Critical Points of Scattering Positrons from Neon, Krypton and Xenon atoms at low energy regions by using dipole polarization potential

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Abstract

The elastic Scattering of positrons from Ne, Kr, and Xe atoms is studied by using a simple model potential, called polarization - correlation potential (PCP) , to represent the interaction between the positron and target atoms. This model contains the static potential and Jain correlation potential. together with the polarization interaction ($-\alpha_D(0)/2r^4$) , where $\alpha_D(0)$ is the dipole target polarisability.

The optical potential of the e^+ - atom system is treated exactly in a partial - wave analysis to extract the scattering parameters. We have calculated the phase shifts, differential cross sections (DCS's), total cross sections (TCS's) and momentum transfer cross sections (MTCS's). Our results gave a good agreement with other experimental and theoretical values. We also discussed the critical points (representing the minima in the differential scattering cross section) in the low - energy e^+ - Ne , Kr and , Xe scattering.

النقاط الحرجة لاستطارة البوزترونات من ذرات النيون ، الكربتون و الزينون عند الطاقات الواطئة بأستخدام جهد الاستقطاب الثنائي

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الخلاصة

تمت دراسة الاستطارة المرنة للبوزترونـات مـن ذرات Ne , Kr و Xe باسـتخدام نموذج جهد بسيط – يسمى جهد الترابط و الاستقطاب (PCP) – يوضح تفاعل البوزترون مع ذرات الهدف . ويتكون هذا النموذج من الجهد الاستاتيكي وجهد ترابط Jain مع جهد الاستقطاب الثنائي $-\alpha_D(0)/2r^4$ ، حيث $\alpha_D(0)$ تمثل الاستقطابية الثنائية للهدف . تمت معاملة الجهـد البصري الكلي لنظام بوزترون – ذرة باستخدام طريقة تحليل الموجة المجزئة لاستخدام معاملات الاستطارة .

حسبت ازاحات الطور ، المقاطع العرضية التفاضلية ، المقطع العرضي الكلية و المقـاطع العرضية للزخم المنتقل . واعطت نتائجنا توافق جيد مع القيم العملية و النظرية لباحثين اخـرين كذلك ناقشنا النقاط الحرجة – التي تمثل اقل قيمة للمقطع العرضي التفاضلي – عنـد الطاقـات الواطئة لاستطارة البوزترون من ذرات Ne , Kr و Xe .

Introduction

The scattering of positrons by inert-gas atoms can be separated into three energy ranges, which are illustrated by measurements of the total scattering cross section at the room temperature gas atom (such as Ne, Kr, Xe, etc.) there are generally pronounced increases in total cross sections when positron energy rises(1,2). The lowest energy region is below the positronium Ps- formation thresholds where only the elastic scattering channel is opened. The highest energy region is typically above a few hundered eV impact energy where the total cross-sections display a monotonically decreasing behavior with increasing energy. An intermediate energy region can be defined as extending from the Ps-formation thresholds up to a few hundered eV impact energy. At low energies, theoretical calculations are the most straight forward because only the elastic scattering channel generally must be considered.

The most obvious consequence of scattering is attenuating of the primary beam . While the total attenuation allows one to measure the total cross section of positron scattering by atoms, provided that the angular discrimination is made as good as possible, it is possible to deliberately make the angular discrimination very poor in order to keep the scattered positrons in the beam with the unscattered positrons (3).

Differential and total cross sections for inert-gas atoms are studied. The method of partial waves along with optical model potential formalism has been employed. For positron scattering only the static and polarisation potentials are used (exchange potential neglected). There are many experimental and theoretical investigations for comparison with e^+-scattering from inert gases (4-9). To check the stability of the cross sections with respect to the model potential we slightly modify in that model and found that the cross sections are indeed quite stable (10).

