L-SHELL X-RAY PRODUCTION CROSS SECTIONS FOR
\( _{20}^{20}\text{Ca} , \ _{28}^{28}\text{Fe} , \ _{28}^{28}\text{Ni} , \ _{29}^{29}\text{Cu} , \ _{30}^{30}\text{Zn} , \ _{31}^{31}\text{Ga} , \ \text{AND} \ _{32}^{32}\text{Ge} \)
BY HYDROGEN, HELIUM, AND LITHIUM IONS.

DISSERTATION

Presented to the Graduate Council of the
University of North Texas in Partial
Fulfillment of the Requirements

For the Degree of

DOCTOR OF PHILOSOPHY

By

Michael Ridge McNeir, B.S.,
Denton, Texas
May, 1992
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L-shell x-ray production cross sections are presented for Fe, Ni, Cu, Zn, Ga, and Ge by 0.5- to 5.0-MeV protons and by 0.5- to 8.0-MeV helium ions and Ca, Fe, Ni, Cu, and Ge by 0.75- to 4.5-MeV lithium ions. These measurements are compared to the first Born theory and the perturbed-stationary-state theory with energy-loss, Coulomb deflection, and relativistic corrections (ECPSSR). The results are also compared to previous experimental investigations.

The high precision x-ray measurements were performed with a windowless Si(Li) detector. The efficiency of the detector was determined by the use of thin target atomic-field bremsstrahlung produced by 66.5 keV electrons. The measured bremsstrahlung spectra were compared to theoretical bremsstrahlung distributions in order to obtain an efficiency versus energy curve.

The targets for the measurement were manufactured by the vacuum evaporation of the target element onto thin foils of carbon. Impurities in the carbon caused interferences in
the L-shell x-ray peaks. Special cleansing procedures were developed that reduced the impurity concentrations in the carbon foil, making the use of less than 5 μg/cm² targets possible.

The first Born theory is seen to greatly overpredict the data at low ion energies. The ECPSSR theory matches the data very well at the high energy region. At low energies, while fitting the data much more closely than the first Born theory, the ECPSSR theory does not accurately predict the trend of the data. This is probably due to the onset of molecular-orbital effects, a mechanism not accounted for in the ECPSSR theory.
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CHAPTER I

INTRODUCTION

The study of inner-shell ionization by fast ions, and the subsequent emission of characteristic x rays, has captured the interest of scientists for the past several decades. This process has been one of the primary tools in the investigation of the atom. It has also found practical applications, through particle induced x-ray emission (PIXE) and through materials analysis in the electronic and manufacturing industries. These applications have promoted a great deal of research over the past 20 years.

The interaction between a fast ion and an electron of a target atom can lead to ionization by several different processes. The three major processes are direct Coulomb ionization, electron capture or charge transfer, and molecular orbital effects or Pauli excitation. The relative importance of these processes depends upon the atomic number of the ion and target atom, $Z_1$ and $Z_2$ respectively, and the relative velocities of the incident ion, $v_1$, and the electron in state $S$ of the target atom, $v_{2s}$.

Direct ionization (DI) occurs when the incident ion transfers energy to the bound electron through the Coulomb force between them. If the energy transferred is greater
than the binding energy of the electron, then the electron enters a continuum state. This process is dominant when the incident ion is much lighter than the target atom, $Z_1 << Z_2$, or the ion is much faster than the orbiting electron, $v_i >> v_{2s}$.

Electron capture (EC) is an interaction where the electron moves from a bound state of the target atom to a bound state in the ion. This process maximizes when the ion and target atom are nearly symmetric, i.e. $Z_1 \approx Z_2$, and the velocities of the ion and electron match, $v_1 = v_{2s}$. Though EC is a large effect in this region, DI can still give a significant contribution to the total cross section.

Molecular orbitals are produced when the electron has sufficient time to adjust its orbit in response to the presence of an incident ion. The ion-atom system forms a short lived quasi-molecule during the collision. When these orbitals form, the Pauli exclusion principle becomes an ionization mechanism; electrons are promoted from filled molecular shells. This process dominates in near symmetric collisions when the electron completes many orbits during the process; $Z_1 \approx Z_2$, and $v_1 << v_{2s}$.

The subject of inner-shell ionization is generally separated into the low velocity regime, $v_1 << v_{2s}$, and the high velocity regime, $v_1 \geq v_{2s}$. In the low velocity region, the electron is able to adjust its orbit in response to the ion, forming molecular orbitals. The incident ion has
kinetic energy in the eV/u range. In the high velocity range, the electron wave function is only slightly perturbed by the incident ion. The ion scatters from the target electron, and the energy of the ion is in the MeV/u range. This work deals with the high velocity region, thus only the DI and EC contributions shall be discussed in detail in this work.

The DI process has been modeled by several different methods. The earliest model for inner-shell ionization was the free electron model, considering the collision between the ion and a "free" electron. The presence of the target nucleus was completely ignored, except to impose a minimum requirement on the energy transferred. Since the ion is much more massive than the electron, very little of the initial energy is transferred. Thus, according to this model, the ion would require an energy several hundred times the binding energy of the electron in order for ionization to occur.

Later this model was replaced by several others. The classical treatment of DI is known as the binary encounter approximation (BEA).\(^1\)\(^-\)\(^3\) The quantum mechanical treatment of this process is the plane wave Born approximation (PWBA),\(^4\)\(^-\)\(^7\) treating the scattering of a plane wave from a bound state electron in a first Born calculation. The semi-classical approximation (SCA)\(^8\)\(^,\)\(^9\) treats the electron quantum mechanically but the ion is treated as a classical particle
describing a hyperbolic trajectory. An extension beyond the PWBA is the ECPSSR theory,\textsuperscript{10-16} which includes the energy loss and Coulomb deflection of the ion, with the relativistic velocity and perturbed wave function of the electron.

The EC process was originally calculated by Brinkman and Kramers\textsuperscript{17} following an idea of Oppenheimer\textsuperscript{18} (OBK). This model may be used to calculate the cross section for a single electron transferring from a hydrogenic wave function of the atom to a hydrogenic wave function of the ion. Nikolaev\textsuperscript{19} introduced a semi-empirical scaling function in order to match the theory with experimental results (OBKN). When Lapicki et al.\textsuperscript{20,21} applied the ECPSSR theory to the EC process, they were able to match experimental results without this semi-empirical function.

These various theories calculate the ionization cross section, the probability that the ion will produce a vacancy in the target atom. While these processes cannot be observed directly, they can be observed through the vacancy filling mechanisms: x rays and Auger electrons. Thus, a prime tool for the investigation of ionization cross sections is the measurement of x-ray production cross sections.

Chadwick\textsuperscript{22} was the first to observe characteristic x rays produced by alpha particle bombardment. His results showed that ionization occurred at much lower energies than the free electron model predicted. Gerthsen\textsuperscript{23} was able to
produce x rays with protons at very low energies. As Gerthsen noted, an increase in the effective mass of the electron would increase the energy transferred through a collision, lowering the incident energy required to ionize the electron. The binding energy of the electron provides this increase in the effective mass. The binding of the electron is of overriding importance in the DI process.

A description of the process that included the binding of the target electron was developed using the quantum mechanical collision theory. For this theory, the ion was treated as a free particle of charge $Z_1e$, with free particle wave functions (plane waves). The target electron was considered to have a nonrelativistic hydrogenic wave function, unperturbed by the incident ion. The other electrons only served to screen the nucleus, thus the nuclear charge, $Z_2e$, was replaced by $Z_2 - 0.3$ for the K-shell and $Z_2 - 4.15$ for the L-shell. The cross section was then calculated using the Born approximation. This procedure became known as the plane wave Born approximation (PWBA).

In order to make the calculations possible, further simplifying assumptions were introduced. The internuclear potential was neglected; the incident ion was assumed to follow a straight line path. Also, the energy transferred to the electron was assumed to be negligibly small compared to the energy of the incident ion. Considering the ion as a
bare nucleus following a straight line trajectory limits the PWBA to light ions on heavy targets, $Z_1/Z_2 << 1$. The assumptions that the electron wave function is unperturbed and the energy transferred is small restricts the PWBA to fast ions, $v_1/v_2 >> 1$. Fortunately, it is in these areas that the DI contribution is dominant.

The results of the PWBA may be summarized as follows. The cross section is proportional to $Z_1^2$. It is also dependent only upon the incident velocity of the ion, but not explicitly on the mass. The target dependence is more complex, though the cross section is generally proportional to $Z_2^4$. The ionization cross section is very strongly dependent on the binding energy of the electron in the PWBA.

