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Model for structural defect characterization of metals based on positron beam technique

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Abstract

In this work, a model for the structural characterization of metals using positron beam technique was developed and tested. The developed model was tested using experimental data obtained from a positron beam laboratory. The model was based on the Doppler spectrum obtained in the Dopper broadening technique. The model considered specific positron annihilation characteristics in metals. Also, the model considered the properties of positrons as they diffuse through the metals. The S and W- parameters; types of defects can be simulated from the model for any given incident photon energy and for any metal. The results obtained revealed that the S-parameter, the W-parameter and structural defect simulated using the model is in one to one agreement with the experimental values. The model can be used in place of experiments for the structural characterization of defects in metals.

Keywords
Positrons, S and W-parameters, defects, characterization and metals.

1.0 Introduction

Positron beams are very useful in the study of surfaces and near surface properties of materials. Various positron processes at and near the surface can be used for material characterisation [1]. Positrons are known as sensitive self seeking probes of defects in materials and can provide detailed information on the electronic structure of defects or bulk materials such as morphology of Fermi surfaces [2]. Also, positrons are used for the characterization of metals, nano-crystalline materials and polymers among others [3-4].

When a positron annihilates with an electron in a material, two gamma photons each of energy 511keV are emitted. The energy, direction of emission and time of emission provides information about the material in which the positrons annihilates [5]. Positron annihilation in materials provides information about the momentum distribution of the electrons in the materials. The Doppler broadening of the annihilation line is a measure of the momentum-density distribution of the annihilating electrons. The determined line-shape parameters are defect specific, since they are determined by the local electronic environment of defects. The momentum distribution is reflected in the Doppler broadening of the 511keV annihilation peak. Positron annihilation with low-momentum valence or conduction electrons results in a small Doppler shift contributing to the centre of the peak. Positron annihilation with high-momentum

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core electrons results in a large Doppler shift contributing to the wings of the 511*keV* annihilation peak. The shape of the 511*ke*V peak is characterized by the *S* and *W*-parameters. The *S*-parameter indicates the relative contribution from valence electrons while the W parameter represents the relative contribution from core electrons. The *S* and *W*-parameters are specific bulk property of every material.

Positron annihilation technique using the Doppler broadening is a very sensitive method for characterization and study of different properties of materials [6-9]. In positron annihilation spectroscopies, positron annihilation parameters and characteristics can be modelled to serve as a guide or alternative to experiments. Elcher and Krause-Rehberg [10] developed a model for theoretical spectra of different vacancy clusters in silicon. Britton et al.,[11] applied the Fermi's Age theory to model and explain the penetration of positrons in solids. Since positron beams are not generally available and accessible, there is the need to develop a model for the structural characterization of metals based on positron beam techniques to serve as alternative to experimental works. In this work, a model for the defect structural characterization of metals based on the slow positron beam technique is developed and tested.

2.0 Theory

The Doppler spectrum is obtained by integrating the total momentum density along the two directions (p_x, p_y)

$$P(p_z) = \iint \rho(p)\, dp_x\, dp_y \qquad (2.1)$$

where p_x and p_y are the directions of the annihilation gamma-quanta which make up the Doppler shifted energy spectrum in the Doppler-broadened spectra. P_z is the longitudinal momentum component of the annihilating electron-positron pair. The *S*-parameter is the ratio of the area of the central low-momentum part of the spectrum to the total area of the whole curve after subtracting for the background radiation expressed as

$$S = \frac{A_s}{A_0} = \frac{\int_{E_0 - E_s}^{E_0 + E_s} N_D\, dE}{\int^{E_0 + E_s} N_D\, dE} \qquad (2.2)$$

The *S*-parameter is taken as the ratio between the numbers of counts in the centre (511±0.8*keV*) to the total peak area of the annihilation area where every kind of positron annihilation site yields characteristic *S* parameter. The *S* parameter is defined to parameterise the Doppler broadening of the positron annihilation [10] as

$$S = \frac{\int_{511keV - I_I}^{511keV - I_I} F(E)\, dE}{\int^{peak} F(E)\, dE} \qquad (2..3)$$

where $F(E)$ is the convoluted spectrum of energy and I_s is the interval limit of the calculation of the line shape parameter. Experimentally, the measured *S* parameter is given [12] as

