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Transmission and Backscatter Coefficients of 1 to 160 keV Positrons incident on a semi-crystalline polymer target film

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ABSTRACT

The aim of this research is to investigate the behavior of the backscattering, transmitted and absorbed coefficients as a function of the positrons beam primary energy. The absorbed, backscattering and transmitted probability coefficients has been calculated and studied graphically via Monte Carlo simulation technique PsMCS (positronium Monte Carlo Computer Simulation) for a high energetic positrons from 1 to 160 keV, implanted normally into a semi - crystalline Polytetrafluoroethylene target (PTFE) with it's the two components of the target. Comparison with available references yields good quantitative agreement for dynamics factors.

Index Terms

Absorbed coefficient, Backscattering coefficient, Monte Carlo Simulation, PTFE, Transmitted coefficient.

I. INTRODUCTION

The positron interaction with the matter especially polymers has been studied theoretically and experimentally for different energies [1-4]. Monte Carlo simulation technique designed to be used for the simulation of particle transport across an absorber material by following each incident particle through the subsequent collisions it undergoes and applying specific rules each time one of the expected interaction processes occurs. The positron undergoes elastic and inelastic collisions through its trajectories. Elastic scattering describes the interactions of it with the potential field of an atomic nucleus[5] because a nucleus is more massive than the positron, the energy transfer involved here is usually negligible. Inelastic scattering is the main energy loss mechanism for positrons interacting with the PTFE sample. These interactions usually include core ionization and excitation [1]. For the positron, it has some possibility of annihilating with an electron or making positronium atom.

There are two parameters to describe inelastic collision: the inelastic mean free path and the stopping power. Gryzinski [6-8] models that usually applied to describe inelastic scattering used a semi quantum-mechanism treatment to describe the scattering off individual atom in medium by the electron binding energy. The Monte Carlo programs used in the models of the implantation profile of electrons and positrons have been developed first by Adesida et al. [9], Valkealahti and Nieminen [10] and Jensen and Walker [11], All of these programs have a similar structure.

The accuracy of the model which is being used depends on the modeling of scattering processes included the most dominant interactions elastic and inelastic processes. The program used in this paper Positron Monte Carlo Simulation PsMCS, was designed to have a good flexibility to determine many factors for Polytetrafluoroethylene PTFE target such as absorbed coefficient, transmitted coefficient, backscattered coefficient, mean penetration depth, angle of scattering, etc. and simulated the trajectory of the positron starting from time zero and energies range from 1-160 keV.

II. THEORY

A Monte Carlo simulation program has been established consisting many steps for showing how the positron particle moves through its track .When it inters the matter, undergoes many interactions (elastic and inelastic collisions) with the matter PTFE in which it consists of two major components, Carbon and Fluoride atoms and step by step lose most of its energy until it get thermalized and pick up an atomic electron to form positronium atom[12]. Therefore the ejected positron have many probabilities for losing its energy through inelastic collisions inside the target; it is either annihilated from a bulk state within material or trapping in surface state [13] followed by either annihilation or thermal absorption as positronium [14], other two probabilities are direct emission as positronium [15] or direct reemission as a free positron. Therefore elastic and inelastic cross sections for interactions must be found using the differential elastic scattering cross section which can be calculated by the so-called relativistic partial wave expansion method, corresponding to the Mott cross-section which approximated with the screened Rutherford formula. The differential cross is:

$$\frac{d\sigma_{el}}{d\Omega} = \left(\frac{{Z_i}^2 e^2}{2{E_p}^2} \right)^2 \frac{1}{(1-\cos\theta + 2\alpha_i)^2} \qquad (1)$$

And the total elastic scattering cross section σ_{el} is

$$\sigma_{el} = \int \frac{d\sigma_{el}}{d\Omega} d\Omega \qquad (2)$$

θ is scattered particle angle with solid angle Ω and α is the atomic screening parameter as suggested by Nigam et al.[16], M.Dapor [17] and later by I.Kyriakou et.al. [18] defined as

(3)

$$\alpha_i = 0.51\left(\frac{m_e e^2 \pi}{h}\right)^2 \frac{Z_i^{2/3}}{mE_p} \quad (3)$$

Where m_e is an electron mass, Z_i is the charge of target i with mass m, h is Planck constant and E_p is the energy of incident positron.