In this paper, our aim to present calculations for the elastic scattering of positrons by rare-gas atoms through polarisation correlation potential (PCP).The phase shifts δ_l of the first few partial waves $\delta_0 \longrightarrow \delta_3$ depending upon the incident projectile energy have been calculated exactly different. The results are obtained at incident projectile energies in order to explore the suitability of the present method by comparing these results with the available differential cross-section (DCS) measurements. The TCS's are also obtained at these energies but no other results (theoretical or experimental)are available for comparison to our knowledge. Furthermore , we discussed the critical points (E_c, θ_c) which represented minima in the differential cross section as a function of incident energy and the scattering angle.

In the next section, we described the theoretical model Section.3A, represents results and discussion on the differential total and momentum transfer cross sections. While the results on the critical points are described in section 3B. The final concluding remarks are made in section.4. We employ atomic units throughout this paper.

Calculation Model

In this paper, we adopt the correlation potential of Jain (7), and the polarisation potential which we have used the O' Connel and Lane (11) as:

$$V_{pol}(r) = \begin{cases} V_{cor}^{SR}(r) & r \le r_0 \\ V_{pol}^{LR}(r) & r > r_0 \end{cases} \quad \ldots\ldots\ldots\ldots(1)$$

where r_0, is the crossing point between $V_{cor}^{SR}(r)$ and $V_{pol}^{LR}(r)$. $V_{cor}^{SR}(r)$ is the correlation potential at short distances and $V_{pol}^{LR}(r)$ is the polarization potential at long distances which is usually taken as:

$$V_{pol}^{LR}(r) = -\frac{\alpha_D^{(0)}}{2r^4} \quad \ldots\ldots\ldots\ldots\ldots(2)$$

where $\alpha_D(0)$ is the static dipole polarisability of the target.

For the correlation potential ,we have employed the formula of Jain (7):

$$2V_{cor}(r) = \begin{cases} \frac{-1.82}{\sqrt{r_s}} + (0.05 \ln r_s - 0.115) \ln r_s + 1.167 & ; for \quad r_s \le 0.302 \\ -0.92305 - \frac{0.09098}{r_s^2} & ;\text{for } 0.302 \le r_s \le 0.56 \\ \frac{8.7674\, r_s}{(r_s + 2.5)} - 0.6298 & ;\text{for } 0.56 \le r_s \le 8.0 \end{cases} \quad ---(3)$$

where $r_s=[3/4\pi\rho(r)]^{1/3}$

For the calculation of the static and correlation - polarisation potentials, we have used the Hartree - Fock wave function given by Clementi and Roetti (12).

For $\alpha_D(0)$ we have used the values $\alpha_D(0)$ =2.66 (Ne), 16.73 (Kr) and 27.26 (Xe) as given by Miller and Bederson(13) ,(all quantities are in atomic units). Elastic electron scattering from Ne , Kr and Xe atoms at low energies are calculated by using the CAVLEED program (Titterington and Kinniburgh(14) modified to optimise step sizes) and some programs of Ali(15) and Hussain (16).

In figures (1 a,b), we plot the calculated r . $V_{cor}^{SR}(r)$ as a function of the radial distance , r. It is clear that the point r_0 always falls in the low density region ($r_s(r_0)$ >>l), and larger than r_0 where the $V_{cor}^{SR}(r)$ is unimportant. In our calculation ,we always choose the r_0 point to be the point of a minima for the function r. $V_{cor}^{SR}(r)$ as evaluated by the following equation:

$$r_o = \frac{V_{cor}^{SR}(r)}{d/d\,(V_{cor}^{SR}(r))} \qquad r = ro \qquad \ldots\ldots\ldots\ldots\ldots (4)$$

