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Research Paper

Monte Carlo Dynamic Transmission Calculations For High Energetic Positrons Implanted Into A Semi-Crystalline Polymer Target Film (Polytetrafluoroethylene)

Physics

KEYWORDS : Backscattering coefficient, transmitted coefficient, Monte Carlo Simulation, PTFE.

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ABSTRACT

In this work, backscattering and transmitted probability coefficients with mean penetrating depth has been calculated via Monte Carlo simulation technique PsMCS (positronium Monte – Carlo Computer Simulation) for positrons with different energies starting by high energies and finishing with very slow energy (from 0.15MeV to 70 eV) ,implanted normally and with different angles , into a semi finite Polytetrafluoroethylene target (PTFE) . Comparison with available references yields good quantitative agreement for dynamics factors.

Introduction

The positron interaction with the matter especially polymers has been studied theoretically and experimentally for different energies [1-4]. Many procedures has been used for this purpose , one of them is a Monte Carlo simulation technique , in which 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 an inelastic collisions through its trajectories. Elastic scattering describes the interactions of it with the potential field of an atomic nucleus [5]. The nucleus is more massive than the positron; therefore 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 for both materials carbon and fluoride [1]. For the positron, it has some possibility of annihilating with an electron or making positronium atom depending on its energy.

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 Positonium Monte Carlo Computer Simulation PsMCS, was designed to have a good flexibility to determine many factors for the polymer PTFE target such as transmitted coefficient, backscattered coefficient, absorbed coefficient, mean penetration depth, angle of scattering, etc. , and simulated the trajectory of the positron starting from time zero and energies range from 0-160 keV.

Theory:

A Monte Carlo simulation program has been established consisting many steps for showing how the energetic positron particle moves through its track .When it inters the matter, undergoes many interactions (elastic and inelastic collisions) with the matter Polytetrafluoroethylene 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]. PTFE is a semi-crystalline polymer and was chosen in this study for several reasons, including its use as a common engineering material for small high-performance parts and its availability from several manufacturers. While studied extensively in the past, it has received little attention in the open literature for the last years.

Therefore the ejected positron has 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 Ps[14], other two probabilities are direct emission as Ps[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 elastic collision cross section is

$$\frac{d\sigma}{d\Omega} = \left(\frac{z_i^2 e^2}{2E_p^2}\right)^2 \frac{1}{(1-\cos\theta+2\alpha_i)^2} \quad \text{.................................. (1)}$$

and the total elastic scattering cross section can be written as

$$\sigma = \int \frac{d\sigma}{d\Omega}\, d\Omega \quad \text{.................................. (2)}$$

in which θ is scattered particle angle, Ω is a solid angle which may be calculated over all angles from zero to π, 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] in which it ;must be determined in order to obtain the total elastic scattering cross-section by the program, defined as

$$\alpha_i = 0.51 \left(\frac{m_e e^2 \pi}{h}\right)^2 \frac{Z_i^{2/3}}{m\, E_p} \quad \text{.................................. (3)}$$

Here m_e is an positron mass, Z_i is the atomic number of target i with mass m , h is Planck constant and E_p is the energy of incident positron. Integrating eq(1) over all solid angles allow us to obtain the total cross section σ

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$$\sigma = \left(\frac{Z_i e^2}{2E_p}\right)^2 \frac{\pi}{\alpha_i(1+\alpha_i)}$$

.... (4)

and many random numbers are generated to calculate the angles of scattering by dividing the right side of equation (2) by σ and making the integral equals to the random number R_1 and by using the above equations, we can find angles of scattering started from zero to π for each random number from one to zero, beside that for knowing the type of scattered particle either carbon or fluoride, another random number R_2 must be used to do this job as follow:

$$K = \frac{F_i\,\sigma_i/A_i}{\sum_i (F_i\sigma_i/A_i)}$$

.... (5)

in which *k* is the range of scattering between zero and one, that's mean if the range is

between (o-*k)*, the particle may be scattered by fluoride, otherwise if it is (*k*-1),its scattered by carbon.

The other part of the positron interaction, is the inelastic collision case. We used Gryzinski[6-8] excitation function in which the differential cross section for the energy transfer have been measured by the program. Our purpose is to determine the mean penetrating depth of the positron starting from high energetic particle until it reaches thermal equilibrium, beside that the coefficients of transmission or absorption and the ratio of the recoil particles must be calculated.

If the positron collides with a matter, it will transfer some of its energy to the matter and its direction will be changed, this collision will cause a little energy loss. The basic mechanism of positron energy loss via collisions is also valid in applying Bethe-Bloch equation in which it must be modified.