$$S(E) = j_{ep}(E) s_{ep} + \left(1 - j_{ep}(E)\right) s(E) \qquad (2.4)$$

where j_{ep} is the epithermal positron fraction reaching the surface and it is expressed as

$$j_{ep} = \int_0^\infty (z, E) \exp\left(-\frac{z}{I_{ep}}\right) dz \qquad (2.5)$$

where $p(z, E)$ is the stopping distribution for positrons incident on a solid surface and is given [13] as

$$p(z,E) = -\frac{z^{-1}}{z_0}\exp\left[\left(-\frac{z}{z_0}\right)\right] \qquad (2.6)$$

where z is positron implantation depth, and z_0 is the positron implantation profile. The positron implantation depth is related to the incident positron energy through the expression

$$z = -\frac{\alpha}{\rho}E^n \qquad (2.7)$$

where ρ is density and E is implantation energy of the positrons, and α and n are material dependent constants.

The S parameter obtained from variable implantation energy positron beam for a defect free sample is given as [14]

$$S(E) = j_{ep}s_s + (1 - j_s)s_b \qquad (2.8)$$

where

$$j_s = \int_0^\infty (z,E)\exp\left(-\frac{E}{L_+}\right)dz \qquad (2.9)$$

and $p(z, E)$ is the positron implantation profile, L_+ is the positron scattering length in the material. The positron scattering length in a material is expressed as

$$L_+ = \frac{3D_+}{\sqrt{\frac{3k_BT}{m*}}} \qquad (2.10)$$

where $m*$ is the rest mass of positron which is 1.5 electronic mass, k_B is the Boltzmann constant, T is temperature and D_+ is the positron diffusion coefficient expressed [12] as

$$D_+ = \frac{\gamma k_BT}{m*} \qquad (2.11)$$

where γ is positron scattering relaxation time. In equation (2.8), Ss is the surface S-parameter contribution to $S(E)$, j_s is the surface annihilation fraction and j_b is the bulk positron annihilation fraction.

The W- parameter is the area of the Doppler curve in a fixed energy interval divided by the area under the whole curve so

$$W = \frac{\int_{-E_s}^{E_s} N_D dE}{\int^{Peak} N_D dE} \qquad (2.12)$$

The W-parameter is the sum of the area under the wings of the spectrum. Equation (2.12) can be written as

$$W = \frac{\int_{511KeV - I_w - \Delta I_w}^{511KeV - I_w} F(E)dE + \int_{511KeV + I_w}^{511KeV + I_w - \Delta I_w} F(E)dE}{\int^{Peak} F(E)dE} \qquad (2.13)$$

where I_w is the interval limit of the calculation of the line shape parameters. Experimentally for a defect free sample

$$W(E) = j_s w_s + (1 - j_s)w_b \qquad (2.14)$$

where w_s is the surface *W*-parameter and w_b is the *W*-parameter for the bulk. A model was developed for the simulation of *S* and *W*-parameters for metals. The developed model was tested using experimental data for aluminum metal obtained from Positron Beam Laboratory of the Department of Physics, University of Cape Town, South Africa.

3.0 Results and discussion

The model developed using the equations stated in section 2 above was tested using experimental data for aluminium metal obtained from the Positron Beam Laboratory of the University of Cape Town, South Africa [15]. Aluminium metal was used because of it industrial and technological applications and because it is readily available.

Figure 3.1 shows the variation of experimental and modelled S-parameter with positron penetration depth in aluminium. As shown in figure 3.1, both the modelled and experimental S-parameters vary in the same manner with penetration depth. As shown in figure 3.1, apart from the surface and near surface regions, (penetration depth ≤ 44.91*nm*), the modelled and experimental *S*-parameters are in one to one agreement. This confirms the Spearman's correlation of 0.96 obtained between the modelled and experimental *S*-parameters of positrons annihilating in aluminum metals.

Figure 3.2 depicts the variation of modelled and experimental W-parameters with penetration depth d for aluminium. Figure 3.2 reveals that in the surface and near surface regions, (d ≤ 91.53*nm*), there is no agreement between the modelled and experimental W parameters. But in the bulk region, d > 91.53*nm*, there is a good agreement between the modelled and experimental *S*-parameters. The modelled and experimental *S*-parameters exhibit the same trend, but the experimental *S*-parameter fluctuates, this may be due experimental conditions such as fluctuations in the voltage supply or sudden change in the temperature of the laboratory.