Also , we adopt eq.(2) of $V_{pol}^{LR}(r)$ for large distances, then, we have satisfied the following relation by taking all regions r:

$$\vee_{pol}^{LR}(r_0) = V_{cor}^{SR}(r_0)$$

The quantity describing the scattering process is defined to be the differential total, and momentum transfer cross sections by using the following relations:

$$\frac{\partial\sigma}{\partial\Omega} = \frac{1}{4K^2}\left|\sum_{l=0}^{l\max}(2l+1)\left[S_l(k)-1\right]p_l(\cos\theta)\right|^2 \qquad \ldots\ldots\ldots\ldots\ldots(5)$$

where : $S_l(k)\exp(2i\,\delta_l)$,

δ_1 = is the phase shift,

$P_1(\cos\theta)$:is a legender polynomial of order 1.

$$\sigma_1 = \frac{}{K^2}(2l+1)\left|1-S_1(k)\right|^2$$

or,

$$\sigma_1 = \frac{4\pi}{K^2}\sum_l(2l+1)\sin^2\delta_1 \qquad \ldots\ldots\ldots\ldots\ldots\ldots (6)$$

and are evaluated from the integration of eq.(5) with a weighting factor of (1- $\cos\theta$).

$$\sigma_m = 2\pi\int_0^{\pi}\frac{d\sigma}{d\Omega}Sin\,\theta(1-\cos\theta)d\theta$$

or ,

$$\sigma_m = \frac{4\pi}{K^2}\sum_l(l+1)Sin^2(S_l - S_{l+1}) \qquad \ldots\ldots\ldots\ldots..(7)$$

We do not need a large number of partial waves , i.e. $l_{\max}$; a value of $l_{\max}$ = 9 is sufficient for well-converged DCS at the highest energy considered here.

Results and Discusston

The present calculations contain two parts:

A Differential , total and momentum transfer cross – sections:

We get our theoretical differential cross sections (DCS's) by using the polarisation correlation potential (PCP) model for e^+ - atom elastic scattering at low energies (5).

Figures (2 a, b) display our DCS at incident energies 13.6 and 20 eV for neon atoms These are compared with theoretical calculations of Nakanishi et al. (17) and Bartschat et at (18) and experimental values of Smith et al (19) and Kauppila et al. (1) respectively. Figures (3 a,b) explain the DCS for the elastic scattering of positrons from krypton for the incident energies 6.67 and 10 eV. For these energies, we compare our results with the theoretical values of szmytkowski (20) and experimental measurements of Dou' et al. (21). Also for the scattering of positrons from xenon atoms for the incident energies 5, 10, 40 and 100 eV. Our results are compared in figures (4 a,b,c,d) to the theoretical calculation of McEachran et al (22) and Hasenburg et al. (23) also we compared it with experimental values of Kauppila et al.(l). From these figures we clearly see that our calculations are in a good a greement with those data of other investigators.

We compared our calculations of total cross sections (TCS's) as shown in figures (5 a,b,c) for Ne, Kr and Xe atoms with many theoretical and experimental works (24,25, 26, 27, 28, 29) .Also the momentum transfer cross sections (MTCS's) are displayed in figures (6 a,b,c) and compared only with theoretical calculations of McEachran et al. (22,29).

B Critical points:

The differential cross section becomes a minimum with respect to both the incident positron energy E and the scattering angle θ. The combination of the impact energy and the angle are known as critical points and are represented by E_c (critical energy) and θ_c (critical angle) (30). Therefore, in the present investigation we have selected the Ne , Kr and Xe - atoms (Z= l0,36 and 54) respectively which is a closed -shell atom. Finally, the critical points are evaluated by employing the partial wave method (15).

We take the differential cross section

$$\frac{d\sigma}{d\Omega}(E_c,\theta_c) = f_1^2 + f_R^2 = 0$$

without any significant error. Therefore at the critical points one may take real as well as imaginary parts of the scattering amplitude represented by f_R and f_l, respectively separately equal to zero.

In the present low-energy regions ,the position and magnitude of the minimum in the DCS are highly sensitive to polarization potential (see figs7(a,b)). However, the higher partial waves mostly ($l > 2$) are not affected by the details of the polarisation potential in the target region.