The partial differential cross-section with the energy difference for a positron giving its energy E_p to an electron of inner shell is given by [6-8]:

$$\frac{d\sigma}{d\Delta E} = [\frac{\sigma_o}{E_p}] \frac{E_B^{5/2}}{[(\Delta E)^2 (E_p + E_B)]^{3/2}} \quad \text{X}$$

$$\{ \frac{\Delta E}{E_B}(1 - \frac{E_B}{E_p}) + \frac{4}{3}\ln[2.7 + (\frac{E_p - \Delta E}{E_B})^{1/2}] \} \; (1 - \frac{\Delta E}{E_p})^{(\frac{E_B}{E_B + \Delta E})} \quad (4)$$

Where $\sigma_0 = 6.56 \times 10^{-14} Z^2$[19,20].

Scattering angle after each collision is calculated by choosing a uniform random number R_1 in which it lies between zero and one, and then finding the value of scattering angle from the cross-section data which satisfies the screening Rutherford equation. We can generate another random number R_2 to choose the part of interaction in which the particle will interacts with it, to decide if it is carbon or fluoride in the target, therefore the probability of interaction is:

$$P(i) = (f_i \sigma_i / A_i)/(\sum_i f_i \sigma_i / A_i) \quad (5)$$

Where f_i represents the atomic specie i with atomic mass A_i . Therefore if R_2 is in the range between zero and P_i , the interaction is done by the atom i and the probability of the other specie is done between P_i and one. For each inelastic scattering interaction, the energy loss is calculated by choosing another uniform random number R3 to find the value of decrement or:

(4)

$$rnd_3 = \int_{\Delta E_B}^{E_p} (d\sigma_i / d\Delta E) X (d\Delta E / \sigma_i) \qquad (6)$$

Finally the distance traveled between collisions s is obtained by generating another uniform random generator $0 \leq R_4 \leq 1$ and also R_5 is generated to classify the processes whether an individual event is due to elastic scattering , inelastic core electron scattering , or inelastic valence electron scattering in which its ranges are between 0 and one.

When a particle beam impinges on a solid target, some particles, after a number of elastic and inelastic collisions with the atoms of the target, transmitted through the matter , while other particles are absorbed and annihilated or, final process is backscattering far from it. The backscattering coefficient depends on the type of particles, on their primary energy, on the target mean atomic number, and on the incidence angle. In this paper, we consider high energy positrons interacts with both atoms of the polymer.

The backscattering coefficient defined as the ratio of the number of backscattered positronsns to the number of incident positrons. The bulk backscattering of positrons from surfaces in the energy ranges 10 keV to 1 MeV for a target of Z<30 materials indicates a significant increase of the backscattering coefficient, and it is increasing with increasing target thickness until saturation is reached at a thickness around half the practical range of the incident positrons this means that the backscattered positrons are increased at low energies of incident particles.

The transmission coefficients increases with electron energy for a given target thickness but it decreases with increasing effective atomic number Z of the target material as in our target, the primary reason for the smaller transmission coefficient for materials of high Z is that, on the average, the angular deflections of the positrons during interactions or collisions with such materials are greater than the angular deflections of positrons interacting with materials of low Z[21].

The conservation of the total number of particles entails that, for a given thickness t,

$$\eta_A(t) + \eta_B(t) + \eta_T(t) = 1 \tag{7}$$

The implantation or penetration profile $P(z, E)$ of monoenergetic positrons having an energy E travelled a distance z from the surface of the material in the direction of the incoming beam, is given by:

$$P(z,E) = \frac{mz^{m-1}}{z_0^m} exp\,[-(\frac{z}{z_0})^m] \tag{8}$$

with

$$z_0 = \frac{A\,E^r}{\rho\Gamma(\,1+\frac{1}{m})} \tag{9}$$

m is known as shape parameter, r and A are empirical material related parameters, ρ is the mass density of the sample and Γ is the gamma function[22].