The energy loss of a high-energy charged particle in matter due to its interactions with the electrons present in the matter is given by the Bethe-Bloch equation[19]:

$$-\left(\frac{dE}{dx}\right) = \frac{K\rho Z}{2A\beta^2}\left[ln\left(\frac{\tau^2(\tau+2)}{2(I/m_e c^2)^2}\right) + F(\tau) - \delta - \frac{2C}{Z}\right]$$

.... (6)

Where

$$F(\tau) = 2ln2 - \frac{\beta^2}{12}\left(23 + \frac{14}{\tau+2} + \frac{10}{(\tau+2)^2} + \frac{4}{(\tau+2)^3}\right)$$

.... (7)

Where

dE/dx: energy loss of particle per unit length

is the positron kinetic energy in units of m_0c^2

K = 4πm$_e$ = 0.307075 MeV g^{-1} cm^2

: Avogadro's number

A: Atomic mass of absorber g /mol

r_e: Classical electron radius = 2.81794 fm

I: Mean excitation energy of the target medium eV

δ: Density effect correction to ionization energy loss

Z: charge of the particle

c: velocity of light

βγ: relativistic particle velocity, v/c

ρ: density of the material

δβ: density-dependent term that attenuates the logarithmic rise of the cross section at very high energy.

C/Z: Shell corrections, constitute a large correction to positron stopping powers in the energy range of 1-100 MeV, with a maximum correction of about 6%. It corrects the Bethe-Bloch theory requirement that the particle's velocity is far greater than the bound electron velocity [20].

The energy loss for the compound:

For any compound such as Teflon, a good approximation value can be found by averaging each element (carbon or fluoride) weighted by the fraction of electrons belonging to each element. Thus

$$\frac{1}{\rho}\frac{dE}{dx} = \frac{w_1}{\rho_1}\left(\frac{dE}{dx}\right)_1 + \frac{w_2}{\rho_2}\left(\frac{dE}{dx}\right)_2$$

.... (8)

Where w_1 and w_2 are the fraction by weight of elements 1 and 2, ρ_1 and ρ_2 are densities of the tow matters.

Since particles lose energy when travelling in a medium, they will eventually have lost all their kinetic energy and come to rest. The distance travelled by the particles is referred to

as the range. As the particle penetrates in the medium, its energy loss per unit length will change. The range, R, of a particle entering a material can be found as follows:

$$R = \int_{E_0}^{0} \frac{dE}{dE/dx}$$

.... (9)

Our goal in this work is to develop a general model using the Monte Carlo method based on the interactions that the positron undergoes when traversing through the polymer. For the calculation of positron trajectory, the Monte Carlo approach has a good flexibility and high accuracy for following the paths of particle movements through its track.

Scattering angle after an inelastic collision is expressed by the expression of binary collision model given as follows:

$$\theta = \sin^{-1}\left(\sqrt{\frac{\Delta E}{E}}\right)$$

.... (10)

The transmission probability is defined as the ratio between the numbers of transmitted particles to the incidental ones. The transmission probability has been written and calculated for three types, absorbed, transmitted and backscattered. The backscattering coefficient may be obtained by using the analytical expression of Dapor[21] given by:

$$\eta = 1 - \frac{1+3\varepsilon(E)\sqrt{z-1}}{\left(1+\varepsilon(E)\sqrt{z-1}\right)^{3}}$$

.... (11)

where

$$\varepsilon(E) = \begin{cases} 0.0811 + 0.007E & for\ \ 2 \le E \le 6.7keV \\ 0.1051 + 1.078X10^{-4}E & for\ \ 6.7 \le E \le 45keV \end{cases}$$

.... (12)

We know that reduced depth y=x/R where x is the distance along x-axis and the angle of scattering is related to it by, cosθ =y/1-y , therefore: R=x(1+cosθ) and the transmitted particles is calculated from the following relation[22] after some algebra:

$$\eta_T = e^{-0.187\, Z^{2/3} \cos\theta}$$

.... (13)

And at the end of all of this we can calculate the residual ratio or the absorbed number of the

particles into the matter η_A by adding the transmitted to the backscattered and subtracting from one the remainder may be the absorbed ratio.

Results and discussions:

The backscattered positrons coefficient represents the ratio of the number of particles that return back when emerges the target surface and the beam impinges on the target PTFE to that of incident positrons. The figure (1) represents the backscattered coefficient of the polymer PTFE for the two components C and F versus the positron energy. We see that the backscattered positrons ratio was decrease strongly for energies in between 0.5keV and 3keV and after that its ratio reduces slowly for energies over 3keV to 15keV.We can explain this behavior by saying that for a small energies, the maximum value of the positrons can be returns back in different angles, but for high energies the most of it can enter the matter without more obstructions.