We see that the higher order phase shifts ($l > 2$) do not penetrate the target region and scatter mainly with the asymptotic polarisation potential, which is known correctly. The values of the critical parameters (angle , θ_c ; energy, E_C; DCS,s) are shown in fig.(7 a,b).

Conclusion

In this paper, we have employed polarisation - correlation potential (PCP) model to investigate the low - energy collisions of positrons with Ne, Ar, Kr and Xe – atoms. The PCP model is determined from correlation energy E_{corr} of one positron in a homogeneous electron gas. The E_{cor} is simpley a function of the target electronic density and very easy to calculate computationally. At large distances the correlation term is replaced by the correct asymptotic form of the polarisation potential ($-\alpha_D(0)/2r^4$) by following the crossing point procedure suggested first by O' Connel and Lane (11). We also reported our results on the critical points in the DCS and found that there the PCP model is in reasonable agreement with previous estimates.

FIGURE CAPTIONS

Fig. (1 a,b): Variation of $rV_{cor}(r)$ as a function of radial distance r for Ne- Kr- and Xe-atoms.

Fig. (2 a,b): Differential cross sections (a_0^2/sr) for the elastic scattering of positrons from Neon atoms for the incident energies 13.6 and 20eV.

Fig. (3 a,b): Differential cross sections (a_0^2/sr) for the elastic scattering of positrons from Krypton atoms for the incident energies 6.67 and 10 eV.

Fig. (4 a,b,c,d): Differential cross sections (a_0^2/sr) for the elastic scattering of positrons from Xenon atoms for the incident energies 5, 10, 40 and 100 eV.

Fig. (5 a,b,c) : The total cross sections (in a_0^2) for the elastic scattering of positrons from Ne, Kr- and Xe-atoms.

Fig. (6 a,b,c): The momentum transfer cross sections (in a_0^2) for the elastic scattering of positrons from Ne-, Kr- and Xe-atoms.

Fig. (7 a,b): Critical points results for Ne-, Kr- and Xe-atoms.

a : The relation between the differential cross sections (a_0^2/sr) and scattering angle.

b : The relation between the differential cross sections (a_0^2/sr) and incident energies.

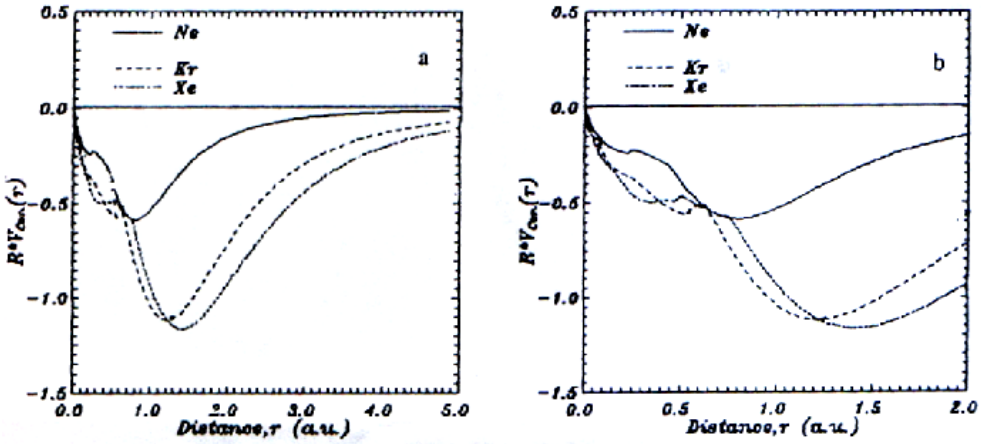

Fig. (1 a,b)

