ELECTRON IMPACT ELASTIC SCATTERING OF STRONTIUM USING DISTORTED WAVE METHOD

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NOVEMBER, 2018

DECLARATION

This thesis is my original work and has not been presented for a degree in any other University or any other award.

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DEDICATION

This thesis is dedicated to my wife Tabitha and our daughters Veronica and Ruth and son David for the encouragement and the sacrifices they made for me in the whole process of my studies.

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ABBREVIATIONS, ACRONYMS AND SYMBOLS

AES	Auger-Electron Spectroscopy
CCC	Convergent Close Coupling
CC2	Two-State Close-Coupling
CPB	Coulomb Projected Born
DCS	Differential Cross Sections
DHF	Dirac-Hartree-Fock
DW	Distorted Wave
DZ	Double Zeta wave functions
DWBA	First-Order Distorted Wave Born Approximation
DWBA1	e – H inelastic scattering Computer Program
eV	Electron Volt
FBA	First Born Approximation
ICS	Integral Cross-Sections
MCS	Monte-Carlo Simulation
OMPM	Optical Model Potential Method
RHF	Roothan Hatree Fock
RVP	Relativistic Variable Phase
Sr	Strontium
XPS	X-ray Photoelectron Spectroscopy
a_0	Bohr radius
A	Antisymmetrizing operator
E_i	Energy for intial state of projectile

f	Direct amplitude
f_B	Born approximation
g	Exchange amplitude
G^+	Total Green's function
H_a	Hamiltonian of isolated atom
k_i	Intial wave vector
k_f	Final wave vector
N_n	Factor of normalization
T	Kinetic energy operator of the projectile
T_{if}	Transition matrix
U_f	Arbitrary distortion potential
V	Interaction potential
Y_{lm}	Spherical harmonics
Ψ_i^+	Total wave function
$\phi_{i,f}$	Atomic wave functions for initial and final state respectively
β_i	Plane wave for an initial-state of the projectile
Ω	Solid angle
ψ_i	Initial atomic wave function
χ_i^+	Initial distorted wave
δ_l	Elastic scattering phase shift

ABSTRACT

Differential and integral cross sections for electron-atom are useful for interpretation and understanding of electron contact with the targets and for determining dynamics of the collision processes. They are useful in X-ray photoelectron spectroscopy (XPS), upper atmosphere dynamics, Monte-Carlo simulation (MCS), Auger-electron spectroscopy (AES), in gaseous-exchange, laser development, plasma physics and fluorescent lighting. For elastic scattering of strontium very few calculations have been performed and currently there are no known results using the present method. Also the available theoretical results do not have other results to be compared with so it makes it important to obtain results to compare them and to be compared with future experimental results. In calculation of differential and integral cross section for elastic scattering of electron by strontium atom, first-order distorted wave born approximation method has been used to determine DCS and ICS at impact energies of 10eV to 200eV and scattering angles ranging from 0^0 to 180^0. Also in this study at the initial state, both initial and final channel distortion potential of elastic scattering of electron by a strontium atom are taken as the static potentials since it is an elastic scattering. The distorted waves are expanded in terms of radial wavefunctions and spherical harmonics, Numerov method was then used to solve the radial equations to obtain the radial wavefunctions. The Madison and Bartschat computer program DWBA1 for e^- - H scattering was modified to perform the mathematical computations for e^- - Sr scattering and the results for differential and integral cross sections are calculated and compared with the available results. The integral cross sections (ICS) results agree well qualitatively with the other theoretical results. At lower incident energies (10-30 eV), the present differential cross section (DCS) results disagree with results obtained from optical potential method. This is because the first order distorted wave method gives poor results at low impact energies and also the nature of the distortion potential used. At intermediate and higher energies (60-200 eV), the present DCS results agree well with the results obtained from optical potential method. In conclusion, the DWBA was developed and applied to $e-$ - Sr scattering, changes on the DWBA1 computer program were made for strontium, differential cross section (DCS) and integral cross section (ICS) at impact energies 10-200eV for elastic scattering of electron-strontium were determined using DWBA at intermediate and high energies and the results compared with the other available results. From this work it was recommended that some experimental studies on electron impact elastic scattering of strontium should be made to give results for comparison with the calculated results, more theoretical studies using other methods should be conducted on DCS and ICS for purposes of comparison with the present results, a distortion potential that incorporates the polarization potential, exchange potential and absorption potential should be used in the calculation and the present method incorporating all the distortion potentials should be extended further for electron impact elastic scattering of other alkaline earth metals such as beryllium, cesium, ytterbium, and radium.

CHAPTER ONE

INTRODUCTION

1.1 Background to the study

Differential and integral cross sections for electron-atom are useful for interpretation and understanding of electron contact with the targets and deciding dynamics of the collision processes. Ramsauer (1921), conducted the first electron-atom scattering experiment and he made an observation that low energy elastic scattering with projectile energy of about 0.7eV by noble gas atoms full of transparency showed almost zero scattering. It contradicts classical mechanics which tries to determine a monotonic gain in the number of scattered electrons as falling electron energy diminishes. To investigate this, experiments on scattering have been carried out with various impact energies with different projectiles and target atoms for both elastic and in elastic processes. Cross-section data set for electron – atom elastic scattering are useful in X-ray photoelectron spectroscopy (XPS), upper atmosphere dynamics (Jablonski *et al*., 2004), Monte-Carlo simulation (MCS), Auger-electron spectroscopy (AES) (Jablonski *et al*., 2004), in gaseous-exchange, laser development (McCarthy and Weigold, 1995), plasma physics and fluorescent lighting. It is therefore evident that the knowledge of atomic collisions is important for calculations and also experimental approach in atomic physics.

In atomic collisions signals transmitted along a narrow path of free projectile act together with target and detector takes the record of particles scattered in the relating to the region. There are two types of collision processes: - elastic and inelastic. In elastic scattering, energy is conserved after the interaction between the target and the projectile electron. In inelastic scattering energy is not conserved. After the interaction of the target and projectile electron, inelastic scattering results into positronium, ionization, target excitation or annihilation. (Ali and Soding, 1988).

Atomic collision study methods are further classified into two approaches either quantum mechanical approaches or semi-classical approaches. Quantum mechanical approaches are the one that uses the principle of quantum mechanics entirely; which is also classifieds into non-perturbative method and perturbative method. Examples of the non-perturbative methods are R-Matrix, the close coupling and other variational methods which employ the non-perturbative approach of close-coupling. The perturbative approaches are based on the expansion of the Born series or the distorted wave Born series. Examples of the perturbative methods are the eikonal series, the many-body theory, Born-Approximation and distorted wave born approximation (DWBA), While non-perturbative approaches are based on the close coupling approach that expands the test wave functions into a set of basic functions.

Semi - classical approaches borrows from both classical and quantum mechanics. Some of the examples of the methods are semi – classical impact parameter method, eikonal approximation, classical trajectory Monte Carlo method and Glauber Approximation.

In the experiment of electron atom scattering, it gives results for differential cross section (DCS). DCS are determined by considering azimuthal (ϕ) angles and the polar (θ), as illustrated by the figure 1.1 (McCarthy and Weigold, 1995). A parallel beam of single energy channel electrons of momentum $\vec{k}$ falling on target atoms. After the interaction between the incident electron and target, the incident projectile electrons were then turned away from their initial course retaining their original energy. This phenomenon describes elastic scattering.

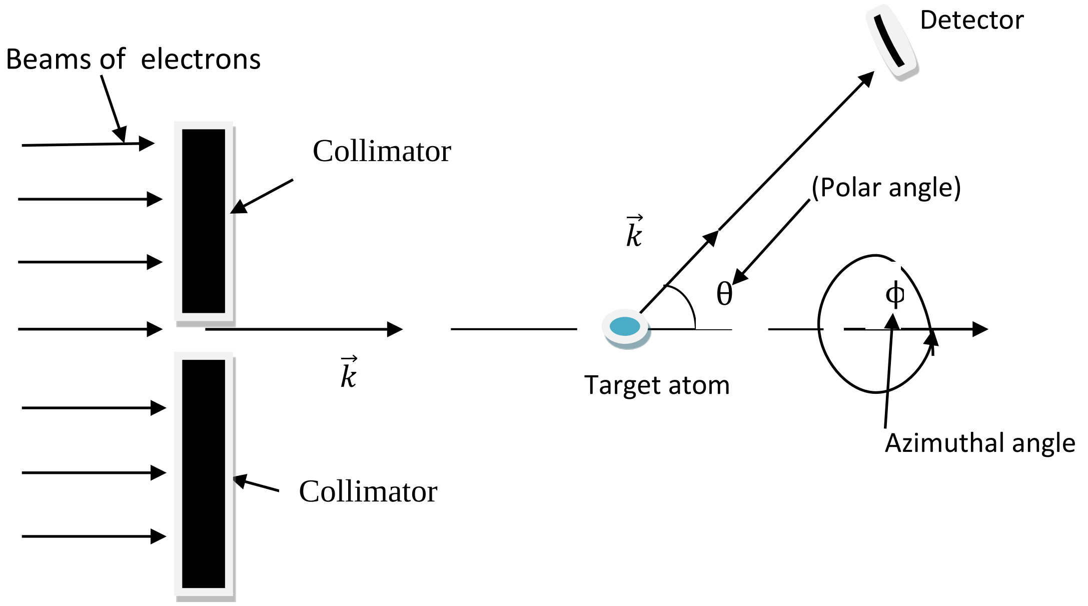

Figure 1.1: A diagram showing electron-atom scattering experiments

The azimuthal and polar angles $\emptyset$ and θ respectively defines the direction in which the projectile electrons were deflected after interaction and which also determined the differential cross sections. Differential cross sections (DCS) results were obtained from this electron-atom scattering experiments. Theoretically, the scattering problem for the wave function ψ representing the system is approached by trying to solve the Schroedinger equation of the projectile and the target and hence calculating the differential cross section. From differential cross sections, integral cross sections (ICS) may also be determined through calculation.

In the study of electron-atom scattering theory the main aim is to investigate the characteristic of electron-atom body in the asymptotic region. Many methods have been formulated for the computation of cross sections. These methods are the R-Matrix method (Burke and Berrington, 1993), the close-coupling (CC) method (McCarthy and Weigold, 1995) and the distorted-wave Born approximation (DWBA) (Joachain, 1975). R-matrix method is taken to be composed of more than one part through theory of atomic structure. In the CC approach, the wavefunction of the electron-atom system is expanded in terms of known target-atom states and unknown scattered-electron states.

Differential cross sections (DCS) in relation with integral cross sections (ICS) look at the feature of interaction potential and depends more on the target wave function and the estimated approach used in computation (Zhong *et al*., 1997). DCS for one scattering procedure if known with certainty can also be used to modify data belonging to different collisions processes (Scott and Taylor, 1979).

The first order distorted wave Born approximation method (DWBA) is the technique chosen to evaluate cross sections in this study since it is rather marked with a favorable outcome in interpreting different characteristics for an elastic process and in giving results which agreed well with other theoretical data for intermediate and high incident energy regions (Katiyar and Srivastava, 1988). This method uses an arbitrary distortion potential in the determination of distorted waves and also in the evaluation of transition matrices. Transition matrices cannot be evaluated exactly without making some approximations. The approximations made in this study range from the total wave function where only first order term has been taken, the target wave function has been approximated and is treated as two electron system. The incident and scattered electrons continuum wave functions were calculated using static potential of the target.

1.2 Statement of research problem

For the intermediate energy region both differential and integral cross section for elastic scattering of electrons for strontium have been determined using first-order distorted wave Born approximation (DWBA) method in this study.

For elastic scattering of strontium very few calculations have been performed and currently there are no known results using the present method. Also the available theoretical results do not have other results to be compared with so it makes it important to obtain results to compare them and to be compared with future experimental results.

DWBA is a perturbative method which has been marked by favorable outcome; it is used to determine both differential and integral cross sections at intermediate and high incident energies for electron-atom collisions. Hence, DWBA at intermediate energy region 10eV to 200eV for elastic scattering of electron strontium and for scattering angles from 0^o to 180^o has been used in this study.

1.3 Rationale of study

Elastic scattering of electron by a strontium atom has been studied both experimentally (Romanyuk, 1980) and theoretically (Fabrikant, 1980, Yuan and Zhang, 1990, Szmytkowski and Sienkiewicz, 1994) for low energy level below 10eV. As a result, this study of differential and integral cross sections for elastic scattering of electron strontium was calculated using distorted wave method for a range of 10-200eV in an attempt of providing result for comparing with the only available theoretical differential cross section results in the range of 10-200eV (Adibzadeh and Theosodiou, 2004) which were obtained using optical potential scattering method.

1.4 Objectives

1.4.1 General objective

The general objective was to use the distorted wave Born approximation method (DWBA) to the elastic scattering of electrons by strontium atom at intermediate energies.

1.4.2 Specific objectives

i. To develop the DWBA applied to $e-$ - Sr scattering.
ii. To make changes on the DWBA1 computer program for strontium.
iii. To determine differential cross section (DCS) and integral cross section (ICS) at impact energies 10-200eV for elastic scattering of electron-strontium.
iv. To use obtained results to do comparisons with other available results and to make judgments on the validity of DWBA for strontium.

CHAPTER TWO

LITERATURE REVIEW

2.1 Experimental studies on electron- strontium elastic scattering

From the experimental data of Romanyuk *et al.* (1980) the total cross sections for strontium at low energies of 0.2 to 10eV was obtained using electron trap method in which a collision chamber was used as a collector of scattered electrons and the entire electron optical system was placed in a parallel magnetic field required for velocity selection of the electron monochromator and for collimation of electron beam.

The electrodes, whose potentials are close to the cathode potential, were mounted at the entrance to the collision chamber and at its exit. This formed a trap for the electrons that lose some of their energy due to change of their direction as a result of collision with an atom. The scattered electrons oscillate between these electrodes along the magnetic field until they settled in the collision chamber, thus the differential cross section were measured. Romanyuk *et al.* (1980) tabulated the values of DCS from their experiments which they used atomic beam modulation at low energies of 0.2–10 eV.