The positron implantation profile is called a Makhov profile, named after Makhov's original electron implantation experiments[23]. The parameters of this profile can be obtained theoretically from Monte-Carlo simulations [10,19]. Ghosh[24] showed by several Monte-Carlo calculations. The transmission

probability could be written in the following form as follow[25]:

$$\eta_T(t) \cong exp\,[-(\frac{z}{z_0})^m] \tag{10}$$

The general form of the η_T of the incident potential relation is similar to the Lindhard et al. law in which related with the total number of atoms per unit volume in the target and also with the total scattering cross section[26]:

When a positron beam impinges on a solid target, a fraction of the beam is absorbed, another fraction is backscattered, and the remaining one is transmitted. The sum of these fractions is equal to unity. Their values depend on the beam quality, the nature of the target and its thickness. The backscattering phenomena is usually described by the backscattering coefficient. The backscattering coefficient depends on the type of particles, on their primary energy, on the target mean atomic number, and on the incidence angle. In this paper, we study the dependence of it on the target mean atomic number, positron incidence angle, and primary energy[27].

In order to obtain the value of Backscattered coefficient for the arbitrary atomic number Z of the target and incident kinetic energy E of the positrons, it would be convenient to use the following equation which well reproduces the most probable values given by the existing data for the energy region from about 1 to 160 keV[28-29].

Therefore we can find backscattered coefficient as a function of z and distance x, $\eta_B(z,x)$

$$\eta_B = 1.2\gamma\int_0^x \frac{W}{S^{1.16}}dx - 0.673\int_0^x \left\{[1 - W - \frac{1}{\gamma^2}[S^2W - 1] - \frac{1}{\gamma}[SW - 1]]\right\}dx \tag{11}$$

Where $\gamma = 0.355z^{2/3}$, W= exp(- γx/S) and S=1-x

The residual positrons are absorbed in a solid target and the absorbed positron coefficient calculated by subtracting the transmitted with absorbed positron coefficients from one.

Monte Carlo method calculation has been used in this research for describing the energy distribution of transmitted positrons. This method can offer the most accurate solutions for the positron transmission problems in bounded medium and applicable to any energy range of positrons and to any geometry. Statistical nature of inelastic scattering processes, as well as the elastic scattering process, is taken into account.

The Monte Carlo program simulation is constructed in such away and many restrictions to give probabilities of positron interaction with the two parts of the medium (Carbon and Fluoride). At the first moment of interaction, the positron must be interacts with the Fluoride atom or the Carbon atom, otherwise it remains in its direction till it met another molecule of the polymer and repeat the same procedure. If the particle interacts with the Fluoride atom, this interaction may be of coarse elastic or inelastic interaction in which the two parts also divided into two parts core or valence interaction.

III. RESULTS AND DISCUSSION

1 – Backscattered coefficients: Backscattered positron coefficient is the ratio between the number of positron beam that return and emerge from a target surface when the beam impinges on a solid to that of incident positron. Figure (1) represents the Backscattered coefficient BSC of the energetic positrons from the target Polytetrafluoroethylene PTFE verses its energy .It has been seen that the back scattered positrons are increased with the positron energy decreasing because the particle has a low energy and the probability of colliding with another particle to return back is too high [30].

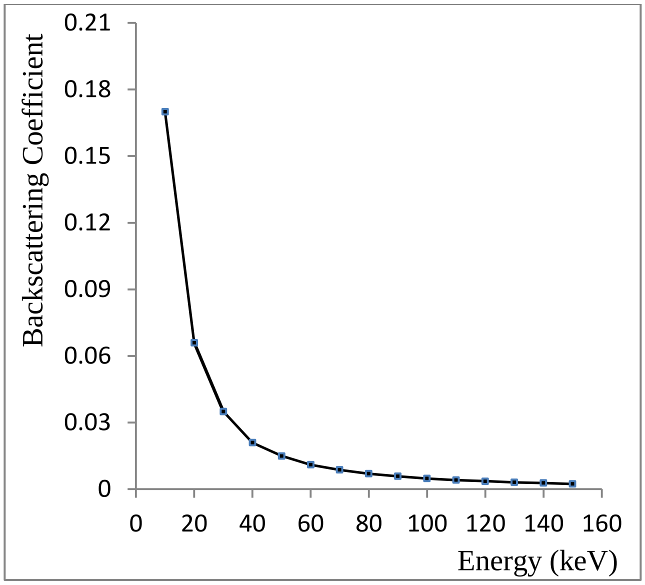

Fig1: Backscattered coefficient of Polytetrafluoroethylene PTFE verses positron primary energy.