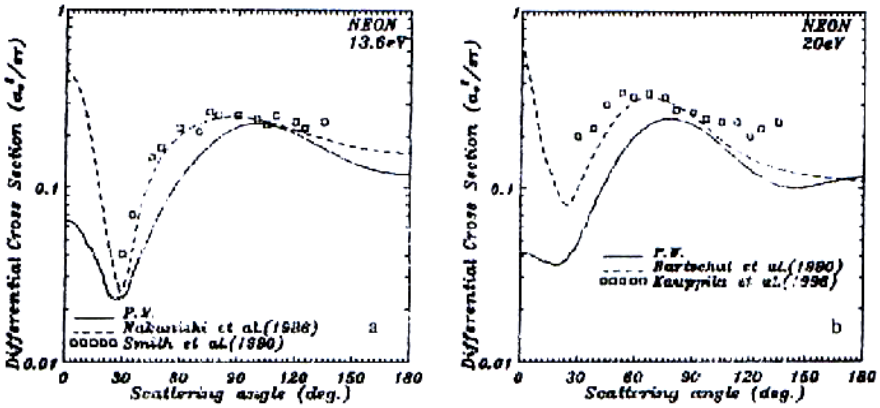

Fig. (2 a , b)

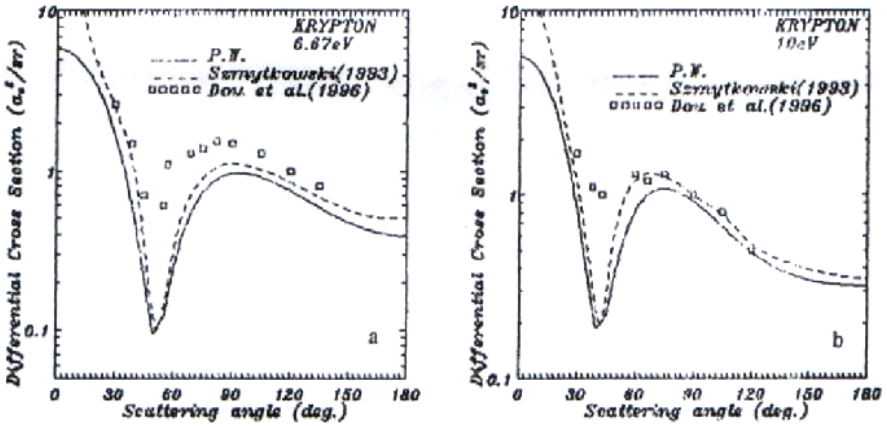

Fig. (3 a , b)

