Positron interaction with matter and study the effects of Low resolution on its lifetime spectrum

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ABSTRACT

The positron lifetime spectrum is the convolution of decay function with resolution function in the generating of positron lifetime spectra several parameters affect the spectrum. The main parameter that affected it is the resolution. In this work we study the effect of resolution for single Gaussians on one, two and three lifetime components spectra. We generate theoretically the decay function for three-components and time resolution function for one Gaussians then convoluted them and superimposed with random coincidence (background (B.G)). Different values of resolution for One-Gaussian components ware convoluted with constant values of lifetime component for 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.G) fixed at 0.001% of the peak. We concluded that the increasing of resolution lead to difficult analysis, when the resolution increase leads to difficult in the decomposition (analysis) of positron lifetime spectrum. We notice that the effect of single component lifetime spectrum is disappeared when the resolution function arises to 200ps, and the effect of second component disappeared when resolution function arises to 300ps and the effect of third component is vanish when the resolution arise to400ps.

KEY WORDS: Positron, Lifetime, Resolution Function, Gaussian.

1. INTRODUCTION

Our understanding of many important mechanical and electrical properties of the material is limited by our knowledge of the microstructure and defects.

There are many techniques that can identify the species and size impurities (Dlubec, 1999). There are few however that can detect open volume defects such as atomic vacancies or voids (Muhamad, 2007). Using positron annihilation lifetime spectroscopy determines the size or charge of defects in metals, semiconductors and molecular or organic compounds.

Positron annihilation lifetime spectroscopy measures the electron density at the annihilation site (Howel, 1998). In metals and some compounds the correlations between lifetimes and defect size can be calculated from the first principles with sufficiently high accuracy to differentiate between major defect classes such as vacancies, vacancy clusters and voids (Lynn, 1987).

The correlation between low local electron density and larger size defect leads to longer positron lifetimes for larger defects (Thraenert, 2006), the generated spectra involve smaller and longer positron lifetimes.

Experimentally positron annihilation lifetimes can be measured by the difference between the time of positron entry the sample and the later time of annihilation (Liu, 1993).

To obtain these spectra theoretically required to generate the resolution function and decay function by represent the mathematical models for both functions.

The generated spectra contain three components of decay function convoluted with one component of Gaussian functions and superimposed with random coincidence (background) to generate the positron lifetime spectrum.

The experimental spectra include a number of distinct positron lifetime, so that the analysis of such spectra requires their decomposition into a sum of exponential decay term (Somieski, 1996). So that the narrower the lifetime lie together, the more difficult in the analysis.

A lot of sources of errors raised in the analysis of lifetime spectra such as (Sormann, 1983).

- The wrong number of exponential decay function in the model.
- The use of insufficient model of the resolution function.
- An instability of the time zero point of the spectrometer.
- Statistical errors due to statistical fluctuations of the count number of the channels of the spectra.

In this work we take one lifetime component (τ_1) fixed at 100ps and the resolution vary from 50 to 400ps, secondly we take two lifetime components fixed at τ_1=100ps and τ_2=250ps with resolution vary from 50 up to 400ps, at last we study the effect of resolution on three lifetime components fixed at τ_1=100ps, τ_2=250ps, τ_3=350ps with resolution vary from 50 to 400ps. The spectra additionally contain random coincidence (background) contributions as well as annihilation events in the positron source. In this work the background fixed at 0.001% of the peak. The fraction of the annihilations in the source is not only determined by the source itself, but it is also a fraction of atomic number of the sample and increases due to multiple positrons backscattering through the source. In decomposition, the source correction has to be performed after background subtraction. This means subtracting the characteristic lifetime spectrum of the source. The determination of this source spectrum is rather complicated and usually carried out in such a way that a single – component spectrum of a defect free sample is analyzed. The source components are varied using a single – component fit to get the best fit i.e. the smallest variance (Freeman and March, 1998), since the source component is weak so we neglected its effect.

All components were taken equal intensities, where the possibility of decomposition the positron lifetime spectra depends essentially on the number of lifetime components in the spectrum and its intensities (Puff, 1983).

2. MATHEMATICAL MODEL

The time-dependent positron decay spectrum N(t) is given by

$$N(t) = \sum_{i=1}^{k+1} I_i \exp(-\frac{t}{\tau_i}) \quad (1)$$

k different defect type contributing to the positron trapping are related to k+1 components in the spectra with the individual lifetime τ_i and intensities I_i , as we take three components, i.e. two type of defect were studied, so k=2

The spectrum is shifted on the time scale to time zero t_z, and consequently the time t in Eq. (1) has to be replaced by $t-t_z$.

The theoretically obtained spectra are the convolution of decay function with one Gaussian of time resolution function $G_i(t)$

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

Where σ is the standard deviation related to full width at half maximum (FWHM) of prompt are by (FWHM/2.356). Δt_i is the shift in the centroid position and t_z is the time zero channel number.

