1.

Differential Cross-Sections and Critical Points For Elastic Scattering Of Electrons by Krypton Atoms in the range (2-110) eV by using an Optical Potential Model .

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Abstract

The effect of scattering potential are tested by using the partial wave method for low and intermidiate energies in elastic scattering of electrons from krypton atom.Roothaan- Hartree-Fock atomic wave functions are used to performing these calculations. In this paper a model for correlation potential we derive from Armiento-Mattsson (2003) correlation energy function , this model used to constructing the optical (full) scattering potential that used to performing our calculations and this can serve as new addition in this field.This optical scattering potential model consists of the sum of the energy dependent electron gas exchange potential (Hara version) plus the energy independent electron gas correlation potential (derived in this work) plus the long range polarization potential (Miller-Bederson version) plus the well known static potential .We present a modify results for differential cross sections and critical positions for electrons scattering from krypton atom in the energy range (2-110eV).Our model and the corresponding results can serve as a new addition in this field . The results obtained in this paper are in good agreement with the available theoretical results of other investigators .

Keywords : Density Functional Theory ; Scattering Potential ; Electron-Krypton Scattering ; Differential Cross Section ;Critical Position

حساب المقاطع العرضية التفاضلية والنقاط الحرجة للاستطارة المرنة للالكترونات بواسطة ذرات الكربتون عند مدى طاقة (2-110) الكترون فولت باستخدام نموذج جهد بصري

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الخلاصة

ان تاثير جهد الاستطارة تم اختباره باستخدام طريقة الموجة المجزئة للاستطارة المرنة للالكترونات من ذرة الكربتون عند الطاقة الواطئة والمتوسطه حيث استخدمت الدوال الموجية الذرية للباحثين (روثان-هارتري-فوك) لانجاز هذة الحسابات.في هذا البحث تم اشتقاق نموذج لجهد الترابط من دوال طاقة الترابط للباحثين (ارمينتو-ماتسون)(2003).هذا النموذج استخدم لتركيب جهود الاستطارة الكلية التي استخدمت لانجاز الحسابات، حيث نوقشت النتائج التي تم الحصول عليها في نموذج جهد الاستطارة الكلي الذي يتكون من مجموع جهد التبادل للغاز الالكتروني المعتمد على الطاقة (نموذج هارا) مضافا اليه جهد الترابط للغاز الالكتروني غير المعتمد على الطاقة (النموذج المشتق في هذا العمل) مضافا اليه جهد الاستقطاب ذو المدى الطويل (نموذج ميلر-بيدرسون) مضافا اليه الجهد المستقر (الاستاتيكي) المعروف.لقد تم الحصول على نتائج معدلة للمقاطع العرضية التفاضلية والمواقع (النقاط) الحرجه للاستطاره المرنه للالكترونات بواسطة ذرة الكربتون.ان النموذج المستخدم والنتائج المستخلصة يمكن اعتبارها اضافة جديدة في هذا المجال.ان النتائج التي تم الحصول عليها في هذا البحث في حالة اتفاق جيد مع نتائج الباحثين الاخرين.

Introduction

The study of electron-atom scattering has grown considerably during the last twenty five years. The aim of this paper is to apply the model of correlation potential we derive from density functional theory to construct the scattering potential model that consist of a static, exchange, correlation and polarization effects and to apply at low and itermidiate impact energies for electron-krypton collision processes to get a modify results of differential cross sections and critical positions for electron-krypton scattering.

Introductory Remarks

The theoretical complexity of the electronic structure or electron-scattering dynamics of atoms is due to electron exchange and correlation effects [1,2]. Electron exchange effects are due to the Pauli exclusion principle and the consequence that the total wave function of the system must be antisymmetric with respect to the interchange of the coordinates (spatial and spin) of any two electrons[3] . Thus a variety of exchange approximations has been devised to permit the study of large atoms and molecules and other forms of condensed matter[4,5].On the other hand ,in the static-exchange approximation ,the theory takes into account only the static and exchange interactions of the electron with an unperturbed ground electronic state of the target .There is no allowance for polarization or other correlation effects,where exchange effects preventing two electrons of like spin from being found near one another because of Each bound electron is surrounded by a Fermi hole where the repulsive Coulomb interaction between two electrons of like spin vanishes[5].

