COMPUTATION OF POSITRON IMPLANTATION PROFILE IN SOLIDS

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ABSTRACT
Positron implantation profile in solids is very vital in understanding the process of positron annihilation in solids. In this work, a model for positron implantation profile in solids is presented; a computer program for computing and analyzing positron implantation profile in solids based on the model was developed and implemented. The program was used to compute and analyze positron implantation profile in aluminium, copper, steel and silicon. The results obtained revealed that the height of the positron implantation profile depends inversely on the incident positron energy while the implantation depth depends directly on the incident positron energy. Also, positron implantation profile depends directly on the nature of the solid. The results obtained in this work are in one to one agreement with the experimental positron implantation profiles in solids showing the predictability power of the model.

Key words: Positrons, solids, implantation profile, penetration depth, computing.

INTRODUCTION

Positron annihilation spectroscopy is a very vital, non-destructive and non-evasive technique for studying different properties of materials (Coleman, 1999). In positron spectroscopic studies, the techniques used are positron life time or annihilation rate, Doppler broadening technique and momentum distribution study (Kruase-Rehberg and Leipner, 1999).

Brusa et al. (2000) studied the formation of vacancy clusters in He-implanted silicon using slow positron annihilation spectroscopy. They found the appearance of vacancy clusters whose size increases with depth in He-implanted silicon. Positron lifetime technique was used by Ling et al. (1999) to investigate the electric field distribution in Au-semi insulating GaAs contact. They found that the interface-trapped positrons revealed that the electric field strength in the depletion saturates at applied biases above 50 V. They used two theoretically derived electric field profiles together with an experimentally based profile to estimate positron mobility of 95±35 $cm^2v^{-1}s^{-1}$ under the saturation field.

Porto et al. (1997) used positron lifetime and Doppler broadening spectroscopies to study the inhibition of positronium formation in binary molecular solid solutions of metal acetyla-cetonate complexes. They observed no positronium quenching reactions and obtained positron inhibition constants for the different complexes.

Chen et al. (2000) used positron lifetime distribution to discriminate defects in semi-conductors. They used positron lifetime study to discriminate the negative vacancy-type defects in GaAs and InP with different conduction types showing that the life time distribution can give more detailed information on the negative defects. Charkraverty et al. (2005) used positron annihilation studies to identify the transformation of the inverse spinel structure of $NiFe^2O^4$ to the normal phase, with tetrahedral sites being occupied by the divalent Ni^{2+} ion and the Fe^{3+} ion transferred to the octahedral sites. Cizek et al. (2005) used positron lifetime and coincidence Doppler broadening techniques to understand tin interaction and its influence on the diffusion of tin atoms. Positron lifetime annihilation characteristics in $BaTiO^3$ perovskite single crystals were measured at room temperature up to 873K and also measured at room temperature after quenching from 473K. Positron lifetime dependence on temperature was found to be reversible after annealing above 550K (Macchi et al., 2001).

Bandzuch et al. (2000) computed the free volume fraction in amorphous polymers using positron lifetime measurements based on a model they presented. They also computed temperature dependence of fraction of free volume, Vogel temperature. They compared the results they obtained with the ones obtained using other methods. Osiele et al. (2004) used positron beam to characterize defects in P3HT and P3HT:PCBM blends. They found that the P3HT polymer has relatively broad electron momentum distribution and blending it with PCBM narrows the momentum distribution.

Osiele and Akpomedaye (2009) developed and tested a model for structural characterization of metals using positron beam technique. The model was used to simulate the S and W-parameters and defects in metals for any given incident photon energy. When compared with experimental values, it was found that the model was in one to one agreement with experimental values.

In the applications of positrons to study solids, the observed signal reaching the surface after the annihilation of the positron carries information about the material. Slow positron implantation spectroscopy based on the generation, implantation and subsequent annihilation of mono-energetic positrons in a sample are used to study depth dependent properties of the material and in particular the depth profile of the vacancy type damage (Grunszpan et al., 2007).

