TOTAL CROSS SECTIONS FOR ELASTIC SCATTERING OF POSITRONS FOR SILICON, GALLIUM AND ANTIMONY ATOMS

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ABSTRACT

In this paper, elastic total cross sections of positrons which is scattered by bound silicon, gallium and antimony atoms have been calculated. The calculation of elastic scattering cross section for E<10 keV made with the partial wave expansions. The total elastic cross section have been taken for positrons of silicon, gallium and antimony calculated by Öztürk, Williamson and Antolak in the energy region 10 eV - 10 keV. In this article the screened Rutherford cross section with the spin-relativistic factor have been used for elastic scattering in the energy region 10 keV - 4 MeV.

Key Words: positron, elastic scattering, cross section, scattering angle.

1.İNTRODUCTION

Due to its importance for positron annihilation spectroscopy the study of the interaction of positron beams with solid targets has been approached in the last few years by several investigators. An accurate knowledge of elastic and inelastic scattering processes is essential for modeling particle beam behavior inside solid targets if the particle history is simulated by the Monte Carlo method and purely theoretical descriptions are undertaken. A quantity that plays a very important role is the elastic differential cross section that describes the effects of angular deflections due to elastic scattering processes.

In the penetration of positrons through a solid material, it is primarily the elastic collisions with the target atoms that cause the angular spread of the incident beam. Due to the lack of reliable experimental data, relatively little theoretical work has been done to calculate the inelastic and

elastic differential cross sections and total cross section for positron scattering.

In this paper continuous expressions of the total elastic cross section have been calculated as a function of E in the range 10 eV - 4 MeV for silicon, gallium and antimony.

2. METHODS OF CALCULATIONS

For the elastic scattering the screened Rutherford cross section with the spin-relativistic factor have been used [1]

$$\frac{d\sigma(\theta,E)}{d\Omega} = \frac{d\sigma_{Ruth}(\theta,E)}{d\Omega} K_{scr}(\theta,E) K_{rel}(\theta,E) \tag{1}$$

$$\frac{d\sigma_{Ruth}}{d\Omega} = Z^2 r_e^2 \frac{1-\beta^2}{\beta^4} \frac{1}{(1-\cos\theta)^2} \tag{2}$$

where θ is the scattering angle, E is the incoming positrons kinetic energy, Z atomic number, r_e is the classical electron radius and β is the speed of positron in units of c. In equation (1) the screening correction K_{scr} is simply

$$K_{scr}(\theta,E) = \left(\frac{1-\cos\theta}{1-\cos\theta+2\eta} \right)^2 . \tag{3}$$

In Moliere's work [2,3] all the effect of the deviation from the first Born approximation on the distribution function for multiple scattering is contained in the quantity
which depends only on the screening angle χ_α. The screening angle χ_α, for the scattering of a charged particle by the screened Coulomb field of an atom is given by [4,5]

$$\lambda n \frac{2}{\chi_\alpha} - \frac{1}{2} = \int_0^1 \frac{q(y)}{y} dy \qquad , \qquad y = \sin(\chi/2)$$
$$q(y) = \sigma(y) / \sigma_R(y) \tag{4}$$

where χ is the angle of scattering and q(y) is the ratio of the scattering cross section (with screening) to the Rutherford cross section (no screening) for single scattering. The screening angle χ_α is defined such that in the first Born approximation, when

$$q(y) = \sigma_B(y)/\sigma_R(y),$$
$$\chi_\alpha \rightarrow \chi_0 = \eta\lambda/p \tag{5}$$

for the scattering of an electron of momentum p by an exponentially screened potential $V(r)= - (Ze^2/r)\exp(-\lambda r)$. In Moliere's paper the potential used is $V(r)= - (Ze^2/r)w(r\lambda_0)$ where the Thomas Fermi function $w(r\lambda_0)$ is represented by a sum of three exponentials and $\lambda_0=Z^{1/3}/0.885a_0$, a_0 being the Bohr radius. In the first Born approximation, this Thomas Fermi field gives, upon numerical integration,

$$\chi_\alpha \rightarrow \chi_0 \cong 1.12(\eta\lambda_0/p). \tag{6}$$

In the paper of Nigam *et al*.[3], the calculations are carried out by using Dalitz's [6] relativistic formula, derived in the second Born approximation, for the scattering of a spin 1/2 particle of charge z (z= -1 for an electron) by an exponentially screened Coulomb field

