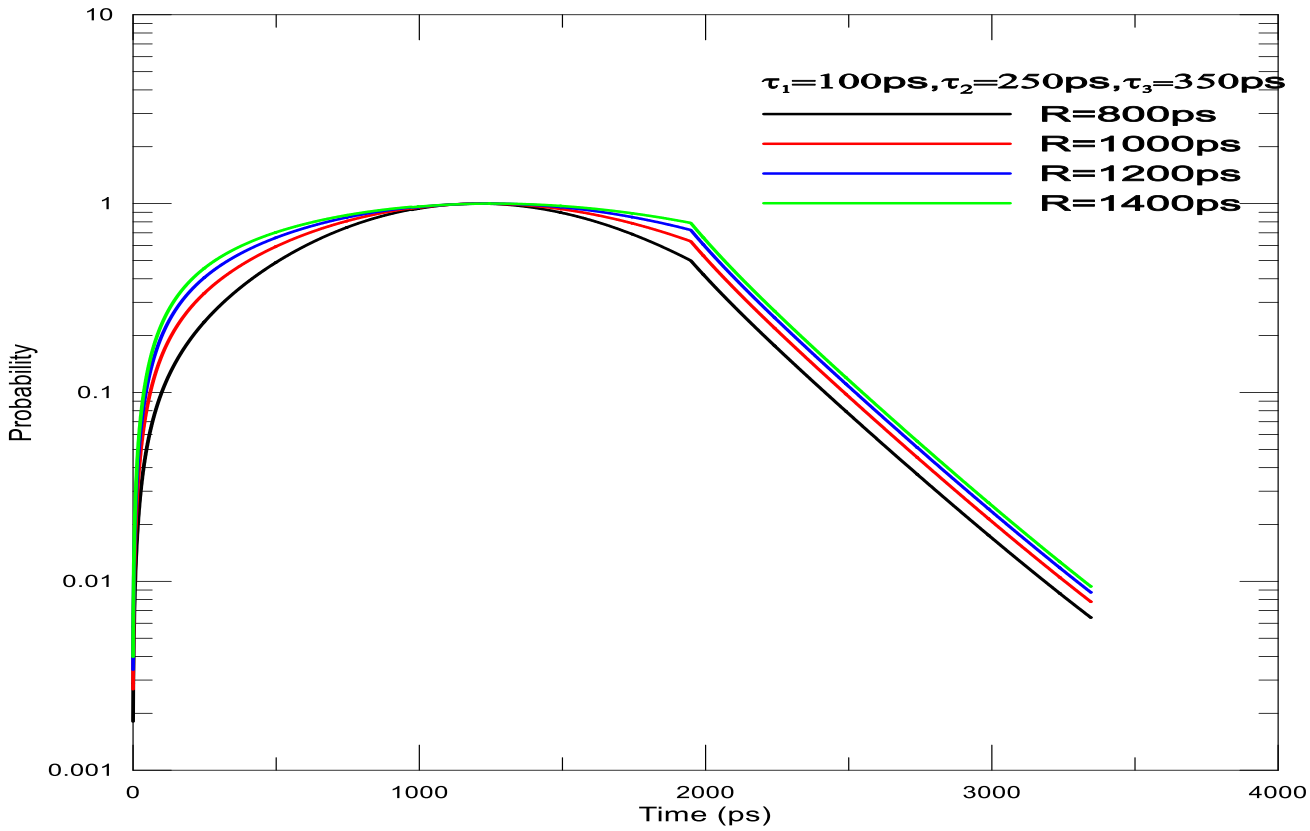

Fig. (3.7) Illustrate the effect of high resolution(R) on three positron lifetime components

3.9 The Effect of Short Lived Component on the Spectrum

Different values of short lived component (τ_1) ranged between 80ps to200ps of positron decay function are convoluted with time response function with fixed resolution (R=200ps). In order to study the of short-lived component on the spectral shape as shown in Fig.(3.8), it is clear that from Fig.(3.8) the right hand side approach to linear shape when τ_1 increase, also the background decrease as τ_1 increase because the some values of background are linked with time response function.