The positron implantation profile plays a very vital role in the annihilation of positrons. The implantation profile determines how far the positrons penetrate the material before annihilation. Also, it accounts for the type of electrons that the positrons annihilate with.

A good and accurate knowledge of the implantation profile is very essential for the analysis of positron beam experiments and predicting positron annihilation characteristics in solids. This necessitates the development of a model and computer program for the study and analysis of positron implantation profile in solids.

THEORETICAL CONSIDERATION AND CALCULATIONS

The mean penetration depth of positrons of energy, E in a solid is given as (Saleh et al., 1999):

$$\overline{Z} = AE^n \qquad (1)$$

where E is energy of incident positrons, n is a dimensionless constant, A is the thickness of the material which can be expressed as:

$$A = \frac{\alpha}{\rho} \qquad (2)$$

where α is a material dependent constant and ρ is the density of the material. Positron implantation profile can be expressed as:

$$P(\overline{Z},E) = -\frac{d}{d\overline{Z}} \exp\left(\frac{-\overline{Z}}{z_0}\right)^m \qquad (3)$$

where z_0 is expressed as (Taylor et al., 1999):

$$z_0 = \frac{AE^n}{\Gamma\left(1+\frac{1}{m}\right)} \qquad (4)$$

where A, m and n are Makhovian function parameters that are material dependent (Puska and Nieminen, 1994).

RESULTS AND DISCUSSION

Positron implantation profile for different energies for aluminium, copper, steel and silicon were obtained using the computer program. These materials were chosen based on the availability of data for computation, technological applications and availability of experimental data. Figure 1 shows the variation of positron implantation profile with depth for different positron incident energies for aluminum. As revealed in Figure 1, when the incident positron energy is 5 keV, the implantation profile is high at the surface and near the surface region of the metal. When the incident energy of the positrons is 10 keV, the implantation profile is highest in the bulk region and decreases towards the substrate region.

Positrons with incident energy of 15 keV probe the bulk, the interface between the bulk and the substrate region. Although the implantation profile for the 15 keV incident positrons is the smallest, they have the highest penetration depth. This shows that the positron implantation profile is profile is inversely proportional to the penetration