In the Hartree -Fock approach each electron is assumed to move in the average self-consistent field of the other electrons, taking into account only the Coulomb energy and the Pauli exclusion principle .Thus ,correlation is the correction of this average interaction to allow electrons to avoid one another ,not only "on the average" but in every region of configuration space .Thus, in addition to the "Fermi hole" each electron surrounds itself with a "Coulomb hole" from which other electrons are excluded[3].

The polarization is an important correlation effect found to be particularly important in low energy electron scattering .When an electron slowly approaches the target atom, the bound electrons are influenced by the electric field of the external charge, and an adiabatic redistribution of bound electronic density occurs, resulting in an (indused) dipole moment on the target atom .The adiabatic change in energy due to the slow approach of the electron exhibits the asymptotic form[5]:

$$V_{pol.}(r) - \overrightarrow{r \longrightarrow \infty} \frac{\alpha_d}{2r^4} \qquad \text{----------(1)}$$

where α_d is the electric dipole polarizability of the inner charge distribution depends on the direction of the external electric field and hence the position vector of the electron. Equation (1) represents a dipole approximation and breaks down as the electron closely approaches the target .Moreover ,the adiabatic effect breaks down at high energies and near the nuclei, where the electron has a large local kinetic energy[5].

The purpose of this paper is to report a simple and accurate model of scattering potential for electron-atom system .The approach represents a hybridization of free-electron-gas (FEG) theory and the long range polarization interaction theory , some what along the lines of Armiento-Mattsson[6] of the short range correlation interaction theory .Our approach is to adopt the static potential plus Hara's modification [7] of the free-electron-gas exchang potential plus the short range correlation potential (derived in this work from Armiento-Mattsson (2003) correlation energy function[6]) plus the long range polarization potential of Miller-Bederson [8] where the short range correlation potential becomes equal to the long range polarization potential at the crossing point r_o when $r = r_o$ .Thus requires only the electron density and polarizabilities of the target . The approach described in this paper is similar to that used by O,Connell and Lane [3] .However, the choice of correlation –polarization potential model used to perform the calculations is quite different.

In sec.3 ,the forms of exchange and correlation potentials used in this paper are described .In sec.4,the computational method used in present work is discussed. While sec.5 deals with the results and discussion obtained from application of elastic electrons scattering from krypton atom ,the conclusions are given in sec.6 .

Exchange and Correlation Potentials:

3.1: Hara-Free-Electron-Gas (HFEG) Exchange potential:

The free electron gas exchange potential form used is [5]:

$$\mathbf{V}_{FEG}^{ex}\mathbf{(r)} = \frac{2}{\pi} - \mathbf{k}_F\mathbf{(r)F}\left[\eta(r)\right] \qquad \text{----------(2)}$$

Where $k_F(r)$ is related to the charge density of the target atom $n(r)$ by :

$$k_F(r) = [3\pi^2 n(r)]^{1/3} \qquad \text{----------(3)}$$

and $F[\eta(r)]$ is given by :

$$F[\eta(r)]=\frac{1}{2}+\ln\frac{1-\eta^2}{4\eta}\left|\frac{1+\eta}{1-\eta}\right| \quad \text{----------(4)}$$

with:

$$\eta(r)=k(r)/k_F(r) \quad \text{----------(5)}$$

defined in terms of the "local momentum" k(r) of the projectile electron and the "local fermi momentum" $k_F(r)$. In equation (5) , Hara [5] , suggested that the momentum k(r) of the scattered electron should be referred to the same energy base as that of the bound electrons in the gas .Thus the variation of k(r) with r arises from $k_F(r)$ according to:

$$k^2(r)=k_F^2(r)+2I+k^2 \quad \text{----------(6)}$$

where I is the ionization potential of the target atom and $k^2/2$ is the incident kinetic energy of the projectile electron. In the present study the Hara free electron gas (HFEG)exchange potential of equation (2) with the help of equation (6) has been adopted.