2 – Transmitted coefficients: For a million particles we notice from Fig.(2) that the transmitted positrons increased with the increasing of its energy because of the high energy of the positrons ranged from (1 to 160 keV). This is true for both atoms Fluoride and Carbon atom. We can see that transmitted coefficient reaches the saturation region 99.41% after about 90 keV positron energy.

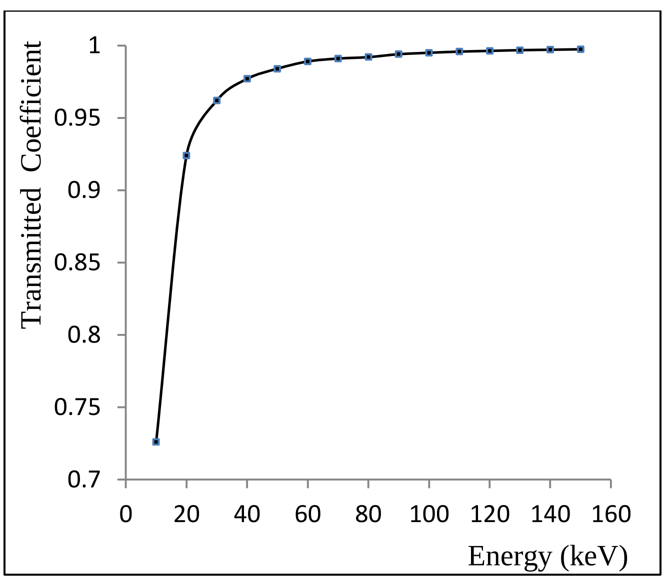

Fig2: Transmitted coefficient of Polytetrafluoroethylene PTFE versus positron primary energy.

3 – Absorbed coefficients: Figure (3) represents the variation of the ratio of absorbed particles (absorption coefficient) with its energy for all number of positrons. It has been seen that the absorbed positrons are decreased with its energy bellow 40 keV (transmitted coefficient is 0.078 %) and its ratio is near zero for high energies and reaches saturated region bellow this energy because its may be collides with any one of the components (Fluoride or Carbon) as follow:

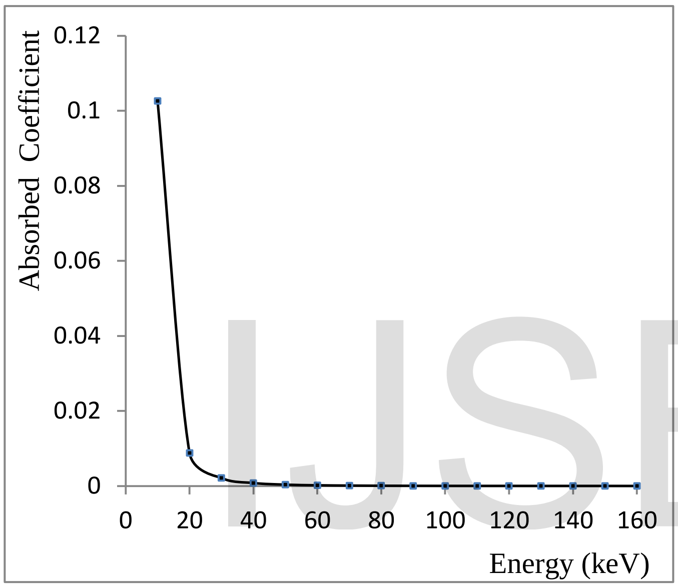

Fig3: Absorbed coefficient of Polytetrafluoroethylene PTFE versus positron primary energy.