$$V(r) = (zZe^2/r)e^{-\lambda r} \tag{7}$$

where the screening parameter $\lambda= \mu\lambda_0$, μ being an adjustable parameter of the order of unity. The parameter μ is introduced to compensate for the use of a single exponential as the screening factor of the Coulomb field of an atom instead of a sum of three exponential as done by Moliere. The expression for the screening angle χ_α is then obtained by calculating the angular distribution function [4,5]

$$f(\theta,t) = \sum_{l=0}^{\infty}\left(\lambda+\frac{1}{2}\right)P_\lambda(\cos\theta)\exp\left\{-Nt\int_0^\pi d\chi\sin\chi\sigma_0(\chi)\left[1-P_\lambda(\cos\chi)\right]\right\} \tag{8}$$

where $f(\theta,t)\sin\theta\, d\theta$ is the actual number of scattered particles between θ and $\theta+d\theta$; t is the thickness of the foil. The expression for the screening angle χ_α is obtained by calculating the integral in the exponential of equation (8) and combining all the contribution from the small angles into a single term. This gives

$$\chi_\alpha = \chi_0\left\{1+2\alpha\chi_0\left[\frac{1-\beta^2}{\beta}\lambda n\chi_0+\frac{0.2310}{\beta}+1.448\right]\right\} \tag{9}$$

where

$$\chi_0=\mu\frac{\eta}{p}\left(\frac{Z^{1/3}}{0.885a_0}\right), \quad \alpha=-zZ/137\ ,\ \beta=v/c\ ,\ p=m_0c\left[\beta^2/(1-\beta^2)\right]^{1/2} \tag{10}$$

η is the Planck constant divided by 2π, μ =1.12 , m_0 is the electron rest mass and c is the speed of light.

The corresponding expression in Moliere's theory is

$$\chi_\alpha = \chi_0 \left\{ 1.13 + 3.76\alpha^2 / \beta^2 \right\}^{1/2} \quad . \qquad (11)$$

Notice that since in equation (9), χ_α depends on α , we will get different values of the screening angle for electron (z=-1) and positron (z= + 1) scattering. In Moliere's theory χ_α depends on α^2 , equation (11) and there is no difference in electron and positron scattering.

The screening angle η for positrons has been calculated by Nigam *et al.* [2,3] using the
second Born approximation

$$\eta = \frac{1}{4}\chi_0^2 \left\{ 1 + 2\alpha\chi_0 \left[\frac{1-\beta^2}{\beta} \lambda n \chi_0 + \frac{0.2310}{\beta} + 1.448 \right] \right\}^2 \quad .(12)$$

The screening angle given in equation (12) does not behave smoothly for E<10 keV , so equation (12) have been used for the calculation of the total elastic cross section only in the region 10 keV - 4 MeV.

We need on analytical expression of the $K_{rel}(\theta,E)$ to calculate the total elastic cross section by integrating the equation (1) and (2) . $K_{rel}(\theta,E)$ is equal to the ratio of the Mott cross section to the Rutherford cross section, and its values for several energies and scattering angles have been tabulated by Doggett and Spencer [7] , Idoeta and Legarda [8]. The relativistic correction factor has not been calculated for silicon, gallium and antimony atoms (Z=14,31,51) by Doggett and Spencer, Idoeta and Legarda. Therefore aluminum, copper and tin (Z=13,29,50) has been used instead of for silicon, gallium and antimony respectively. To obtain an analytic expression for $K_{rel}(\theta,E)$, first the coefficients p_1, p_2, p_3, p_4 have been determined by fitting, and then

$$K_{rel}(\theta,E) = p_1 + p_2\,\theta + p_3\theta^2 + p_4\theta^3 \qquad (13.a)$$

expansion for E=0.05 , 0.1 , 0.2 , 0.4 , 0.7 , 1 , 2 , 4 MeV to the values given by Doggett and Spencer [7] (Table 1) for Al, Cu, Sn , where θ is given in radian units. Then the energy dependence of each p_i in equation (13.a) have been found by fitting the expressions given below for the values of p_i , obtained with the angle dependence fits:

Table 1. The ratio σ/σ_R of the Mott to the Rutherford cross section: positron scattering

E (MeV) θ°	4	2	1	0.7	0.4	0.2	0.1	0.05
				Z=-13				
0	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
15	0.941	0.942	0.943	0.948	0.953	0.963	0.973	0.982
30	0.878	0.881	0.886	0.895	0.909	0.930	0.952	0.968
45	0.792	0.797	0.807	0.822	0.848	0.887	0.924	0.953
60	0.688	0.696	0.714	0.736	0.776	0.836	0.893	0.935
75	0.573	0.584	0.612	0.640	0.697	0.781	0.860	0.918
90	0.454	0.469	0.506	0.542	0.616	0.725	0.826	0.900
105	0.338	0.356	0.402	0.446	0.537	0.671	0.794	0.883
120	0.331	0.253	0.308	0.359	0.465	0.622	0.765	0.868
135	0.1398	0.1649	0.227	0.284	0.404	0.582	0.741	0.856
150	0.0707	0.0979	0.1654	0.228	0.357	0.549	0.723	0.846
165	0.0280	0.0561	0.1270	0.1924	0.328	0.530	0.711	0.840
180	0.0130	0.0417	0.1139	0.1803	0.319	0.523	0.707	0.838
				Z=-29				
0	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
15	0.920	0.921	0.926	0.931	0.938	0.952	0.967	0.979
30	0.837	0.840	0.850	0.858	0.878	0.908	0.938	0.963
45	0.740	0.746	0.763	0.777	0.810	0.859	0.908	0.946
60	0.635	0.644	0.669	0.690	0.737	0.809	0.877	0.929
75	0.524	0.537	0.570	0.599	0.663	0.758	0.848	0.914
90	0.412	0.429	0.471	0.508	0.589	0.709	0.820	0.900
105	0.305	0.325	0.376	0.422	0.518	0.663	0.794	0.887
120	0.208	0.231	0.291	0.344	0.456	0.622	0.772	0.877
135	0.1268	0.1531	0.220	0.278	0.404	0.588	0.753	0.868
150	0.0652	0.0936	0.1660	0.229	0.364	0.563	0.740	0.862
165	0.0265	0.0562	0.1321	0.1981	0.339	0.547	0.732	0.859
180	0.0136	0.0438	0.1208	0.1880	0.331	0.542	0.729	0.857
				Z=-50				
0	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
15	0.900	0.902	0.908	0.914	0.926	0.945	0.964	0.978
30	0.802	0.807	0.820	0.831	0.856	0.895	0.934	0.962
45	0.698	0.706	0.727	0.745	0.784	0.845	0.904	0.947
60	0.592	0.603	0.632	0.658	0.713	0.797	0.875	0.931
75	0.485	0.500	0.537	0.571	0.643	0.750	0.849	0.918
90	0.379	0.398	0.445	0.486	0.575	0.707	0.825	0.906
105	0.280	0.302	0.359	0.408	0.514	0.668	0.805	0.896
120	0.191	0.217	0.282	0.339	0.459	0.635	0.787	0.888
135	0.1171	0.1456	0.218	0.281	0.415	0.608	0.774	0.882
150	0.0613	0.0921	0.1704	0.238	0.382	0.588	0.764	0.877
165	0.0264	0.0586	0.1406	0.212	0.362	0.576	0.758	0.874
180	0.0147	0.0475	0.1306	0.203	0.355	0.572	0.756	0.873

Silicon

$$p_1(E)=1.00044+0.00638809E-0.000488317E^{2}-0.0121958E^{0.5}$$
$$p_2(E)=-0.011104+0.10783E-0.00842815E^{2}-0.19685E^{0.5}$$
$$p_3(E)=0.0901381+0.24731E-0.0162897E^{2}-0.52713E^{0.5} \qquad (13.b)$$
$$p_4(E)=-0.0191456-0.0570709E+0.00381289E^{2}+0.12036E^{0.5}$$