For correlation potential in density functional theory, there is a correlation function used to perform our calculations:

3.2:Armiento–Mattsson correlation function:

Armiento and Mattsson[6] have shown that the local values of the conventional exchange energy per particle cannot be described by an analytic expansion in the density variation . They construct an alternative separation in which the exchange part is made well behaved by screening its long-ranged contributions ,and the correlation part is adjusted accordingly .They demonstrate functional development based on this approach by creating and deploying a local-density-approximation-type xc functional . Armiento and Mattsson[6] present results by separating the xc energy in an alternative way and show this results to hold for systems of effective potentials by introduces $\vec{K}_y$ as the Yakawa wave vector which effectively is an inverse screening length for the coulomb potential that may dependent on r . A corresponding correlation like term $E_{cor.-y}$ is defined by the relation $E_{ex.+y}+E_{cor.-y}=E_{xc}$ [6],where E_{xc} is the total exchange-correlation energy per particle. This can be seen as moving a term E_y from correlation to exchange[6]. So,

$$E_{ex.+y}=E_{ex.}+E_y \quad \text{----------(7)}$$

And,

$E_{cor.-y} = E_{cor.} - E_{y}$ ----------(8)

This is an alternative way of partitioning E_{xc} without introducing any new approximations .This approach is fundamentally different from other previous approaches in that the screening of the exchange is compensated for by redefining correlation to keep the total E_{xc} constant[6].In the present work, the exchange part of the alternative separation is neglected after the correlation part is adjusted accordingly(i.e, We used only the correlation part).Thus ,there is a correction model of Armiento-Mattsson correlation energy function for local density approximation in density functional theory [6] used to performing our calculations.

Armiento–Mattsson [6] gives an explicit expression for $E_{cor.-y}^{LDA2}$,(all equations used in the following in mRy. atomic units),the result is [6]:

$$E_{cor.-y}^{LDA2}(r_s) = \frac{e_1 r_s + e_2 \sqrt{r_s} + e_3}{r_s^{\,2} + e_4 r_s^{3/2} + e_5 r_s + e_6 \sqrt{r_s}} \qquad \text{----------(9)}$$

Of the six parameters , $e_1 - e_6$ where, $r_s = [3/4\pi n(r)]^{1/3}$ (a.u.) is the charge density parameter. With

$e_1 = -1.81942, e_2 = 2.74122, e_3 = -14.4288, e_4 = 0.537230, e_5 = 1.28184$ and $e_6 = 20.4048$ .These parameters is compared with the Ceperley–Alder [9] data and other xc parametrizations currently in use [10].Then we extract the correlation potential $V_{cor.}(r)$ from the flowing relation [10]:

$$V_{cor.}(r) = E_{cor.}(r_s) - \frac{r_s}{3}\frac{\partial E_{cor.}(r_s)}{\partial r_s} \qquad \text{----------(10)}$$

Thus ,the result from equations (9) and (10) is:

$$V_{cor.}^{LDA2}(r) = E_{cor.-y}^{LDA2}(r_s) - \frac{r_s}{3}\left(\frac{c_1.c_2 - c_3.c_4}{c_5}\right) \qquad \text{----------(11)}$$

where,

$c_1 = r_s^{\,2} + e_4 r_s^{3/2} + e_5 r_s + e_6 \sqrt{r_s}$ ----------(12)

$c_2 = e_1 + \frac{e_2}{2\sqrt{r_s}}$ ----------(13)

$c_3 = e_1 r_s + e_2 \sqrt{r_s} + e_3$ ----------(14)

$$c_4 = 2r_s + \frac{3e_4\sqrt{r_s}}{2} + e_5 + \frac{e_6}{2\sqrt{r_s}} \qquad \text{----------(15)}$$

$$c_5 = \left(r_s^{\,2} + e_4\, r_s^{3/2} + e_5\, r_s + e_6\sqrt{r_s}\right)^2 \qquad \text{----------(16)}$$

where $e_1 - e_6$ as given previously , Armiento & Mattsson[6] make sure that there is no major difference between this correlation energy function and the other LDA correlation functionals. I.e. Perdew–Zunger[11],Vosko–Wilk–Nusair[12],Perdew–Wang[10].In the present study the correlation potential represent by equation (11)with the help of equations (12–16) are adopted in order to construct our scattering potential model to performing the calculations of this work.On the other hand, the long range polarization potential is defined by the relation(Miller–Bederson version)[8]:

$$V_{pol}^{LR}(r) = -\frac{\alpha_d}{2r^4}\left\{1 - \exp\left[-\left(\frac{r}{R_c}\right)^6\right]\right\} \qquad \text{----------(17)}$$

where α_d represent the electric dipole polarizability of the target atom and R_c is a cut-off parameter which is important in which it gives correction for correlation effects at low distance from the atom .The full correlation potential ,then ,is obtained by continuously joining of the short-and long-range forms at the crossing point r_o where $V_{cor.}^{SR}(r)$ and $V_{pol}^{LR}(r)$ are cross at the crossing point r_o ,thus obtaining :

$$V_{cor.}(r) = \begin{cases} V_{cor.}^{SR}(r) & , r \le r_o \\ V_{pol}^{LR}(r) & , r > r_o \end{cases} \qquad \text{----------(18)}$$

This is the simplest prescription for joining the correlation and polarization potential. This treatment similar to that used by O'Connell–Lane[3] in the local density functional theory.However,the choice of correlation and polarization potentials is quite different.