2.2 Theoretical studies on electron-strontium elastic scattering

Two-state close-coupling (CC2) method was also used in calculations of DCSs of electron strontium scattering for energies below 10eV (Fabrikant, 1980). The relativistic correlation – polarization potential calculations of Yuan and Zhang (1990) are restricted to energies below 10 eV. Yuan and Zhang (1990) have also calculated the Sherman function. Three-Channel Close-Coupling Approximation calculations. Dyson's approach to the many-body theory calculations (Gribakin *et al*,1991) give results for elastic e – Sr scattering and static- exchange plus parameter correlation- polarization potential calculations (Kumar *et al*,1994). Szmytkowski and Sienkiewicz (1994) calculated differential cross sections for elastic scattering of electron strontium at lower and intermediate energies of 0.2 to 100eV using relativistic polarized orbital approximation. By solving Dirac-Hartree-Fock (DHF) equations for isolated target, a static part of the projectile target interaction potential was generated and polarization potential by solving coupled DHF equations for the target by projectile and including only the dipole term in scattering calculation for polarization potential. Kelemen *et al*. (1995) have investigated elastic scattering of electron with strontium using phenomenological complex optical potential at impact energies less than or equal to 200eV. In the polarization potential, the values of adjustable variables were found using known electron attraction to the strontium atoms. Adibzadeh and Theosodiou (2004) used the optical potential method to calculate DCS at 10-200eV.

This study of differential and integral cross sections for elastic scattering of electron strontium has not been calculated using distorted wave Born approximation (DWBA) method before, therefore this work aims to investigate the differential and integral cross sections for elastic scattering of electron strontium by applying the distorted wave Born approximation (DWBA) method.

CHAPTER THREE

THEORIES OF ATOMIC COLLISION

3.1 Introduction to Approximation Methods in Atomic Collisions

It is difficult to obtain exact results for atomic collision cross sections, in most instances the necessary atomic wave functions are not known exactly and the approximate wave functions on which we must rely are frequently not orthogonal. Evidently, as the structural complexity of the colliding atoms increases, the difficulty of obtaining good wave functions also increases and more complex reactions become possible. Calculations on molecular systems are particularly difficult. Furthermore, the structure of the equations to be solved is such that approximate methods must be used even if the necessary wave functions are completely and exactly known (McDaniel, 1989).

Approximation methods to scattering can be basically classified into quantum mechanical methods and semi-classical methods. In quantum mechanical methods, concept of quantum mechanics are used fully. They are categorized into close coupling methods and perturbative methods. Examples of perturbative methods are the distorted wave series, Coulomb Projected Born approximations and the Born series while close coupling methods include R-matrix and convergent close coupling.

In the semi-classical methods both quantum mechanics and classical mechanics are used. Examples of these methods are classical trajectory Monte Carlo method, eikonal approximation, the semi-classical impact parameter method and Glauber approximation.

3.2 Quantum Mechanical Approximations

3.2.1 The Born Approximation

In this approximation the amplitude is given as

$$f = -\frac{1}{4\pi}\left\langle \psi_{k_f} \middle| U + UG_0^+U + UG_0^+UG_0^+U + \cdots \middle| \psi_{k_i} \right\rangle \qquad (3.1)$$

where U represents the interaction potential, $\psi_{k_f}=\varphi_f.\ e^{ik_i.r}$ is the product of final target wave function and final plane wave of the projectile $\psi_{k_i} = \varphi_i.e^{ik_f.r}$ is the product of initial atomic wave function and initial plane wave of the incident particle and G_0^+ is the outgoing Green's function written as

$$G_0^+(k, r, r') = -\frac{1}{4\pi}\frac{e^{ik|r-r'|}}{|r-r'|} \qquad (3.2)$$

From equation (3.1) the Born approximation to the amplitude are given as

$$f_{B_1} = -\frac{1}{4\pi}\left\langle \psi_{k_f} \middle| U \middle| \psi_{k_i} \right\rangle \qquad (3.3)$$

$$f_{B_2} = -\frac{1}{4\pi}\left\langle \psi_{k_f} \middle| UG_0^+U \middle| \psi_{k_i} \right\rangle \qquad (3.4)$$

so $f_{B_2} = f_{B_1} + f_{B_2}$ (3.5)

up to f_{B_n} which is also obtained through the same procedure. Where f_{B_1}, f_{B_2} up to f_{B_n} is the first Born approximation, second Born approximation up to n^{th} Born approximation respectively to the scattering amplitude.

3.2.2 Coulomb Projected Born (CPB) Approximation

This method according to Geltman (1971) looks at the electron nucleus interaction term in the electron-atom scattering. In this method the total Hamiltonian (H) can be split into two parts perturbation (V) and an unperturbed part (H*o*). In the unperturbed part of the Hamiltonian a term $\frac{-1}{\mathrm{r}^2}$ is included which is the electron – nucleus interaction term, as shown below

$$H_0 = H_A - \frac{1}{2}\nabla_2^2 - \frac{1}{r^2} \tag{3.6}$$

and

$$V = r_{12} = \frac{1}{|r_1 - r_2|} \tag{3.7}$$

The transition matrix T_{if} is written as

$$T_{if} = \left\langle \psi_f \middle| \frac{1}{|r_1 - r_2|} \middle| \Psi_i^+ \right\rangle \tag{3.8}$$

where

$$\psi_f = \varphi_f(r_1)\chi_f(r_2) \tag{3.9}$$

In equation (3.9) χ_f is the coulomb wave of the projectile electron in the field of the nuclear charge of the hydrogen atom while φ_f is the final atomic wave function. The CPB approximation is obtained from (3.9) by approximating Ψ_i^+ as $exp(ik.r_2)\phi(r_1)$. Hence the contribution of the electron-nucleus interaction has been taken into account through the coulomb wave χ_f, which is in the transition matrix.

3.2.3 Convergent Close Coupling (CCC) Method

CCC is applicable at all impact energies for both elastic and inelastic scattering. This method depends mostly on close coupling to solve coupled equations with no approximations. The cross section is obtained by putting an ever increasing set of states.

Resolving target Hamiltonian in an orthogonal Laguerre basis, target states are determined for completeness to be reached as the basis size increases. In this method the distinct and continuum parts of the target are treated through close coupling to allow credibility of this method and independence of projectile energy (Fursa and Bray, 1995).

3.2.4 The Optical Model Potential Method (OMPM)

In this method elastic scattering of an atom is analyzed from a complicated target. The optical potential or pseudo potential replaces the difficult interactions for projectile and target particle in which the falling particle moves. After optical potential is calculated, the initial many body problems reduce to a single body. This potential is complex hence approximations are needed (Joachain, 1975).

3.2.5 The R-Matrix Method

The (N+1) electron-atom system arrangement is formed by two parts, inner part ($r < a$) and the other is the outer part ($r > a$). This is done by considering the displacement between the atomic nucleus and the projectile electron. There is strong interaction in the internal region and the exchange of the electron is useful. Collision in the external region is illustrated by coupled differential and exchange in this region is neglected. The linear sum of the incident and the slater orbitals, gives pseudo and target eigen states contracted in terms of rectangular orbitals which fulfill boundary specifications on the outer part of the sphere. The Hamiltonian is then diagonalized in an appropriately chosen basis in the internal region and the cross sections calculated by solving the asymptotic problem in the external region (Burke, 2011).

3.2.6 The Distorted Wave Methods (DWM)

Distorted wave method was developed as a result of failures from first Born approximation (FBA). It works well since it is one of perturbative methods, the transition between final and initial elastic state is obtained and at high and intermediate energies, DCS for electron excitation of atoms are calculated (Itikawa, 1986). The distorted wave series converges faster than in Born series. DWM is more useful in the study of atom ionization, heavy particles collision processes among heavy particles and collision of electron molecules. It is more useful in interpreting excitation processes, the consequences of certain distortion potentials (Katiyar and Srivastava, 1988).

3.2.7 Distorted Wave Formula Using Two Potential Scattering Model

Let H be the total Hamilton of the projectile electron and N-electron target atom. Then we can write

$$H = H_0 + V \tag{3.10}$$

where $$H_0 = H_a + T \tag{3.11}$$

Therefore $$H = H_a + T + V$$

where $$V = -\frac{N}{r_0} + \sum_{i=1}^{N} \frac{N}{r_{0i}} \tag{3.12}$$

where V, T and H_a, represents interaction potential, function for kinetic energy and Hamiltonian target respectively. In this case interaction potential is divided into two parts the approximate and the exact part. That is

$$V=U + W \tag{3.13}$$

It is assumed that

$$H\chi = E\chi \tag{3.14}$$

where $H = H_0 + U$, can be evaluated exactly i.e. we are able to evaluate the Lippmann- Schwinger's equation

$$\chi^{\pm} = \phi + \frac{1}{E-H_o+i\varepsilon} U\chi \tag{3.15}$$

where U is the distortion potential chosen in such a way that V - U = W, is a small perturbation and χ is the distorted wave corresponding to the free wave ϕ distorted by the availability of the distortion potential. E represents the system total energy. Where the subscripts (+) and (-) shows the outgoing and incoming wave boundary conditions respectively. For elastic scattering the transition matrix is written as

$$T_{if}=\langle\phi_f|V_f|\Psi_i^+\rangle \tag{3.16}$$

where Ψ_i^+ is the total initial wave function and fulfills the Schroedinger equation

$$H\Psi_{\mathrm{i}}^+ = E\Psi_{\mathrm{i}}^+ \tag{3.17}$$

We assume the following relationship

$$V_f = U_f + W_f \ , \quad V_i = U_i + W_i \tag{3.18}$$

so that

$$H = H_i + V_i = H_f + V_f \tag{3.19}$$

where i is initial and f is final channel. From equation (3.18), T_{if} can be written as

$$T_{if} = \langle \phi_f | U_f + W_f | \Psi_i^+ \rangle \tag{3.20}$$

Making use of the relation

$$\chi_f^- = \phi_f + \frac{1}{E + \overline{H}_f + i\varepsilon} U_f \phi_f \tag{3.21}$$

we get

$$\langle \phi_f | = \langle \chi_f^- | - \langle \phi_f | U_f \frac{1}{E_{f-}\ \overline{H}_{f+i\varepsilon}} \tag{3.22}$$

where we have taken into consideration the transition on the energy shell so that E= E_i= E_f

$$\overline{H}_f = H_o + U_f \tag{3.23}$$

Now T_{if} becomes

$$T_{if} = \langle \phi_f | U_f | \Psi_i^+ \rangle + \langle \chi_f^- | W_f | \Psi_i^+ \rangle - \left\langle \phi_f \middle| U_f \frac{1}{E_{f-\overline{H}_f+i\varepsilon}} \middle| \Psi_i^+ \right\rangle \tag{3.24}$$

The third term on the right hand side can be changed using equation below

$$|\Psi_i^+\rangle = |\phi_i\rangle + \frac{1}{E_{i-H+i\varepsilon}} V_i|\phi_i\rangle \tag{3.25}$$

Considering that on the energy shell

$$\langle\phi_f|U_f + W_f|\phi_i\rangle = \langle\phi_f|V_f|\phi_i\rangle = \langle\phi_f|V_i|\phi_i\rangle \tag{3.26}$$

so (3.24) simplifies to

$$T_{if} = \langle\chi_f^-|V_i - W_f|\phi_i\rangle + \langle\chi_f^-|W_f|\Psi_i^+\rangle \tag{3.27}$$

The relation (3.26) is the two potential formulae of Gellman and Goldberger. The relation (3.27) is simplified once we assumes $V_i = V_f = V$; $U_i = U_f = U$ and

$W_i = W_f = W$ to

$$T_{if} = \langle\chi_f^-|U|\phi_i\rangle + \langle\chi_f^-|W|\Psi_i^+\rangle \tag{3.28}$$

By using the two potential scattering models the relation (3.28) is obtained which is the distorted wave formula. Here potential U distorts the wave function. When using the distorted wave method (3.28), U has to be determined first. It is the choice of this distortion potential that brings different forms of the distorted wave approaches.

3.2.8 The Bethe-Born Approximation

Bethe, H.A. (1939) proposed a modification of the Born approximation in which he made the additional assumption that if the product of the momentum transfer and the range of interaction is small, then the exponential term in the Born approximation for scattered amplitude can be expanded and the integration carried out term by term. A series of terms corresponding to the atomic transition moments is obtained (i.e. electric dipole, electric quadrupole)

3.3 Semi Classical Approximations

3.3.1The Glauber Approximation

Glauber *et al* (1959) while seeking a high energy scattering approximation more satisfactory than the first Born approximation, proposed an Eikonal method, in which all states of the perturbation expansion were added, with the leading term being the Born approximation. The Glauber *et al* (1959) approximation was introduced for nuclear problems and was not applied to atomic collision until 1968. However, it has subsequently been used extensively in calculations on elastic and inelastic collisions of electrons with atoms and molecules, at intermediate and high energies. One of its useful features is that it satisfies the optical theorem, thereby being applicable in certain situations where the potential is large for the Born approximation to be acceptable.

3.3.2 The Eikonal approximation

When the wavelength of the projectile is little comparably with the distance through which the scattering potential varies to a noticeable degree, (Joachain, 1975), the study of a classical trajectory gets meaning. If r_0 is the extent of the potential, the condition can be stated as,

$$kr_0 \gg 1 \qquad (3.29)$$

This condition is the basis of semi-classical scattering approximations, which have been very useful for heavy particle, and also for electron, scattering. Further, if the energy of the projectile, E, is large compared with a typical value of the potential V_0, so that

$$\frac{V_0}{E} \ll 1 \qquad (3.30)$$

the Eikonal approach to scattering problems becomes feasible.

3.3.3 The Classical Trajectory Monte Carlo Method

This method provides a means of evaluating collision cross sections. The equations governing the relative motion of the collision partners are integrated step by step on a computer for a large number of different impact parameters. The final states of the particles are determined, and the outcome of the collision is recorded. A Monte Carlo method is used for random selection of the impact parameter and the relevant target parameters (such as the position and momentum of the bound electrons). Thousands of collisions are studied and cross sections are determined from the relative probabilities of the different values.

3.3.4 The Semi Classical Impact Parameter Method

Many cross section calculations on systems for which the concept of a well-defined trajectory is valid for the relative motion have been made in the impact parameter formulation. The trajectory is taken to be rectilinear, and the impact parameter plays the role of angular momentum. Quantum mechanics is used to treat the electronic motion, so the impact parameter method is semi classical. This method is most successful for high energy, heavy particle collisions and low energy transfers. An alternative approach is to integrate numerically the classical equations of motion to obtain the trajectory, or to apply classical perturbation theory to calculate it. The latter technique is applicable for large impact parameters and small energy transfers.

