Calculation of Dynamic Coefficients for High Energetic Positrons Implanted into a Semi-Crystalline Polymer Target Film

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Received 28 March 2015 ; Accepted 6 December 2015

Abstract

In this work absorbed , backscattering and transmitted probability coefficients has been calculated via Monte Carlo simulation technique PsMCS (positronium Monte Carlo Computer Simulation) for a high energetic positrons implanted normally into a semi finite Polytetrafluoroethylene target (PTFE) with its two components. Comparison with available references yields good quantitative agreement for dynamics factors.

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

حساب المعاملات الداينميكية لبوزترونات ذو طاقة عالية تغرزفي رقيقة بوليمر شبه بلورية

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الخلاصة

في هذا العمل معاملات احتمالية الامتصاص والارتداد والنفوذ حسبت بواسطة تقنية محاكاة مونت كارلو (مختصر لمحاكاة بالحاسبة للبوسترونيوم بطريقة مونت كارلو) لبوسترونات ذو طاقات عالية تغرز عموديا" في هدف شبه محدود من مادة البولي تترافلوروواثيلين وذلك للمركبين. تمت المقارنة مع المصادر المتاحة لنا وتبين لنا ان النتائج تعتبر جيدة لهذه المعاملات الداينميكية .

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الكلملت المفتاحية : معامل الارتداد ، معامل النفوذ ، معامل الامتصاص ، محاكاة مونت كارلو ، بولي تترافلورواثيلين

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 0-160 keV.

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:

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

And the total elastic scattering cross section is

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

θ is scattered particle angle 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

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

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.

According to Gryzinski[6-8], the differential cross-section for an energy transfer from a positron with an energy E_p to an electron of the k^{th} inner shell is given by:

$$\frac{d\sigma_{inel}(\Delta E, E_p, E_B)}{d\Delta E} = [\frac{\sigma_0}{(\Delta E)^3}]\, g_\sigma(\frac{E_p}{E_B};\frac{\Delta E}{E_B})$$

$$g_\sigma(\frac{E_p}{E_B},\frac{\Delta E}{E_B}) = \Theta\Re\,\frac{E_B}{E_p}\{\frac{\Delta E}{E_B}(1-\frac{E_B}{E_p})+\frac{4}{3}\ln[2.7+(\frac{E_p-\Delta E}{E_B})^{1/2}]\} \quad \ldots\ldots\ldots\ldots\ldots\ (4)$$

Where

$$\Theta(E_B, E_p) = (\frac{E_B}{E_P + E_B})^{3/2} \quad \ldots\ldots\ldots\ldots\ (5)$$

$$\Re(E_B, E_p, \Delta E) = (1-\frac{\Delta E}{E_p})^{(\frac{E_B}{E_B+\Delta E})} \quad \ldots\ldots\ldots\ldots\ (6)$$

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

Scattering angle after each collision is calculated by selecting a uniform random number R_1 where $(0 \le R_1 \le 1)$ and then finding the value of θ from the cross-section data which satisfies the screening Rutherford equation. The atom specie i which scatters the incident positron in a mixed target (PTFE) is also chosen in a Monte Carlo fashion by generating another uniformly distributed random number R_2. The probability that the positron will be scattered by an atom i (carbon or fluoride) is simply the fractional cross-section:

$$p_i = \frac{C_i\sigma_i / A_i}{\sum_i C_i\sigma_i / A_i} \quad \ldots\ldots\ldots\ldots\ (7)$$

Hence if R_2 is in the range $(0 - p_i)$, the positron is assumed to be scattered by that specie of an atom. If R2 is in the range $(p_i - 1)$, scattering is caused by another specie of an atom. At each inelastic scattering event, the energy loss is calculated by selecting a uniform random number R3 and then finding a value of ΔE that satisfies:

$$R_3 = \int_{\Delta E_B}^{E_p} \frac{d\sigma_{inel}(\Delta E)}{d\Delta E} \frac{d\Delta E}{\sigma_{inel}} \qquad \text{.......... (8)}$$

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. The positron interaction with the matter classified into three types; transmitted through it, absorbed and annihilated or, final process is backscattering far from the matter.

The bulk backscattering of positrons from surfaces in the energy ranges 10 – 1000 keV for a target of Z<30 materials indicates a significant increase of the backscattering coefficient defined as:

$$\eta_B = \frac{number\ of\ backscattered\ positrons}{number\ of\ incident\ positrons} \qquad \text{.......... (9)}$$

with decrease of energy this means that the backscattered positrons are increased at low energies of incident particles .