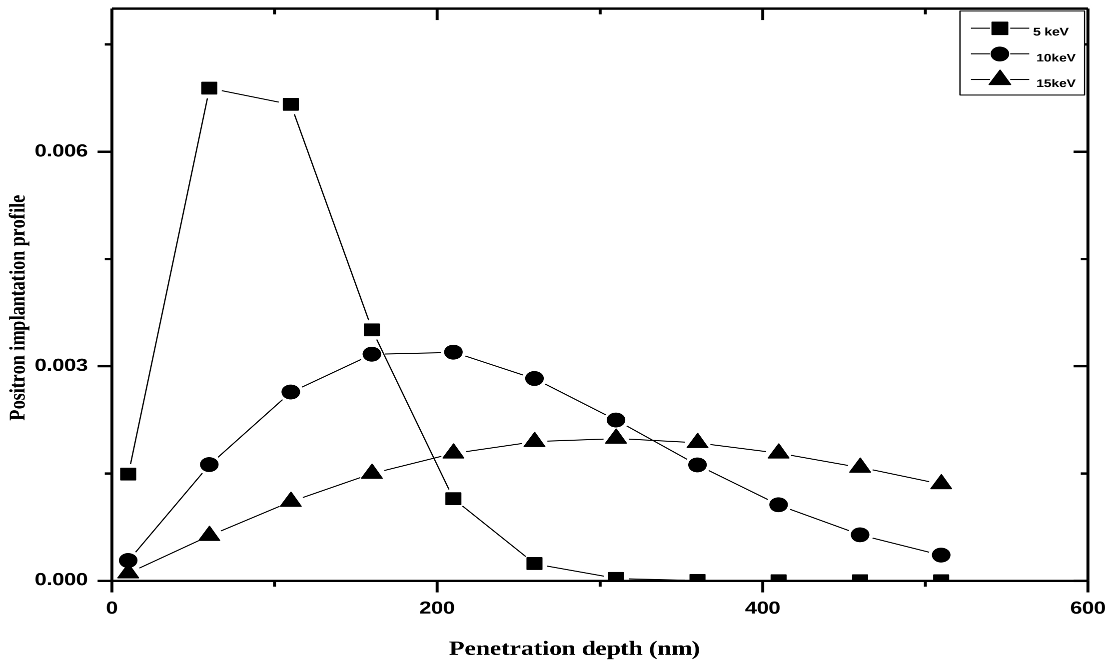

Figure 1. Variation of Positron implantation profile with penetration depth for aluminium.

penetration depth.

The positron implantation profile for copper and steel are shown in Figures 2 and 3. As revealed in the figures, the positron implantation profile for copper and steel when the incident energy of the positrons is 5 keV could not penetrate beyond a depth of 110 nm. This could be due to the high densities of the metals which make it difficult for low energy positrons to travel far in the metals. At incident positron energy of 10 keV, the positrons will annihilate in the bulk without penetration to the substrate. But for positrons with incident energy of 15 keV, the implantation profile for copper and steel are Gaussion is shape and these positrons penetrate up to a depth of 300 nm.

Figure 4 shows the variation of positron implantation profile with penetration depth for silicon. As revealed in Figure 4, the higher the incident of the energy of the positrons, the

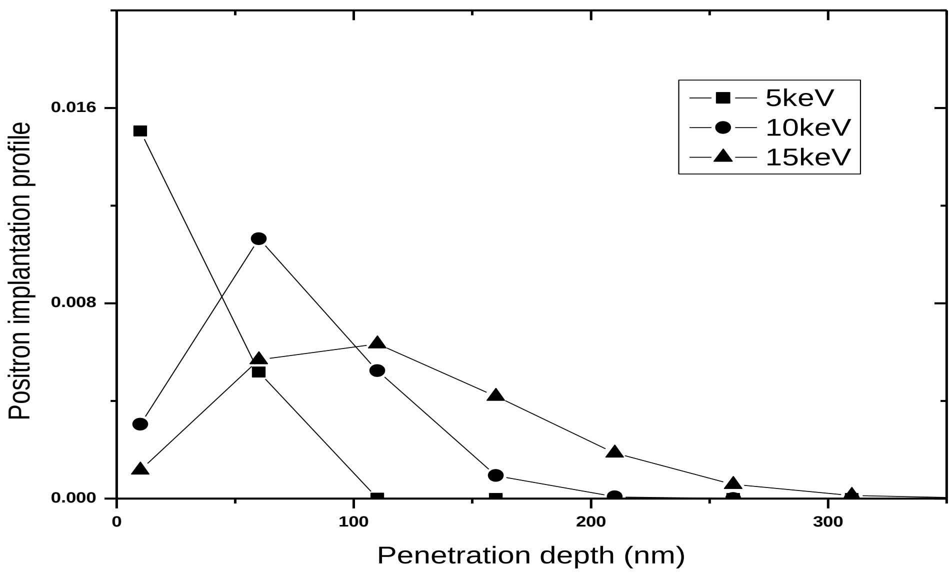

Figure 2. Variation of positron implantation profile with penetration depth for copper.