The development of accelerator technology led to the ready availability of light ions within a wide energy range. Thus, a large body of experimental data began to accumulate. Originally, scintillation detectors$^{25,26}$ were used to measure hydrogen and helium induced x rays. Through the 1960's, gas proportional counters were used to measure x rays.$^{27-31}$ Most of the experiments concentrated on hydrogen and helium inducing K-shell x rays of relatively light targets.$^{29-31}$ The introduction of the Si(Li) detector, with a greatly improved resolution, allowed the measurements to be performed with much greater precision. Due to protective windows that shielded the detector face, these detectors were unable to measure low energy x rays. Thus, the emphasis shifted to
heavier target elements. Over the past few decades, a large body of measurements for K-shell$^{32,34}$ and L-shell$^{35,36}$ x rays, induced by a variety of ions, have been published. As the measurements began to accumulate, discrepancies between the PWBA predictions and the data became apparent.

Several investigators concentrated on ionization induced by low velocity protons to determine the limit of $v_1/v_2$, at which the theory began to fail. Khan and Potter$^{37}$ measured K-shell x rays with 60 to 500 keV protons, with the data falling significantly below the PWBA. The same was seen by Hart et al.$^{38}$ with 20 to 100 keV protons on oxygen. Brandt et al.$^{39,40}$ studied low energy $^1$H, $^4$He on Mg, Al, and Cu, finding the data approaching a factor of 5 below the PWBA predictions. Similar results were obtained with the measurement of Au L-shell x-ray production cross sections by hydrogen and helium.$^{41-42}$ The data at low ion velocity tended to fall well below the theoretical predictions.

A significant discrepancy between the PWBA predictions and experiment came to light when measurements were taken by different isotopes of the same element. Brandt et al.$^{39}$ found that measurements by protons on aluminum were up to a factor of two lower than the same measurement with deuterons, with the difference increasing at lower ion velocity. Shima et al.$^{44,45}$ found a similar effect, first with protons and deuterons$^{44}$ and then with $^3$He and $^4$He ions,$^{45}$ on the L-shell of Mo and Ag. Heavier isotopes of an element
were found to have larger cross sections than the lighter isotopes. This mass dependence became known as the isotope effect.

The $Z_i^2$ dependence of the cross section was examined by Lewis et al.\textsuperscript{46} using 3 to 20 MeV/u deuterons and alpha particles impinging upon the K-shell electrons of elements from Cl to Cu. At ion velocities slightly higher than the target electron velocity, the cross section was seen to increase faster than $Z_i^2$. Awaya et al.\textsuperscript{47} observed a similar increase comparing nitrogen ions to alphas. A comparison of high energy oxygen to hydrogen induced L-shell x rays by Chaturvedi et al.\textsuperscript{48} yielded similar results. This effect was also observed for the copper K-shell x rays induced by protons, Be, C, and O ions by Andersen et al.\textsuperscript{49} This group concluded that an additional $Z_i^3$ dependent term was present, becoming increasingly important at higher energy.

With the experimental data indicating the regions where the PWBA inadequately described DI, attempts were made that aimed to relax the assumptions upon which the theory was based. The deflection of the ion due to the internuclear interaction was included by a new model, the semi-classical approximation (SCA).\textsuperscript{8,9} This model still treated the atom quantum mechanically, but assumed that the ion was a point particle following a hyperbolic path. The SCA is an impact parameter dependent model that calculates the differential ionization cross section, $d\sigma/dE_i$, where $E_i$ is the kinetic
energy of the ionized electron. Integration over all possible electron energies yields the total ionization cross section. The results of this model were below those of the PWBA at lower ion velocities.

The SCA showed an important impact parameter dependence. For low velocity ions, low impact parameter collisions contributed most to the total cross section. Ionization by low velocity ions were predominately from collisions where the ion was within the target electron shell. High velocity collisions had the greatest contribution from high impact parameter collisions. In this range, ionization occurred by ions moving predominantly outside the electron shell.

This impact parameter dependence led to the inclusion of two new effects\textsuperscript{10,13} in the PWBA. The first was a correction for low velocity ions.\textsuperscript{10} As these ions penetrated the electron shell, they would attract the electron into a tighter orbit around the now augmented nuclear charge. The presence of the ion would increase the binding energy of the electron. This effect would serve to lower the cross section for low velocity ions. The second correction was applied for high velocity ions.\textsuperscript{13} These ions, passing outside of the electron shell, would polarize the electron orbit. This polarization would serve to increase the cross section by adding a term proportional to $Z_i^{3 \alpha}$. These two effects appeared to explain the deviance
between the PWBA and the observed data.

Bethe\textsuperscript{50} showed the equivalence of the PWBA and the SCA in the limit of a straight line projectile motion. Basbas et al.\textsuperscript{10,39} were then able to extract from the SCA a Coulomb deflection correction that they then applied to the PWBA. This correction lowered the theoretical cross section at lower ion velocities. Also, since the magnitude of the deflection depends upon the mass of the ion, the isotope effect was included in the theory.

Basbas et al.\textsuperscript{11} determined that the hydrogenic wave functions used to describe the electrons in the PWBA were insufficient. They derived new wave functions that included the incident ion as a perturbing influence. Using these perturbed stationary states (PSS), they were able to reproduce the binding and polarization effects, earlier appended to the PWBA. Inclusion of the Coulomb deflection correction (C) created the CPSS model of DI.

Experiments showed that the CPSS theory was a great improvement to the PWBA theory in the low ion velocity regime. However, studies with heavy ions began to indicate that further improvements were necessary. Winters et al.\textsuperscript{51} studied the K-shell x rays of Ar with varying charge states of C, N, O, and F ions. This group found that, for ions with four or more electrons, the cross section was independent of the charge state. However, as the number of electrons decreased, the cross section rose. McDaniel et
al.\(^{52}\) found the same effect for L-shell x rays of Nd, Ho, and Au with highly charged F and Si ions. The increase was due to the capture of inner shell electrons to the K-shell of the ion. The EC effect was no longer negligible.

Electron capture was treated using the first Born approximation by Brinkman and Kramers\(^{17}\), following an idea of Oppenheimer\(^{18}\). This model described the transition of an electron from a hydrogenic wave function of the target to a hydrogenic wave function of the ion. A maximum in the cross section was predicted when the velocity of the ion matched the velocity of the electron during symmetric collisions. Nikolaev\(^{19}\) extended this model to calculate capture from completely filled shells. He also introduced a semi-empirical factor that matched the theory to experiment. This calculation was the OBKN approximation. Together with the PWBA, it makes up the first Born theory.

Lapicki and coworkers\(^{20,21}\) applied the CPSS theory to the electron capture process. Using the perturbed stationary states, they were able to reproduce the OBKN cross section without the introduction of any semiempirical scaling factors. The new CPSS theory included both DI and EC ionization cross sections summed to give the total ionization cross section.

Problems were, however, found for experiments using heavy targets. Burch et al.\(^{53}\) examined K-shell ionization of lead by 50 to 100 MeV Cl ions. Their data did not match
the CPSS theory, but was in good agreement with the PWBA. The addition of the relativistic nature of the target electron provided a correction that canceled the binding and Coulomb deflection effect at the ion velocities employed. Tarawa et al.\textsuperscript{54} found that CPSS theory plus a relativistic correction provided a good fit to Ta L-shell x-ray production by 1 to 4.4 MeV protons.

Rather then recalculate the Born theory with relativistic wave functions, as was done by Chen and Crasemann,\textsuperscript{55} Brandt and Lapicki\textsuperscript{14} included another correction factor to the CPSS calculations. They replaced the electron's mass by a larger relativistic mass in the low velocity limit of the CPSS cross section. The relativistic correction (R) slightly increased the cross section. The CPSSR theory was closer to the experimental measurements.

The last remaining assumption of the PWBA was that the energy loss of the ion was very small. For low velocity ions, though, the energy lost is an appreciable fraction of the initial energy and may no longer be neglected. Brandt and Lapicki\textsuperscript{16} provided an additional corrective factor that accounted for the energy loss (E). The inclusion of this factor completed the ECPSSR theory.

The ECPSSR theory has been tested by several experiments. For light ions in the velocity range $v_1 > v_2$, the theory is in excellent agreement with experimental data for both the K-shell\textsuperscript{56-59} and the L-shell\textsuperscript{60-63}. Recent focus
has concentrated in determining where the theory begins to fail. Work has concentrated on two areas: the low velocity regime, $v_1 < v_{2s}$, and the heavy ion regime, $Z_1 + Z_2$.

L-shell x-ray production by low velocity protons, deuterons, and alpha particles have been examined recently. Sarter et al.$^{64}$ examined the $Z_2$ dependence of the x-ray production cross section with low velocity protons. While elements with $47 < Z_2 < 82$ matched well or were slightly higher than the ECPSSR, data from heavier elements were well below the ECPSSR predictions. Lighter $Z_2$ elements were investigated by Marble et al.$^{65}$ using low energy protons, with the ECPSSR generally overpredicting the data. Jesus et al.$^{66,67}$ have investigated proton, deuteron, and alpha particle induced ionization of elements from Ta to U. This group found slight underpredictions by the ECPSSR, matching the conclusion of a review of earlier work by Mukoyama and Sarkadi.$^{68}$

L-shell x rays induced by heavier incident ions, up to $Z_1 = 20$, have also been investigated. Sarkadi and Mukoyama$^{69}$ investigated gold L-shell x-ray production by H, He, C, N, and O ion bombardment. The total cross section was in agreement with the ECPSSR. Bauer et al.$^{70}$ examined H, He, N, and Ne ions and found good agreement between the ECPSSR theory and the data. Jitschin et al.$^{71}$ have investigated ionization of the L-shell of gold by He, Li, Be, C, O, Si, and S impact from 0.23 to 6.7 MeV/u. This group found some
discrepancy between the CPSSR theory and their data. They concluded that the atomic wave functions were insufficient in describing the collision process.