Computational method

In this section ,the elastic scattering of electrons by krypton atom is described. Atomic unit will be used throughout but unless otherwise stated , we will assume the target nucleus to be infinitely heavy compared with the electrons so that we may work in the center of mass frame with the origin of coordinates fixed at the nucleus.

The Z-axis will be defined as the direction of the incoming electron .We have used the partial wave method to calculate the phase shifts and then differential cross sections and critical positions for the elastic scattering of electrons by krypton atom. For the spherically symmetric atomic targets, the radial partial wave functions satisfy the radial equation [13]:

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+k^2-\frac{l(l+1)}{r^2}-2V(r)\right]R_{kl}(r)=0 \qquad \text{----------(19)}$$

where $V(r)$ is the full electron–atom potential energy model ,including the static potential $V_s(r)$,the exchange $V_{FEG}^{ex}(r)$ and correlation–polarization $V_{cor.}(r)$ potentials as described by the following expression:

$$V(r)=V_s(r)+V_{FEG}^{ex}(r)+V_{cor.}(r) \qquad \text{----------(20)}$$

where $V_{cor.}(r)$ represent the correlation–polarization potential which is given by equation (18) with the help of equations (11) and (17).Therefore ,the correlation potential $V_{cor.}(r)$ which we have been adopted in precent work ,can be represent by the model:

$$V_{cor.}(r)=\begin{cases} V_{cor.}^{SR}(r) & ,r\le r_o \quad \text{of equation (11)} \\ V_{pol}^{LR}(r) & ,r>r_o \quad \text{of equation (17)} \end{cases} \qquad \text{----------(21)}$$

Where $V_{FEG}^{ex}(r)$ is Hara's modification of FEG exchange potential (HFEG) [7] represented by equation (2) with the help of equation (6) we have been adopted for the calculations reported in this paper and $V_s(r)$ is the static coulomb potential is simply given by [14]:

$$V_s(r)=-\int\frac{n(r')}{|r-r'|}d^3r' \qquad \text{----------(22)}$$

The bound atomic orbital function $\Phi_i(r)$ are taken to be the analytic Hartree–Fock functions of Clementi–Roetti [15].Thus the radial electron density is given in terms of these orbitals by [3]:

$$n(r)=\frac{1}{4\pi r^2}\sum_{i=1}^{N}\Phi_i^2(r) \qquad \text{----------(23)}$$

where N represent an electrons of target atom .The radial equation (19) where solved numerically in the internal region $(r<a)$ by using Numerov's algorithm [16] where a is called the matching radius at which the

continuously occur between the solutions in the internal $(r < a)$ and external $(r > a)$ regions by matching the internal solution to the external ones at $(r = a)$ where $r * V(r) \to 0$ [It must note that the matching radius a differ from the crossing point r_o where a is related with the solution of the radial equation represent by equation (19) while r_o is the point at which $V_{cor.}^{SR}(r) = V_{pol.}^{LR}(r)$,also the parameter $r_s = [3/4\pi n(r)]^{1/3}$ (a.u.) is the charge density parameter which is related to the charge density of the target atom $n(r)$].Therefore, the asymptotic boundary conditions at $(r > a)$ [17]:

$$R_{kl}(r) = B_l(k)\left[j_l(kr) - \tan\delta_l(k) \cdot n_l(kr)\right] \qquad \text{----------(24)}$$

where $B_l(k)$ is real constant equal to one which is independent of r while $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and spherical Neumann functions respectively .Thus,

by using the solutions in the internal $(r < a)$ and external $(r > a)$ regions at $(r = a)$ we get the result of phase shifts $\delta_l(k)$ [3].Thus, the scattering amplitude is given by the expression [17]:

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\exp(2i\delta_l(k) - 1)P_l(\cos\theta) \qquad \text{----------(25)}$$

where $P_l(\cos\theta)$ are the Legendre polynomials and θ is the scattering angle .The elastic differential scattering cross section (DCS's) is given by [18]:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \qquad \text{----------(26)}$$

after this stage we have been calculated critical positions for elastic scattering of electrons by krypton atoms,where at some incident electron energy and scattering angle ,the differential scattering cross section become a minimum with respect to both the incident electron energy and the scattering angle.The combination of the impact energy and the angle are known as critical positions (points) and are represented by E_C (critical energy) and θ_C (critical angle)[19].In this work,since,there is no acurate method for calculating critical positions for atoms having atomic number Z >10, the critical positions (E_C , θ_C)are evaluated by a method consist of computing the differential scattering cross sections in the energy range (0.2-150eV) and angles between (0.00^o-180.00^o) with an energy step of 0.2eV,and angular step of 0.01^o by using aproprate code with large accuracy

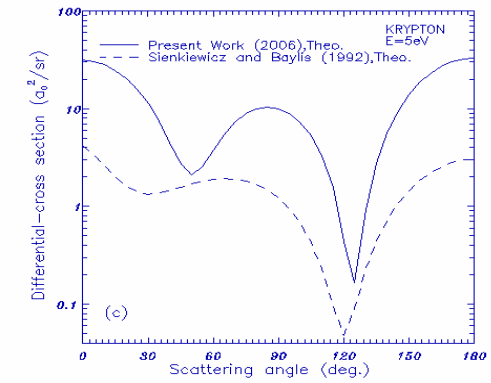
written for this purpose.The results obtained by this method are compared with the available theoretical results of Kelemen [20].Our results are in good agreement with other theoretical results.

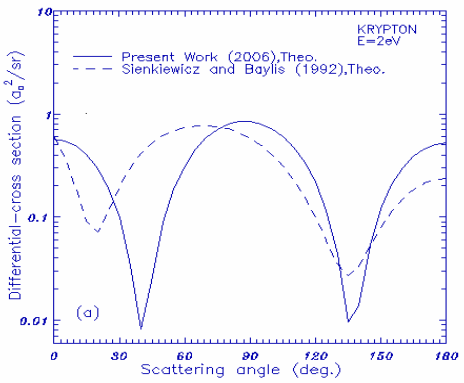
Results and Discussion

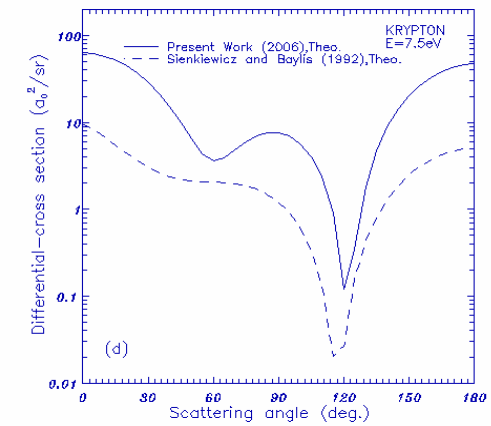
The ionization potential used for krypton atom is I=13.9997eV [21] , and the electric dipole polarizability used in this calculations are $\alpha_2(0) = 16.74\, a_o^3$ [8], while the crossing point $r_o = 2.422\ a_o$ and the cut-off parameter $R_c = 2.0\ a_o$ .Figure (1) shows the results of the differential cross-sections (a_o^2 / sr) for the elastic scattering of electrons from krypton atom for an incident electron energy (a) 2eV, (b) 3eV, (c) 5eV, (d) 7.5eV, (e) 10eV, (f) 20eV, (g) 25eV, (h) 30eV, (i) 40eV, (j) 50 eV, (k) 75eV and (l) 100eV.For these energies we compare our results with the theoretical results of Sienkiewicz and Baylis [22].From these results we note that there is a slightly difference between our results and the results of Sienkiewicz and Baylis [22] as shown in figures (1a–d) for a small and large angles because these angles is dominated by the long range polarization and short range static potential respectively.As the impact energy increases the results of our model are slightly agree with the results of Sienkiewicz and Baylis [22] ,but it seems higher as shown in figures (1e–l).This behavior depend on scattering potential model used where at small impact energies the scattering potential model become much sensitive than at large impact energies because the effects of correlation,polarization and exchange effects become nigligible at high energies as shown in figures (1i–l). While figure(2) shows the results of critical positions (points) (E_C, θ_C) for energy range (0.2-150eV) and angles range between (0.00^o-180.00^o) by using the model adopted in present work. We compare our results of critical positions with the available theoretical results of Kelemen [20] as shown in table (1).From these results we note that there is a slightly agreement between our results and the results of Kelemen [20] , and the reason is the same as discuss in figure (1).