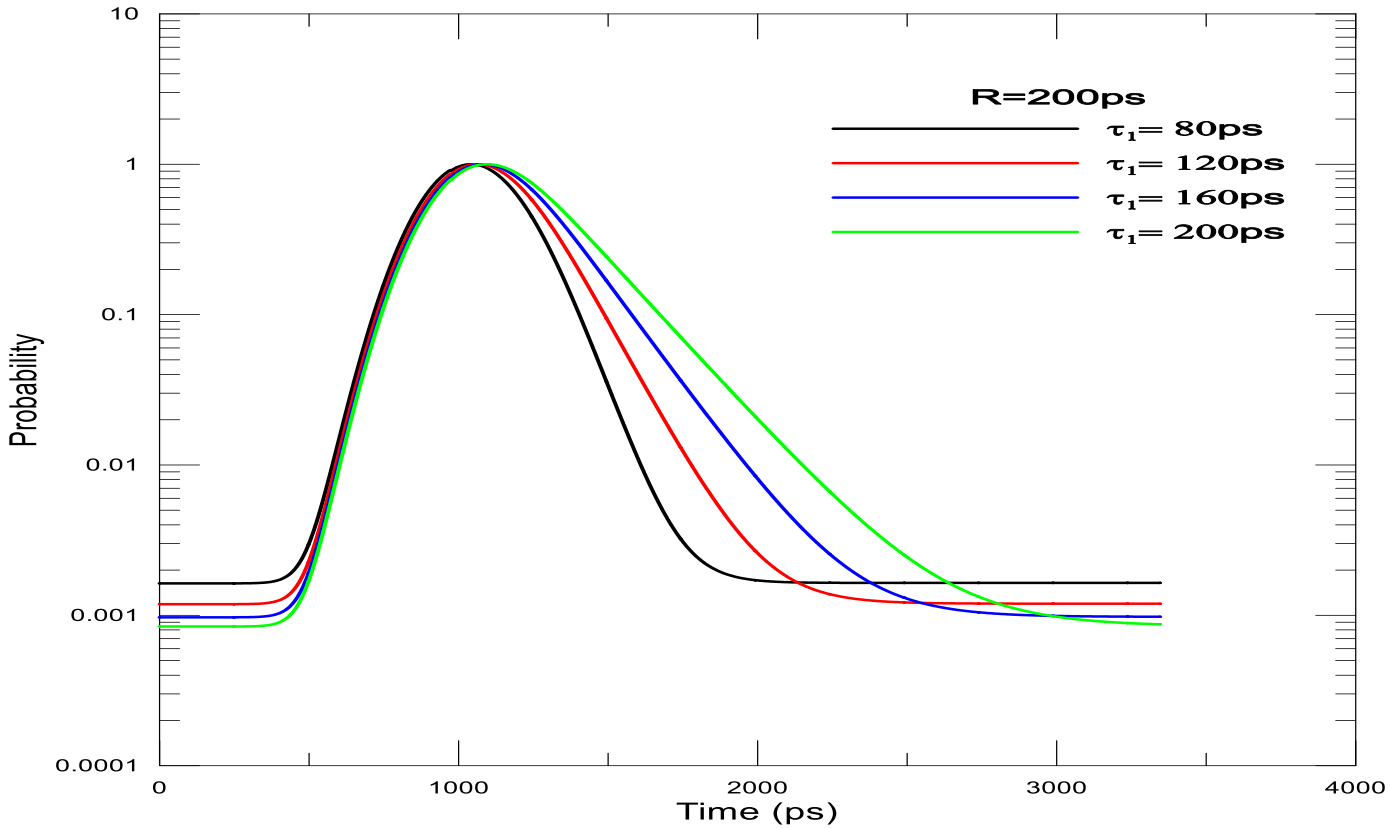

Fig. (3.8) Single-component lifetime spectra with different lifetime values and R=200ps

CONCLUSIONS

1- The positron tends to annihilate in defects.

2- τ_1 does not affect on background, τ_2 has little effect on background and τ_3 has large effect on background.

3- As the resolution increase the spectrum approach to time response shape and as the resolution R decrease the right hand side of spectrum approach to linear shape.

4- The high resolution leads to difficult in decomposition.

5- As τ_1, τ_2 and τ_3 increase the right hand side of spectrum approach to linear shape.

6- Background is completely disappear at three components of lifetime spectrum.

Future Work

1- using two time response function to study its effects on resolution of lifetime spectra.

2- study the effects of intensity of positron beam on the lifetime spectra.

3- study the effects of random coincidence such as background on the positron spectrum.

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الخلاصة

في هذه الدراسة تضمنت محاكاة لتفاعل البوزترون مع المادة حيث ولد طيف زمن عمر البوزترون بواسطة توليد داله الاستجابة الزمنية مع داله الانحلال ومتداخلة مع التطابق العشوائي (الخلفية الإشعاعية). الدراسة تضمنت محاكاة تفاعل البوزترون مع المادة النقية والمادة ذات العيوب ودراسة تأثير بعض العوامل على طيف زمن العمر مثل الاستجابة العالية والواطئة ومركبات القصيرة - المتوسطة - الطويلة.

ودرست قيم مختلفة لمركبة كاوس الواحدة (دالة الاستجابة الزمنية) ولفت مع قيم ثابتة من زمن عمر البوزترون لمركبات واحده- اثنان- ثلاثة (τ_1,τ_2,τ_3) من مركبات زمن العمر. كل هذه المركبات أخذت شدات متساوية لإظهار تأثير داله الاستجابة على هذه المركبات وكذلك التطابق العشوائي (الخلفية الإشعاعية) ثابت عند 0.001% من الذروة حيث مدى الاستجابة من -500 1400 ps

تم الاستنتاج ان البوزترون يميل الى الإبادة في العيوب والخلفية الإشعاعية تختفي تماما عند المركبات الثلاثة لطيف زمن العمر ايضا كذلك عندما تزداد داله الاستجابة الزمنية ان الطيف يكون مقارب لشكل كاوس وكذلك أيضا عندما تزداد قيم τ_1 و τ_2 و τ_3 فان الجانب الأيمن من الطيف يكون مقارب الى الشكل الخطي. كذلك لوحظ ان الاستجابة الزمنية العالية تؤدي الى تشويه في شكل طيف زمن عمر البوزترون.

جمهورية العراق

وزاره التعليم العالي والبحث العلمي

جامعه بابل

كليه التربية للعلوم الصرفة

قسم الفيزياء

دراسة فناء البوزترون في المعادن

رسالة مقدمة

الى مجلس كلية التربية للعلوم الصرفة في جامعة بابل

وهي جزء من متطلبات نيل درجة الدبلوم العالي

تربية / فيزياء المواد وتطبيقاتها

من قبل

علي محمد هاشم چلاب

بكالوريوس علوم الفيزياء

جامعة المستنصرية (٢٠٠٦) م

بأشراف

أ.م.د. مهند حسين عليوي

كلية التربية للعلوم الصرفة

قسم الفيزياء

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