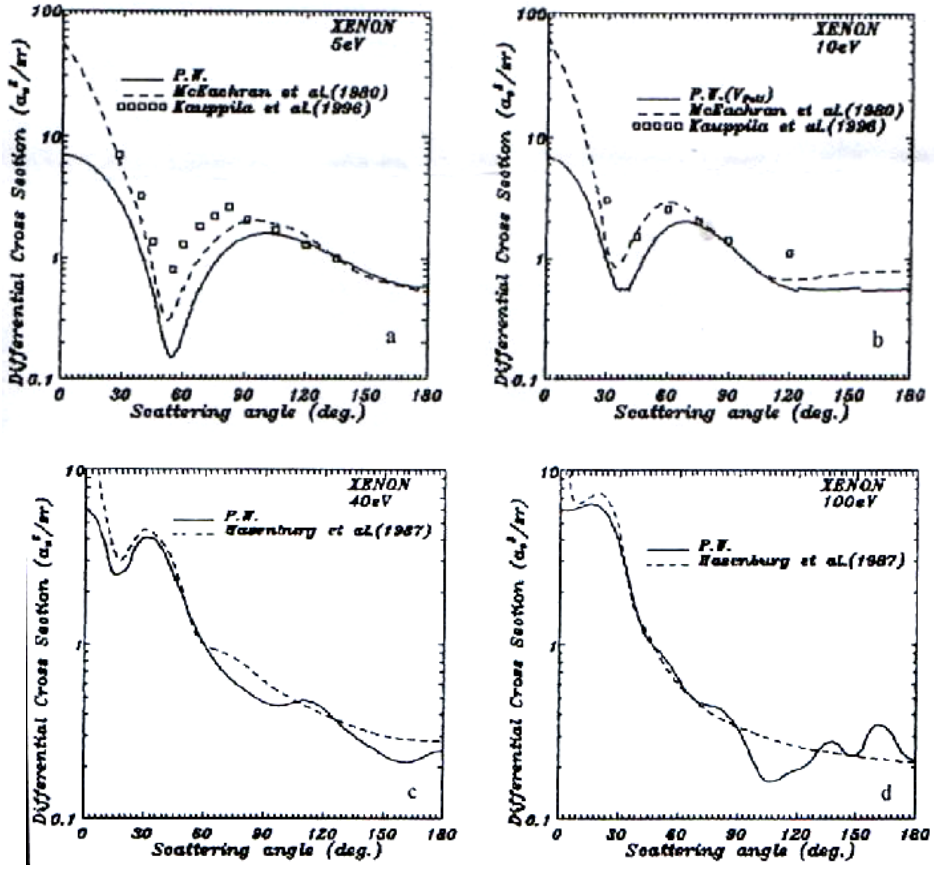

Fig. (4 a, b, c, d)

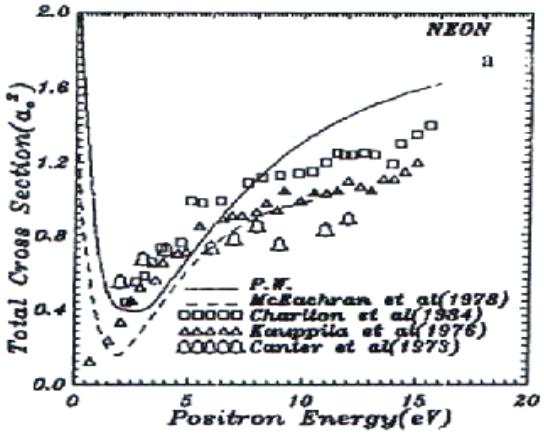

Fig. (5 a)

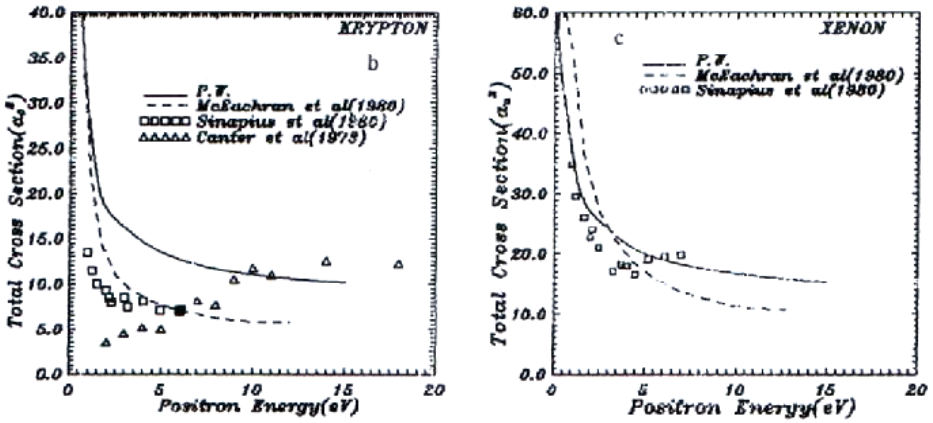

Fig. (5 b, c)