CHAPTER FOUR

MATERIALS AND METHODS

4.1 The distorted wave method (DWM)

There exist variants of DWM based on how the distortion for the electron wave has been introduced. The DWM was brought in due to the drawbacks experienced in the first Born approximation (FBA) (Madison and Bartschat, 1996). The FBA gave results in harmony with experimental data for the higher energies. This was realized using the plane waves for projectile electron; though it gave poor results for low impact energies and large angle differential cross sections, this necessitated the development of the Distorted Wave Method. In the DWM the plane wave is replaced by a distorted wave.

In the two – potential approach the T – matrix (as given in equation 3.28) for electron – atom (N – electron atom) scattering takes the following form (Madison and Bartschat, 1996) (where χ is replaced by the product of projectile and target wave functions and total wave function is written in antisymmetrized form)

$$T_{if} = (N+1)\left\langle \chi_f^-(0)\phi_f(1,\dots.N)\middle| V - U_f \middle| A\Psi_i^+(0,\dots N)\right\rangle$$

$$+\left\langle \chi_f^-(0)\phi_f(1,\dots N)\middle| U_f \middle| \phi_i(1,\dots N)\beta_i(0)\right\rangle \qquad (4.1)$$

where $\phi_{i,f}$ are atomic wave functions for initial and final state respectively, $\beta_i = exp(ik.r_0)$ is plane wave for an initial-state of the projectile and A is the operator for antisymmetrizing given by

$$A = \frac{1}{N+1}\left(1 - \sum_{i=1}^{N} p_{i0}\right) \qquad (4.2)$$

where p_{io} is the exchange operator between 0th and ith electron. Potential U_f is a chosen distorting potential for the projectile, needed to determine the distorted wave χ_f^- by solving the wave equation

$$\left(T + U_f - E_f\right)\chi_f^- = 0 \tag{4.3}$$

using Numerov's method (Madison and Bartschat , 1996).

T and E_f are the operator for kinetic energy of isolated projectile and the energy for final state of projectile respectively. For the total wave function Ψ_i^+ in (4.1) approximations are needed since it cannot be solved fully.

Ψ_i^+ may be written as $\psi_i.\chi_i^+$. Where ψ_i is the atomic wave function (initial) and χ_i^+ is distorted wave (initial). Then a power series expansion can be developed for the interaction, which is taken to be small. For energy E_i of the projectile electron, the initial state distorted wave is a solution of Schröedinger equation

$$(T + U_i - E_i)\chi_i^+ = 0 \tag{4.4}$$

for chosen distortion U_i which diminishes asymptotically. Lippmann – Schwinger solution for the total wave function (Ψ_i^+) in terms of χ_i^+ is written as

$$\Psi_i^+ = [1 + G^+(V - U_i)]\psi_i\chi_i^+ \tag{4.5}$$

where G^+ is given as

$$G^+ = (E - H + i\varepsilon)^{-1} \tag{4.6}$$

By putting a chosen potential U in equation (4.6), the distorted Green's function g^+ is written as

$$g^+ = (E - H_a - T - U + i\varepsilon)^{-1} \tag{4.7}$$

The total Green's function G^+ can be written using the distorted Green's function g^+ as

$$G^+ = g^+ + G^+ (V - U)\, g^+ \tag{4.8}$$

The full Green's function series expansion can be written as

$$G^+ = g^+ + G^+ (V - U)\, g^+ + G^+ (V - U)\, g^+ (V - U)\, g^+ \tag{4.9}$$

If equation (4.5) is put in (4.1) along with equation (4.9), we get

$$T_{if} = T_1 + T_2 + T_3 \ldots\ldots\ldots\ldots \tag{4.10}$$

where

$$\begin{aligned} T_1 = {} & (N+1)\langle \chi_f^-(0)\psi_f(1,\ldots N)\big|V - U_f\big|A\psi_i(1,\ldots,N)\chi_i^+(0)\rangle \\ & + \langle \chi_f^-(0)\psi_f(1,\ldots,N)\big|U_f\big|\psi_i(1,\ldots,N)\beta_i(0)\rangle \end{aligned} \tag{4.11}$$

$$T_2 = (N+1)\langle \chi_f^-(0)\psi_f(1,\ldots,N)\big|\big(V - U_f\big)Ag^+(V - U_i)\big|\psi_i(1,\ldots,N)\chi_f^+(0)\rangle \tag{4.12}$$

and

$$T_3 = (N+1)\langle \chi_f^-(0)\psi_f(1,\ldots,N)\big|\big(V - U_f\big)Ag^+(V - U)g^+(V - U_i)\big|\psi_i(1,\ldots,N)\chi_i^+(0)\rangle \tag{4.13}$$

Equation (4.10) is the distorted wave series for the T- matrix while in this study the first order distorted wave approximation (4.11) was used. Direct and exchange transition matrices were determined from (4.11), where an atom has two valence electrons for elastic scattering, we get

$$T_{if} = T^{d} - T^{ex} \tag{4.14}$$

with

$$T^{d} = \left\langle \chi_f^{-}(0)\psi_i(1,2) \middle| U_f \middle| \psi_i(1,2)\beta_i(0) \right\rangle \tag{4.15}$$

and

$$T^{ex} = -\left\langle \chi_f^{-}(0)\psi_i(1,2) \middle| V - U_f \middle| \psi_i(0,2)\chi_i^{+}(1) + \psi_i(1,0)\chi_i^{+}(2) \right\rangle \tag{4.16}$$

In elastic scattering case the terms containing distorted waves in the direct T-matrix vanishes and one gets T^{d} as given in equation (4.15). Neglecting the terms, with overlap integral between the bound and continuum states (which would be small at intermediate and high energies), we get T^{ex} as

$$T^{ex} = -\left\langle \chi_f^{-}(0)\psi_i(1,2) \middle| V \middle| \psi_i(0,2)\chi_i(1) + \psi_i(1,0)\chi_i(2) \right\rangle \tag{4.17}$$

The partial waves χ_i^{+} and χ_f^{-} are replaced in the transition matrices (4.15) and (4.17) to solve them (Madison and Bartschat (1996) and Singh (2004)).

$$|\chi_i^{+}\rangle = \sqrt{\frac{2}{\pi}}\frac{1}{k_i r}\sum_{l_i m_i} i^{li}\,\chi_{l_i}(k_i, r)Y_{l_{im_i}}(\hat{r})Y^{*}{}_{l_i m_i}\left(\hat{k}_i\right) \tag{4.18}$$

and

$$|\chi_f^-\rangle = \sqrt{\frac{2}{\pi}}\frac{1}{k_f r}\sum_{l_f m_f} i^{l f}\chi_{l_f}^*\left(k_f, r\right)Y_{l_f m_f}(\hat{r})Y_{l_f m_f}^*\left(\hat{k}_f\right) \tag{4.19}$$

where Y_{lm} is the spherical harmonic. In the expansion of χ_f^- the complex conjugate of the radial part χ_{l_f} is taken so that it satisfies the incoming wave boundary conditions. Substituting the above partial wave expansions of the distorted waves equations (4.18) and (4.19) into (4.20) and (4.21)) respectively,

$$(\nabla_0^2 + U_i - k_i^2)\chi_i^+ = 0 \tag{4.20}$$

$$\left(\nabla_0^2 + U_f - k_f^2\right)\chi_f^- = 0 \tag{4.21}$$

where $U_{i,f}$ and $k_{i,f}^2$ are in Rydberg units. The radial distorted wave is a solution of the Schroedinger equation

$$\left(\frac{d^2}{dr^2} - \frac{l_s(l_s+1)}{r^2} - U_s(r) + k_s^2\right)\chi_{l_s}(r) = 0 \tag{4.22}$$

and it is solved by using the Numerov method (Madison and Bartschat, 1996). In the asymptotic region equation (4.22) take the form

$$\lim_{r\to\infty}\chi_{l_s}(k_s, r) = j_{l_s} + B_{l_s}\left(-\eta_{l_s} + i j_{l_s}\right) \tag{4.23}$$

where η_{l_s} is irregular and j_{l_s} is regular Ricatti – Bessel functions and B_l is a complex number given as

$$\mathrm{B}_l = exp(\mathrm{i}\delta_l)\sin\delta_l \tag{4.24}$$

where δ_l is the elastic scattering phase shift.

4.2 Differential cross-section (DCS) and integral cross-section (ICS)

Differential cross section is the probability of finding scattered particles within a given solid angle, determined by the formula

$$\frac{d\sigma}{d\Omega} = 4\pi^4 \frac{k_f}{k_i} [|T^d - T^{ex}|^2] \qquad (4.25)$$

By finding the integral of the differential cross section, integral cross section can be determined as

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \frac{d\sigma}{d\Omega} = 2\pi \int_0^{\pi} \sin\theta \frac{d\sigma}{d\Omega} \qquad (4.26)$$

4.3 Evaluation of Static Potentials

Even if the selection of the distortion potential is subject to individual discretion, the most used selection is the static potential at initial or final state, or both used together (Madison and Bartchat, 1996; Itikawa, 1986). It may also include polarization potential, absorption potential and exchange potential, in order to take account of polarization effects of the incident electron, absorption of particles and exchange effects from the incident channel respectively. Since it is the elastic scattering problem being considered, both static potential and distortion potential are equal ($U_i = U_f$).

$$U_i = U_f = \langle \phi_i | V | \phi_i \rangle \qquad (4.27)$$

The interaction potential (V)

$$V = -\frac{N}{r_o} + \sum_{i=1}^{N} \frac{1}{r_{oi}} \qquad (4.28)$$

where r_0 is the projectile electron atom and r_{0i} is the distance between the projectile and the i$^{\text{th}}$ atomic electron. Since the target atom is being considered as two-electron atom, in the above relation N = 2 for the present case. The relation of the static potentials is given as

$$U_s = \langle \psi_s | V | \psi_s \rangle \tag{4.29}$$

where ψ_s is the final or initial state target wave function and V is the interaction between the target and the projectile. For the target states Hartee- Fock wave functions from Clementi and Roetti (1974) have been used. In these wave functions ψ_s is summed over Slater type orbitals of the basis set as

$$|\psi_s\rangle = \sum_n C_n |\phi_n\rangle \tag{4.30}$$

and

$$\langle \psi_s | = \sum C_{n'}^{*} \langle \phi_{n'} | \tag{4.31}$$

Values of C_n represent the expansion coefficients and ϕ_n are the Slater type orbitals of the basis set. Using equation (4.30) and (4.31) in equation (4.29), the distortion potential can be written as

$$U_s = \sum_n \sum_{n'} C_n C_{n'}^{*} \left\langle \phi_{n'} \middle| V \middle| \phi_n \right\rangle \tag{4.32}$$

$$V = -\frac{2}{r_0} + \sum_{i=1}^{2} \frac{1}{r_{0i}} \tag{4.33}$$

When two electrons atom is considered

$$V = -\frac{2}{r_0} + \frac{1}{r_{01}} + \frac{1}{r_{02}} \tag{4.34}$$

The electron interaction potential $\frac{1}{r_{01}}$ is expanded in terms of spherical harmonics $Y_{lm's}$ as

$$\frac{1}{r_{01}} = \sum\sum \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_{l,m}(r_0) Y_{l,m}^*(r_1) \tag{4.35}$$

where r lesser ($r_<$) or r greater ($r_>$) of r_0 and r_1. In the calculation, the interaction potential (V) have nuclear part on the right hand side of equation (4.34) plus the monopole term ($l = 0$) of the summation of equation (4.35). Because of the effects of the terms that are not spherical is negligible (Madison *et* al., 1996).

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \tag{4.36}$$

In Rydberg units the static potential is given as

$$U_s = 2\sum\sum C_n C_{n'}^* \left\langle \phi_{n'} \middle| \frac{2}{r_>} - \frac{2}{r_0} \middle| \phi_{n'} \right\rangle$$

$$U_s = 4\sum\sum C_n C_{n'}^* \left\langle \phi_{n'} \middle| \frac{1}{r_>} - \frac{1}{r_0} \middle| \phi_{n'} \right\rangle \tag{4.37}$$

The radial wave functions and spherical harmonics Y_{lm} their product gives the slates type orbitals (Clementi and Roetti, 1974) written as

$$\phi_n = N_n r^{\mu_n - 1} \exp(-\xi_n r) Y_{l,m}(\hat{r}) \tag{4.38}$$

where ζ, N_n and μ_n is a constant, factor of normalization and principal quantum number respectively of the n^{th} orbital of the basis set. Where N_n is written as

$$N_n = \frac{(2\xi_n)^{\mu_n + \frac{1}{2}}}{\sqrt{(2\mu_n)!}} \tag{4.39}$$

Substituting the wave function in equation (4.38) putting standard integral to replace Bra and Ket notation, this gives a fully extended static potential as shown

$$U_s = 4\sum_{nlm}\sum_{n'l'm'} C_n C_n^* N_n N_{n'}^* \int_{r_0}^{\infty} r^{\left(\mu_n + \mu_{n'}\right)} \left(\frac{1}{r} - \frac{1}{r_0}\right) exp\left(-\left[\xi_n + \xi_{n'}\right] r_1\right) dr \int Y_{l,m}(r_0) Y_{l'm'}(r) d\Omega \tag{4.40}$$

In equation (4.40) above, partial integration from radial distance 0 to r_0, r_0 is taken to be larger than r and from r_0 to ∞, r is taken to be larger than r_0. The right hand side of equation (4.40) vanishes as a result of spherical harmonics being orthonormal unless $l = l'$ and $m = m'$.

Resulting to

$$U_s = 4\sum_n \sum_{n'} C_n C_{n'}^* N_n N_{n'}^* \int_{r_0}^{\infty} r^{\mu_n + \mu_{n'}} \left(\frac{1}{r} - \frac{1}{r_0}\right) exp(-kr) dr \tag{4.41}$$

where k $= \left[\xi_n + \xi_{n'}\right]$

In this study, the exact static potentials were obtained by solving this integral in order to get the distortion potentials. The total static potential is the addition of elements in $n \times n'$ matrix.

The solutions the equation (4.41) changes according to the sum of the principal quantum numbers μ_n *and* $\mu_{n'}$. This sum changes from (4.50) to (4.58) for the problem that was determined as follows.