In testing the limit of when $Z_1/Z_2$ is large enough for the ECPSSR theory to fail, problems occur when large $Z_1$ ions are employed. Broadening and shifting of the x-ray peaks result from multiple ionization of the target. The effects of multiple ionization on the fluorescent yields of the target are not very well known. Further, heavy ions dramatically increase the background radiation. These effects generally result in large uncertainties when comparing the data to theory.

An alternative method of investigating the high $Z_1/Z_2$ region is to employ light targets with low $Z_2$. The use of light ions drastically reduce the multiple ionization effects. A significant number of measurements have been reported for the K-shell of light targets using gas proportional counters, yet few L-shell measurements have been performed. Measurement with Si(Li) detectors in this region have generally had large uncertainties, up to 30%. Therefore, a need for the investigation of these light targets exists.

This work reports the measurements of L-shell x-ray production cross sections for $^{20}\text{Ca}$, $^{26}\text{Fe}$, $^{28}\text{Ni}$, $^{29}\text{Cu}$, $^{30}\text{Zn}$, $^{31}\text{Ga}$, and $^{32}\text{Ge}$ induced by 0.5 to 5.0 MeV $^1\text{H}$, 0.5 to 8.0 MeV $^4\text{He}$, and 0.75 to 4.5 MeV $^7\text{Li}$ ions. The results are compared
to the first Born theories for DI (PWBA) and EC (OBKN), and
the ECPSSR theory. This work will provide a test for these
theories in the low velocity range, \( v_1 \leq v_2 \). Also, the use
of light target elements will test the theory as the
collisions become less asymmetric, \( Z_1 \) approaches \( Z_2 \).
Measurements will be extended into a region heretofore
unexplored.
CHAPTER II

THEORY

The previous chapter discussed the historical development of the first Born and ECPSSR inner-shell ionization theories. This chapter presents the mathematical derivations of these theories. First, the formalism for calculating cross sections in the Born theory shall be presented. Then the first Born approximation shall be used to calculate the DI contribution (PWBA) and the EC contribution (OBKN). Next the SCA shall be presented, since the ECPSSR theory makes use of the results of this theory. Finally, the derivation of the ECPSSR theory shall be presented.

The ECPSSR theory introduces several effects into the cross section calculation. These effects shall be discussed in the chronological order of development. First, the Coulomb deflection term is extracted from the SCA description. Next, the increased binding and polarization effects are derived, first from the SCA and later through the introduction of the perturbed stationary state wave functions for the electron. Following these effects, the relativistic velocity of the electron is included. The theory is completed with the inclusion of the energy loss of
the ion during the collision.

**Born Approximation**

Consider a particle of mass $M$ and energy $E$ interacting with a potential $V$. The system can be described with a Hamiltonian of the form

$$H = H_0 + V,$$

where $H_0$ is the Hamiltonian for the particle outside of the influence of the potential. If $V$ is weak enough so that it may be considered to be a small perturbation, then the Born approximation can be employed. At high particle energy, this condition is fulfilled by

$$V a \ll \hbar v,$$

where $a$ is the interaction distance and $v$ is the ion's velocity.

The differential cross section for the transition of the particle from some initial state, $\psi_i$, to some final state, $\psi_f$, may be calculated from the scattering amplitude,

$$T_{if} = \langle \psi_f | V | \psi_i \rangle.$$

The wave functions are eigenstates of the unperturbed hamiltonian, satisfying

$$H_0 \psi_n = E_n \psi_n.$$

The cross section is given by
where $v_{i(f)}$ is the initial (final) velocity of the incident particle.

\[
\begin{align*}
\sigma &= \left( \frac{M}{2\pi \hbar^2} \right)^2 \frac{v_f}{v_i} |T_{f}|^2 \, d\Omega, \\
\end{align*}
\]

Figure 1. Direct ionization in the plane wave Born approximation.

**Plane Wave Born Approximation**

The case of direct ionization involves an ion incident upon an electron that is bound in the $S$th state of an atomic system, as shown in figure 1. The quantum mechanical description of the process was presented by Merzbacher and
Lewis. The projectile is treated as a point particle of mass $M_1$ with charge $Z_1$, assumed to be an incident plane wave. The target electron occupies an inner shell of an atom of mass $M_2$ that is initially in the ground state surrounded by $Z_2$ electrons. The interaction between the ion and an electron transfers enough energy to free the electron.

The total Hamiltonian of the system is given by

$$H = H_A + H_p + V,$$

where $H_A$ is the Hamiltonian for an isolated atom and $H_p$ is the Hamiltonian of a free particle. The total interaction potential between the ion and the atomic system is

$$V = \frac{Z_1 Z_2 e^2}{R} + \sum_{n=1}^{Z_2} \frac{Z_1 e^2}{|R-\mathbf{r}_n|}.$$  \hspace{1cm} \text{(II.7)}

However, this is a many body problem whose solution is very difficult. To reduce the problem to a solvable two body problem, the interaction potential is taken only between the ion and the target electron of interest;

$$V = \frac{Z_1 e^2}{|R-\mathbf{x}|}.$$  \hspace{1cm} \text{(II.8)}

This may be done if the internuclear and other electron interactions are considerably weaker than this potential.

To find the scattering amplitude, both the initial and final states of the system must be specified. The unperturbed Hamiltonian is the sum of the atomic and free
particle Hamiltonians. Thus, the eigenstates of $H_0$ are the products of the wave functions for $H_A$ and $H_p$. The initial wave function is

$$\psi_i(R,z) = e^{ik_1 R} \phi_i(z),$$

where $\exp[i k_1 \cdot R]$ represents the incident plane wave and $\phi_i(z)$ is the initial wave function for the orbiting electron. The wave number, $k_1$, is related to the initial momentum of the ion by $p_i = \hbar k_1$. Likewise, the final state is a combination of ion and electron wave functions;

$$\psi_f(R,z) = e^{ik_f R} \phi_f(z).$$

The scattering amplitude becomes, after insertion of the wave functions,

$$T_{IF}^{WBA} = \int \phi_f^*(x) \frac{Z_1 e^{i \exp [i (k_1 - k_f) \cdot R]} |R - x|} \phi_i(x) dR dR.$$

The scattering amplitude may be placed in a more manageable form by the introduction of the change in momentum variable,

$$\hbar \mathbf{q} = \hbar \mathbf{k}_i - \hbar \mathbf{k}_f,$$

which has the property that

$$q^2 = k_1^2 + k_f^2 - 2k_1 k_f.$$

By making this replacement and performing the integration over $R$, one obtains
\[ \tau_{1f}^{\text{PWBA}} = \frac{-4\pi Z_i e^2}{q^2} \int \phi_r^*(r) \exp(iq \cdot r) \phi_f(r) \, dr. \]  

II.14

The integral is usually expressed as the inelastic form factor,

\[ F_{1f}(q) = \int \phi_r^*(r) \exp(iq \cdot r) \phi_f(r) \, dr. \]  

II.15

From equation II.5, the differential cross section becomes

\[ d\sigma_{1f}^{\text{PWBA}} = \left( \frac{2Z_i e^2 M}{\hbar^2} \right)^2 \frac{V_f(q)}{V_i} \left( \frac{F_{1f}(q)}{q^2} \right)^2 \, d\Omega. \]  

II.16

where \( M = M_1 M_2 / (M_1 + M_2) \) is the reduced mass of the system.