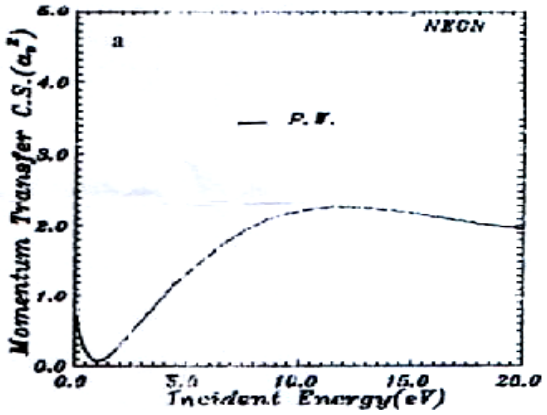

Fig. (6 a)

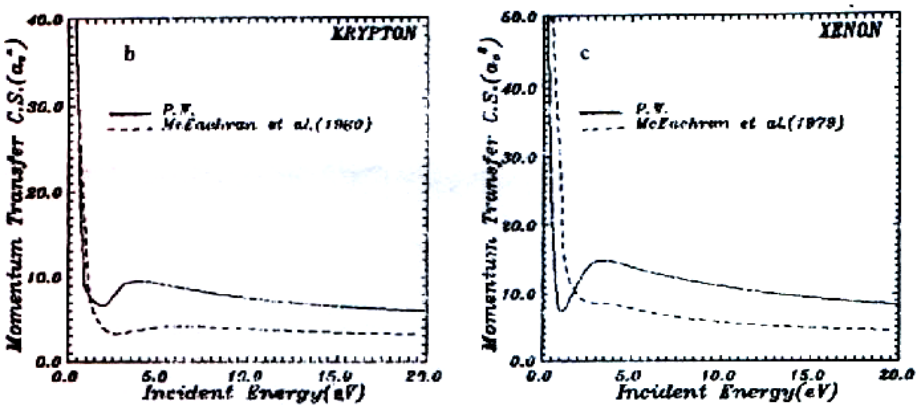

Fig. (6 b, c)

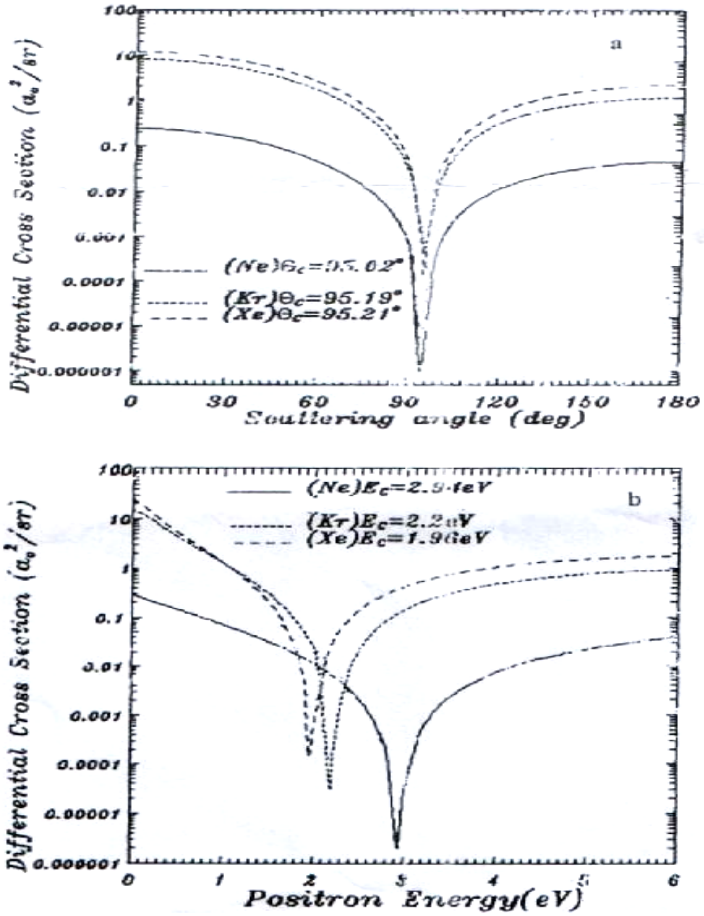

Fig. (7 a, b)

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