The following procedure was followed to determine distortion potential

For r^2
$$v_{ii} = \left\langle \psi_0(\bar{r}_1)\psi_0(\bar{r}_2) \middle| \frac{2}{r_{02}} + \frac{2}{r_{01}} - \frac{4}{r_0} \middle| \psi_0(\bar{r}_1)\psi_0(\bar{r}_2) \right\rangle \tag{4.42}$$

The term associated with $\frac{2}{r_{01}}$ gave

$$\left\langle \psi_0(\bar{r}_1) \middle| \frac{2}{r_{01}} \middle| \psi_0(\bar{r}_1) \right\rangle \tag{4.43}$$

The term associated with $\frac{2}{r_{02}}$ gave

$$\left\langle \psi_0(\bar{r}_2) \middle| \frac{2}{r_{02}} \middle| \psi_0(\bar{r}_2) \right\rangle \tag{4.44}$$

and the term associated $\frac{-4}{r_0}$ gave

$$\left\langle \psi_0(\bar{r}_1)\psi_0(\bar{r}_2) \middle| -\frac{4}{r_0} \middle| \psi_0(\bar{r}_1)\psi_0(\bar{r}_2) \right\rangle = \left\langle \psi_0(\bar{r}_1) \middle| -\frac{4}{r_0} \middle| \psi_0(\bar{r}_1) \right\rangle \tag{4.45}$$

in Rydberg units.

Combining (4.43), (4.44), and (4.45), we get

$$\int_0^\infty R^2 \left(\frac{4}{r_>} - \frac{4}{r_0}\right) r^2 dr = 4\left(\int_0^{r_0} R^2 \left(\frac{1}{r_0} - \frac{1}{r_0}\right) r^2 dr + \int_{r_0}^\infty R^2 \left(\frac{1}{r} - \frac{1}{r_0}\right) r^2 \mathrm{dr}\right) \tag{4.46}$$

where R is the radial part of $\psi_0(\bar{r}_1)$. The first term will become zero and the other one is separated to give

$$\int_{r_0}^{\infty} e^{-kr}\left(\frac{1}{r}-\frac{1}{r_0}\right) r^2 dr = \int_{r_0}^{\infty}\exp(-kr) r^2 \frac{1}{r} dr - \int_{r_0}^{\infty}\exp(-kr)\, r^2 \frac{1}{r_0} dr$$

$$=\int_{r_0}^{\infty}\exp(-kr) r dr - \frac{1}{r_0}\int_{r_0}^{\infty}\exp(-kr) r^2 dr \qquad (4.47)$$

Considering the first term of equation (4.47) above

$$\int_{r_0}^{\infty}\exp(-kr) r\, dr = -\frac{1}{k}\exp(-kr)\, r|_{r_0}^{\infty} + \left[\frac{1}{k}\int_{r_0}^{\infty}\exp(-kr)\, dr\right]$$

$$= \frac{1}{k}\exp(-kr_0)\, r_0 - \frac{1}{k^2}[\exp(-kr]_{r_0}^{\infty}$$

$$=\frac{1}{k} exp(-kr_0) + \frac{1}{k^2}\exp(-kr_0) \qquad (4.48)$$

Now considering the second term of equation (4.47) it can be seen that

$$\frac{1}{r_0}\int_{r_0}^{\infty} exp(-kr) r^2 dr = \frac{1}{r_0}(-\frac{1}{k} exp(-kr) r^2 |_{r_0}^{\infty} + \frac{2}{k}\int_{r_0}^{\infty} exp(-kr) r dr)$$

$$=\frac{1}{r_0}(\frac{1}{k} exp(-kr_0) r_0^2 + \frac{2}{k}\left[\frac{1}{k} exp(-kr_0) r_0 + \frac{1}{k^2} exp(-kr_0)\right])$$

$$= \frac{1}{r_0}(\frac{1}{k} exp(-kr_0) r_0^2 + \frac{2}{k^2} exp(-kr_0) r_0 + \frac{2}{k^3} exp(-kr_0))$$

$$=(\frac{1}{k} exp(-kr_0) r_0 + \frac{2}{k^2} exp(-kr_0) + \frac{2}{k^3} exp(-kr_0) \qquad (4.49)$$

Therefore using equation (4.48) and (4.49) leads to

$$\int_{r_0}^{\infty} exp(-kr)\left(\frac{1}{r}-\frac{1}{r_0}\right) r^2 dr = -exp(-kr_0)\left[\frac{1}{k^2}(2-1) + \frac{1}{k^3 r_0}(2.1)\right]$$

$$=-exp(-kr_o)\left[\frac{1}{k^2}+\frac{2}{k^3 r_0}\right] \qquad (4.50)$$

This is converted to computer code using fortran language as:

```
19 POT=POT+ANCO*(-EXP (-SETA*R)*(1./SETA**2+2./ (SETA**3*R)))
```

Similarly

For r^3

$$\int_{r_0}^{\infty} \exp(-kr)\left(\frac{1}{r}-\frac{1}{r_0}\right) r^3 dr = -exp(-kr_0)\left[\frac{r_0}{k^2}(3-2)+\frac{1}{k^3}(3.2-2.1)+\frac{1}{k^4 r_0}(3.2.1)\right]$$

$$= -exp(-kr_0)\left[\frac{r_0}{k^2}+\frac{4}{k^3}+\frac{6}{k^4 r_0}\right] \qquad (4.51)$$

This is converted to computer code using fortran language as:

```
29 POT=POT+ANCO*(-EXP (-SETA*R)*(R/SETA**2+4./SETA**3+
+6. / (SETA**4*R)))
```

For r^4

$$\int_{r_0}^{\infty} exp(-kr)\left(\frac{1}{r}-\frac{1}{r_0}\right) r^4 dr = -exp(-kr_0)\left[\frac{r_0^2}{k^2}(4-3)+\frac{r_0}{k^3}(4.3-3.2)+\frac{1}{k^4}(4.3.2-3.2.1)+\frac{1}{k^5 r_0}(4.3.2.1)\right]$$

$$= -exp(-kr_0)\left[\frac{r_0^2}{k^2}+\frac{6r_0}{k^3}+\frac{18}{k^4}+\frac{24}{k^5 r_0}\right] \qquad (4.52)$$

This is converted to computer code using fortran language as:

```
39 POT=POT+ANCO*(-EXP (-SETA*R)*(R*R/SETA**2+6*R/SETA**3+
+18./SETA**4+24./ (SETA**5*R)))
```

For r^5

$$\int_{r_0}^{\infty} exp(-kr)\left(\frac{1}{r}-\frac{1}{r_0}\right)r^5dr = \qquad -exp(-kr_0)\left[\frac{r_0^3}{k^2}(5-4)+\frac{r_0^2}{k^3}(5.4-4.3)+\right.$$

$$\left.\frac{r_0}{k^4}(5.4.3.-4.3.2.)+\frac{1}{k^5r_0}(4.3.2.1)\right]$$

$$=-exp(-kr_0)\left[\frac{r_0^3}{k^2}+\frac{8r_0^2}{k^3}+\frac{36r_0}{k^4}+\frac{96}{k^5}+\frac{120}{k^6r_0}\right] \qquad (4.53)$$

This is converted to computer code using fortran language as:

```
49 POT=POT+ANCO*(-EXP (-SETA*R)*(R3/SETA**2+8*R*R/SETA**3+
     36*R/SETA**4+96./SETA**5+120./ (SETA**6*R)))
```

For r^6

$$\int_{r_0}^{\infty} exp(-kr)\left(\frac{1}{r}-\frac{1}{r_0}\right)r^6dr=$$

$$-exp(-kr_0)\left[\frac{r_0^4}{k^2}(6-5)+\frac{r_0^3}{k^3}(6.5-5.4)+\frac{r_0^2}{k^4}(6.5.4-5.4.3)\right.$$
$$+\frac{r_0}{k^5}(6.5.4.3-5.4.3.2)+\frac{1}{k^6}(6.5.4.3.2-5.4.3.2.1)$$
$$\left.+\frac{1}{k^7r_0}(6.5.4.3.2.1)\right]$$

$$=-exp(-kr_0)\left[\frac{r_0^4}{k^2}+\frac{1or_0^3}{k^3}+\frac{60r_0^2}{k^4}+\frac{240r_0}{k^5}+\frac{600}{k^6}+\frac{720}{k^7r_0}\right] \qquad (4.54)$$

This is converted to computer code using fortran language as:

```
59 POT=POT+ANCO*(-EXP (-SETA*R)*(R4/SETA**2+10*R3/SETA**3+

    + 60*R*R/SETA**4+240*R/SETA**5+600./SETA**6+720./ (SETA**7*R)))
```

For r^7

$$\int_{r_0}^{\infty} exp(-kr)\left(\frac{1}{r}-\frac{1}{r_0}\right)r^7 dr =$$

$$-exp(-kr_0)\left[\frac{r_0^5}{k^2}(7-6)+\frac{r_0^4}{k^3}(7.6-6.5)+\frac{r_0^3}{k^4}(7.6.5-6.5.4)\right.$$
$$+\frac{r_0^2}{k^5}(7.6.5.4-6.5.4.3)+\frac{r_0}{k^6}(7.6.5.4.3-6.5.4.3.2)$$
$$\left.+\frac{1}{k^7}(7.6.5.4.3.2-6.5.4.3.2.1)+\frac{1}{k^8 r_0}(7.6.5.4.3.2.1)\right]$$

$$= -exp(-kr_o)\left[\frac{r_0^5}{k^2}+\frac{12r_0^4}{k^3}+\frac{90r_0^3}{k^4}+\frac{480r_0^2}{k^5}+\frac{1800r_0}{k^6}+\frac{4320}{k^7}+\frac{5040}{k^8 r_0}\right] \qquad (4.55)$$

This is converted to computer code using fortran language as:

```
69 POT=POT+ANCO*(-EXP (-SETA*R)*(R5/SETA**2+12*R4/SETA**3+

90*R3/SETA**4+480*R*R/SETA**5+1800*R/SETA**6+4320./SETA**7+5040./
(SETA**8*R)))
```

For r^8

$$\int_{r_0}^{\infty} exp(-kr)\left(\frac{1}{r}-\frac{1}{r_0}\right)r^8 dr =$$

$$-exp(-kr_0)\left[\frac{r_0^6}{k^2}(8-7)+\frac{r_0^5}{k^3}(8.7-7.6)+\frac{r_0^4}{k^4}(8.7.6-7.6.5)\right.$$
$$+\frac{r_0^3}{k^5}(8.7.6.5-7.6.5.4)+\frac{r_0^2}{k^6}(8.7.6.5.4-7.6.5.4.3)$$
$$+\frac{r_0}{k^7}(8.7.6.5.4.3-7.6.5.4.3.2)+\frac{1}{k^8}(8.7.6.5.4.3.2-7.6.5.4.3.2.1)$$
$$\left.+\frac{1}{k^9 r_0}(8.7.6.5.4.3.2.1)\right]$$

$$= -exp(-kr_0)\left[\frac{r_0^6}{k^2} + \frac{14r_0^5}{k^3} + \frac{126r_0^4}{k^4} + \frac{840r_0^3}{k^5} + \frac{4200r_0^2}{k^6} + \frac{15120r_0}{k^7} + \frac{35280}{k^8} + \frac{40320}{k^9 r_0}\right] \tag{4.56}$$

This is converted to computer code using fortran language as:

```
79 POT=POT+ANCO*(-EXP (-SETA*R)*(R6/SETA**2+14*R5/SETA**3+
126*R4/SETA**4+840*R3/SETA**5+4200*R*R/SETA**6+15120*R/SETA**7+352
80./SETA**8+40320./ (SETA**9*R)))
```

For r^9

$$\int_{r_0}^{\infty} exp(-kr)\left(\frac{1}{r} - \frac{1}{r_0}\right) r^9 dr =$$

$$-exp(-kr_0)\left[\frac{r_0^7}{k^2}(9-8) + \frac{r_0^6}{k^3}(9.8-8.7) + \frac{r_0^5}{k^4}(9.8.7-8.7.6)\right.$$

$$+ \frac{r_0^4}{k^5}(9.8.7.6-8.7.6.5) + \frac{r_0^3}{k^6}(9.8.7.6.5-8.7.6.5.4)$$

$$+ \frac{r_0^2}{k^7}(9.8.7.6.5.4-8.7.6.5.4.3) + \frac{r_0}{k^8}(9.8.7.6.5.4.3-8.7.6.5.4.3.2)$$

$$\left. + \frac{1}{k^9}(9.8.7.6.5.4.3.2-8.7.6.5.4.3.2.1) + \frac{1}{k^{10}r_0}(9.8.7.6.5.4.3.2.1)\right]$$

$$= -exp(-kr_0)\left[\frac{r_0^7}{k^2} + \frac{16r_0^6}{k^3} + \frac{168r_0^5}{k^4} + \frac{1{,}344r_0^4}{k^5} + \frac{8{,}400r_0^3}{k^6} + \frac{40{,}320r_0^2}{k^7} + \frac{141{,}120r_o}{k^8} +\right.$$

$$\left.\frac{322{,}560}{k^9} + \frac{362{,}880}{k^{10}r_0}\right] \tag{4.57}$$

This is converted to computer code using fortran language as:

```
89 POT=POT+ANCO*(-EXP (-SETA*R)*(R7/SETA**2+16*R6/SETA**3+
```

```
168*R5/SETA**4+1344*R4/SETA**5+8400*R3/SETA**6+40320*R*R/SETA**7+1
41120*R/ SETA**8+322560./SETA**9+362880./ (SETA**10*R)))
```

And finally

For r^{10}

$$\int_{r_0}^{\infty} \exp(-kr)\left(\frac{1}{r}-\frac{1}{r_0}\right) r^{10} dr =$$

$$\begin{aligned}
-\exp(-kr_0)\Bigg[&\frac{r_0^8}{k^2}(10-9)+\frac{r_0^7}{k^3}(10.9-9.8)+\frac{r_0^6}{k^4}(10.9.8-9.8.7)\\
&+\frac{r_0^5}{k^5}(10.9.8.7-9.8.7.6)+\frac{r_0^4}{k^6}(10.9.8.7.6-9.8.7.6.5)\\
&+\frac{r_0^3}{k^7}(10.9.8.7.6.5-9.8.7.6.5.4)+\frac{r_0^2}{k^8}(10.9.8.7.6.5.4-9.8.7.6.5.4.3)\\
&+\frac{r_0^1}{k^9}(10.9.8.7.6.5.4.3-9.8.7.6.5.4.3.2)\\
&+\frac{1}{k^{10}}(10.9.8.7.6.5.4.3.2-9.8.7.6.5.4.3.2.1)\\
&+\frac{1}{k^{11}r_0}(10.9.8.7.6.5.4.3.2.1)\Bigg]
\end{aligned}$$

$$= -exp(-kr_0)\left[\frac{r_0^8}{k^2}+\frac{18r_0^7}{k^3}+\frac{216r_0^6}{k^4}+\frac{2{,}016r_0^5}{k^5}+\frac{15{,}120r_0^4}{k^6}+\frac{90{,}720r_0^3}{k^7}+\frac{423{,}360r_0^2}{k^8}+\right.$$
$$\left.\frac{1{,}451{,}520r_o}{k^9}+\frac{3{,}265920}{k^{10}}+\frac{3{,}628{,}800}{k^{11}r_0}\right] \qquad (4.58)$$

This is converted to computer code using fortran language as:

```
99 POT=POT+ANCO*(-EXP (-SETA*R)*(R8/SETA**2+18*R7/SETA**3+
```

```
216*R6/SETA**4+2016*R5/SETA**5+15120*R4/SETA**6+90720*R3/SETA**7+4
23360*R*R/SETA**8+1451520*R/SETA**9+3265920./SETA**10
+3628800./(SETA**11*R)))
```

The values of $C_n, \xi_n,\ \mu_n$ and ANCO$_i$ are determined from from Clementi and Roetti (1974) table. This helped to make changes on computer program which develop the needed static potential.