Using the explicit form of \( d\Omega \),

\[ d\Omega = \sin\theta \, d\theta \, d\phi, \]  

II.17

and noting from equation II.13 that

\[ q \, dq = k_i k_f \sin\theta \, d\theta, \]  

II.18

the cross section may be expressed as

\[ d\sigma_{1f}^{\text{PWBA}} = 2\pi \left( \frac{2Z_i e^2}{V_i} \right)^2 \frac{|F_{1f}(q)|^2}{q^2} \, dq. \]  

II.19

Calculation of the cross section depends upon the exact wave functions used in the evaluation of the inelastic form factor, \( F_{1f}(q) \). The PWBA calculations that appear in this work use nonrelativistic hydrogenic wave functions with screened atomic nuclei.\textsuperscript{4-7} The atomic number has been
modified by a screening correction from Slater: $Z_{2K} = Z_2 - 0.3$ for the K-shell and $Z_{2L} = Z_2 - 4.15$ for the L-shell.\textsuperscript{24}

Using a hydrogenic wave function for the electron in state $S$ for the initial state and a continuum wave function as the final state of the electron, the form factor may be evaluated for an energy transfer of $\Delta E$.\textsuperscript{5-7} Assuming the form factor is isotropic, the cross section becomes

$$d\sigma_{\text{PWBA}}^{\Delta E, S} = \frac{8\pi \sqrt{2} e^4 |F_{\Delta E, S}(q)|^2}{v_i^2} dq d\Delta E. \tag{II.20}$$

The total cross section is then found by integration over all possible momenta and energies transferred. The limits of the momentum transfer integration may be found from equation II.13:

$$q_{\text{min}} = k_i - k_f, \tag{II.21a}$$

and

$$q_{\text{max}} = k_i + k_f. \tag{II.21b}$$

These may be expressed as

$$q_{\text{min}} = \frac{E_i - E_f}{\hbar v_i} \left[1 + (1-\Delta)^{1/2}\right]^{-1} \tag{II.22a}$$

and

$$q_{\text{max}} = \frac{E_i - E_f}{\hbar v_i} \left[1 - (1-\Delta)^{1/2}\right]^{-1}, \tag{II.22b}$$

where $\Delta = (E_i - E_f)/E_i$. If the energy transferred in the
collision is small compared to the initial energy, then
\( \Delta = 0 \). The integration limits become

\[
q_{\text{min}} = \frac{E_f - E_i}{\hbar v_i} \quad \text{II.23a}
\]

and

\[
q_{\text{max}} = \infty. \quad \text{II.23b}
\]

For an electron to gain enough energy so that it enters a continuum state from the energy level of state \( S \), the transferred energy must be greater than the electronic binding energy. This limits the minimum momentum transfer to

\[
q_{\text{min}} = q_0 = \frac{\hbar \omega_{2S}}{\hbar v_i}, \quad \text{II.24}
\]

where \( \hbar \omega_{2S} \) is the binding energy for an electron in state \( S \).

The total ionization cross section now becomes

\[
\sigma_{\text{FWRA}}^S = \frac{8\pi Z_i^2 e^4}{v_i^2} \int_{q_0}^{\infty} \frac{dq}{Q^3} \int_{\hbar \omega_{2S}}^{\infty} d(\Delta E) \left| F_{\Delta E, S}(q) \right|^2, \quad \text{II.25}
\]

where the maximum energy transfer is taken to be \( \infty \).

It is usually convenient to express the cross section in terms of dimensionless variables. The momentum transfer is reduced to

\[
Q = \frac{Q^2 \sigma_0^2}{Z_{2S}^2 \hbar^2}, \quad \text{II.26}
\]
where $a_o$ is the Bohr radius and $\mathcal{E}$ is the Rydberg energy.

The energy transfer is likewise replaced by

$$W = \frac{\Delta E}{Z_{2S}^2 \mathcal{E}}. \quad \text{II.27}$$

After these substitutions, the cross section takes the form

$$\sigma_S^{PWA} = 8\pi a_o^2 \left( \frac{Z_1 e^2}{Z_{2S} \hbar V_1} \right)^2 \int_{\omega_{min}}^\omega d\omega \int_{Q_{min}}^\infty \frac{dQ}{Q^2} |F_{WS}(Q)|^2. \quad \text{II.28}$$

where

$$\omega_{min} = \frac{\hbar \omega_{2S}}{Z_{2S} \mathcal{E}}. \quad \text{II.29}$$

and

$$W_{min} = \frac{\hbar \omega_{2S}}{Z_{2S} \mathcal{E}}. \quad \text{II.30}$$

The cross section may be further reduced if one defines

$$\eta = Z_{2S}^2 \left( \frac{V_1}{V_o} \right)^2. \quad \text{II.31}$$

where $v_o$ is the Bohr velocity. The cross section becomes

$$\sigma_S^{PWA} = 8\pi a_o^2 \frac{Z_1^2}{Z_{2S} \eta} \int_{\omega_{min}}^\omega d\omega I(\eta, W), \quad \text{II.32}$$

where

$$I(\eta, W) = \int_{W_{min}}^W \frac{dQ}{Q^2} |F_{WS}(Q)|^2. \quad \text{II.33}$$
is the excitation function for an electron receiving a reduced energy between \( W \) and \( dW \). One further reduction is performed by defining

\[
\theta_s = \frac{\hbar \omega_{2s} n_s^2}{Z_{2s}^2 \mathcal{R}},
\]

where \( n_s \) is the principal quantum number for state \( S \). This parameter takes the ratio of the true binding energy to the energy calculated by treating the atom as hydrogenic. The cross section is finally given as

\[
\sigma_{s}^{\mathrm{PWA}} = 8\pi a_{o}^{2} \frac{Z_{1}^{2}}{Z_{2s} \eta} f_{s}(\theta_{s}, \eta),
\]

where

\[
f_{s}(\theta_{s}, \eta) = \int_{\frac{\eta}{Z_{2s}}}^{\infty} I(\eta, W) dW.
\]

It is possible to obtain analytical forms for the limiting case of low projectile energy. One more reduced variable is the reduced velocity, defined by

\[
\xi_{s} = \frac{2v_{f}}{\theta_{s} v_{2s}}.
\]

The cross section in this form is

\[
\sigma_{s}^{\mathrm{PWA}} = 4\pi a_{o}^{2} \frac{Z_{1}^{2}}{Z_{2s}^{4}} \frac{n_{s}^{2}}{\theta_{s}} \mathcal{F}_{s}(\xi_{s}, \theta_{s}),
\]

where
In the low velocity limit \((\xi_s \ll 1)\) the function \(J_s\) has an exceedingly gradual \(\theta_s\) dependence. In this case, the function may be written in the following asymptotic forms:

\[
J_{\xi_k}(\xi_k) = \frac{2^9}{45} \xi_k^8, \quad \text{II.40a}
\]

\[
J_{\xi_L}(\xi_L) = \frac{2^{12}}{45} \xi_L^6, \quad \text{II.40b}
\]

and

\[
J_{\xi_{L_2},L_3}(\xi_{L_2}, L_3) = \frac{2^{11}}{11} \xi_{L_2,L_3}^{10}. \quad \text{II.40c}
\]

An examination of the approximations involved will give an idea of the limitations of the PWBA. Condition II.2 states the general condition under which the Born approximation may be utilized. Substituting the potential used, \(V\), the condition becomes

\[
Z_1 e^2 \ll \hbar v_i. \quad \text{II.41}
\]

Thus a general range of validity is given by light ions at high incident velocities. This general statement must be refined, however, by the further approximations invoked. The incident ion is treated as a bare nucleus. Since the largest contributions to the total cross section occur when the ion penetrates to about the electron's atomic radius, the ion will appear bare if its electron's orbits are much
larger than the radii of the target electron, \( a_{1K} \ll a_{2s} \). In the Bohr model, the electron radius is given by

\[
a_{2s} = n_s^2 a_o / Z_{2s},
\]

where \( a_o \) is the Bohr radius. Thus, for a K-shell target electron, this condition yields \( Z_1 \ll Z_2 \). The use of nonrelativistic hydrogenic wave functions requires that the electron be undisturbed by the interaction with the ion. If the ion is traveling at high enough velocity, then the electron wave function does not have time to adjust during the collision. This condition imposes that the velocity of the ion be much greater than the orbital velocity of the electron, or \( v_i \gg v_{2s} \). From Bohr's model,

\[
v_{2s} = Z_{2s} v_o / n_o.
\]

where \( v_o \) is the Bohr velocity. The condition of high \( v_i \) is also required for the energy loss of the ion to be neglected. As examination of the various approximations reveals, the conditions under which the PWBA is expected to be valid are

\[
Z_1 \ll Z_{2s} \quad \text{and} \quad v_i \ll v_{2s}.
\]

Examination of the cross section in equation II.35 reveals the properties of the PWBA cross section. The cross section is not explicitly dependent upon the ion's mass, only on the incident velocity. If different isotopes of an ion are employed, then the theoretical cross section will not change. Equation II.35 also shows that the cross section is proportional to \( Z_1^2 \). As discussed previously,
the theoretical cross section does not accurately reflect experimental data at low ion velocities.

Figure 2. Electron capture in the OBKN approximation. The point $C_2$ represents the center-of-mass for the atom-electron system prior to the collision. Similarly, $C_1$ is the center-of-mass for the ion-electron system.

**OBKN Approximation**

Electron capture involves the transfer of an electron from the 2S state of the target atom to the 1S state of the ion. This effect was calculated by Brinkman and Kramers. The coordinates involved are displayed in figure 2. The
position of the electron is denoted by \( r_1 \), the position relative to the ion, and \( r_2 \), the position relative to the target atom. The vector \( \mathbf{R}_j \) represents the position between the ion and the target atom prior to the exchange, measured relative to the center of mass of the target nucleus-electron system. After the collision, \( \mathbf{R}_i \) is the position to the target nucleus from the ion-electron center of mass. As with DI, the EC process will be evaluated using the Born approximation formalism.