Gallium

$$p_1(E)=1.00423-0.000308721E+0.000148887E^{2}-0.0080014E^{0.15}$$
$$p_2(E)=0.10381+0.14443E-0.013828E^{2}-0.45404E^{0.5}$$
$$p_3(E)=0.0772627+0.14419E-0.00765645E^{2}-0.3442E^{0.5} \qquad (13.c)$$
$$p_4(E)=-0.0171256-0.0397789E+0.00234679E^{2}+0.0900239E^{0.5}$$

Antimony

$$p_1(E)=1.00025+0.000213722E+0.000183767E^{2}-0.00422401E^{0.5}$$
$$p_2(E)=0.0636656+0.39473E-0.0308159E^{2}-0.73725E^{0.5}$$
$$p_3(E)=0.0422838-0.0111198E+0.0141341E^{2}-0.11643E^{0.5} \qquad (13.d)$$
$$p_4(E)=-0.0135344-0.0243651E+0.00110866E^{2}+0.0618396E^{0.5}$$

where E is given in MeV units.

The macroscopic total elastic cross section values have been calculated for several values of E in the region 10 keV - 4 MeV by integrating the equations (1),(2) over whole solid angle using equations (12) and (13.a),(13.b),(13.c) ,(13.d) and ,multiplying the integral results by

$$\text{Si} : N=N_0\,\rho/A=5.144\times10^{22}\ \text{atom/cm}^3$$
$$\text{Ga} : N=N_0\,\rho/A=5.103\times10^{22}\ \text{atom/cm}^3$$
$$\text{Sb} : N=N_0\,\rho/A=3.305\times10^{22}\ \text{atom/cm}^3\ , \qquad (14)$$

where N_0 is the Avogadro's number, ρ and A are the density and atomic weight .

3. CONCLUSIONS

In the screened Rutherford cross section with spin relativistic factor are expected errors greater than of the order of 10 % for electrons and positrons at energies below about $0.3Z^{4/3}$ keV [1]. Therefore the calculation have not been made at energies below about 30 keV and 60 keV for gallium and antimony respectively. The calculation results have been tabulated (Table2) for silicon, gallium and antimony. Furthermore, the calculation results have been plotted in figure.1 for Si, Ga and Sb.

Table.2: The calculations of the screened Rutherford cross section with spin-relativistic factor

E(MeV)	μ_{Si} (cm^{-1})	μ_{Ga}(cm^{-1})	μ_{Sb}(cm^{-1})
0.010	$3.6815x10^{+5}$	-	-
0.015	$2.7592x10^{+5}$	-	-
0.020	$2.2278x10^{+5}$	-	-
0.030	$1.6342x10^{+5}$	$3.7355x10^{+5}$	-
0.040	$1.3089x10^{+5}$	$3.1364x10^{+5}$	-
0.050	$1.1031x10^{+5}$	$2.7281x10^{+5}$	-
0.060	$9.6109x10^{+4}$	$2.4314x10^{+5}$	$2.6385x10^{+5}$
0.080	$7.7758x10^{+4}$	$2.0282x10^{+5}$	$2.2833x10^{+5}$
0.100	$6.6360x10^{+4}$	$1.7669x10^{+5}$	$2.0379x10^{+5}$
0.150	$5.0395x10^{+4}$	$1.3921x10^{+5}$	$1.6639x10^{+5}$
0.200	$4.1685x10^{+4}$	$1.1890x10^{+5}$	$1.4525x10^{+5}$
0.300	$3.1644x10^{+4}$	$9.6120x10^{+4}$	$1.2143x10^{+5}$
0.400	$2.5516x10^{+4}$	$8.2224x10^{+4}$	$1.0709x10^{+5}$
0.500	$2.1187x10^{+4}$	$7.1941x10^{+4}$	$9.6428x10^{+4}$
0.600	$1.7921x10^{+4}$	$6.3649x10^{+4}$	$8.7599x10^{+4}$
0.800	$1.3322x10^{+4}$	$5.0769x10^{+4}$	$7.3092x10^{+4}$
1.000	$1.0281x10^{+4}$	$4.1217x10^{+4}$	$6.1474x10^{+4}$
1.500	$6.0203x10^{+3}$	$2.6036x10^{+4}$	$4.1143x10^{44}$
2.000	$3.9335x10^{+3}$	$1.7687x10^{+4}$	$2.8868x10^{+4}$
3.000	$2.0462x10^{+3}$	$9.5421x10^{+3}$	$1.6078x10^{+4}$
4.000	$1.2479x10^{+3}$	$5.9150x10^{+3}$	$1.0108x10^{+4}$