The convolution of the spectra Eq. (2) with Eq. (3) gives the convoluted decay spectrum

$$D_f(t) = \int_{-\infty}^{\infty} N(t-t') F_t(t') dt' \quad (3)$$

The positron decay spectrum is given as

$$D_f(t) = \sum_{i=1}^{3} \frac{I_i}{2} \exp[-\frac{(t-t_z)-\Delta t_i - \sigma^2/(4\tau_i)}{\tau_i}][1-\text{erf}(\frac{1}{2\sigma\tau_i} - \frac{t-t_z}{\sigma})] \quad (4)$$

3. RESULTS AND DISCUSSION

Generation of Deacy Function: Fig. (1) Represent the shape of deacy function different values of one component deacy functions (τ_1). Where τ_1 takes the values 160, 170, 180, 190 and 200ps. As we notice from fig.1, the increase in τ_1 give more shifting in deacy function, also the random coincidence is clear in one component deacy function.

Fig.2, illustrate the shape of two components deacy function, where τ_1 fixed at 200ps and the second component take the values τ_2=250, 260, 270, 280, 290 and 300ps. It is notice that as τ_2 increase, the deacy function increase and smaller values of the random coincidence disappear.

Fig.3, represent of deacy function for three component τ_1, τ_2 and τ_3, where τ_1=200ps, τ_2=300ps, and τ_3 take the values 330,360,390,420,450 and 480ps. It is notice that as τ_3 increase to high value, make the deacy function more divergence. Also the random coincidence completely disappear in this case.

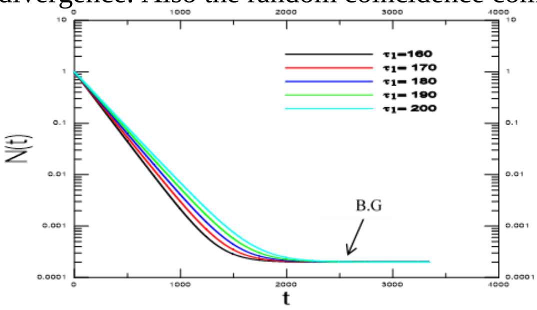

Figure.1. one component positron decay function(τ_1), t in ps

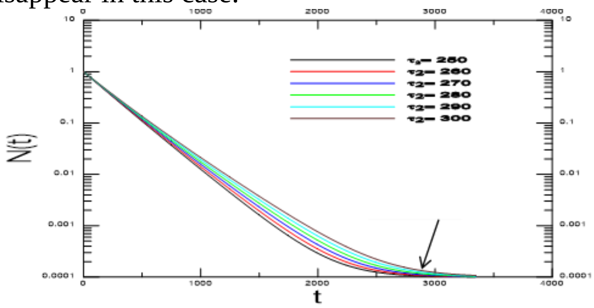

Figure.2. Two components positron decay function (τ_1,τ_2), t in ps

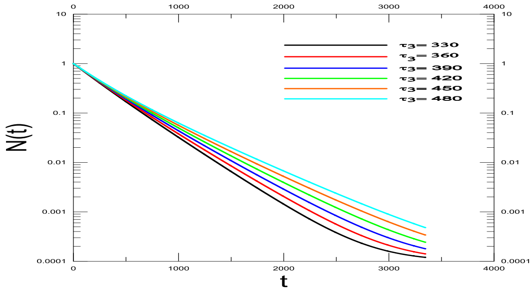

Figure.3. **Three components positron decay function (τ_1,τ_2,τ_3), t in ps**

Generation of Positron Lifetime Spectra:

The Effect of Low Resolution on One Lifetime Component: The effect of low resolution (R) on one positron lifetime component (τ_1) was study. Fig.1, shows the one component positron spectra with different values of resolution (R), different R were convoluted with one lifetime component (R=50, 100, 200, 300 and 400) and τ_1 fixed at 200ps. As notice from fig.4, the τ_1 disappear as R increase when R=50, 100ps the lifetime component is clear beyond these values of R, the lifetime being disappear and the spectrum tends to have a Gaussian shape. Also the random coincidence is clear in this case as shown in fig.4.

