J. At. Mol. Sci.
doi: 10.4208/jams.052611.070611a

Vol. **3**, No. 3, pp. 197-208
August 2012

Spin polarization and differential cross-sections for $e^{\pm}-$ scattering from rhenium atom

Kapil K. Sharma[a,*], Neerja[b], and R. P. Vats[a]

[a] *Department of Physics, M.S (P.G) College, Saharanpur (U.P), India*
[b] *Department of Electronics and Communication, A.B E S Engineering College, Ghaziabad (U.P), India*

Received 26 May 2011; Accepted (in revised version) 6 July 2011
Published Online 18 February 2012

Abstract. Various scattering cross section such as differential, integrated elastic, momentum transfer, total cross-sections and spin polarization parameters for both the elastic and total scattering of electron and positron from Re atoms in the impact energy range between 2.0 to 500 eV using the relativistic Dirac equations are studies. The target-projectile interaction is included by real and complex- free optical potentials for obtaining the solutions of Dirac equation for scattered electrons and positron. The Dirac-Fock wave functions have been used to represent the $e^{\pm}-$Re target atoms. Corresponding theoretical results are obtained from a relativistic approach based on solving the Dirac equation using Hartree-Fock and Dirac-Fock wave functions to calculate cross sections at all the energies measured.

PACS: 34.80Uv, 34.80.Bm

Key words: relativistic calculation, electron- positron scattering

1 Introduction

Recently experimental and theoretical work has been focused on heavier atomic target for e.g. Cs, Fr, Pb, Ag, Cu, etc. Theoretical work has been done using relativistic calculations for including spin-effect and its relativistic calculation play an important role in the spin-dependent phenomenon due to collision between incident particles and atoms [1-2]. Anderson and Bartschat [3] have made extensive studies on scattering of electrons from heavy atoms. Due to the development of efficient polarized electrons sources and accurate polarimeters, spin dependence of scattering processes can be easily studied through the complete scattering experiment. Within the framework of density matrix formalism

*Corresponding author. *Email address:* kapil81_physics@yahoo.co.in(K. K. Sharma)

one can define a set of observables parameters viz. the unpolarized differential cross-section (DCS) and polarization parameters S, T and U. The polarization parameter S is known as Sherman function, which describes the change of polarization produced in the scattered beam due to collision, and the other two T and U parameter give the angle of rotation of the components of the polarization vector in the scattering plane.

Theoretically, Walker and Lam [4–6] studied electron and positron scattering using the relativistic form of the Schrödinger equation, Haberland *et al.* and Bartschat *et al.* have studied scattering processes using the generalized Kohan-Sham type equations, static exchange R-matrix theory and real and complex model potential approach respectively [7–12]. Most of the calculation performed for the positron-atom scattering which are based on model potential approach by using the similar form of polarization and absorption potentials [13–16]. However, the positron offers an altogether different collision process, the possibility of genuine rearrangement -positronium (Ps) formation. If the ionization energy of the atom is greater than 6.8 eV, the positronium channel opens at binding energy. The incident positron sees an attractive field due to the characteristics effect of the Ps-formation on the elastic channel. The close-coupling calculations, which include the Ps-channel explicitly, have been used routinely for positron-hydrogen and alkali systems rather than heavier target [17–23]. Dorn *et al.* [23] carried out calculations for spin polarization of xenon atoms using an optical potential including both polarization and absorption effects. Their results show that absorption potential must be included in the relativistic description for accurate prediction of the S, T, and U parameters. This aspect of electron and positron scattering from heavy atoms has been further examined by Neerja *et al.* [24–26]. Recently, Nikolić and Tančić and Harish Mohan *et al.* [27–28] studied the low energy elastic scattering of positrons by inert target.

This paper involves the detailed study of atomic behavior of Re ([Xe] 6s (2)4f (14)5d (5)) atom using electron and positron scattering. We have used parameter-free model optical potential approach [25, 34] for calculating the DCS, S-parameter, momentum and total cross-sections of electron and positron scattering from Re atom.