The normalization factor N and the expansion coefficient C are the values that makes ANCO$_i$ and all is from Clementi and Roetti (1974) tables.

4.4 ANCO values for the distortion potential elements 5s state

For term with r^2

ANCO $= N_1C_1 * N_1C_1 + 2N_1C_1 * N_2C_2 + N_2C_2 * N_2C_2$

For term with r^3

ANCO $= 2N_1C_1 * N_3C_3 + 2N_1C_1 * N_4C_4 + 2N_2C_2 * N_3C_3 + 2N_2C_2 * N_4C_4$

For the term with r^4

ANCO $= 2N_1C_1 * N_5C_5 + 2N_1C_1 * N_6C_6 + 2N_2C_2 * N_5C_5 + 2N_2C_2 * N_6C_6 + N_3C_3 * N_3C_3 + 2N_3C_3 * N_4C_4 + N_4C_4 * N_4C_4$

For term with r^5

ANCO $= 2N_1C_1 * N_7C_7 + 2N_1C_1 * N_8C_8 + 2N_2C_2 * N_7C_7 + 2N_2C_2 * N_8C_8 + 2N_3C_3 * N_5C_5 + 2N_3C_3 * N_6C_6 + 2N_4C_4 * N_5C_5 + 2N_4C_4 * N_6C_6$

For term with r^6

ANCO = $2N_1C_1 * N_9C_9 + 2N_1C_1 * N_{10}C_{10} + 2N_2C_2 * N_9C_9 + 2N_2C_2 * N_{10}C_{10} + 2N_3C_3 * N_7C_7 + 2N_3C_3 * N_8C_8 + 2N_4C_4 * N_7C_7 + 2N_4C_4 * N_8C_8 + N_5C_5 * N_5C_5 + 2N_5C_5 * N_6C_6 + N_6C_6 * N_6C_6$

For term with r^7

ANCO = $2N_3C_3 * N_9C_9 + 2N_3C_3 * N_{10}C_{10} + 2N_4C_4 * N_9C_9 + 2N_4C_4 * N_{10}N_{10} + 2N_5C_5 * N_7C_7 + 2N_5C_5 * N_8C_8 + 2N_6C_6 * N_7C_7 + 2N_6C_6 * N_8C_8$

For the term with r^8
ANCO = $2N_5C_5 * N_9C_9 + 2N_5C_5 * N_{10}C_{10} + 2N_6C_6 * N_9C_9 + 2N_6C_6 * N_{10}C_{10} + N_7C_7 * N_7C_7 + 2N_7C_7 * N_8C_8 + N_8C_8 * N_8C_8$

For the term with r^9

ANCO = $2N_7C_7 * N_9C_9 + 2N_7C_7 * N_{10}C_{10} + 2N_8C_8 * N_9C_9 + 2N_8C_8 * N_{10}C_{10}$

For the term with r^{10}

ANCO = $N_9C_9 * N_9C_9 + 2N_9C_9 * N_{10}C_{10} + N_{10}C_{10} * N_{10}C_{10}$

All static potential elements are summed up to get V_s (the static potential for initial, $s=i$ and final, s=f states). The distortion potential elements were fed into the DWBA1 computer code by making modifications in the relevant subroutine.

4.5 Computer Program DWBA1

Table 4.1: Input file for e-Sr scattering at 200 eV

```
1,0,1,0,200,                   NI LI NF LF ENERGY
 -1,1                          PROJECTILE CHARGE, TARGET CHARGE
 1, 0                           INIT. STATE STAT. POT. (N L; 0, 0 = PLANE WAVE)
 1, 0                          FINAL STATE STAT. POT. (N L; 0,0 = PLANE WAVE)
 1.E-6,1.E-6,1.E-4,1.E-4      WF ZERO, FORM RATIO ZERO, EXCHANGE RATIO ZERO
 6,15,20,25,55,60,65           # PRINT FLAGS,  PRINT FLAGS
 0,0,0,0,0,16                 TAPE UNITS FOR INPUT AND OUTPUT
 10                           NN
39.13040,27.02730,18.76380,15.79910,9.60271,7.18092,4.16121,2.82050,1.63036,0.96129
                                ZETA
0.00051, 0.01860, 0.02762,-0.09189,0.02284,0.12416,-0.19858,-0.11545,0.50870,0.60912
                               COEFFICIENT
 35,70                          JFIT,JFSTOP
```

4.6 Atomic Wave Functions

Roothan Hartree Fock (RHF) atomic wave function have been used obtained from Clementi and Roetti (1974) table in which the radial orbital $P_{n_a l_a}(r)$ are expressed as,

$$P_{n_a l_a}(r) = \sum_{j=1}^{k} C_{jn_{al_a}} f_{jn_a l_a}(r) \qquad (4.59)$$

where $f_{jn_a l_a}(r)$ are normalized Slater- Type Orbitals (STOs).

The full wave function is written as

$$\psi^n = A\left(\phi_1^{(1)} \ldots . \phi_n^{(n)}\right) \tag{4.60}$$

where ϕ_i^i represent spin orbital, n represent total number of electrons and A represent antisymmetrizing operator, assumption is made that they are all mutually perpendicular.

The orbital $\Phi_{i\eta\gamma}$is written as

$$\Phi_{i\eta\gamma} = \sum_p \chi_{p\eta\gamma}\, C_{i\eta p} \tag{4.61}$$

where $\chi_{p\eta\gamma}$ is the basis functions, p is basis function with correspondence to η and C is constant of expansion.

The $\chi_{p\eta\gamma}$ is the basis functions given as

$$\chi_{p\eta\gamma}(r,\theta,\phi) = R_{\eta p}(r) Y_{\eta\gamma}(\theta,\phi) \tag{4.62}$$

The radial part is written as;

$$R_{\eta p}(r) = N r^{n_{\eta p}-1} e^{-\xi_{\eta p} r} \tag{4.63}$$

The factor of normalization N is given as

$$N = \left((2n)!\right)^{-\frac{1}{2}} \left(2\xi_{\eta p}\right)^{n+\frac{1}{2}} \tag{4.64}$$

where ξ is orbital exponent zeta , n is the principal quantum number and $Y_{\eta\gamma}(\theta,\phi)$ represents normalized complex spherical harmonics. $\mu_{\eta p} \geq \eta + 1$ and $\xi_{\eta p}$ is selected in order to deliver good energy by hard process of optimization (Clementi and Roetti, 1974).

Table 4.2: Values from K(2)L(8)M(18)4S(2)4P(6)5S(2),1S of strontium.

T.E. = -0.313146552D+04, P.E. = -0.626306960D+04, K.E.= 0.3136044D+04,

V.T.=-0.19999556D+01 in atomic units.

Orbital (n)	Zeta ($\xi_{\eta p}$)	5s
1s	39.13040	0.00051
1s	27.02730	0.01860
2s	18.76380	0.02762
2s	15.79910	-0.09189
3s	9.60271	0.02284
3s	7.18092	0.12416
4s	4.16121	-0.19858
4s	2.82050	-0.11545
5s	1.63036	0.50870
5s	0.96129	0.60912

The double- zeta type wave functions for strontium are given as:

$$\phi(5s) = \sum_{p} C_f \phi_f$$

$$\begin{aligned}\phi(5s) = {} & 0.00051\phi_1 + 0.01860\phi_2 + 0.02762\phi_3 - 0.09189\phi_4 + 0.02284\phi_5 \\ & + 0.12416\phi_6 - 0.19858\phi_7 - 0.11545\phi_8 + 0.50870\phi_9 \\ & + 0.60912\phi_{10}\end{aligned}$$

changed in computer code using fortran language as

```
UK=UK+COEFF(I)*PHI(I)
```

where

$$\phi_1 = N_1 r^0(-39.13040)Y_{0,0}(\theta,\phi) \qquad (4.65)$$

$$\phi_2 = N_2 r^0(-27.02730)Y_{0,0}(\theta,\phi) \qquad (4.66)$$

$$\phi_3 = N_3 r^1(-18.76380)Y_{0,0}(\theta,\phi) \qquad (4.67)$$

$$\phi_4 = N_4 r^1(-15.79910)Y_{0,0}(\theta,\phi) \qquad (4.68)$$

$$\phi_5 = N_5 r^2(-9.60271)Y_{0,0}(\theta,\phi) \qquad (4.69)$$

$$\phi_6 = N_6 r^2(-7.18092)Y_{0,0}(\theta,\phi) \qquad (4.70)$$

$$\phi_7 = N_7 r^3(-4.16121)Y_{0,0}(\theta,\phi) \qquad (4.71)$$

$$\phi_8 = N_8 r^3(-2.82056)Y_{0,0}(\theta,\phi) \qquad (4.72)$$

$$\phi_9 = N_9 r^4(-1.63036)Y_{0,0}(\theta,\phi) \qquad (4.73)$$

$$\phi_{10} = N_{10} r^4(-0.96129)Y_{0,0}(\theta,\phi) \qquad (4.74)$$

converted in computer code using fortran language as

```
PHI(I)=AN(I)*X**K*EXP(-ZETA(I)*X
```

and the factors for normalization are written as in equation (4.64) where n is principal quantum number $and\ \xi_n$ is orbital exponents and are written as given in ANCO values for the distortion potential elements 5s state above.

In computer code using fortran language is written as

```
AN(I)=(TWO*ZETA(I)**A/SQRT(REAL(IFAC(2*K))
```

Wave function of double zeta is obtained by adding all the basis functions from Clementi and Roetti table for the radial part. These are based on Roothan – Hartee – Focks (RHF) expansion technique.

4.7 Normalization

For normalization, the equation below must hold

$$\int \psi\psi^* \, d\tau = 1 \tag{4.75}$$

However

$$\int \psi\psi^* \, d\tau = C_1^2 + C_2^2 + C_3^2 + \cdots = k \tag{4.76}$$

where C_i is constant of expansion.

Then we performed the following operation to achieve normalization. Divide the final potent calculation by the factor k, i.e.$\frac{1}{K}$ potent and subsequently divide the atomic wave function [UU(J)] by the square root of k i.e. UU(J) / SQRT (k). Where UU(J) is the wave function.

4.8 Computer code

The computer code DWBA1 for electron-hydrogen scattering written by Madison and Bartschat (1996) was modified to fit the problem of electron-strontium scattering. The areas modified include: Main program-where the sections dealing with the input data, transition matrix, and distortion potential sections were modified to fit our problem. The Subroutine FHYD dealt with atomic wave functions. The hydrogen atom wave functions were replaced by strontium atom wave functions. The subroutine

EXCHANGE dealt with evaluation of the exchange transition matrix and the subroutine POTENT for static potentials. The coefficients fixed in the subroutines were obtained from Clementi and Roetti (1974) for strontium and also they were used to construct the wave functions which were used to formulate distortion potential. The subroutine DW was used to solve radial equations solved using Numerov method. Origin pro 7 was used to analysis the data and representing the data graphically. It is from these graphical results that useful conclusions were made.

CHAPTER FIVE

RESULTS DISCUSSIONS

5.1 Introduction

At intermediate energies differential cross section results for elastic scattering of electron by strontium have been obtained in this study and these will be discussed in part 5.2. At the impact energies 10, 20, 30, 40, 50, 70, 80, 100 and 200eV, differential cross sections (DCS) results are calculated and tabulated as shown in table 5.1. The integral cross section results obtained by DWBA are represented and comparisons done with the only available theoretical results by Adibzadeh and Theosodiou (2004). There are no experimental DCS results to be compared with.

5.2 Differential cross sections

At 10, 20, 30, 40, 50, 70, 80, 100 and 200 eV differential cross section (DCS) are calculated using DWBA by a strontium atom with scattering angles ranging from 0° to 180° and present results tabulated in table 5.1 below and plotted as shown in figures 5.1 to 5.9 and comparing it with calculated results of Adibzadeh and Theosodiou (2004), which is the only available differential cross section result for e-Sr elastic scattering.

Table 5.1: Differential cross sections calculated for the elastic scattering of electrons from strontium atom (in units of a_0^2/sr).