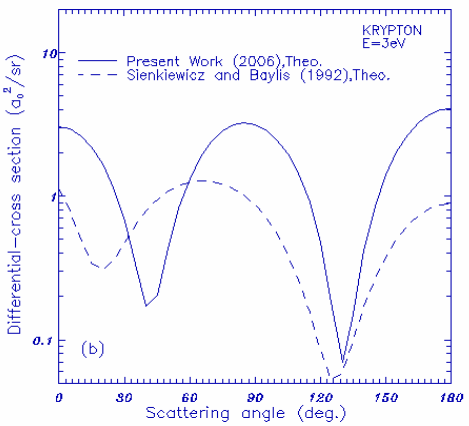
Conclusions

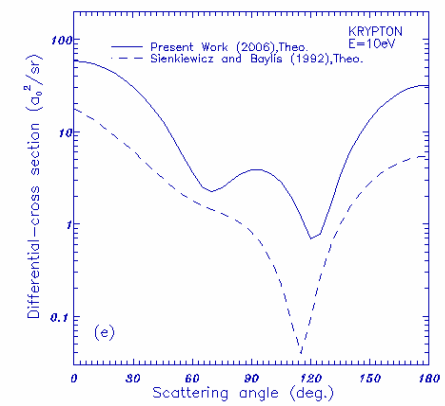
In this paper, we have used our model in electron-krypton scattering .We take the exchange potential to include it in the total scattering potential model because of exchange effects are due to the Pauli exclusion principle ,consequently ,exchange potential prevent two electrons of like spin from being found near one another because it make each bound electron is surrounded by a "Fermi hole" where the repulsive Coulomb interaction between two electrons of like spin vanishes .Also ,we included the correlation potential in the total scattering potential model because each electron is assumed to move in the average self consistent field of other electron ,taking in to account only the Coulomb energy and the Pauli exclusion principle .Thus, the correlation potential is the correction of this average interaction to allow electrons to avoid one another ,not only "on the average' but in every region of configuration space .Thus in addition to the "Fermi hole" caused by the exchange potential ,the correlation potential make each electron surrounds itself with a "Coulomb hole" from which other electrons are excluded when a single electron is removed sufficiently far from the other electrons . However ,the theoretical complexity of the electron scattering dynamics of atoms is due to electron exchange and correlation effects. The comparision of our results of differential (DCS's) and critical positions (E_C, θ_C) that preformed by using our scattering potential model that constructed in this paper with the available theoretical results of other investigator explain the success of our model .The present calculations test more stringently the features of these potentials and suggest that this model can produce reliable differential, total, momentum transfer cross sections and critical positions for electron- krypton scattering at impact energies above the region used to performing our calculations .Therefore we believe that our present model can serve as a good starting point from which to construct a scattering potential model involve an relativistic effects. We intend to extend these calculations by including the relativistic effects in these calculations in future work .

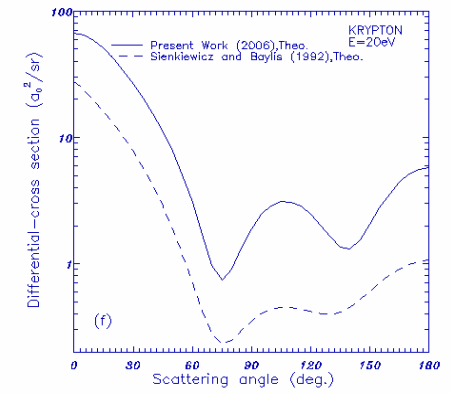

KRYPTON
E=5eV
Present Work (2006),Theo.
Sienkiewicz and Baylis (1992),Theo.
Differential-cross section (a_0^2/sr)
Scattering angle (deg.)
(c)


KRYPTON
E=2eV
Present Work (2006),Theo.
Sienkiewicz and Baylis (1992),Theo.
Differential-cross section (a_0^2/sr)
Scattering angle (deg.)
(a)


KRYPTON
E=7.5eV
Present Work (2006),Theo.
Sienkiewicz and Baylis (1992),Theo.
Differential-cross section (a_0^2/sr)
Scattering angle (deg.)
(d)