2 Theoretical methodology

2.1 Choice of potentials

The total interaction between a particle and the target atom is represented by an effective potential $V(r)$, which is sum of two parts, $V_R(r)$ and $V_A(r)$. For electron scattering, real part of the potential $V_R(r)$ is expressed as sum of three local terms, $V_R(r) = V_{st}(r)+V_{ex}+V_{pol}(r)$, where $V_{st}(r)$, V_{ex} and $V_{pol}(r)$ are static, exchange and polarization potentials respectively. However for positron scattering, $V_R(r) = V_{st}(r)+V_{pol}(r)$. All potential terms are functions of ground state density $\rho(r)$ of the target. The static potential $V_{st}(r)$ and the charge density $\rho(r)$ are obtained using non-relativistic Slater type orbital's of Roothan and Hartree-Fock wave functions as given in McLean [29]. In addition, we have used the compilation of analytical function given by Salvat *et al.* [30], which is

determined by an analytical fitting procedure to Dirac-Hartree-Fock-Slater (DHFS) self-consistent data. In the present calculations, we are using the modified semi-classical exchange (MSCE) potential V_{ex}^{MSCE} given by Gianturco and Scialla [31]

$$V_{ex}^{MSCE}=\frac{1}{2}\left[E-V_{st}(r)+\frac{3}{10}\{3\pi^2\rho(r)\}^{\frac{2}{3}}\right]-\frac{1}{2}\left\{\left[E-V_{st}(r)+\frac{3}{10}\{3\pi^2\rho(r)\}^{\frac{2}{3}}\right]^2+4\pi\rho(r)\right\}^{\frac{1}{2}}. \tag{1}$$

It is important to note that the impinging electron distorts the electronic charge density of target which can further modify this exchange potential. This effect has been taken into account by considering the polarization of the target wave-function by replacing the term $V_{st}(r)$ in equation (1) by $V_D=V_{st}(r)+V_{pd}(r)$. Moreover, the polarization potential $V_{pd}(r)$ is based on the correlation energy by the target atom which has short $V_{SR}(r)$ and long range $V_{LR}(r)$ potentials given by

$$V_{pol}(r)=\begin{cases}V_{SR}(r) & \text{if} \quad r<r_c\\ V_{LR}(r) & \text{if} \quad r\geq r_c\end{cases} \tag{2}$$

where r_c is the point where two forms cross each other for the first time. The short range form of the electron $V_{SR}^{e^-}(r)$ and positron $V_{SR}^{e^+}(r)$ scattering is based on free-electron gas-exchange potential, which is given by

$$V_{SR}^{-e}(r)=\begin{cases}0.0622\ln r_S-0.096+0.018r_S\ln r_S-0.02r_S, & \text{if } r_S\leq 0.7,\\ -0.1231+0.03796\ln r_S, & \text{if } 0.7<r_S\leq 10,\\ -0.876r_S^{-1}+2.65r_S^{-3/2}-2.8r_S^{-2}-0.8r_S^{-5/2}, & \text{if } r_S\leq 10.\end{cases} \tag{3}$$

$$V_{SR}^{+e}(r)=\begin{cases}[-1.82/\sqrt{r_S}+(0.051\ln r_S-0.0115)\ln r_S+1.167]/2, & \text{if } r_S<0.302,\\ (-0.92305-0.09098/r_S^2)/2, & \text{if } 0.302\leq r_S\leq 0.56,\\ [-8.7674r_S(r_S+2.5)^{-3}+(-13.151+0.9552r_S)(r_S+2.5)^{-2} & \text{if } 0.56\leq r_S\leq 8.0,\\ +2.8655(r_S+2.5)^{-1}-0.6298]/2 & \end{cases} \tag{4}$$

where, $r_S=[3/4\pi\rho(r\}]^{1/3}$ and $\rho(r)$ is the electron charge density of the target system. The long-range form of the polarization potential is given by $V_{LR}(r)=-\alpha_d/2r^4$, where α_d is the static dipole polarizability (for Re, $\alpha_d=65.5618$ a.u.) and $r_c=4.981$, 3.232 a.u. for electron and positron scattering respectively. The impact energy range considered in the present calculation exceeds in the first elastic threshold energy ($E_{th}=1.44$ eV), therefore it causes an absorption in the scattered beam. There exist various forms of the absorption potentials for describing all elastic processes during the electron scattering. The electron-atom scattering, absorption potential is given by

$$V_A=-\frac{1}{2}v_{loc}\rho(r)\bar{\sigma_b}, \tag{5}$$

$$v_{loc}=[2(E-V_R)]^{1/2}. \tag{6}$$

In Eq. (6), v_{loc} is the local velocity of the incident electron for $E-V_R \geq 0$. The factor $1/2$ in Eq. (5) is introduced to account for the exchange of the incident electron and bound electrons of the target during the scattering process. $\bar{\sigma_b}$ is the average quasi free binary collision cross section obtained non-empirically by using the free-electron gas model for the target defined by the functional form of the $\bar{\sigma_b}$ is given as