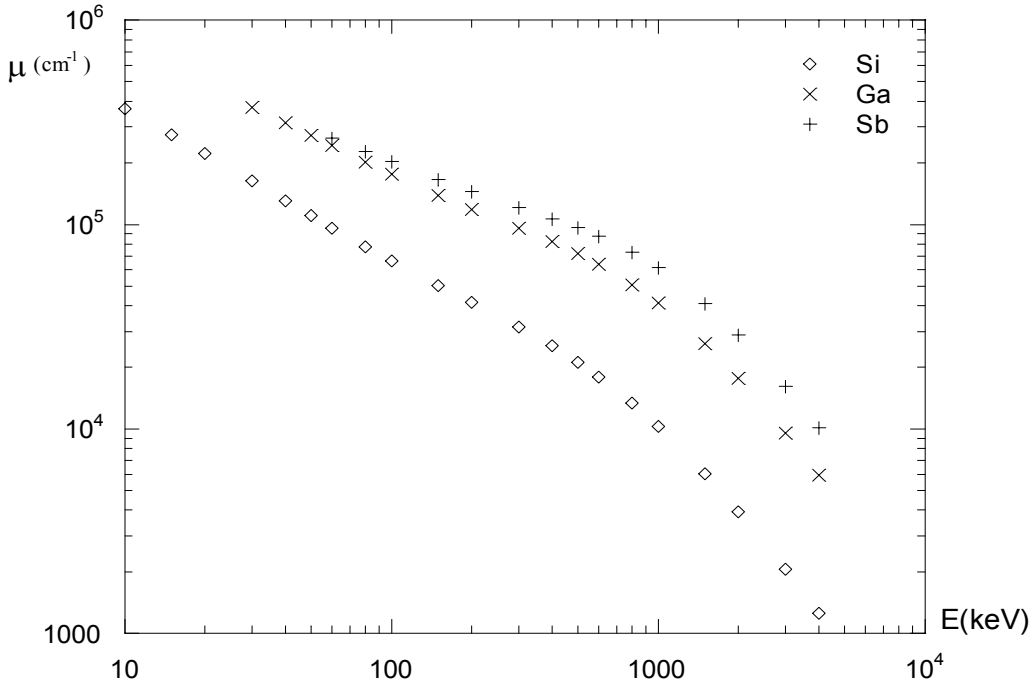

Figure.1 The calculated results of Si, Ga and Sb by the screened Rutherford cross section with spin relativistic factor.

The calculation of elastic scattering cross section for E<10 keV have been made with the partial wave expansions Antolak and Williamson [9], Öztürk, Williamson and Antolak [10], Öztürk, Williamson and Antolak [11] in the energy region for silicon 10 - 500 eV, for gallium and antimony 10 eV - 10 keV. The total elastic cross section have been taken for Si,Ga and Sb calculated by Antolak et al. in the region 10 eV - 10 keV. These values, to obtain in units of cm^{-1} multiplied by N in equation (14).

We need a continuous expression of the total elastic cross section as a function of E in the range 10 eV - 4 MeV. The total elastic cross section is a fast varying function of E, but the logarithm of it is a well behaving function of *ln*E, as can be seen in figure.2, and can be expressed as a simple power expansion. The expression have been found

$$\mu\,(cm^{-1}) = \exp(p_1 + p_2 x + p_3 x^2 + p_4 x^3 + p_5 x^4 + p_6 x^5) \qquad (15)$$

where, $x = ln\,E$ (keV)

Silicon: $\mu(cm^{-1}) = \exp(14.99029 - 0.80021E - 0.0743595E^2 + 0.0139005E^3 + 0.00113381E^4 - 0.000242061E^5)$

Gallium: $\mu(cm^{-1}) = \exp(15.59 - 0.55E - 0.095E^2 + 0.000440039E^3 + 0.00260005E^4 + 0.0000618285E^5 - 0.0000335181E^6)$

Antimony: $\mu(cm^{-1}) = \exp(15.56971 - 0.62975E - 0.097407E^2 + 0.0128209E^3 + 0.00239887E^4 - 0.000334299E^5)$

for the macroscopic total elastic cross section, doing an accurate fit over $(lnE, ln\mu)$ points.