KRYPTON
E=3eV
Present Work (2006),Theo.
Sienkiewicz and Baylis (1992),Theo.
Differential-cross section (a_0^2/sr)
Scattering angle (deg.)
(b)


KRYPTON
E=10eV
Present Work (2006),Theo.
Sienkiewicz and Baylis (1992),Theo.
Differential-cross section (a_0^2/sr)
Scattering angle (deg.)
(e)


KRYPTON
E=20eV
Present Work (2006),Theo.
Sienkiewicz and Baylis (1992),Theo.
Differential-cross section (a_0^2/sr)
Scattering angle (deg.)
(f)

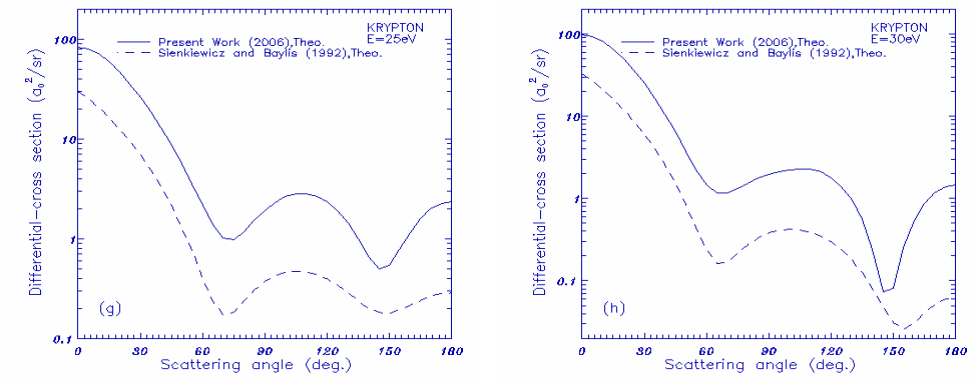
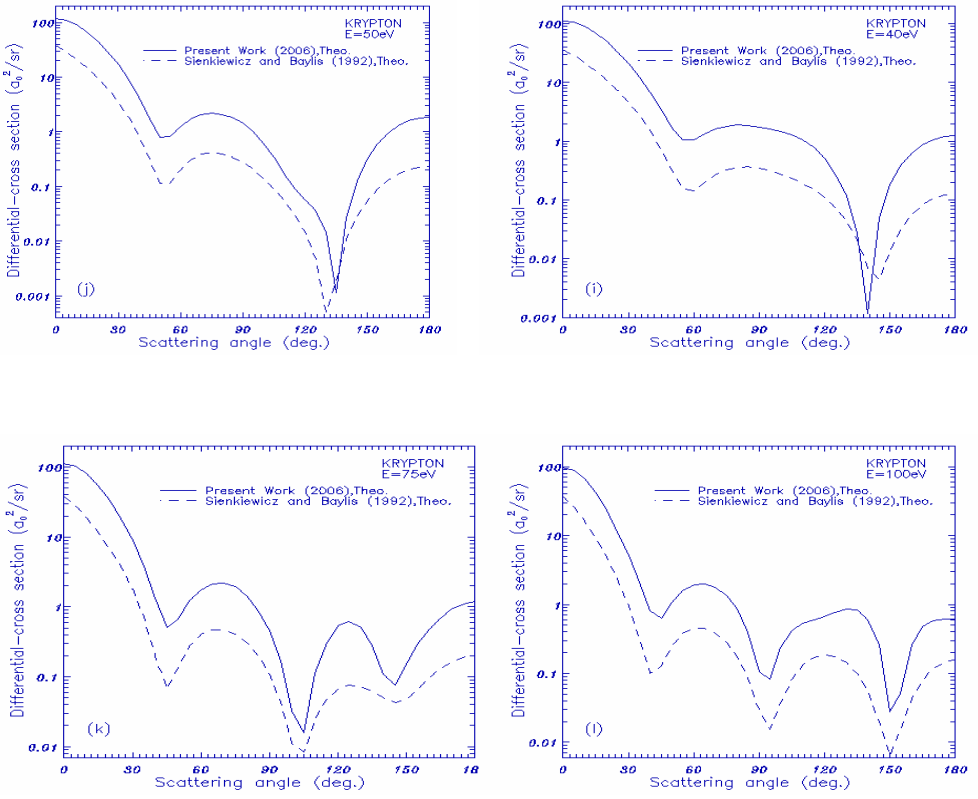


Figure (1):Differential cross-sections (a_o^2 / *sr*) for the elastic scattering of electrons

from krypton atoms for an incident electron energy (a) 2eV, (b) 3eV, (c) 5eV, (d) 7.5eV, (e) 10eV, (f) 20eV, (g) 25eV, (h) 30eV, (i) 40eV, (j) 50 eV, (k) 75eV, (l) 100eV.