$$\bar{\sigma_b} = \begin{cases} \frac{8\pi}{10k_F^3 E}(f_1+f_2) & \text{if } p^2 \geq \alpha+\beta-k_F^2, \\ 0 & \text{if } p^2 < \alpha+\beta-k_F^2, \end{cases} \tag{7}$$

where

$$f_1 = \frac{5k_F^3}{(\alpha-k_F^2} - \frac{k_F^3[5(p^2-\beta)+2k_F^2]}{(p^2-\beta)^2},$$

and

$$f_2 = \begin{cases} 0 & p^2 > \alpha+\beta \\ \frac{2(\alpha+\beta-p^2)^{5/2}}{(p^2-\beta)^2} & p^2 \leq \alpha+\beta \end{cases}$$

where, $k_F = (3\pi^2\rho(r))^{1/3}$ and $p(E) = (2E)^{1/2}$ is incident momentum of the scattering electrons and k_F is the target Fermi momentum. The form of the two parameters α and β introduced in $\bar{\sigma_b}$ depend on, the lowest excitation threshold energy (E_{th}) of the target and the ionization potential energy ($I_p = 7.88$ eV) of the target which are obtained empirically, given by

$$\rho = k_F^2 + 2[E_{th} - (I_p - E_{th})] - V_R, \tag{8}$$

$$\beta = k_F^2 + 2(I_p - E_{th}) - V_R. \tag{9}$$

For positron scattering, $\bar{\rho}(k_F,p)$ the average quasi-free binary collision cross section, is given as

$$\bar{\sigma_b} = \frac{1}{p}\int N(k_F,q)|p-q|dq \times \int \frac{d\rho_b}{d\Omega}\left(\frac{1}{p_0^2}\delta(p_0-p_f)\Theta(q,k_F)\right)dg \tag{10}$$

where p and q are the laboratory frame moment of the incident positron and of the target electron, respectively, before the collision; p' and q' are the laboratory frame moment of the incident positron and of the target electron, respectively, after the collision.

The vectors p_0 and p_f are the initial and final momenta of the positron in the center-of mass frame of the binary system. The function $N(k_F,q)$ is the density per target electron in momentum space; it is given by

$$N(k_F,q) = \begin{cases} N(k_F) & q \leq k_F \\ 0 & q > k_F \end{cases} \tag{11}$$

where, $N(k_F) = \frac{3}{4\pi k_F^3)}$, and $k_F = (3\pi^2\rho(r))^{1/3}$ the Fermi momentum of the target. The momentum transfer vector g is given by $g = p-p' = q-q'$. The function $\Theta(q',k_F)$ in Eq. 10,