IV. CONCLUSION

The paper was focused on the simulation of the interaction of a positron beam with a semi-crystalline polymer target constituted by thin films. Absorption, Backscattered and Transmitted coefficients of positron impinging into polymer material polytetrafluoroethylene PTFE by using positronium Monte Carlo simulation method in the examined energy range (1 – 160) keV and for a million particles has been calculated . We have remarked these coefficients increasing or decreasing for the Polytetrafluoroethylene components (Fluoride and Carbon) and conclude that the both coefficients η_A and η_B are nearly decreased with positron increasing and the last coefficient η_T is increasing with the energy increasing.

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REFERENCES

[1] Carlos A. P. Gomez, 2008. " Some effects on Polymers of low – energy implanted positrons" ; Ghent University.

[2] Jag J. Singh, Gerald H. Mall,and Danny R. Sprinkle, 1988. " Analysis of positron lifetime spectra in polymers", NASA Technical paper 2853.

[3] S.Levin and E. J. Hoffman, 1999. Phys. Med. Biol.44781–799.

[4] S.A.Bigdelo and L.Alamsi, 2011. Aust. J. of Basic and Applied Sciences, 5(12), 1813-1820.

[5] N.F. Mott and H.S.W. Massey, 1950. "The theory of atomic collisions "2nd ed., Oxford, Clarendon Press. 388.

[6] M. Gryzinski, 1965. Phys. Rev. A 138 , 305.

[7] M. Gryzinski, 1965. Phys. Rev. A 138 , 322.

[8] M. Gryzinski, 1965. Phys. Rev. A 138 , 336.

[9] I. Adesida, R. Shimizu, T.E. Everhart, 1980. J. Appl. Phys.51, 5962.

[10] S. Valkealahati, R.M. Nieminen, 1984. Appl. Phys. A35, 51.

[11] K.O. Jensen, A.B. Walker, 1993. Surf. Sci.292, 83.

[12] A. Ore and J. L. Powell, 1949. Phys. Rev , 75 , 1696.

[13] R. M. Nieminen and M. J. Manninen, 1979. " in Positron Solids", Edited by P. Hautojärvi, Springer, New York.

[14] K.G.Lynn, 1979. Phys.Rev.Lett. 43 , 391.

[15] A.P.Mills, 1978. J.Phys.Rev.Lett.41 , 1828.

[16] B. P. Nigam , M. K. Sundaresan and Ta- You Wu, 1959. Phys. Rev. 115, 491.

[17] M. Dapor, 2003. “Electron-Beam Interactions with Solids”; Springer.

[18] I. Kyriakou, D. Emfietzoglou, A. Nojeh and M. Moscovitch, 2013. J. App. Phys. 113, 084303.

[19] S. Valkealahti and R.M. Nieminen, 1983. Appl. Phys. A32,95-106.

[20] J. Mäkinen, A. Vehanen, P. Hautojärvi, H. Huomo and J. Lahtinen, 1986. Surf. Sci. 175, 385-414.

[21] Berger, Martin J., 1963.” Monte Carlo Calculation of the Penetration and Diffusion of Fast Charged Particles. Methods in Computational Physics, Vol. 1 -Statistical Physics, Berni Alder, Sidney Fernbach, and Manuel Rotenberg, eds., Academic Press, pp. 135-215.

[22] A. Vehanen, K Saarinen, P. Hautojärvi, and H. huomo, 1987. Phys. Rev. B,35(10):4606.

[23] A.F. Makhov, 1961. Sov. Phys. Solid State, 2, 1934.

[24] V. J. Ghosh, 1955. Appl. Surf. Sci. 85, 187.

[25] A.Bentabet, 2010. Revue des Sciences et de la Technologie – RST.,V. 1,2.

[26] J. Lindhard, M. Scharff and H. E. Schiott; K.Danske Vidensk, Selsk, 1963.Math-Fys.Meddr.33, 1-42.

[27] M. Dapor and A. Miotello, 1998. Scanning Microscopy Vol. 12, 1, 131.

[28] T. TABATA, R. ITO and S. OKABE, 1971.Nuclear, Instruments & Methods Vol. 94, 3, 509.

[29] K. Kanaya and S. Okayama, 1972. J. Phys.D :Appl.Phys. 5, 43.

[30] L.H.Cai, B Yang, C C Ling, C D Belling and S Fung, 2011. Journal of Physics: Conference Series 262, 012009.