	DIFFERNTIAL CROSS SECTION WITH RESPECTIVE SCATTERING ENERGY (eV)								
Energy / **Angles**	**10**	**20**	**30**	**40**	**50**	**70**	**80**	**100**	**200**
0	123.67	73.708	61.261	56.214	54.282	54.174	54.852	56.732	66.265
10	107.89	59.219	46.15	39.996	36.677	33.274	32.234	30.629	24.945
20	72.224	31.725	21.12	16.2	13.489	10.658	9.8148	8.631	5.8512
30	37.93	12.11	6.616	4.6074	3.7772	3.2452	3.1588	3.0582	2.4922
40	16.055	3.1956	1.3273	1.0488	1.146	1.436	1.5284	1.6096	1.3
50	5.5058	0.36419	0.2589	0.5564	0.8083	1.0467	1.0741	1.0425	0.6619
60	1.4726	0.20237	0.7185	0.9844	1.0631	0.9836	0.9071	0.7522	0.3376
70	0.40902	0.92357	1.4283	1.4286	1.2707	0.9195	0.7772	0.5687	0.2217
80	0.47903	1.5992	1.7952	1.5309	1.2115	0.745	0.5992	0.4188	0.2181
90	0.826	1.8222	1.6644	1.2461	0.8860	0.4742	0.3739	0.2781	0.2458
100	1.0732	1.5603	1.1606	0.7341	0.4431	0.1960	0.1625	0.1623	0.2556
110	1.1264	1.0094	0.5569	0.2485	0.0918	0.0333	0.0545	0.1155	0.2345
120	1.0677	0.44478	0.1406	0.0337	0.0234	0.0938	0.1318	0.1861	0.1965
125	1.0414	0.23281	0.0690	0.0793	0.1320	0.2272	0.2542	0.2750	0.1788
130	1.0397	0.09422	0.1064	0.2367	0.3409	0.4295	0.4327	0.4005	0.1615
135	1.0745	0.03772	0.2527	0.5010	0.6431	0.6946	0.6619	0.5595	0.1643
140	1.1521	0.06257	0.4977	0.8585	1.0236	1.0105	0.9321	0.7456	0.1754
145	1.2717	0.15943	0.8215	1.2863	1.4604	1.3614	1.2302	0.9505	0.1929
150	1.4252	0.31197	1.1975	1.7549	1.9272	1.7279	1.5397	1.1634	0.2152
155	1.5987	0.49897	1.5946	2.2311	2.3942	2.0882	1.8433	1.3724	0.2392
160	1.7745	0.69656	1.9794	2.6814	2.8293	2.42	2.1231	1.5649	0.2619
165	1.934	0.88063	2.319	3.0724	3.2027	2.7037	2.3611	1.729	0.2807
170	2.0608	1.0294	2.5839	3.3742	3.4901	2.9208	2.5423	1.855	0.2930
175	2.1422	1.1259	2.7518	3.5638	3.6725	3.0558	2.657	1.9336	0.2930
179	2.169	1.1579	2.8069	3.6258	3.7327	3.0994	2.695	1.959	0.2967

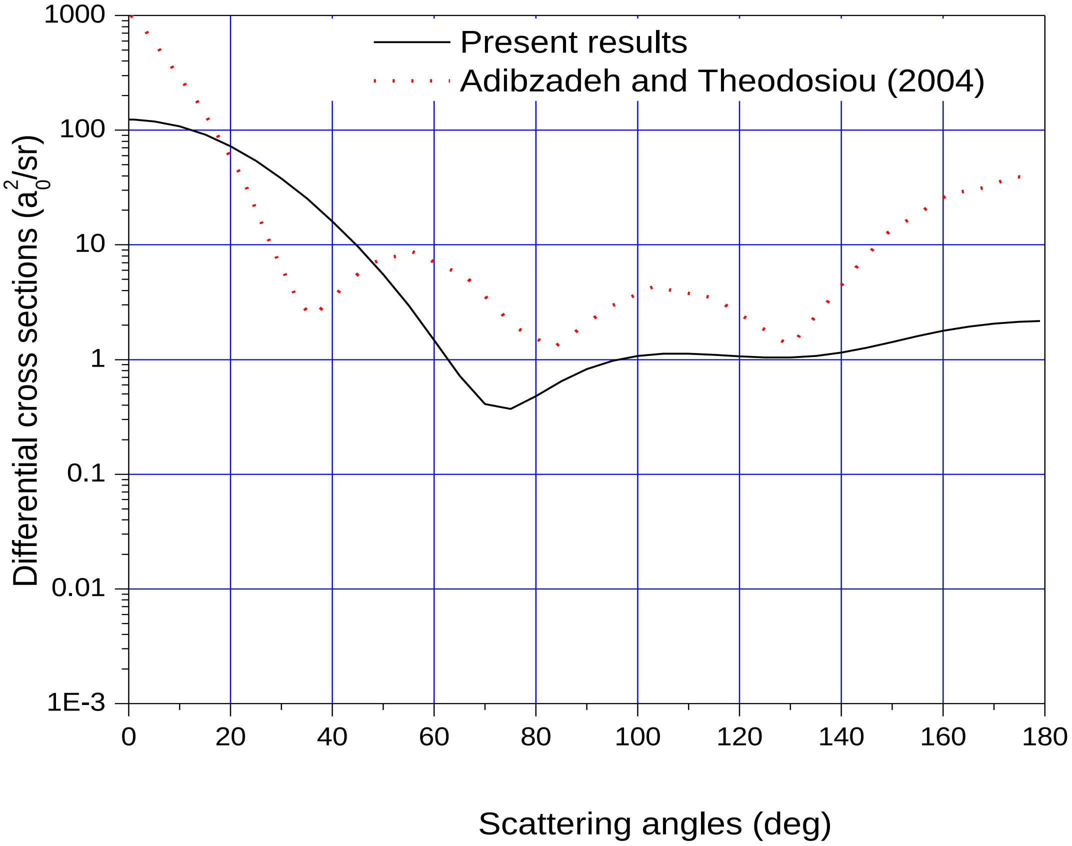

Figure 5.1: Graph of differential cross sections against scattering angles at incident energy of 10 eV for a strontium atom. ——— Present results, ………..Adibzadeh and Theodosiou (2004).

From figure 5.1, differential cross sections at 10 eV for present results disagree with the Adibzadeh and Theodosiou (2004) theoretical results. The present results have two minima at 70° and 130° (at 130^0 it is very shallow) whereas calculated results of Adibzadeh and Theodosiou (2004) using optical potential method have three minima at around 35^0, 85^0 and 130^0. But the values of the cross sections for both the cases are in the same range. The disagreement could be because DWBA does not work well at lower impact energies and also the nature of the distortion potential used in this method.

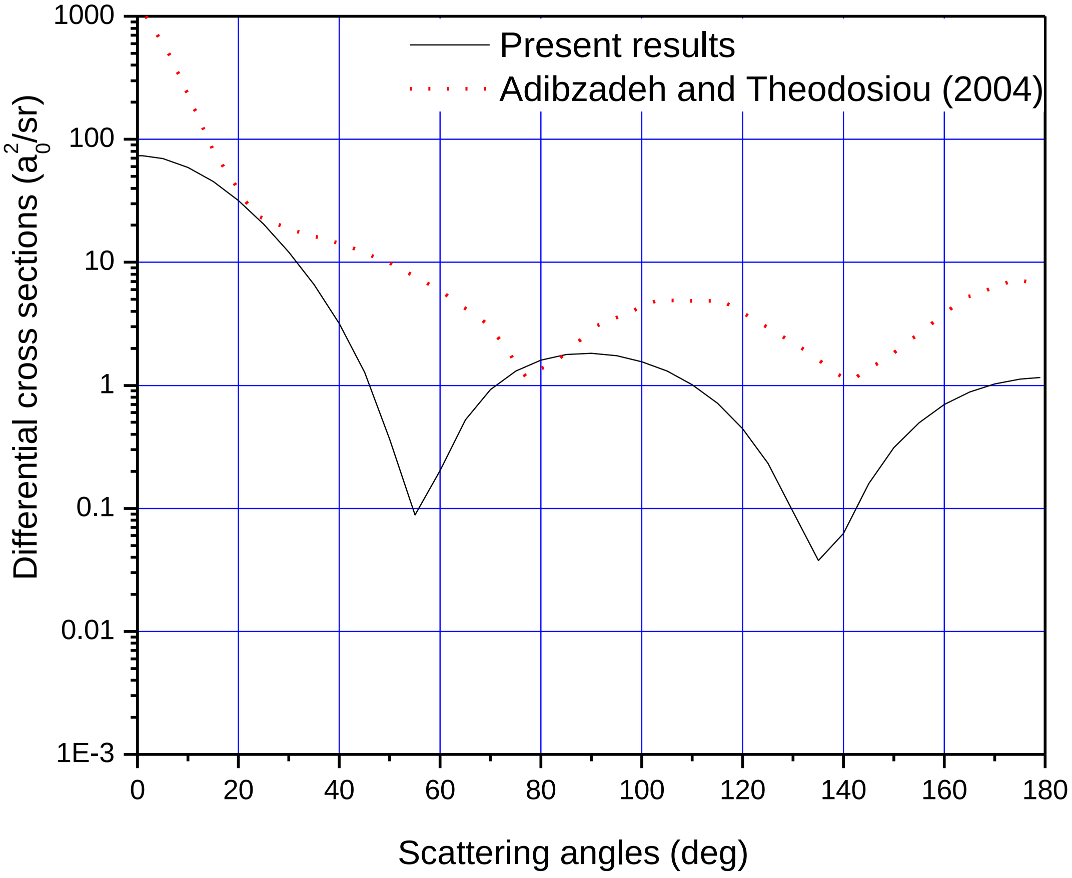

Figure 5.2: Graph of differential cross sections against scattering angles at incident energy of 20 eV for a strontium atom. ——— Present results, ………… Adibzadeh and Theodosiou (2004).

From figure 5.2, it shows that the present results disagree with the results of Adibzadeh and Theodosiou *(*2004). The present results had two minima at 45^0 and 135° whereas results of Adibzadeh and Theodosiou *(*2004) had two minima at 75^0 and 140^0 which were shifted to the right with respect to the present minima positions. It can be said that the two results agree qualitatively (since both have two minima) but disagree quantitatively. The discrepancy can also be attributed to the difference in the distorting potential between the two methods.

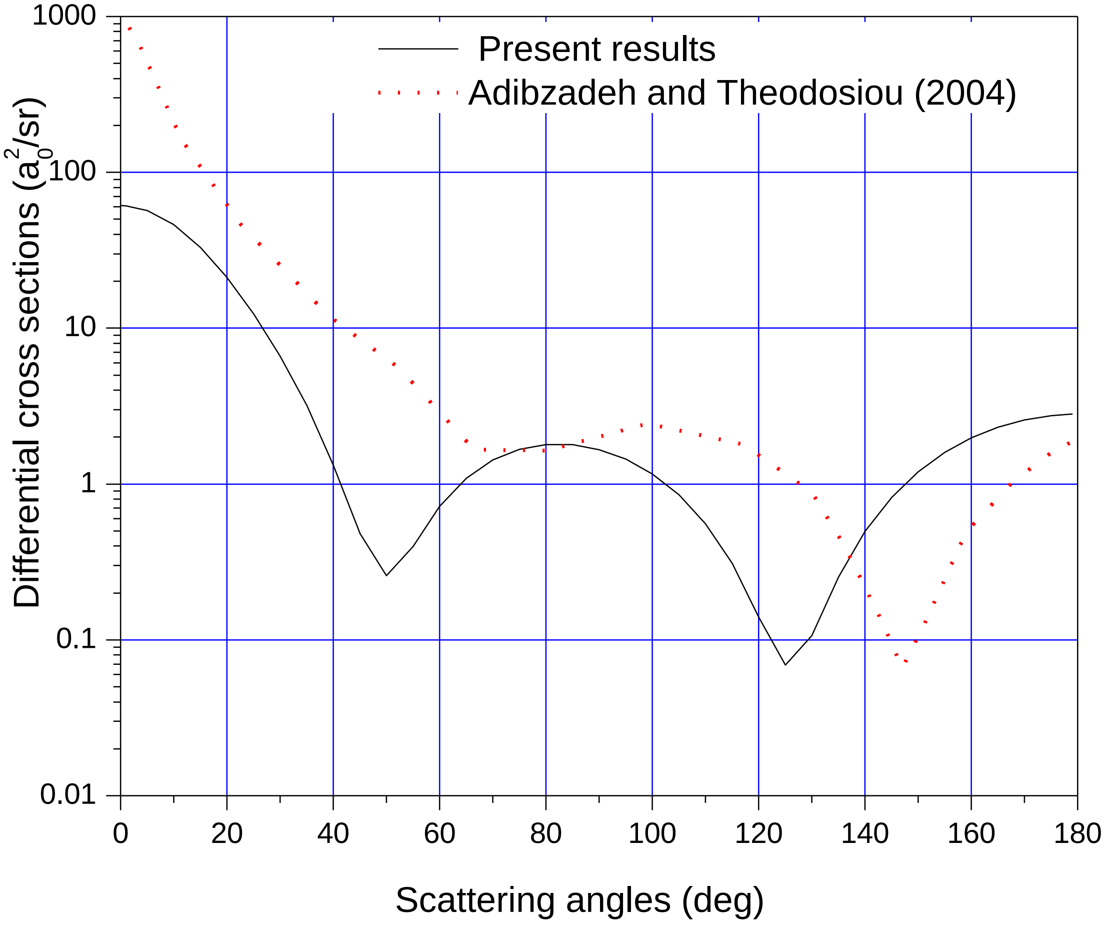

Figure 5.3: Graph of differential cross sections against scattering angles at incident energy of 30 eV for a strontium atom. ——— Present results,·········Adibzadeh and Theodosiou (2004).

In figure 5.3, it was seen that at 30 eV the present results agree qualitatively since the present result has two minima at 50^0 and 125^0 and that of Adibzadeh and Theodosiou (2004) has also two minima at 65^0 and 150^0 which are shifted to the right. Though both results seem to disagree quantitatively, both lie within the same range of values.