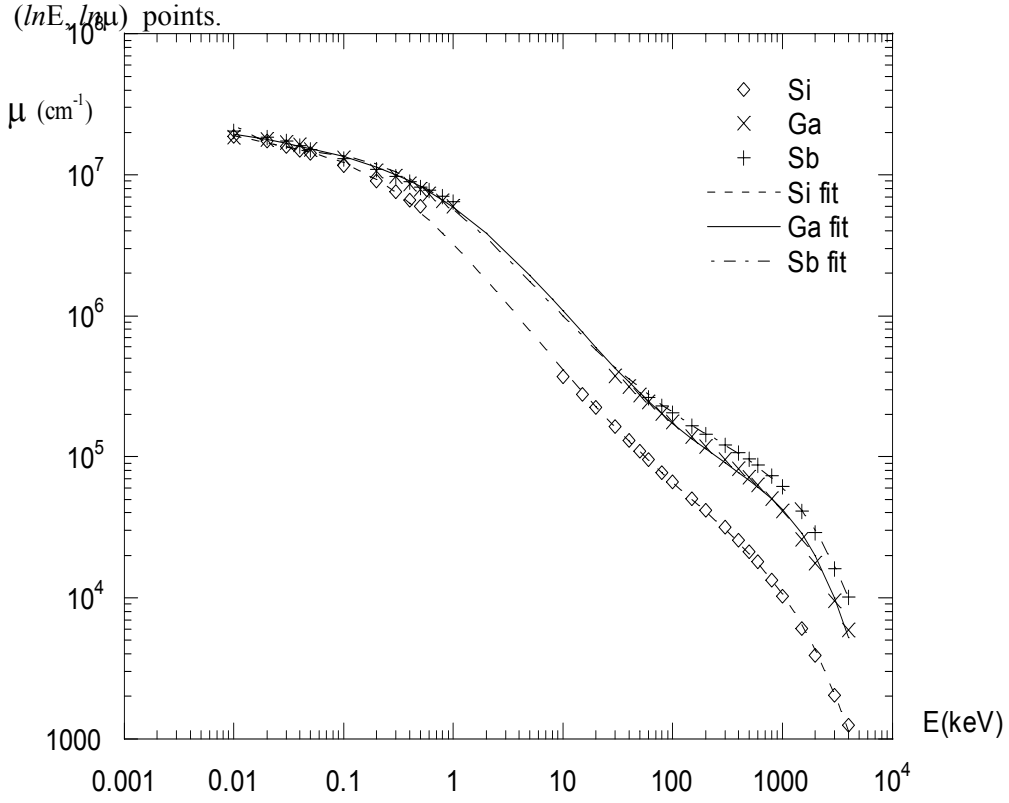

Figure 2 Variation of elastic cross section with incident positron energy. The dots represent total elastic cross section values, determined by the methods explained in the text. The curves that fit to the dots is given in Eq.(15).

4.RESULTS AND DISCUSSIONS

Using the method of partial waves in the energy region 10 eV - 10 keV, elastic differential and total cross section for electrons and positrons scattered by bound silicon and germanium have been calculated by Antolak *et al.* [9, 10, 11]. The screened Rutherford cross section with the spin - relativistic factor have been used for the elastic scattering in the energy region 10 keV - 4 MeV . To obtain a continuous expression of the total elastic cross section as a function of E in the 10 eV - 4 MeV, an accurate fit have done over (lnE , ln μ) points. The total elastic cross section have been shown in figure.2 as a function of E for three different media. So the continuous expression of the total elastic cross section as a function of E have been obtained in the large range of 10 eV - 4 MeV for silicon, gallium and antimony.

This method used to calculate the macroscopic total elastic cross section because this method can be used in wide energy range (10 eV -4 MeV) and it is practical. Before this study, the elastic scattering the cross sections calculated with the same method have been used to simulate the transport of positrons in aluminum, copper, tin, gold, silver, lead. The calculated results are compared with experimental data and those of other Monte Carlo calculations and good agreement is observed [12, 13, 14].

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