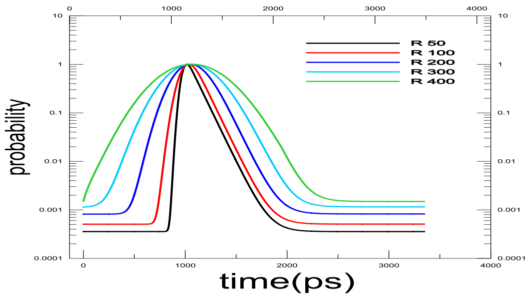

Figure.4. illustrate the effect of R on one positron lifetime component

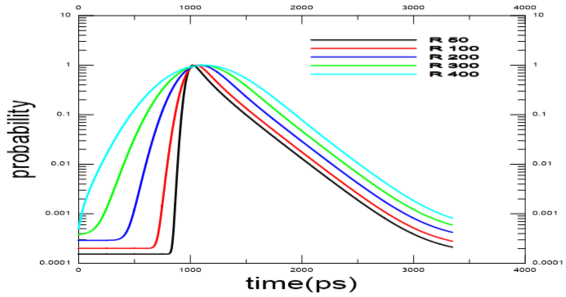

Figure.5. The effect of different R on the spectral shape of two positron lifetime components

The Effect of Low Resolution on Two Lifetime Component: Fig.5, illustrate the effect of increasing of R on two components positron lifetime spectra. In which R=50, 100, 200, 300, 400ps, τ_1=200ps and τ_2=250ps. It is clear that the positron lifetime spectra beyond R=300ps is disappear.

The Effect of Low Resolution on Three Lifetime Component: In this case three positron lifetime component are convoluted with different values of resolution function as in fig.6. Where R=50, 100, 200, 300 and 400ps, and τ_1=200ps, τ_2=250ps, τ_3=400ps. As shown in fig.6, the three positron lifetime components (τ_1, τ_2, τ_3) is clear for all values of R and the random coincidence completely disappear.

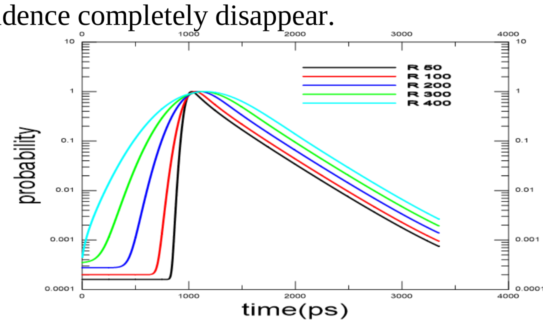

Figure.6. The effect of different R on the spectral shape of three positron lifetime component

4. CONCLUSIONS

The difficult in the decomposition get when the resolution increase more than 300ps, and this explain the difference between the effect increase of resolution on the spectrum, where the high resolution provided a broadening in the prompt curve. We also concluded that as the resolution increase, the lifetime component τ_1 disappear and this lead to different to decomposition. We also conclude that the effect of single component lifetime spectrum (τ_1) disappear when the resolution function raised to 200ps and the effect of second component (τ_2) disappear when resolution function raised to 300ps.

The effect of third component (τ_3) is clear for all values of R. Also the random coincidence disappear only in two and three lifetime component. Also as the number of positron lifetime component increase the decomposition become available.

REFERENCES

Dlubec, Hubner Ch and Eichler S, Do MELT or CONTIN programs accurately reveal the o-Ps lifetime distribution in polymers, Phys. Stat. Sol, 172. 1999, 303-315.

Freeman R, March H, Fragmentation patterns of organic molecules by low energy positrons, Molec. Phys. 93, 1998, 847.

Howell R.H, Asoka-Kumar P, Stoeffi W, Hartley J and Sterne P, Materials analysis using positron beam lifetime spectroscopy. Sci. Instrum. 59, 1998, 228-230.

Liu J, Deng Q and Jean Y.C, Free volume distribution of polystyrene probed by positron annihilation. Macromolecules, 26, 1993, 7149-7155.

Lynn K.G and McKay T, Trapping of nonthermal positrons in metals. Phys. Rev. 36, 1987, 7107-7110.

Muhamad Qasim sheikh, Hassan E.M and Reinhard Krause-Rehberg, Free volume of an oligomeeric epoxy resin and its relation to structural relaxation; Evidence from positron lifetime and pressure-volume-temperature experiments. Phys. Rev. E, 75, 2007, 1-13.

Puff W, A new version of a program for analyzing positron lifetime spectra with non-Gaussian prompt curve, Comput. Phys. Commun, 30, 1983, 359-368.

Somieski B, Staab T.E.M and Kranse-Rehberg, R. The data treatment influence on the spectra decomposition in positron lifetime spectroscopy. Nucl. Instur and Meth in Phys. Res. A, 381, 1996, 128-140.

Sormann H, Kindl P and Puff W, Investigation on the reliability of a multi-component analysis of positron lifetime spectra using a new method of producing computer-simulated test spectra, Nucl. Instur and Meth., 206, 1983, 203-209.

Thraenert S, Hassan E.M and Krause-Rehberg R, Ortho-positronium lifetime measurement-positron source activity and statistics. Nucl. Instur. and Meth. in Phys. Res B, 248, 2006, 336-339.