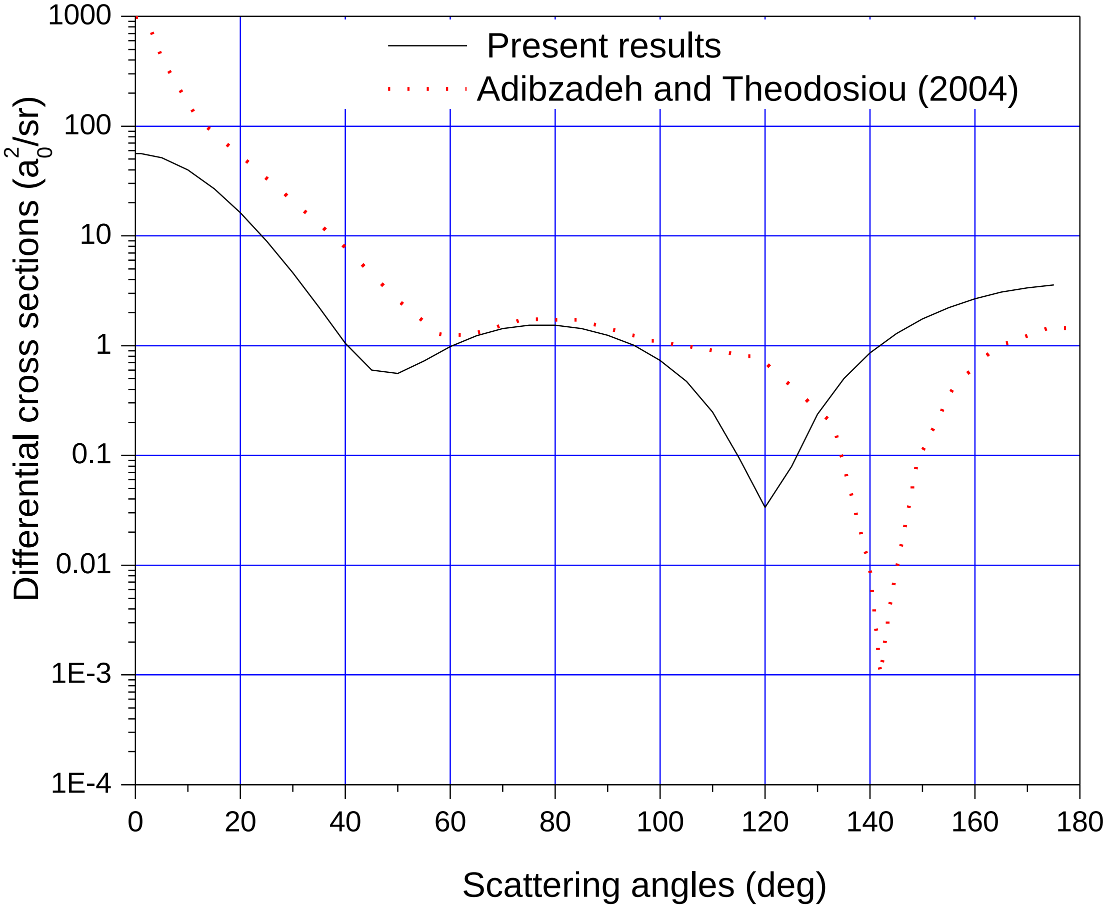

Figure 5.4: Graph of differential cross sections against scattering angles at incident energy of 40 eV for by a strontium atom. ——Present results,⋯⋯⋯Adibzadeh and Theodosiou (2004).

From figure 5.4, the present result has two minima at 45^0 and 120^0 whereas the result of Adibzadeh and Theodosiou (2004) has minima at 60^0 and 145^0. The present results agree well qualitatively and quantitatively with results of Adibzadeh and Theodosiou (2004) below 120^0 compared to what it was at lower energies.

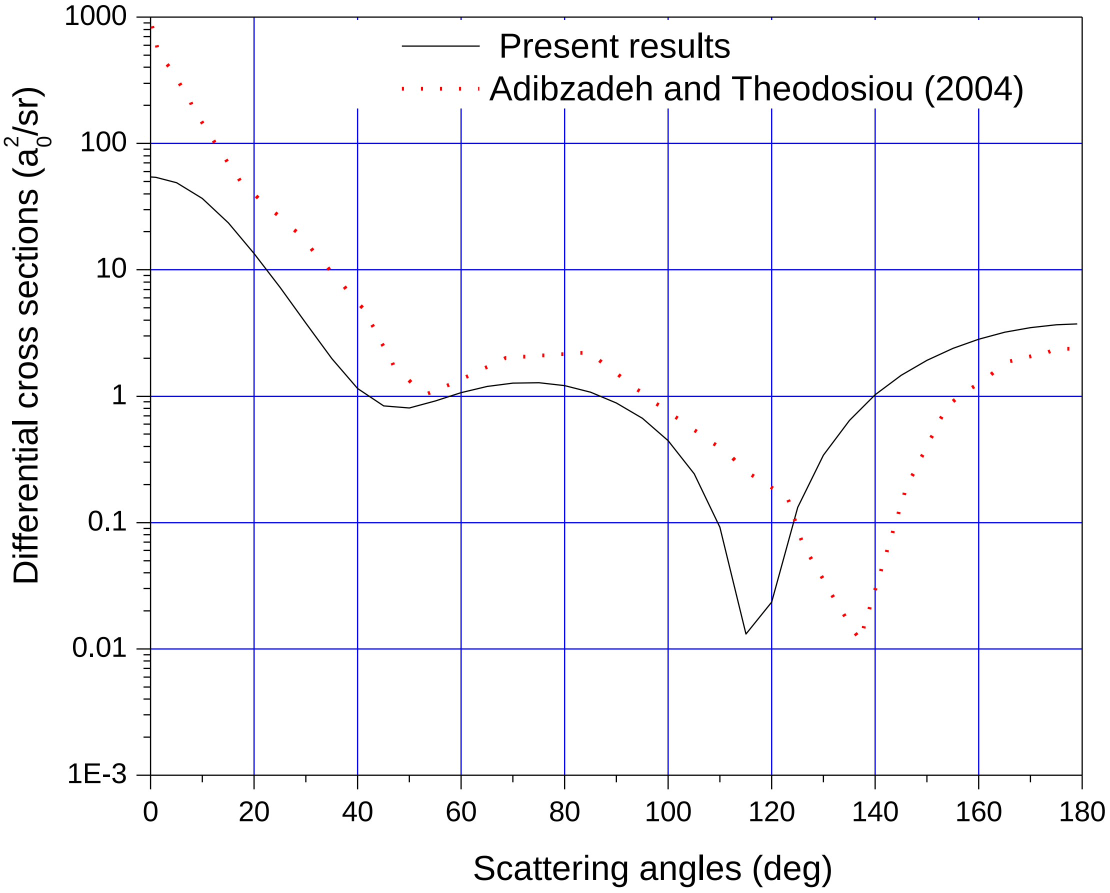

Figure 5.5: Graph of differential cross sections against scattering angles at incident energy of 50 eV for a strontium atom. ——— Present results,⋯⋯⋯ Adibzadeh and Theodosiou (2004).

From figure 5.5, the present result has two minima at 50^0 and 115^0 just like calculated results of Adibzadeh and Theodosiou *(*2004) which has minima at 55^0 and 135^0. It is only that the second minimum of the current results is shifted to the left. The present results agree qualitatively and quantitatively with theoretical results of Adibzadeh and Theodosiou *(*2004) compared to the agreement at lower energies.

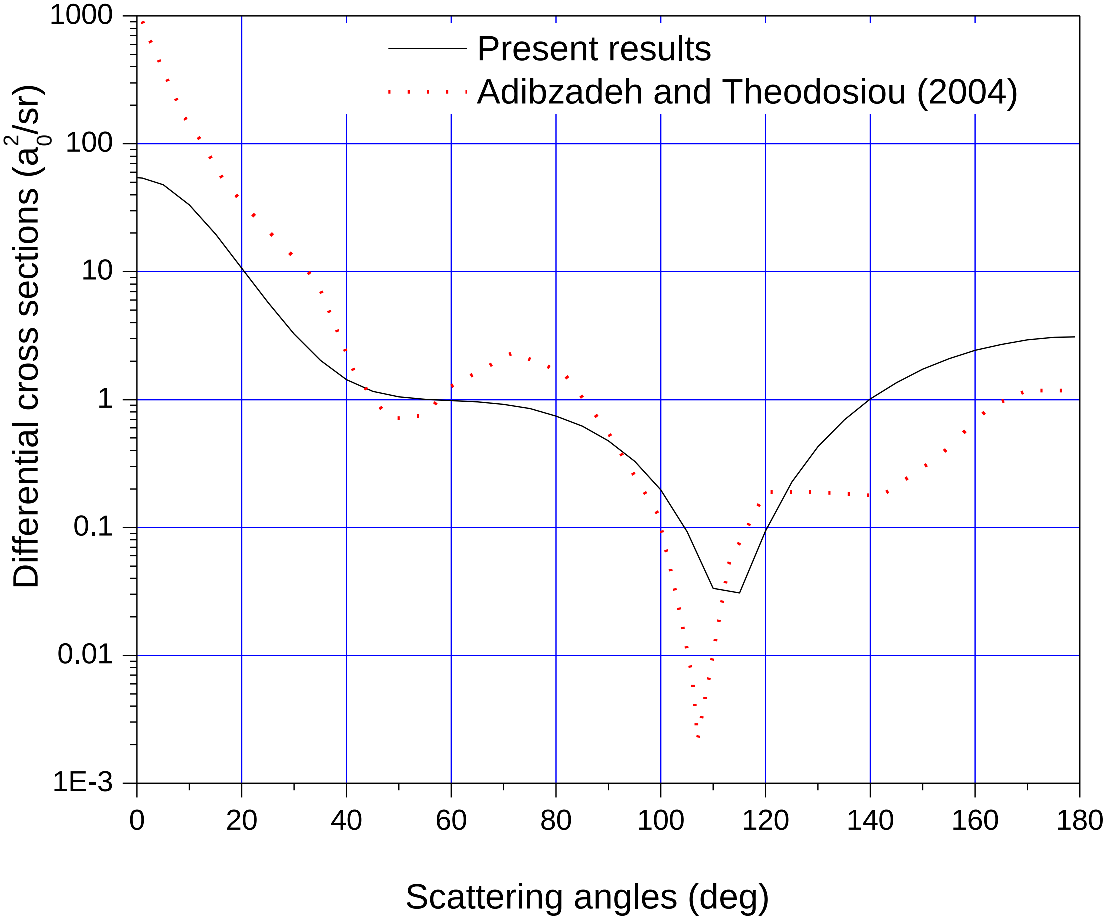

Figure 5.6: Graph of differential cross sections against scattering angles at incident energy of 70 eV for a strontium atom. ——— Present results, ··········Adibzadeh and Theodosiou (2004).

From figure 5.6, the present result again has two minima at 45^0 and 110^0 and that of Adibzadeh and Theodosiou (2004) has two minima at 50^0 and 110^0.The present results agree well qualitatively and quantitatively with theoretical results of Adibzadeh and Theodosiou (2004) compared to the agreement at lower energies.

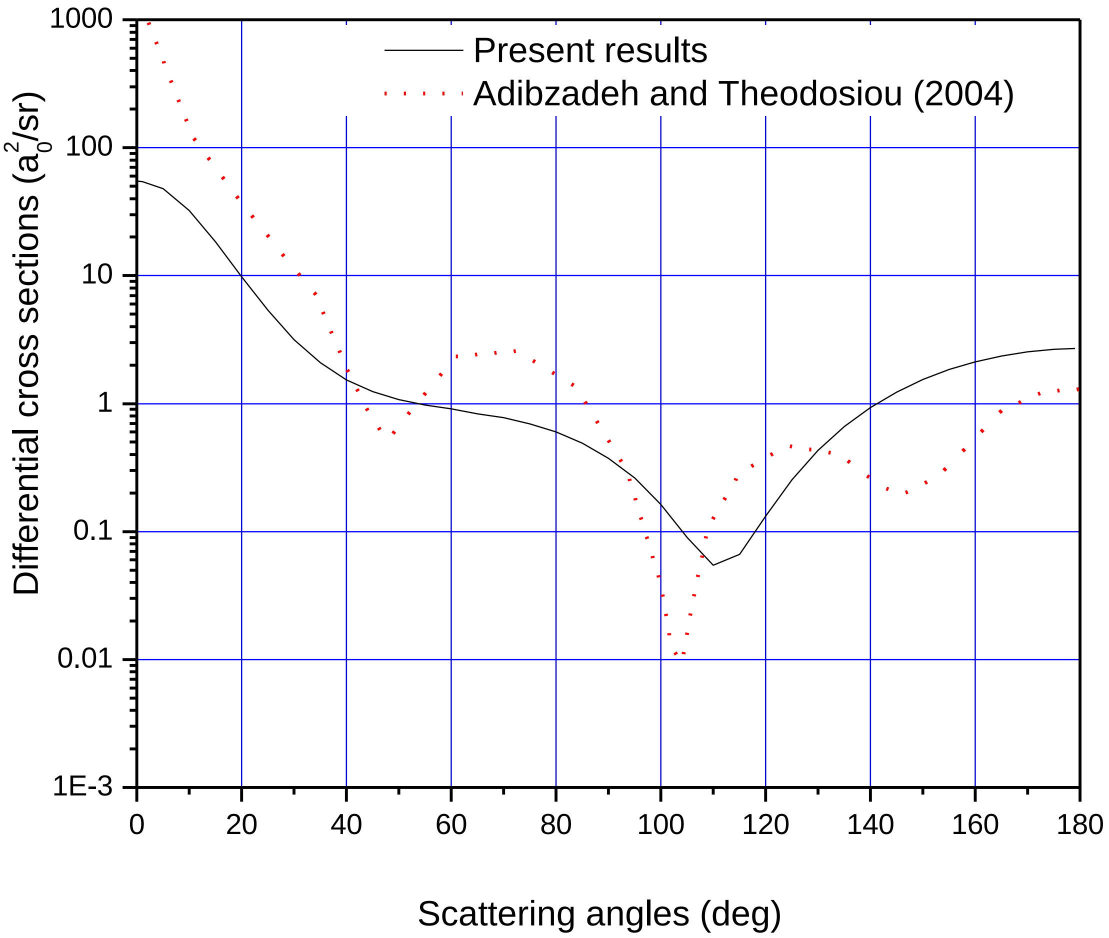

Figure 5.7: Graph of differential cross sections against scattering angles at incident energy of 80 eV for a strontium atom. ——— Present results,………… Adibzadeh and Theodosiou (2004).

From figure 5.7, the present result has one minimum at 110^0 and that of Adibzadeh and Theodosiou (2004) has three minima at 45^0, 105^0 and 150^0. The present results disagree qualitatively with those of Adibzadeh and Theodosiou (2004), even if the DCS are within the same range.