The Hamiltonian for this system may be expressed as

\[
H = H_p + H_A + V,
\]

where \( H_p \) is the free particle Hamiltonian for the incident ion, \( H_A \) is the Hamiltonian for the target atom, and \( V \) is the interaction potential. As in the case for direct ionization, only the ion-electron interaction is considered;

\[
V = \frac{Z_1 e^2}{r_1}.
\]

The initial state of the system has a point particle of charge \( Z_1 \) and an atom with an electron in the \( n_2s \) shell. The initial wave function is

\[
\psi_i = e^{i \mathbf{k}_i \cdot \mathbf{r}_2} \phi_i(r_2),
\]

where \( \phi_i(r_2) \) is the hydrogenic wave function of the electron in the target atom and \( \hbar \mathbf{k}_i = M_i \mathbf{v}_i \) is the initial momentum of the ion. The final state of the ion is
\[ \Psi_f = e^{i k f \cdot R} \phi_f (x_1), \]  

where \( \phi_f (r_1) \) is the hydrogenic wave function for the electron in the incident ion and \( \hbar k_f = M_i v_f \) is the momentum of the ion-electron system after the collision. Here, \( M_i \) and \( M_f \) are the reduced mass of the ion before and after the collision, respectively.

Substituting the wave functions into equation II.3, the scattering amplitude becomes

\[ T_{if} = \int e^{-i k f \cdot R} \phi_r^* (x_1) \frac{Z_1 e^2}{r_1} \phi_i (x_2) e^{i k f \cdot R} dR_1 dR_2. \]  

This integral is placed into a more convenient form by noting from figure 2,

\[ R_2 = \frac{M_2}{M_2 + m} \ x_2 - x_1 \]  

and

\[ R_1 = \frac{M_1}{M_1 + m} \ x_1 - x_2. \]

Then the scattering amplitude may be rewritten as

\[ T_{if} = \int e^{-i k r_1} \phi_r^* (x_1) \frac{Z_1 e^2}{r_2} dR_1 \int e^{i k r_2} \phi_i (x_2) dR_2, \]  

where
\[ A = k_i - \frac{M_2}{M_2 + m} k_f \]  
\[ B = \frac{M_1}{M_1 + m} k_i - k_f. \]

The wave function, \( \phi_f \), must satisfy

\[
\left[ -\frac{\hbar^2}{2M_f} \nabla^2_f + \frac{Z_1 e^2}{r_1} \right] \phi_f = \epsilon_f \phi_f. \]

Substituting this expression into equation 11.51,

\[ T_{if} = \int e^{-iBx_i} \left( \frac{\hbar^2}{2M_f} \nabla^2_f - \epsilon_f \right) \phi_f^* dx_i \int e^{iA} \phi_i dx. \]

Evaluation of this integral by parts twice yields

\[ T_{if} = -\left( \frac{\hbar^2 B^2}{2M_f} + \epsilon_f \right) \int e^{-iBx_i} \phi_f^* dx_i \int e^{iA} \phi_i dx. \]

Noting the Fourier transforms in the above equation, it may be rewritten as

\[ T_{if} = -\left( \frac{\hbar^2 B^2}{2M_f} + \epsilon_f \right) \phi_i(A) \phi_f^*(B). \]

Placing the scattering amplitude into equation II.5 will give the Brinkman-Kramers result,\(^{17}\) which calculates the cross section for a single electron in the target atom to transfer to a particular shell of the ion. Nikolaev\(^{18}\) generalized this result to find the cross section for a
completely filled target shell to a state within the ion. 
The total probability is assumed to be the sum of the 
individual probabilities. Thus, summing over initial and 
final states,

\[ |T_{\text{DOEN}}^{\text{DOEN}}|^2 = \sum_n \sum_m (2\pi)^{12} \left( \frac{\hbar^2}{2M_i} + \epsilon_f \right)^2 |\phi_i(A)|^2 |\phi_f(B)|^2. \]  

II.58

The summation over orbital and magnetic quantum numbers for 
a particular principal quantum number using hydrogenic wave 
functions has been carried out by May;\(^79\)

\[ \sum_{l=0}^{n-1} \sum_{m=-l}^{l} |\phi_{nm}(q)|^2 = 2^6 \pi \frac{(Z/n\alpha_0)^5}{[q^2 + (Z/n\alpha_0)^2]^4}, \]  

II.59

where \( \alpha_0 = \frac{\hbar^2}{e^2 m_e} \) is the Bohr radius. Performing the 
summations yields the probability for an electron transition 
from the \( n_i \) shell of the target atom to a the \( n_f \) shell in 
the ion;

\[ |T_{\text{DOEN}}^{\text{DOEN}}|^2 = 2^{12} \pi^2 n_i^2 n_f^2 \frac{(Z_i/n_f\alpha_0)^5(Z_i/n_i\alpha_0)^5[\hbar^2 B^2 / 2m_e + \epsilon_f]^2}{[B^2 + (Z_i/n_f\alpha_0)^2]^4[a^2 + (Z_i/n_i\alpha_0)^2]^4}. \]  

II.60

Noting that the binding energy of a hydrogenic electron is 
given by,

\[ \epsilon_f = \frac{m_e Z^2 e^4}{2n_f^2 \hbar^2}, \]  

II.61

the above differential cross section may be written as
\[
d\sigma = \frac{\left(\frac{M_e}{2\pi \hbar^2}\right)^2 \left(\frac{V_f}{V_i}\right)^2 2^{10} \pi^2 n_1^2 n_2^2 \left(\frac{\hbar^2}{m_0}\right)^2 \left(\frac{Z_1}{n_1^2 \alpha_0}\right)^5 \left(\frac{Z_2}{n_2^2 \alpha_0}\right)^5}{\left[B^2 + (Z_1/n_1 \alpha_0)^2\right]^2 \left[A^2 + (Z_2/n_2 \alpha_0)^2\right]^4} \ d\Omega. \]
\]

The total cross section is found by integrating the differential cross section. The momenta in equations II.52 and II.53 may be expanded to give,

\[
A^2 = \left[\frac{(e_f - e_i)}{\hbar V_f} + \frac{m_e V_i}{2\hbar}\right]^2 + 4M^2V_i^2\sin^2\theta/2, \quad \text{II.63a}
\]

and

\[
B^2 = \left[\frac{(e_f - e_i)}{\hbar V_f} - \frac{m_e V_i}{2\hbar}\right]^2 + 4M^2V_i^2\sin^2\theta/2. \quad \text{II.63b}
\]

Using the relation, \(a_0^{-1} = v_0 m_e / \hbar\), the total cross section is

\[
\sigma = \frac{2^3 \pi \alpha_0^2 \left(n_1 n_f\right)^2 \left(V_{1n_f}\right)^5}{5 \left(V_{2n_f}\right)^5} \left(\frac{\Phi_4(\beta \xi^2)}{[1 + \beta \xi^2]^3}\right). \quad \text{II.64}
\]

Here,

\[
\xi = V_{2n_f} \left[V_{1n_f}^2 + q_{n_f n_f}^2\right]^{-1/2}, \quad \text{II.65}
\]

where

\[
q_{n_f n_f} = \frac{1}{2} \left[V_f + \left(V_{2n_f} \theta n_f - V_{1n_f}^2 \right) / V_{1}\right] \quad \text{II.66}
\]

is an approximation to the minimum momentum transferred by the capture process. The observed binding energy of the electron is \((1/2)m_e v_{2s}^2 \theta_s\). The function \(\Phi_4\) is given by
The cross section of equation II.64 was found to be greater than the experimental cross sections by a factor of two to three. Nikolaev introduced a semi-empirical corrective factor,\(^1\)

\[ R(t) = 0.3 \left[ \left( \frac{7}{9} t \right) + \frac{7}{9} t \right], \quad \text{II.68} \]

where \( t = Z_2 v_0 / n_t v_i \). This factor multiplied by equation II.64 gives reasonable agreement between the OBKN cross section and experimental data.

Semi-Classical Approximation

The SCA relaxes the restrictions on the PWBA by considering the Coulomb deflection of the charged particle. In order to accomplish this, the particle is considered to follow a classical hyperbolic orbit, while the electron is still treated quantum mechanically.\(^5\) The ion may be treated classically if its wavelength is large compared to the internuclear distance during scattering, on the order of the atomic radius. Thus the SCA is expected to hold for

\[ k_i a_{2s} \gg 1, \quad \text{II.69} \]

where \( \hbar k_i \) is the momentum of the ion and \( a_{2s} \) is the radius of the target electron. Figure 3 is a schematic diagram of the scattering event. \( R(t) \) denotes the position of the ion, and \( r \) denotes the position of the electron.
Figure 3. Schematic diagram of the collision process in the SCA description.

The SCA is an impact parameter dependent model. The cross section is given by

$$\sigma_{\text{SCA}} = \int_0^\pi I(b) 2\pi b db.$$  \hspace{1cm} \text{II.70}

Here, $I(b)$ is the ionization probability for a given impact parameter $b$, given by

$$I(b) = \int_0^{E_{f}} \frac{dT(b)}{dE_f} dE_f,$$  \hspace{1cm} \text{II.71}

where $E_f$ is the final energy of the electron. The
differential ionization probability is found from the square of the transition amplitude,

$$\frac{dI(b)}{dE_i} = |T_{if}^{SCA}|^2.$$ \text{II.72}

In order to find the cross section, the transition amplitude must be specified.