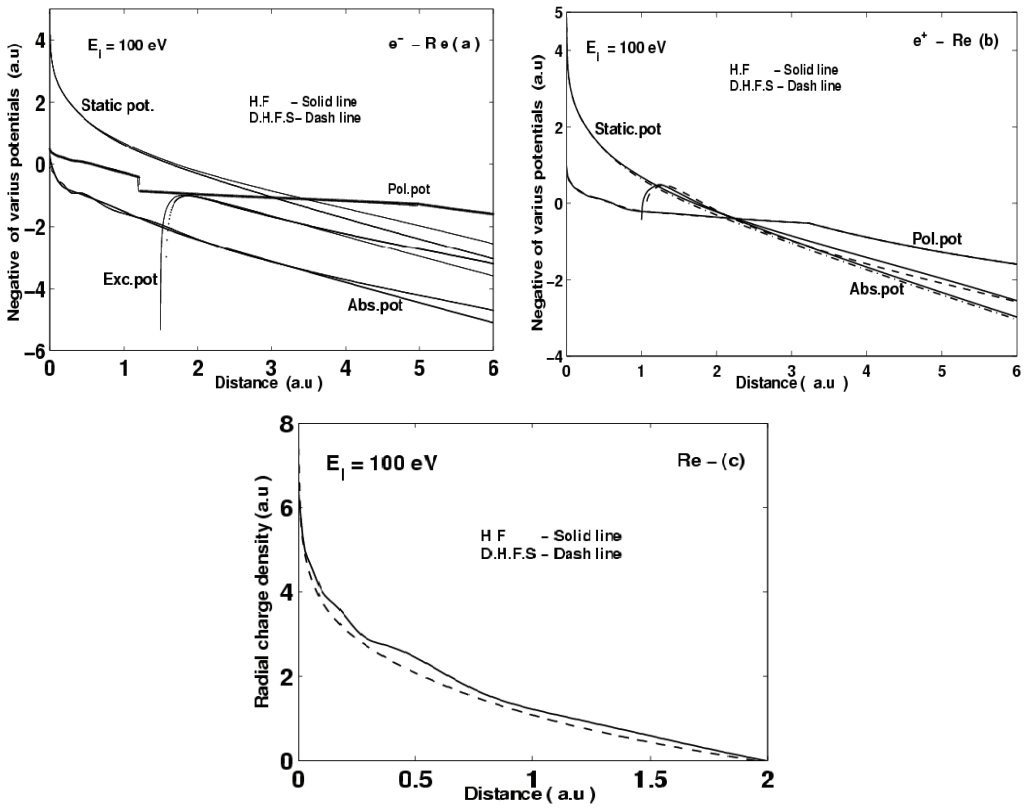

Figure 1: (a-b) Negative of various interacting potentials V_s (static), V_p (pol), V_{ex} (exchange), and V_{ab} (absorption) for $e^{\pm}$ - Re scattering at impact energy 100 eV. The curves represent the absolute values of the potentials which are all negative except V_s of positive.1 (c) spherical charge density of the Re atom.

is unity for allowed final states of the binary collision and zero for final states that are not allowed because of the Pauli exclusion principle. For positron-atom scattering this function is

$$\Theta(q',k_F) = H(q'^2, -k_f - \omega), \tag{12}$$

where ω is given $\omega = 2\Delta$ with Δ the energy gap between the target ground-state energy and the final energy of the originally bound target electron; $H(q'^2, -k_f - \omega)$ is the Heaviside unit step function, which equals 1 when the arguments non-negative and zero otherwise.

2.2 Radial shapes

The various components of the interaction terms and charge density as obtained using the non-relativistic HF wave function of McLean [29] are displayed in Fig. 1(a-c) for e–Re and e+-Re respectively In general, it is found that the static interaction dominates all other

interactions i.e. exchange and polarization for e^--Re in Fig. 1(a) and polarization for e^+-Re in Fig. 1(b) at small values of $r \sim 3.5$ a.u. and $r \sim 2.5$ a. u. and thereafter the correlation polarization takes over all other interactions. In e^--Re, the energy dependent exchange interaction V_{ex}^{MSCE} at $E=100$ eV remains weaker than the static interaction up to very large values of r. Fig. 1(c) shows the radial electronic charge density for Re atom using both HF and DHFS wave function respectively. The number of small peaks exhibited by the charge density curve indicates various shell contributions associated with the atom. The calculated density obtained by the analytical fitting procedure to DHFS wave function as given by Salvat *et al.* [30] shows a reasonable agreement with the HF wave function. It is noted that the analytical density curve only partially reproduces the small peaks of the non-relativistic density associated with different shell contributions. Theoretical shapes of various terms of the potential and density for Re, with both wave-functions are quite similar in nature.

3 Results and discussion

3.1 Angle-integrated elastic cross sections and contribution of partial waves in the low energy region ($E < 10$ eV)

We have performed calculations in different models potential, which are described as follows. For electron scattering, we consider SEP (Static + Exchange + Polarization) and SEPa (SEP + absorption) model potential. However, for positron, SP corresponds to the Static plus Polarization and SPa corresponds to SP plus absorption potential. In the present study, we have reported the calculation in these models using McLean [29] HF wave functions. The maximum in the d-wave cross-sections arises from shape resonance at energies $E_r \approx 2.4$ eV for e^-- Re and $E_r \approx 4.5$ eV for e^+- Re scattering respectively. The total cross-sections are also plotted in the figure under this model. Each curve shows a narrow low-energy peak followed by sharp fall of the cross-sections up to the first inelastic threshold.

It is observed from figure that first inelastic threshold energy E_{th}, s and p wave partial cross-sections contributes maximum to σ_{el} and near and above to E_{th}, d wave dominates. However, the situation is different for e^- and e^+ scattering above to the E_{th}. This difference appears because of an additional effect known as positronium formation.

3.2 Differential cross-sections and spin polarization parameter

In Fig. 3 we present elastic DCS and S-parameter for e^--Re and e^+-Re for both the real and the complex potentials. Figs. 3(a-d) correspond to the DCS and S-parameter at incident electron energies 10, 50, 100, and 200 eV respectively. It is seen that the present theory predicts the forward peak, minima and maxima at middle angles and enhanced backward slopes of the DCS. To illustrate the importance of the absorption effect we have displayed the DCS in the SEPa model. Figs. 4(a-d), show the DCS and S-parameter