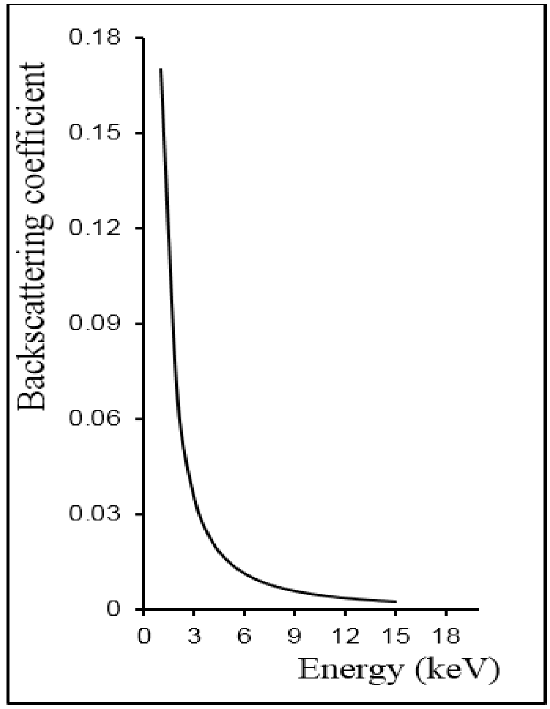

Fig 1. Backscattering coefficient of PTFE versus the incident positron energy.

The ratio of the transmitted positrons into the target PTFE has been sketched in the figure (2) in which it has seen that for lower energies between (1keV and 4keV), the number of the transmitted particles is growing strongly for a little changing in energy, this is because the positron can straggling in between the two components of the target surface and its components without interaction, for these energies. But for energies above 4keV until reaches 16keV, we notice that this ratio almost stays the same value at about 98% because of its high energy.

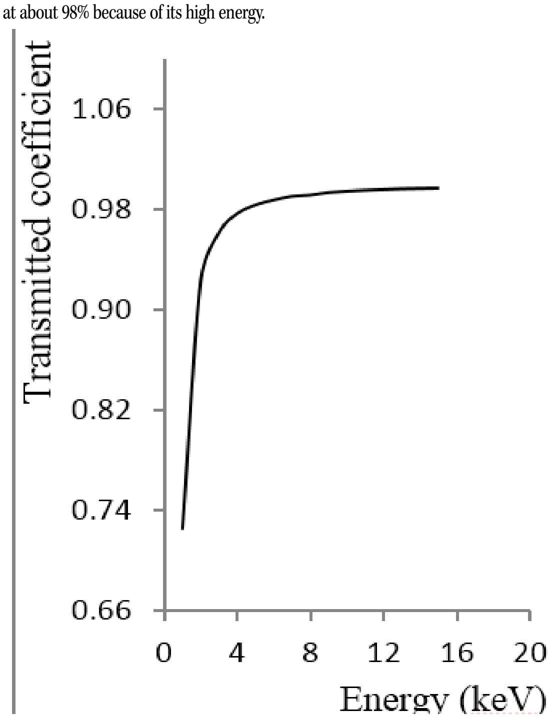

Fig 2. Transmitted coefficient of PTFE versus positron primary energy.

With solving equations of stopping power besides the reduced depth y we can find from the program the distance x along x-axis in which positron can traveling for all energies starting from high energies of about 17.5keV until reaches low energies 1keV. We can see that the more energy of the positron increases, the more particles can go further into the target, this is because of its small mass and due to its high energy. The maximum value of the mean penetrating depth for maximum energy 17.5keV is 0.09×10^8 A^0 (0.9mm).

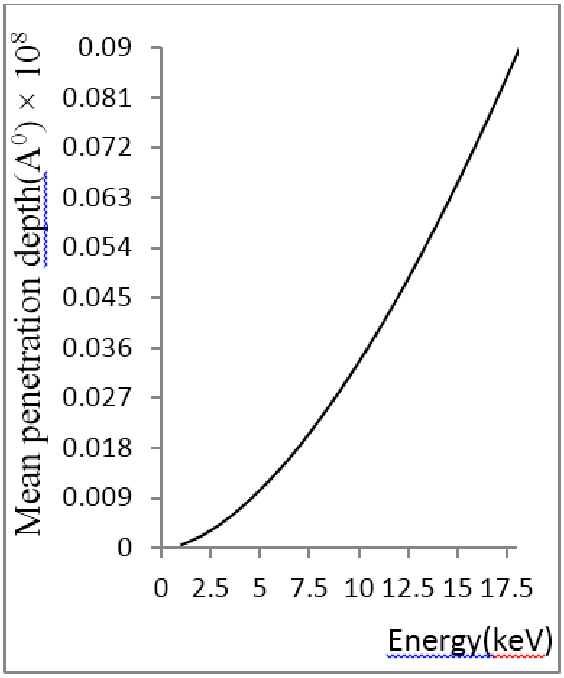

Fig 3. Mean penetration depth versus positron energy

Conclusion

In conclusion, we have calculated the backscattering coefficient, transmitted coefficient and the mean penetration depth of positrons impinging into Polytetrafluoroethylene PTFE polymer target by using our simulation program PsMCS in the examined energy ranges 1-17.5keV.We have remarked that backscattering coefficient was decrease sharply for energies below 3keV and the transmitted is begins growing above this value, therefore it is better to study positron behavior through this matter at this energy and greater.

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