The transition amplitude in the SCA is similar to the first Born transition amplitude,

$$T_{if}^{SCA} = \frac{-i}{\hbar} \int_{-\infty}^{\infty} e^{i\omega_{if}t}(\phi_i|V(t)|\phi_f)dt,$$ \text{II.73}

where $\omega_{if} = (E_f - E_i)/\hbar$. The potential is again taken to be the interaction between the ion and the target electron,

$$V(t) = \frac{Z_1e^2}{|x-R(t)|}.$$ \text{II.74}

This may be placed in a more manageable form by substituting the Fourier transform of $V(t)$,

$$V(q) = \frac{Z_1e^2}{2\pi^2} \int \frac{\exp[iq \cdot (x-R(t))]}{q^2} dq.$$ \text{II.75}

Thus the scattering amplitude may be rewritten as

$$T_{if}^{SCA} = \frac{-i}{\hbar} \frac{Z_1e^2}{2\pi^2} \int \frac{F_{if}(q)}{q^2} I(\omega_{if}, q) dq,$$ \text{II.76}

where the integral $I(\omega_{if}, q)$ is defined by

$$I(\omega_{if}, q) = \int_{-\infty}^{\infty} \exp[i(\omega_{if}t-q \cdot R(t))] dt.$$ \text{II.77}

The scattering amplitude has been separated into a factor
containing the quantum mechanical aspects, $F_{if}(q)$, and a factor containing the classical trajectory of the ion, $I(\omega_{if}, q)$.

The scattering amplitude may be calculated for a straight line trajectory. Here, the path of the projectile may be written as

$$R(t) = bj + \nu_i t k, \quad \text{II.78}$$

for an appropriately aligned coordinate system. Performing the integral in equation II.77,

$$I(\omega_{if}, q) = 2\pi \exp[i b q_y] \delta(\omega_{if} - \nu_i q_x), \quad \text{II.79}$$

The delta function specifies the component of the momentum transfer parallel to the trajectory of the ion. Thus, the minimum momentum transfer is limited to

$$q_{\min} = \frac{\omega_{if}}{\nu_i} = q_o, \quad \text{II.80}$$

the same quantity found in the PWBA. The scattering amplitude may be expressed as

$$T_{if}^{SCA} = \frac{i Z_i e^2}{\pi \nu_i} \int F_{if}(q_x, q_o) \left[ \frac{e^{-iq_x b}}{(q_x^2 + q_o^2)} \right] dq_x, \quad \text{II.81}$$

where $q_x$ is the component of the momentum transfer perpendicular to the ion's trajectory. If the momentum transfer is expressed in polar coordinates and the form factor written explicitly, then this integral may be evaluated;
where $K_0$ is a modified Bessel function of the second kind and $r_1 = [x^2 + (y-b)^2]^{1/2}$.

Bethe and Jackiw\textsuperscript{50} showed that if equation II.81 is used to find the total cross section, including summing over the spins, then

\[
\sigma_{\text{SCA}}^R = \frac{8\pi Z^2 e^4}{V_i^2} \int \frac{F_0(q)}{q^3} dq d\Delta E.
\]

This result matches equation II.25, the result of the PWBA. Thus the total cross section in the straight line approximation of the SCA is equivalent to the PWBA.

Coulomb Deflection

The ECPSSR theory incorporates several factors into the formalism of the first Born theory that were neglected by the PWBA and OBKN theories. The first of these factors accounts for the Coulomb deflection of the incident ion. Basbas et al.\textsuperscript{10} extracted a factor from the SCA by comparing the cross section calculated with a hyperbolic trajectory to the cross section calculated with a straight line trajectory,

\[
C = \left( \frac{d\sigma}{dE_f} \right)^{\text{HYP}} / \left( \frac{d\sigma}{dE_f} \right)^{\text{SL}}.
\]
Evaluation of the integral, \( I(\omega_f, q) \), led them to

\[
C = \exp[-\pi dq_0],
\]

where \( q_0 \) is the minimum momentum transferred defined by equation II.24 and \( d \) is the half distance of closest approach,

\[
d = \frac{Z_1 Z_2 e^2}{Mv_i^2}.
\]

Integrating this expression over the electron energy, \( E_f \), gives the Coulomb deflection factor for the total cross section,

\[
C_s(dq_0) = v E_{v+1}(\pi dq_0),
\]

where \( v = 9 \) for the K and L\text{I} shells and \( v = 10 \) for the L\text{II} and L\text{III} shells. The function \( E_v \) is an exponential integral function.

The Coulomb deflection term always satisfies \( C_s < 1 \), and it approaches 1 as \( v_i \) approaches \( \infty \). Thus, this factor lowers the cross section at low ion velocity. Further, the \( dq_0 \) dependence introduces a dependence upon the mass of the incident particle. The Coulomb deflection explained the isotope effect, and it also improved the theory at low ion velocity.

**Binding Effect**

The biggest effect at low ion velocity, however, was the increased binding of the electron due to the presence of
the ion within the atomic shell. Basbas et al.\textsuperscript{10} calculated the increase in binding energy using first order perturbation theory. This increase is given as

\[ \Delta \varepsilon_{2s} = \left\langle \phi^* (r) \left| \frac{Z_1 e^2}{|R-r|} \right| \phi (r) \rightangle. \]  \hspace{1cm} \text{II.88} 

Using nonrelativistic, hydrogenic wave functions, the increase is

\[ \Delta \varepsilon_{2s} = 2 \left( \frac{Z_1}{Z_{2s}} \right) Z_{2s}^2 \frac{g_s}{y} g_s (y), \]  \hspace{1cm} \text{II.89} 

where \( y = R(t)/a_{2s} \). The function \( g_s (y) \) is a weighting function derived from the SCA scattering amplitude, given by

\[ g_k (y) = 1 - (1+y) e^{-2y}, \]  \hspace{1cm} \text{II.90a} 

for the K-shell and

\[ g_{L_i} (y) = 1 - e^{-y} \left( 1 + \frac{3}{4} y + \frac{1}{4} y^2 + \frac{1}{72} c_{L_i} y^3 \right), \]  \hspace{1cm} \text{II.90b} 

for the L-shell, where \( c_{L_i} \) is 9, 7, and 4 for the \( L_1, L_2, \) and \( L_3 \) shells, respectively.

The binding correction is included in the screening parameter, \( \theta_s \). The cross section is now given by

\[ \sigma_s^{\text{PMAB}} = 8 \pi a_0^2 \frac{Z_1^2}{Z_{2s}^4 \eta} f_s (e_s \theta_s, \eta), \]  \hspace{1cm} \text{II.91} 

where

\[ e_s = 1 + N_s \left( \frac{Z_1}{Z_{2s} \theta_s} \right) g (y) \]  \hspace{1cm} \text{II.92} 

with \( N_s \) representing the number of electrons in the \( n_s \)
Polarization Effect

The Coulomb deflection and binding effect improved the PWBA at low ion energy; however, an adjustment at high energy was still necessary. Thus the polarization effect was included.\textsuperscript{11}

Since the greatest contribution to the ionization cross section occurs for large impact parameters at high energy, only distant collisions need be considered. Hill and Merzbacher\textsuperscript{80} calculated this effect by treating the electron as an isotropic harmonic oscillator. The potential between the ion and the electron is still

\[ V(t) = -\frac{Z_1 e^2}{|r-R(t)|} . \] II.93

This may be expanded to give

\[ V(t) = -Z_1 e^2 \left[ \frac{1}{R(t)} + \frac{r-R(t)}{R(t)^3} + \frac{1}{2} \left( \frac{3r-R(t)}{R(t)^5} - \frac{r^2}{R(t)^3} \right) + \ldots \right] . \] II.94

Then the Hamiltonian of the system may be written as

\[ H = H_o + V_1 + V_2 . \] II.95

where the unperturbed hamiltonian represents the harmonic oscillator,

\[ H_o = \frac{\mathbf{p}^2}{2\mu_o} + 1/2\mu_o \omega^2 r^2 . \] II.96

The perturbation is given by the dipole and the quadrupole
terms of equation II.94, expressed in spherical polar coordinates,

\[ V_1 = -Z_1 e^2 \frac{r}{R^2} P_1(\hat{r} \cdot \hat{r}) \]  

(II.97)

and

\[ V_2 = -Z_1 e^2 \frac{r^2}{R^2} P_2(\hat{r} \cdot \hat{r}), \]  

(II.98)

where \( P_1(x) \) are the Legendre polynomials. The transition amplitude from the ground state to a state designated by quantum numbers \( nlm \) is

\[
T_{nlm} = \frac{i}{\hbar} \int_{-\infty}^{\infty} dt \langle nlm | V'(t) | 000 \rangle e^{i\omega_{nlm} t} \\
- \frac{1}{\hbar^2} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \sum_{n'lm'} \langle nlm | V'(t) | n'lm' \rangle \\
x \langle n'lm' | V'(t') | nlm \rangle e^{i\omega_{nlm} t + i\omega_{n'l'm'} t'},
\]

(II.99)

where \( V'(t) = V_1 + V_2 \) and \( \hbar \omega_{nlm,n'l'm'} = E_{nlm} - E_{n'l'm'} \).