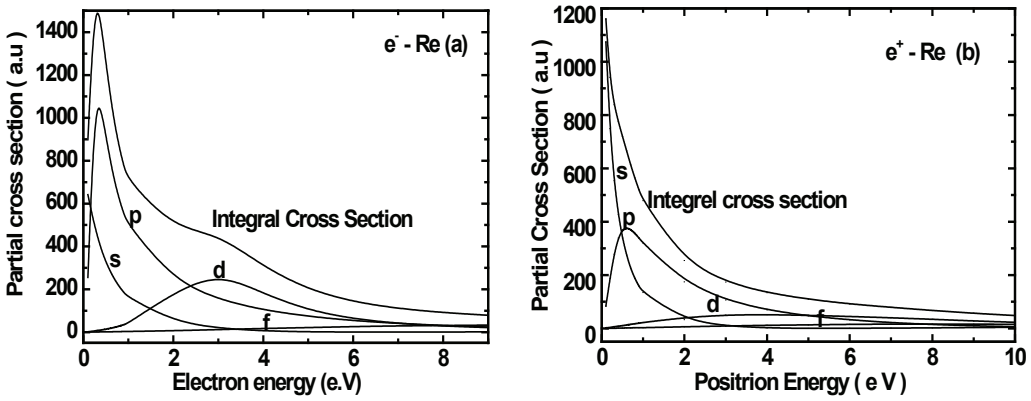

Figure 2: Partial Cross-Sections in the unit of a_o^2 for elastic scattering of $e^{\pm}$ - Re. Present calculation s, p, d, and f wave; summed partial wave cross section.

for positron scattering in SP and SPa models. The calculated angular variation in DCS exhibits deeper minima, which occur at slightly lower scattering angles for Spa model compared to SP model with real potentials. These figures also show the spin-polarization

Table 1: Elastic (σ_{el}), absorption, (σ_{abs}), and total (σ_t) cross-sections (a_o^2) in SEP_a model with absorption effect. σ'_{el} is the elastic scattering cross section without absorption effect for $e^{\pm}$ - Re scattering.

E(eV)	σ-Re				σ^+-Re			
	σ'_{el}	σ_{el}	σ_{abc}	σ_t	σ'_{el}	σ_{el}	σ_{abc}	σ_t
2	490.078	490.078	0	490.078	275.372	257.372	0	257.372
5	206.345	206.345	0	206.345	115.384	115.384	0	115.384
10	86.392	86.366	0.151	86.516	66.012	58.82	24.313	83.132
15	73.586	73.21	1.377	74.587	48.924	40.674	43.699	84.373
20	70.275	69.354	2.731	72.085	40.19	34.385	45.427	79.812
25	68.965	67.507	3.781	71.287	34.819	30.702	43.757	74.46
30	68.024	66.1	4.535	70.635	31.14	28.07	41.534	69.604
50	63.89	60.794	5.831	66.624	23.252	21.825	34.086	55.91
100	53.071	49.239	5.772	55.011	16.434	15.217	24.769	39.985
150	44.271	40.73	5.146	45.876	13.878	12.172	20.343	32.515
200	37.265	34.186	4.598	38.874	12.372	10.366	17.649	28.015
250	32.011	29.331	4.137	33.468	11.365	9.155	15.787	24.942
300	28.148	25.795	3.758	29.553	10.619	8.279	14.4	22.679
350	25.274	23.181	3.438	26.62	10.027	7.612	13.313	20.926
400	23.061	21.189	3.164	24.353	9.546	7.085	12.432	19.516
450	21.31	19.625	2.926	22.55	9.141	6.655	11.697	18.352
500	19.896	18.367	2.719	21.086	8.791	6.297	11.072	17.369

parameter at the same energies. At lower energy, the present phenomenological absorption potentials does not make any change in the calculated values, however, at higher energy DCS and S-parameter exhibit a rapid variation with scattering angles.

3.3 Elastic, total and momentum transfer cross sections

The results of our present integrated elastic, total and momentum-transfer cross sections for Re atoms are presented in Tables 1 and 2. Table 1 shows the compilation of cross-sections with and without absorption effects, σ_{el} and σ'_{el} respectively along with the absorption cross section σ_{abs} and total cross section σ_t. The momentum transfer cross section σ_m for each case is presented in Table 2. We know that electron and positron experience repulsive and attractive potential respectively while coming closer to an atom. This leads to the absorption of incident positron in the electron gas of the target atom, which in turn enhances the absorption cross section in the case of positron scattering as compared to the electron scattering.

Table 2: Momentum -transfer cross-section (σ_{mt}) (a_o^2) for e^- -Re and e^+- Re scattering.