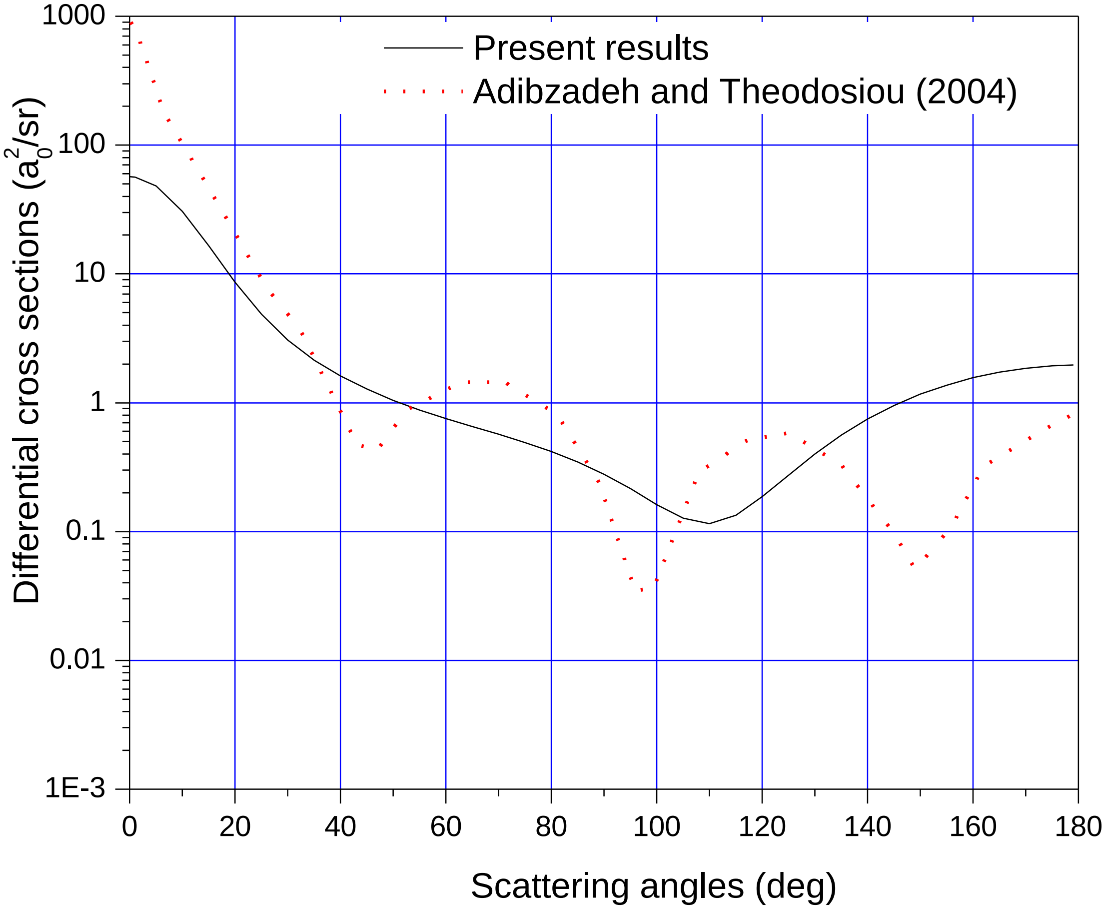

Figure 5.8: Graph of differential cross sections against scattering angles at incident energy of 100 eV for a strontium atom. ——— Present results, ·········· Adibzadeh and Theodosiou (2004).

From figure 5.8, the behaviors of these results are the same as at 80eV. The present result has one minimum at 110^0 and that of Adibzadeh and Theodosiou *(*2004) had three minima at 45^0, 95^0 and 150^0. The two results disagree qualitatively though they are in the same range.

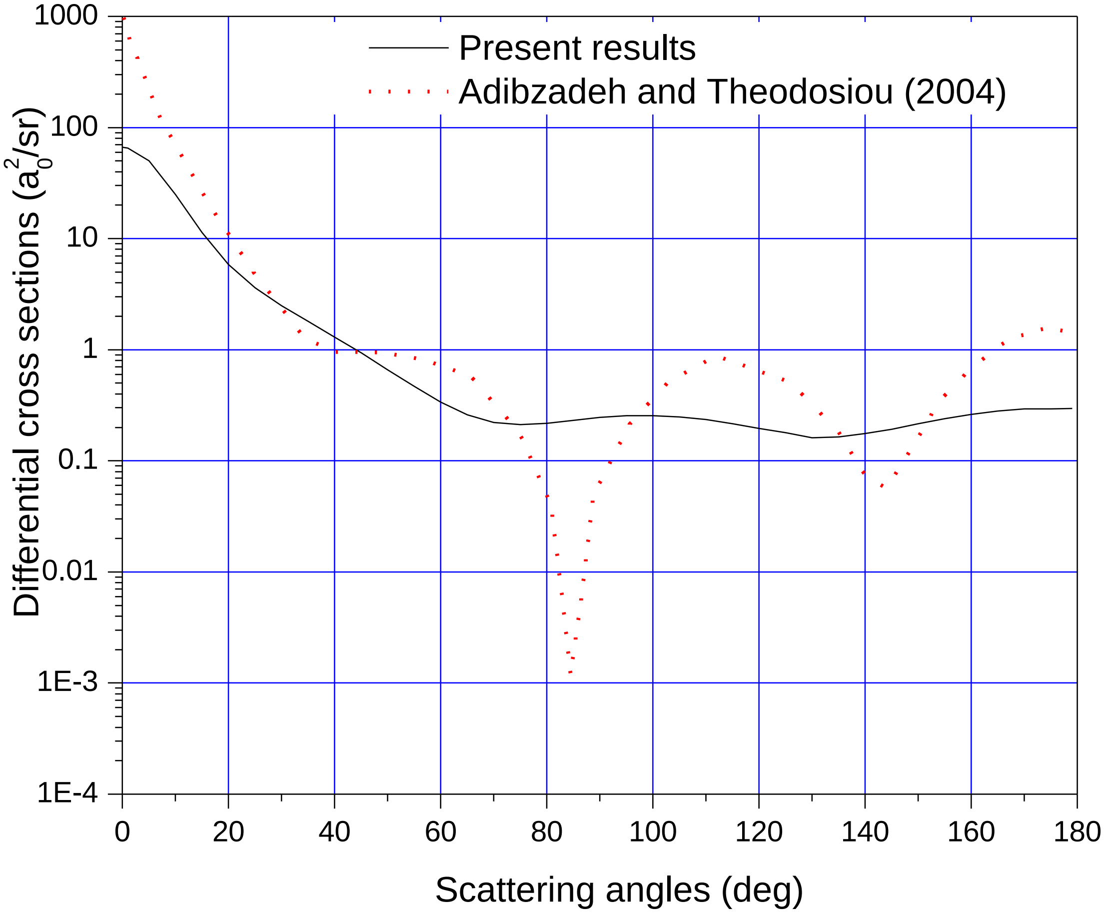

Figure5.9: Graph of differential cross sections against scattering angles at incident energy of 200 eV for a strontium atom. ——— Present results,··········· Adibzadeh and Theodosiou (2004).

From figure 5.9, the present result has two shallow minima at 70^0 and 130^0 and that of Adibzadeh and Theodosiou *(*2004) has minima at 40^0, 85^0 and 145^0. The mimimum at 85^0 is very deep. The present results disagree qualitatively with the results of Adibzadeh and Theodosiou *(*2004). But except for a sharp minimum at 85^0 for the Adibzadeh and Theodosiou *(*2004), both results seem to lie within the same range.

Though the present results disagree qualitatively and quantitatively agree well to Adibzadeh and Theodosiou *(*2004), both results are almost at all scattering angles and at all impact energies in the same range. The minima represent the direction in which the electrons are least likely to be deflected while the maxima represent the direction to which the electrons are most likely to be deflected. It can be concluded from figures 5.1-5.9, that the present DWBA calculated results are reliable for differential cross sections at the intermediate energies. The difference between the present results and the results of Adibzadeh and Theodosiou *(*2004) is because present DWBA has only considered a restricted form of static potential as the distortion potential whereas for the Adibzadeh and Theodosiou *(*2004) they have included static, exchange and polarization potentials this cause the main discrepancies at lower angles since polarization potential has a great effect at lower angles.

5.3 Integral cross sections

Integral cross sections have been calculated from 10eV to 200eV for elastic scattering of electrons by a strontium atom using present distorted wave method. The results are tabulated in the table 5.2.

Table 5.2: Integral Cross Section results (in units of a_0^2) calculated for the elastic scattering of electrons by strontium atom.

Energy	**Present**	**Adibzadeh and Theodosiou (2004)**	**Kumar *et al* (1995)**	**Kelemen *et al* (1995)**
10	96.51	196	96.6	145
20	42.37	138	43.5	104
30	32.75	123	25.93	
40	28.34			
50	25.55	99.3	13.5	62
60	23.55			
70	22			
80	20.73			
90	19.67			
100	18.75	66.9	8.53	39
110	17.93	59.9		
120	17.21			
130	16.56			
140	15.98			
150	15.44	49.3	7.4	29
160	14.95			
170	14.49			
180	14.07			
190	13.68			
200	13.32	40.56	6.4	25

The above data is plotted on a graph of ICS against electron energy as shown in figure 5.10.

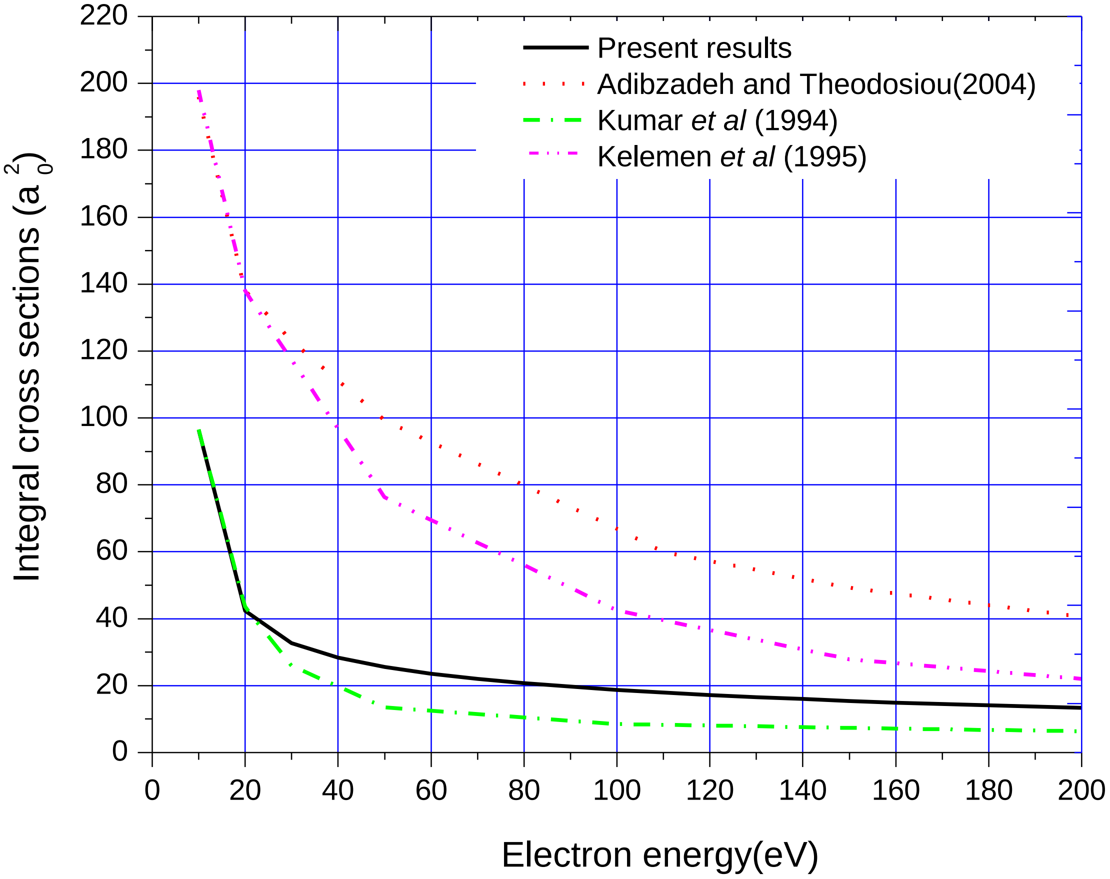

Figure 5.10: Graph of integral cross sections against electron energy for a strontium atom.——— present values of DWM, – · – · – Kumar *et al* (1994), — · · · Kelemen *et al* (1995) and - - - - - Adibzadeh and Theosodiu (2004).

It can be seen from figure 5.10 that the pattern of all the results are the same. At low energies the integral cross section is high and decreases with increase of the impact energy since the interaction time for the target atom and incident electrons reduces as the impact energy is increased. The present result is almost the same to that of Kumar *et al* (1994) where he used real potential.

In the absence of any experimental result it is hard to say which is better than the other.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Introduction

Using the first-order distorted wave Born approximation (DWBA) method differential cross sections (DCS) and Integral cross sections (ICS) have been calculated for elastic scattering of electron strontium atom scattering at intermediate energies. In the initial state of strontium atom both initial and final channel distortion potentials were taken as static potential. Double zeta Roothan-Hartree-Fock wave functions were used in the calculations as wave functions for the strontium atom as compiled by Clementi and Roetti (1974).

6.2 Conclusions

From this study the following observations were made:

i. The DWBA was developed and applied to $e-$ - Sr scattering.

ii. Changes on the DWBA1 computer program were made for strontium.

iii. Differential cross section (DCS) and integral cross section (ICS) at impact energies 10-200eV for elastic scattering of electron-strontium were determined.

iv. At energies between 10-30 eV, the present DCS results disagree with the only available calculated results of Adibzadeh and Theodosiou *(*2004) for differential cross section. This is because the first order distorted wave method gave poor results at low impact energies and also the nature of the distortion potential used in this work.

v. At energies of 60-200 eV, the present DCS results agreed well with calculated results of of Adibzadeh and Theodosiou *(*2004) though at 200eV the agreement is not so good.
vi. The integral cross section (ICS) graph structure for the present results agreed well qualitatively with theoretical results of Kumar *et al* (1994), Kelemen *et al* (1995) and Adbizadeh and Theodosiou *(*2004). Quantitatively, it is in better agreement with Kumar *et al* (1994) result compared to Kelemen *et al* (1995) and Adibzadeh and Theodosiou *(*2004).
vii. The present DWBA can be used to calculate DCS and ICS at intermediate energies.

6.3 Recommendations

From the results of DWBA using elastic scattering of electrons by strontium atom the following were recommended:

i. Some experimental studies on electron impact elastic scattering of strontium should be made to give results for comparison with the calculated results.
ii. Theoretical studies using close-coupling and R-matrix methods should be conducted on DCS for purposes of comparison with the present results.
iii. A distortion potential that incorporates the polarization potential, exchange potential and absorption potential should be used in the calculation.
iv. The present method incorporating all the distortion potentials should be extended further for electron impact elastic scattering of other alkaline earth metals such as beryllium, cesium, ytterbium, and radium.

v. Finally an alternative atomic wave function that is based on the multi zeta functions should be used to determine the correlation between atomic wave function and the graph structure.

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