The transition probability, \( |T_{nlm}|^2 \), caused by the perturbation is limited by the selection rules for the dipole and quadrupole transition. The dipole transition will yield a probability proportional to \( Z_1^2 \), as in the PWBA. The dipole-quadrupole interference term will be proportional to \( Z_1^3 \). This term may be related to the PWBA through the oscillator model.

Calculating the transition amplitude for all states
permitted by the selection rules, the correction to the
cross section may be written as

\[ \sigma_{\text{PWBAP}} = \sigma_{\text{PWBAP}} + \int \! dw \, w(\omega) \left( 2\pi \int \! P_3(\omega, b) \, b \, db \right), \tag{II.100} \]

where \( w(\omega) \) is the differential oscillator strength. \( P_3(\omega, b) \)
is the ionization probability given by

\[
P_3(\omega, b) = \frac{2(Z_1 e^2)^3}{\hbar \omega m^2 v_1^4 b^3} \left( -K_1(u) \int_{-\infty}^{\infty} \frac{dv \cos(\Omega v)}{(1 + v^2)^{5/2}} \left[ (v^2 - 2) F_1(u, v) - 3v F_2(u, v) \right] 
+ K_0(u) \int_{-\infty}^{\infty} \frac{dv \sin(\Omega v)}{(1 + v^2)^{5/2}} \left[ 3v F_1(u, v) - (1 - 2v^2) F_2(u, v) \right] \right), \tag{II.101} \]

where \( u = \omega b/v_1 \),

\[
F_1(u, v) = \int_{-\infty}^{\infty} \frac{dv \sin[u(v-y)]}{(1+y^2)^{3/2}}, \tag{II.102} \]

and

\[
F_2(u, v) = \int_{-\infty}^{\infty} \frac{dv \sin[u(v-y)]}{(1+y^2)^{3/2}}. \tag{II.103} \]

Integration over all impact parameters yields

\[
2\pi \int \! P_3(\omega, b) \, b \, db = \frac{4\pi(Z_1 e^2)^3}{\hbar m^2 v_1^5} I \left( \frac{\omega a}{v_1} \right), \tag{II.104} \]

where \( a_\omega \) is a target dependent radius limiting the collision to distant impact parameters.

The binding effect and polarization effect may be combined if the increase in energy transfer occurring due to
polarization is applied as an effective decrease in the binding energy. Modifying equations II.91 and II.92 to include the polarization effect, the cross section may be written as

\[ \sigma_{\text{PSS}} = 8\pi a_o^2 \frac{Z_1^2}{Z_{2s}^4} f_s(\zeta_s \theta_s, \eta) \quad \text{II.105} \]

or

\[ \sigma_{\text{PSS}} = 8\pi a_o^2 \frac{Z_1^2}{Z_{2s}^4} \frac{n_s^2}{\theta_s} \mathcal{F}(\xi_s/\zeta_s, \zeta_s \theta_s). \quad \text{II.106} \]

The modification to the reduced energy is given as

\[ \zeta_s = 1 + \frac{2Z_1}{Z_{2s} \theta_s} \left[ g_s(\xi_s; c_s) - h_s(\xi_s; c_s) \right], \quad \text{II.107} \]

where \( c_s \) is a parameter limiting the binding correction to lower ion energy and the polarization correction to higher ion energy. The polarization correction is

\[ h_s(\xi_s; c_s) = \left( 2n_s/\theta_s \zeta_s^2 \right) I(c_s n_s/\xi_s). \quad \text{II.108} \]

With the inclusion of the Coulomb deflection factor, these two corrections make up the CPSS theory.

**Relativistic Correction**

The next step in the evolution of the ECPSSR theory was the inclusion of a correction for the relativistic velocity of the electron. Rather than recalculating the cross section with relativistic wave functions, Brandt and Lapicki\(^{14}\) decided to introduce a corrective factor into the
CPSS calculations. In the low velocity limit, the cross section is proportional to the maximum electron kinetic energy,

\[ \sigma \propto E_{\text{max}}^4 = \left( \frac{1}{2} m_e v_i^2 \right)^4. \]

Brandt and Lapicki replaced the electron's mass with an effective mass that accounted for the relativistic speed.

The relativistic mass takes the form

\[ m^*(r) = m_e [1 + (Z_2s/2rc^2)^2]^{1/2} + Z_2s/2rc^2, \]

where \( r \) is the distance from the target nucleus. This distance is chosen to be the mean value between the target and the projectile, \( r = \langle R(t) \rangle \). This value is related to the impact parameter by

\[ \frac{1}{\langle R(t) \rangle} = \frac{1}{\sinh(1)b}. \]

The relativistic mass is averaged over all impact parameters with weighting functions, \( W_s(bq_0) \), derived from the SCA,

\[ m_s^F(\xi_s) = \int_0^\infty m^F(ab) W_s(bq_0)bq_0d(bq_0). \]

The result of this integration is

\[ m_s^F(\xi_s) = (1 + \beta x_s^2)^{1/2} + x_s, \]

where
\[ x_{K,L_1} = \frac{0.40(Z_{2s}/c)^2}{\xi_{K,L_1}} \]  
\[ x_{L_2,L_3} = \frac{0.15(Z_{2s}/c)^2}{\xi_{L_2,L_3}} \]

and \( \beta \) is a constant. A value of \( \beta = 1.1 \) agrees to within 3% of the numerical integration of equation II.112.

**Energy Loss**

The last effect included in the ECPSSR formulation is the inclusion of the energy loss of the ion. This effect is important at very low ion velocity. From the low velocity formulae for the SCA, the inclusion of the energy loss yields

\[ \frac{d\sigma_{SPWBA}}{dE_p} = \frac{d\sigma_{SPWBA}}{dE_f} \left[ \left( \frac{q_{\alpha}}{q_{\min}} \right)^{\nu+1} - \left( \frac{q_{\alpha}}{q_{\max}} \right)^{\nu+1} \right], \]

where \( \nu = 9 \) for the K and L\(_1\) shells and \( \nu = 11 \) for the L\(_2\) and L\(_3\) shells. Integrating over the final states yields the total cross section,

\[ \sigma_{SPWBA}^{FPA} = \sigma_{SPWBA}^{PWA} \frac{V_{\Delta \nu}}{2^{\nu+1} \Lambda_\nu} \int_{\Lambda_\nu}^{1} \left[ \frac{1 + (1-\Delta)^{1/2}}{\Delta} - \frac{1 - (1-\Delta)^{1/2}}{\Delta} \right] d\Delta, \]

where \( \Delta_\nu = \hbar \omega_{2s}(M_1/M)E_i \) is the minimum kinetic energy loss. Evaluation of the integral leads to

\[ \sigma_{SPWBA}^{FPA} = \sigma_{SPWBA}^{PWA} \sigma_{SPWBA}^{PWA}. \]

The energy loss correction is
\[ \mathcal{E}_s(z) = 2^{-\nu} [(\nu z - 1)(1+z)^\nu + (\nu z + 1)(1-z)^\nu], \quad \text{(II.118)} \]

where \( z = (1-\Lambda s)^{1/2} \).

The energy loss also affects the Coulomb deflection term, \( C(\pi d q_o) \). The argument must be replaced by

\[ C^g = C \left( \frac{2d q_o}{(1-\Delta)^{1/2} [1+(1-\Delta)^{1/2}]} \right). \quad \text{(II.119)} \]

After again integrating over all final states, the energy loss may be factored into a straight line factor and a Coulomb deflection factor,

\[ \mathcal{E}'_s(z, d q_{os}) = C_s \left( \frac{2d q_{os}}{z(1+z)} \right) \mathcal{E}_s(z), \quad \text{(II.120)} \]

where \( q_{os} = q_o \Lambda s / \Lambda \).
CHAPTER III

EXPERIMENT

As mentioned in chapter I, measurement of low energy L-shell x rays has received scant attention. This is primarily due to two experimental difficulties that are usually encountered. The first is the relatively large attenuation of low energy x rays occurring when the standard Si(Li) detectors are used. The second problem stems from low energy K-shell x rays from impurities interfering with the target L-shell x rays. These problems inhibit the high precision x-ray production cross section measurements for low Z₂ targets.

The description of the experimental apparatus is divided into three parts, with emphasis on the solutions to the problems mentioned above. First, the equipment and geometry used in this experiment are described. Second, special attention is devoted to the windowless Si(Li) x-ray detector, which was used to make the measurement of the low energy x rays. Last, the method by which the ultra-clean targets used in this experiment were fabricated is presented.