E(eV)	σ^--Re		σ^+-Re	
	SEP	SEPa	SP	SPa
2.0	170.745	170.745	84.033	84.033
5.0	172.082	172.082	29.598	29.598
10.0	83.284	83.237	17.429	13.575
15.0	54.615	54.098	13.763	5.949
20.0	41.783	40.752	11.811	3.381
25.0	34.311	32.902	10.477	2.301
30.0	29.104	27.468	9.454	1.748
50.0	16.855	15.202	6.881	0.985
100.0	6.377	5.401	4.495	0.55
150.0	4.237	3.431	3.465	0.383
200.0	4.017	3.21	2.857	0.292
250.0	4.077	3.278	2.442	0.236
300.0	4.08	3.309	2.137	0.199
350.0	4.021	3.289	1.904	0.173
400.0	3.93	3.24	1.717	0.154
450.0	3.822	3.178	1.565	0.139
500.0	3.707	3.707	1.439	0.127

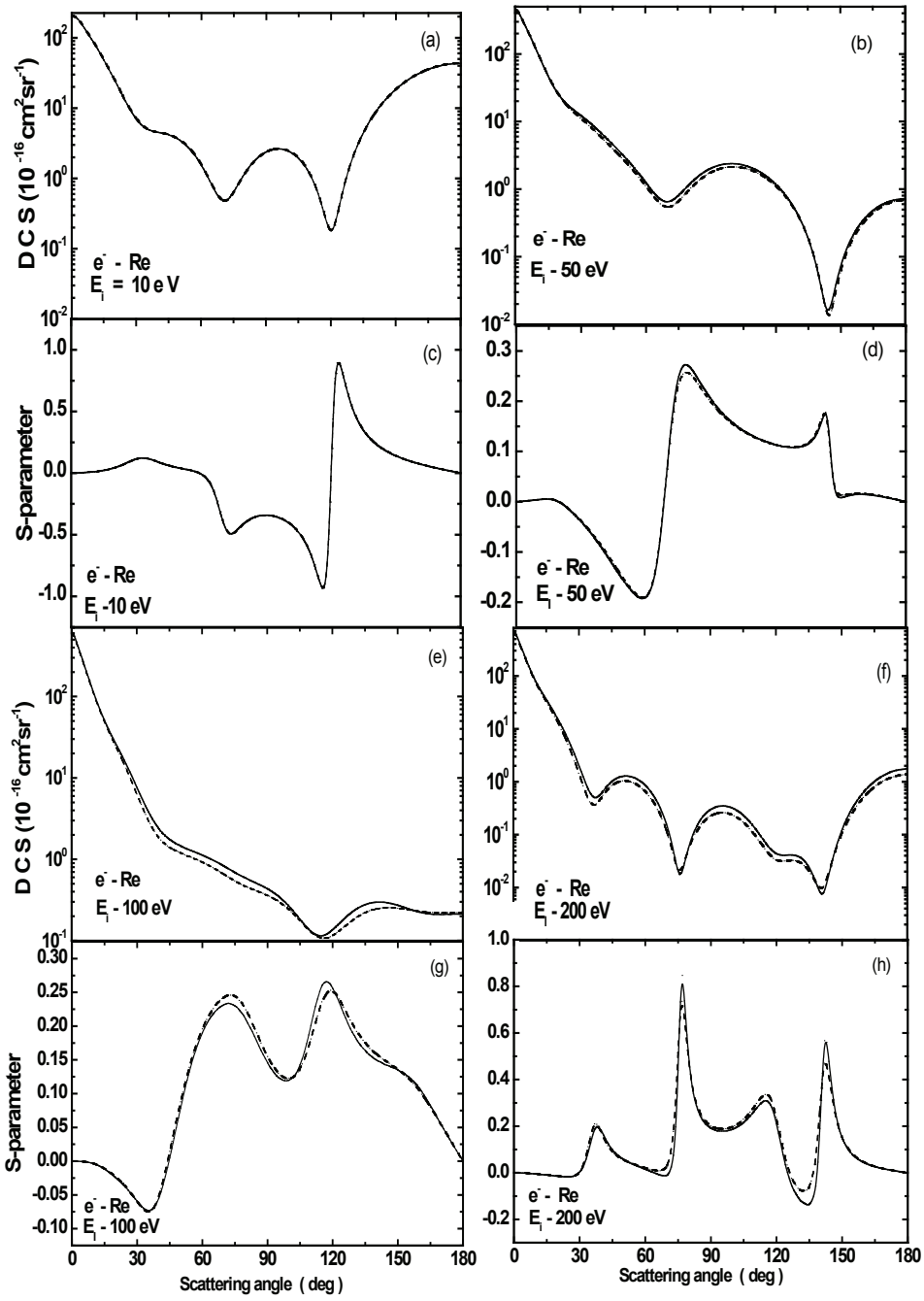

Figure 3: Differential cross section of elastic scattering and S-parameter for e^--Re scattering in units of (a_2^0 sr^{-1}). Present calculation: – with complex potential (SPA); - - - - with real potential (SP)