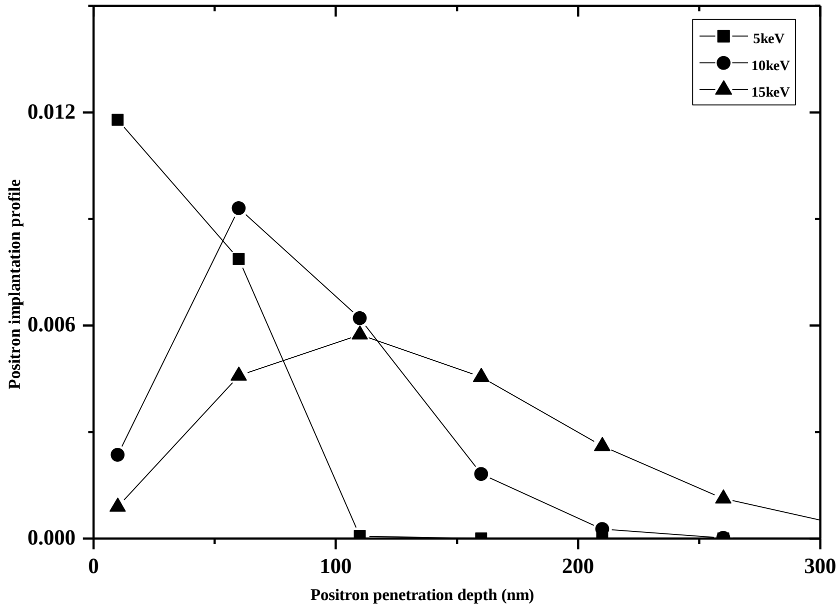

Figure 3. Variation of positron implantation profile with penetration depth for Steel.

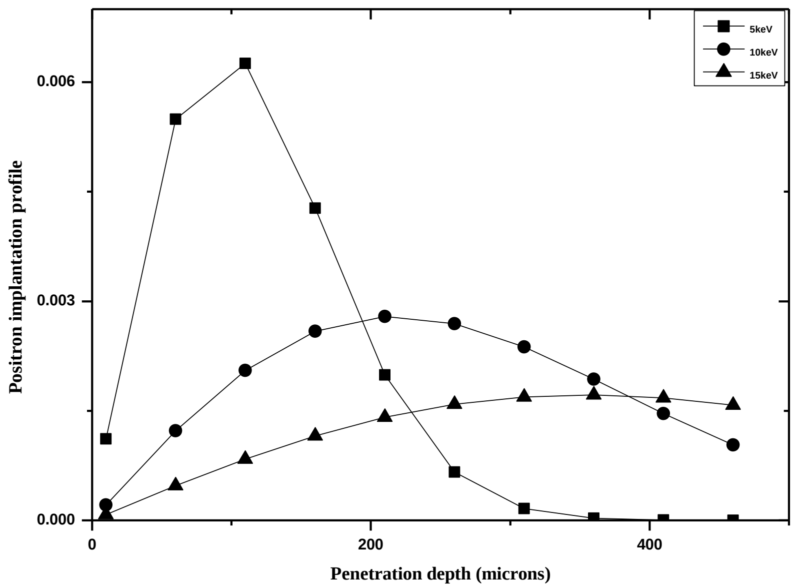

Figure 4. Variation of Positron implantation profile with penetration depth for silicon.

higher the depth reached by the positron profile. Positrons with incident energy of 5 keV could penetrate up to 400 nm in silicon while positrons with incident energy ≥10 keV penetrate up to a depth of 500 nm. The positrons reaching this depth could annihilate with electrons in the bulk and interface regions.

The positron implantation profile for aluminium and silicon obtained in this work can be compared with the implantation profile of the materials obtained experimentally and theoretically (Puska and Nieminen, 1994). This shows that the present computer code can be used to simulate and study positron implantation profile in materials.

Conclusion

In this work, a model for computing and predicting positron implantation profile in solids was developed and implemented. From the study, it was found that positron implantation profile in solids depends on the nature of the material. For hard materials or materials of high density, the incident positron energy should be ≥ 10 keV, but for soft materials, or materials of low density, the incident positron energy should be ≤ 15 keV. The penetration depth of the profile depends directly on the incident positron energy while the height of the implantation profile depends inversely on the incident positron energy.

Conflict of interest

The authors have not declared any conflict of interest.

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