The general form of the η_T (transmitted positron coefficient) of the incident positrons which is

transmitted into the matter may obey an exponential relation similar to the Lindhard et al. law [21]:

$$\eta_T = \exp(-N\sigma_n x) \qquad \text{.......... (10)}$$

where N is the number of atoms per unit volume in the target, x is the depth of traveling and σ_n is the total scattering cross section. Many experimental measurements have been carried out on the bulk backscattering of positrons from surfaces in the energy ranges 10 – 1000 keV [22-27] at normal Incidence. Almost all the experimental data indicates a significant increase of the backscattering coefficient with decrease of energy this means that the backscattered positrons are increased at low energies of incident particles. On the contrary, almost all the empirical relations and analytical theoretical expressions assume an energy independent backscattering coefficient [22]. The residual positrons are absorbed in a solid target and the absorbed positron coefficient calculated according to the following relations:

$$\eta_A = 1 - (\eta_T + \eta_B) \quad \ldots\ldots (11)$$

Attempts have been made to satisfactorily describe the energy distribution of transmitted positrons using Monte Carlo MC calculations. The most successful so for is the direct technique which has been used in the present project. In this technique, the statistical nature of inelastic scattering processes, as well as the elastic scattering process, is taken into account. The program Positronium Monte Carlo Simulation PsMCS constructed in such away and many restrictions to give probabilities of positron interaction with the two parts of the polymer (CF2-CF_2). At the first moment of interance, 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 (CF2) 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.

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 [28].

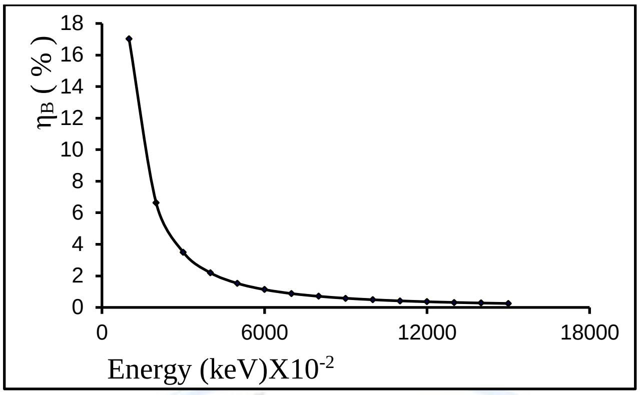

Fig1: Backscattered coefficient of Polytetrafluoroethylene PTFE verses positron primary energy.

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 its high energy ranged from (0 to
18000 eV). This is true for both atoms Fluoride and Carbon atom.

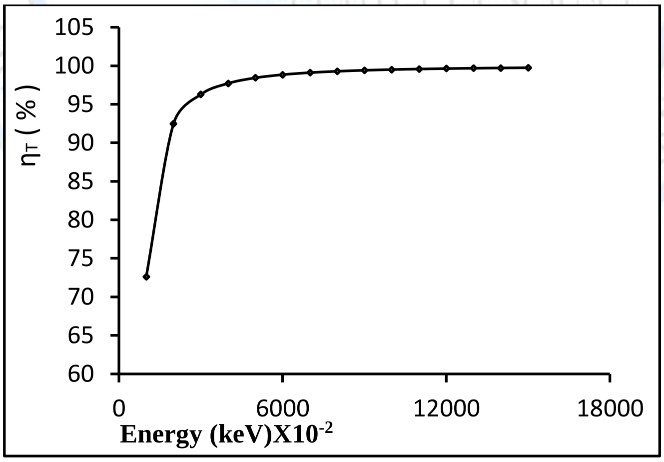

Fig2: Transmitted coefficient of Polytetrafluoroethylene PTFE versus positron primary energy.

3 – Absorbed coefficients: Figure (3) represents the variation of the absorbed particles with its energy for all positrons. It has been seen that the absorbed positrons are decreased with its energy bellow 2500 keV and its ratio is near zero for high energies because its may be collides with one of the components (Fluoride or Carbon) as follow:

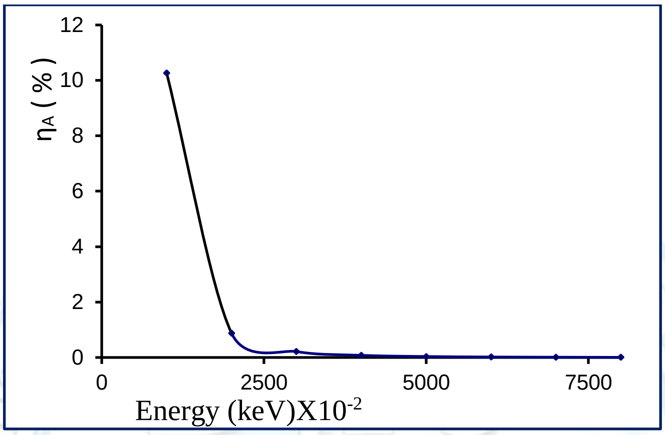

Fig3: Absorbed coefficient of Polytetrafluoroethylene PTFE versus positron primary energy.

Conclusion

Absorption, Backscattered and Transmitted coefficients of positron impinging into polymer material Polytetrafluoroethylene PTFE by using Positronium Monte Carlo simulation method PsMCS 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 PTFE components (Fluoride and Carbon).

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