Figure 3.3 shows the variation of *S*-parameter with *W*-parameter with energy as the running variable for both the modelled and experimental values. Figure 3.3 reveals that there is a single type of defect in the surface and near surface regions while there are no defects in the bulk [7]. This defect must have been introduced during the machining process. Figure 3.3 reveals that there is a one to one agreement between the modelled structural defect and the one obtained experimentally for the surface, near surface and in the bulk regions. But for *W* parameter greater than 0.185, the modelled and experimental values are not in good agreement. The experimental values are scattered. The scattering of the experimental values may be the collision of the positrons with impurities and phonons in the metal before annihilating with an electron.

4.0 Conclusion

We have successfully developed and tested a model for the structural characterization of defects in metals using positron beam technique. The model can successfully reproduce S-parameter, *W*-parameter structural defect and the type of defects in metals. The results obtained with the model compares very well with the results obtained with the model of Elcher and Krause-Rehberg [10]. Also, the results of the developed model follows the same trend with the results obtained for the simulation of positron annihilation characteristics in multi-layer structure [1]. The S-parameter, *W*-parameter and structural defects obtained with the model are in one to one agreement with experimental values. The developed model can be used as a substitute for experimental works.

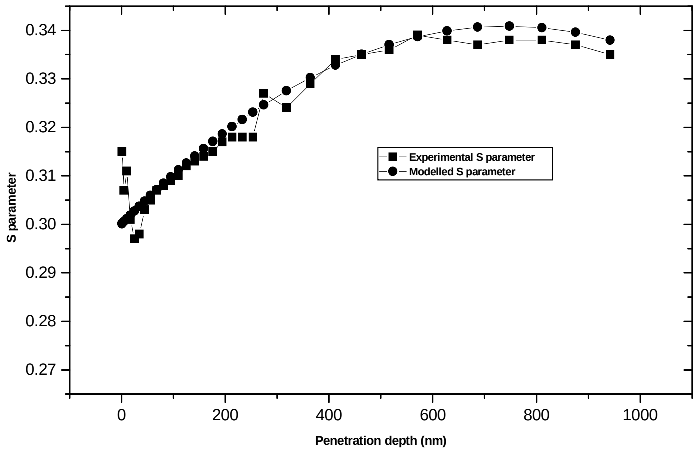

Figure 3.1: Variation of experimental and modelled S- parameter with penetration depth for aluminum

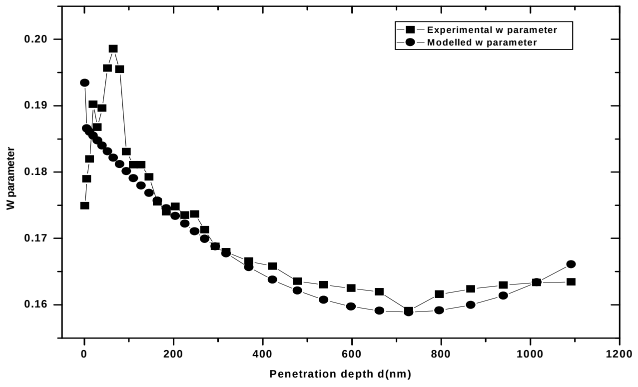

Figure 3.2: Variation of experimental and modelled *W*- parameter with penetration depth for aluminum

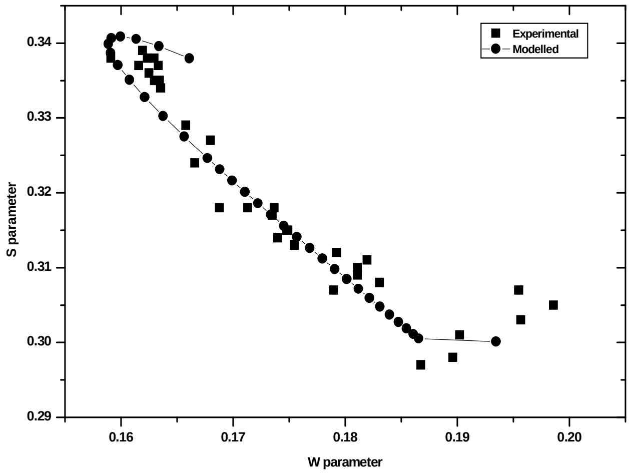

Figure 3.3: Variation of modelled and experimental *S* parameter with *W* parameter for aluminum metal.

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