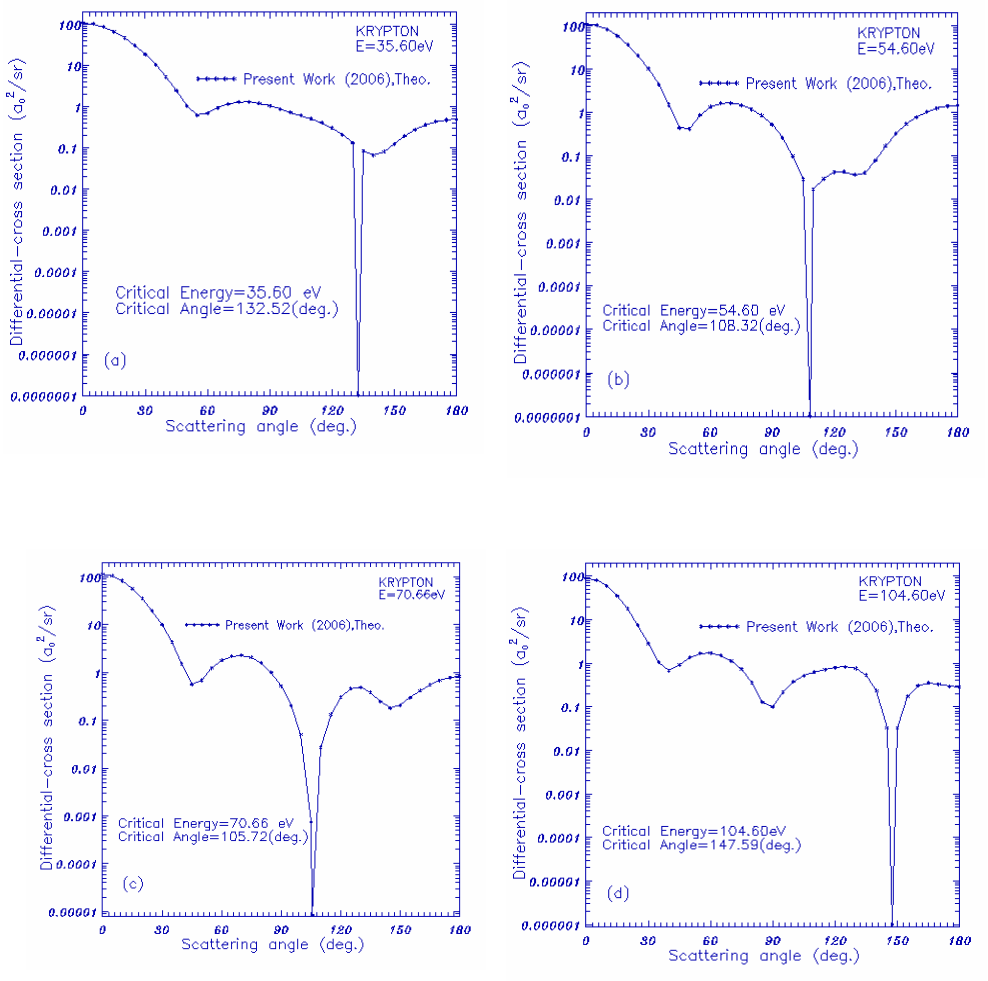


Figure (2):Critical Positions (E_C , θ_C) for elastic scattering of electrons by krypton

atoms : (a) (35.60eV,132.52^o) , (b) (54.60 eV,108.32^o),
(c) (70.66eV,105.72^o) , (d) (104.60eV,147.59^o).

Table (1): Results of Critical Positions (E_C , θ_C) for elastic scattering of electrons by Krypton atoms.

Our Calculation		Other results (ref.[20])	
E_C (eV)	θ_C (deg.)	E_C (eV)	θ_C (deg.)
35.60	132.52	35.90	149.70
54.60	108.32	53.60	128.15
70.66	105.72	61.40	114.14
104.60	147.59	116.50	150.71

[20]:V.I.Kelemen (2004).Theo.

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