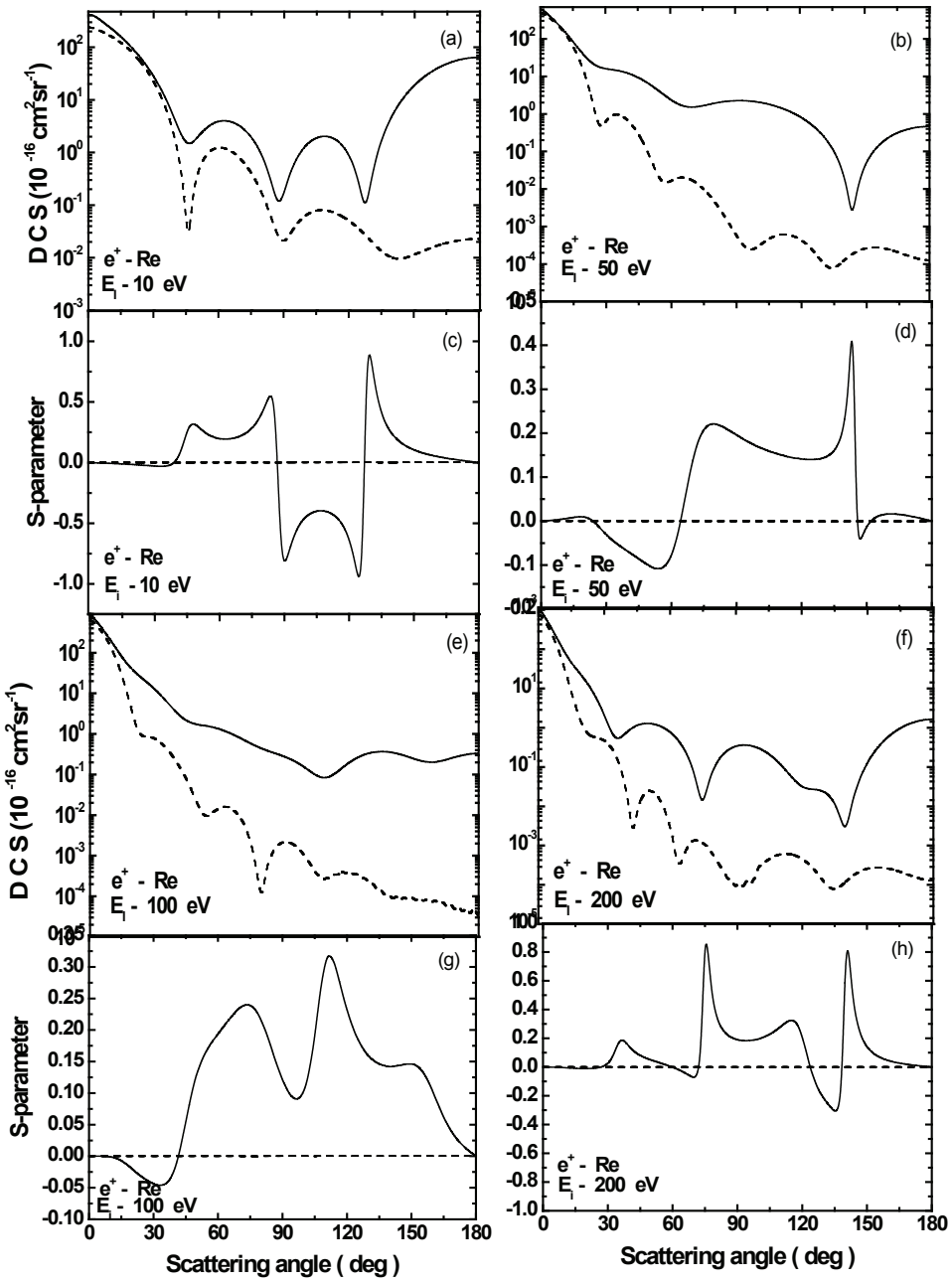

Figure 4: Differential cross section of elastic scattering and S-parameter for e^+ -Re scattering in units of (a_2^0 sr^{-1}). Present calculation: – with complex potential (SPA); - - - - with real potential (SP)

4 Conclusions

We have presented the result for DCS and the angular variation of spin polarization parameter- S for electrons and positrons, scattered from Re-atom at energies between 2.0 to 500 eV. This calculation has been performed using two differential models-without and with absorption potential. Results show that there is a significant amount of spin polarization in the scattered beam of electrons at various scattering angles. However, for positron scattering, the present result shows that the relativistic effects are important and the spin polarization is hardly influenced by the spin-orbit coupling, which is consistent with earlier results. Moreover, Re atom could be a good target for positron scattering as it takes into account the Ps formation. We expect that the importance of relativistic effects will be substantial for such heavy atoms like Re. We hope new experimental results will be reported in the light of our calculations for $e^{\pm}$ - Re elastic scattering.

References

[1] J. Kessler, Adv. At. Mol. Opt. Phys. 27 (1991) 81.
[2] J. Kessler, Polarized Electron, 2nd ed (Springer-Verlag, Berlin, 1985).
[3] N. Andersen and K. Bartschat, Adv. At. Mol. Opt. Phys. 36 (1996) 1.
[4] W. Walker, Adv. Phys. 20 (1971) 257.
[5] W. Walker, J. Phys. B 2 (1969) 356.
[6] L. S. F. Lam, J. Phys. B 15 (1982) 119.
[7] R. Haberland and L. Fritsche, J. Phys. B 20 (1987) 121.
[8] K. Bartschat, H. J. Goerss, and R. P. Nordbeck, Z. Phys. D 17 (1990) 25.
[9] K. Bartschat, J. Phys. B 20 (1987) L 815.
[10] R. P. McEachran and A. D. Stauffer, J. Phys. B 19 (1986) 3523.
[11] S. N. Nahar and J. M. Wadehra, Phys. Rev. A 43 (1991) 1275.
[12] S. N. Nahar and J. M. Wadehra, Phys. Rev. A 35 (1987) 2051.
[13] P. Kumar, A. K. Jain, A. N. Tripathi, and S. N. Nahar, Phys. Rev. A 49 (1994) 899.
[14] J. E. Sienkiewicz and W. E. Baylis, Phys. Rev. A 55 (1997) 1108.
[15] M. W. Bromley, J. Mitroy,and G. Ryzhikh, J. Phys. B 31 (1998) 4449.
[16] D. Reid and J. M. Wadehra, Phys. Rev. A 57 (1998)2583.
[17] R. K. Gangwar, A. N. Tripathi, L. Sharma, and R. Srivastava, J. Phys. B 43 (2010) 085205.
[18] M .T. McAlinden, A. A .Kernoghan, and H. R. Walters, J. Phys. B 30 (1980) 1543.
[19] M. Basu and A. S. Ghosh, Phys. Rev. A 43 (1991) 4746.
[20] F. Ghosh and W. A. King, Can. J. Phys. 74 (1996) 449.
[21] R. P. McEachran, A. D. Stauffer, and L. E. M. Campbe, J. Phys. B 13 (1980) 1281.
[22] S. N. Nahar and J. M. Wadehra, Phys. Rev. A 43 (1991) 1275.
[23] D. A. Elliot, J. Lower, S. F. Mazevet, R. P. McEachran, I. E. McCarthy, and E. Weigold, J. Phys. B 31 (1998) 547.
[24] Neerja, A. N. Tripathi, and A. K. Jain, Phys. Rev. A 61 (2000) 032713.
[25] Neerja and A. N. Tripathi, Eur. Phys. J. D 13 (2001) 5.
[26] Neerja and A. N. Tripathi, Indian J. Phys. B 4 76 (2002) 511.
[27] M. R. Nikolić and A. R.Tančić, Phys. Chem. Technol. 3 (2005) 141.
[28] H. Mohan, A. K. Jain, and S. Sharma, J. Phys. :Conf. Ser. 199 (2010) 012023.

[29] A. D. McLean and R. S. McLean, At. Data Nucl. Data Tables 26 (1981) 197.
[30] F. Salvat, J. D. Martinez, R. Mayol, and J. Parellada, Phys. Rev. A 36 (1987) 467.
[31] F. A. Gianturco and S. Scialla, J. Phys. B 20 (1987) 3171.
[32] A. K. Jain, Phy. Rev. A 41 (1990) 2437.
[33] K. K. Sharma, Neerja, and R. P. Vats, J. At. Mol. Sci. 2 (2011) 304.
[34] R. T. Sugohara, M. G. P. Homem, I. P. Sanches, A. F. de Moura, M.-T. Lee, and I. Iga, Phys. Rev. A 83 (2011) 032708.