Experimental Apparatus

This experiment was performed at the Ion Beam
Modification and Analysis Laboratory at the University of North Texas. The 9SDH-2 Pelletron accelerator system, a 3 MV tandem accelerator produced by National Electrostatic Corporation, provided ions in the 0.5 to 5.0 MeV range. The hydrogen and lithium ions were produced in the source of negative ions by cesium sputtering (SNICS II ion source), while helium was obtained from the Alphatross RF oscillator, charge exchange ion source. The ions were first passed through a selection magnet, then through a mass analyzing magnet prior to injection into the accelerator. After acceleration, the ions were passed through an analyzing magnet, defining apertures, and into the target chamber.

The target chamber (see figure 4) was designed to perform a variety of applications in a UHV environment, including nuclear reaction analysis, Rutherford back-scattering analysis, and inner-shell ionization measurements. A cryopump, mounted atop the chamber, maintained a base pressure of ~10⁻⁸ Torr. In the center of the chamber, an aluminum target holder held the target foils perpendicular to the incoming ion beam. The ion beam was defined by two pairs of carbon slits. These adjustable slits were set to produce a 1 mm square beam spot on the target, with an angular divergence less than 0.15°. The x-ray detector was located at 135° to the incoming ion beam direction. Surface barrier detectors were placed at 45°, 135°, and 173° to the incoming ion beam direction. These
Figure 4. Schematic diagram of the target chamber used for atomic collision studies.
detectors measured the scattered ions simultaneously with the x-ray measurements. A Faraday cup was located at the back of the chamber to measure the current through the target foil. Integration of this current provided the number of incident ions.

**X-ray Detector**

A high resolution Si(Li) detector from LINK Analytical was used to detect x rays. This detector could be operated in three configurations: with a beryllium window, an ultrathin aluminum-formvar window, or no window. When used in windowless mode, these detectors can measure x rays with energy ~200 eV. For all of the x-ray measurements taken in this report, the detector was in the windowless mode. In this configuration, the silicon crystal is vulnerable to energetic scattered particles. To reduce this background radiation, a pair of permanent magnets, mounted in front of the crystal face, deflected lower energy charged particles away from the x-ray detector.

For lower energy x-ray measurements, electronic noise is a significant concern. A signal produced by an x-ray carries voltage noise from the input FET amplifier and 1/f noise from the surrounding insulating material. In order to reduce the noise from these sources, the detector was equipped with the LINK Analytical 2040 pulse processor. This processor filtered incoming pulses, giving better
resolution, and provided pulse pile up rejection, allowing higher count rates.

A crucial problem in this experiment was the determination of the detector efficiency. Previously, the efficiency of windowless Si(Li) detectors in this region have been found by determining the attenuation of photons through the gold contact layer and the silicon dead layer associated with the detector. This method involves the calculation of the thicknesses of these layers by employing radioactive sources with high energy x rays. Due to the exponential dependence of the efficiency on x-ray energy, small errors at high energy are magnified when extrapolated to low energy. This makes precise determination of the efficiency difficult for x-ray energies below 1 keV.

In this experiment, a method of efficiency determination using the atomic-field bremsstrahlung produced by electrons passing through thin foils was employed. This method has previously been used to calibrate Si(Li) detectors equipped with beryllium windows, and it offers distinct advantages over other methods. The atomic-field bremsstrahlung is a smoothly and slowly varying function of photon energy, yielding precise determination of the efficiency. Also, a continuous efficiency curve as a function of energy may be obtained with one measurement, instead of extrapolating a curve from several discrete measurements. This procedure was used to calculate the
intrinsic efficiency, the ratio of x rays detected to x rays that impinge upon the detector.

For the atomic-field bremsstrahlung method, electrons of 66.5 keV energy impacted upon thin self-supporting foils of aluminum, silver, and gold (see figure 5). Three separate targets were used to compensate for the interference of characteristic x rays from the target with the bremsstrahlung spectra. The resulting photon yield is given by

\[ \gamma_{\text{net}} = \varepsilon(k) \Delta\Omega \Delta k \int_0^h dx \frac{d^2\sigma}{d\Omega dk} \exp[-\mu(k) x \cot \psi], \]

where \( k \) is the photon energy, \( \varepsilon(k) \) is the detector efficiency, \( \Delta\Omega \) is the solid angle subtended by the detector, \( \Delta k \) is the energy width of each PCA channel, \( h \) is equal to \( t/\cos \psi \) for target thickness \( t \), \( \psi \) is the angle between the target normal and the beam axis, \( d^2\sigma/d\Omega dk \) is the doubly differentiated cross section for bremsstrahlung production, and \( \mu(k) \) is the photon attenuation coefficient for the material.

If the target is thin enough to allow the energy loss of the electron to be neglected, then the differential bremsstrahlung cross section can be treated as a constant. The integral in equation III.1 may then be evaluated. Solving the resulting equation for \( \varepsilon(k) \) yields
Figure 5. Bremsstrahlung spectra by 6.5 keV electron bombardment of a thin silver target. The characteristic x-rays between 2.8 and 3.8 keV obscure the bremsstrahlung distribution.
\[ e(k) = \frac{Y_{net}}{\Delta \Omega \Delta k \frac{d^2 \sigma}{d\Omega dk} hT(k)}. \]  

The evaluation of the integral in III.1 leads to the average photon transmission from all depths in the target;

\[ T(k) = \frac{1 - \exp\left[-\mu(k) t / \sin \psi\right]}{\mu(k) t \sin \psi}. \]

As seen in equation III.2, the determination of the efficiency at energy \( k \) relies on the knowledge of the differential cross section, \( \frac{d^2 \sigma}{d\Omega dk} \). The angular and energy dependence of the cross section may be separated by

\[ \frac{d^2 \sigma}{d\Omega dk} = s \frac{d\sigma}{dk}, \]

where \( s(\theta) \) is the shape function containing the angular distribution and \( d\sigma / dk \) contains the energy distribution for a photon of energy \( k \) emitted at angle \( \theta \) relative to the incident electron. These two functions have been tabulated based on a model describing the bremsstrahlung process as a single electron transition in a self-consistent central potential.\(^89\) For electrons greater than 1 keV, the exact details of the central potential used do not greatly influence the final results; the particular potential used was a Kohn-Sham potential.\(^90\) The results were obtained by the numerical evaluation of an expansion in partial waves. These tabulations were used to determine the differential cross section.
Figure 6. Intrinsic efficiency of the LINK Si(Li) detector in windowless mode. The absolute efficiency is found by scaling this curve by the geometric factor.
Figure 6 shows the intrinsic efficiency calculated by the atomic-field bremsstrahlung. Once the intrinsic efficiency is determined, the absolute efficiency for the experimental arrangement of the detector may be determined. The absolute efficiency, the ratio of x rays detected to x rays produced, is the product of the intrinsic efficiency and the geometric factor. The geometric factor was calculated using standard radioactive sources by the same method as the solid angle determination for the surface barrier detectors.

Target Preparation

The targets were made by the evaporation of the target element onto thin self-supporting carbon foils. Thin targets were chosen for three reasons. With thin targets, the energy loss of the ion as it passes through the target is minimized. Self-attenuation of the x rays produced below the surface of the target is also minimized. Most importantly, the alteration of the charge state of the incoming ion is minimized. While not an important consideration for protons, this requirement necessitated the use of target foils that were less than 5 μg/cm² for the lithium experiments. The target thicknesses are listed in tables I-III.

The targets were made by evaporation of the pure element onto carbon foils, with two exceptions. Pure zinc
Table I. Target thicknesses for $^1$H ions.

<table>
<thead>
<tr>
<th>Element</th>
<th>Material</th>
<th>Thickness ($\mu g/cm^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{26}$Fe</td>
<td>Fe</td>
<td>33</td>
</tr>
<tr>
<td>$^{28}$Ni</td>
<td>Ni</td>
<td>67</td>
</tr>
<tr>
<td>$^{29}$Cu</td>
<td>Cu</td>
<td>22</td>
</tr>
<tr>
<td>$^{30}$Zn</td>
<td>ZnP</td>
<td>58</td>
</tr>
<tr>
<td>$^{31}$Ga</td>
<td>Ga</td>
<td>11</td>
</tr>
<tr>
<td>$^{32}$Ge</td>
<td>Ge</td>
<td>55</td>
</tr>
</tbody>
</table>
Table II. Target thicknesses for $^4$He ions.

<table>
<thead>
<tr>
<th>Element</th>
<th>Material</th>
<th>Thickness ($\mu g/cm^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{26}$Fe</td>
<td>Fe</td>
<td>20</td>
</tr>
<tr>
<td>$^{28}$Ni</td>
<td>Ni</td>
<td>9.8</td>
</tr>
<tr>
<td>$^{29}$Cu</td>
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</tr>
<tr>
<td>$^{30}$Zn</td>
<td>ZnP</td>
<td>12</td>
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<tr>
<td>$^{31}$Ga</td>
<td>Ga</td>
<td>12</td>
</tr>
<tr>
<td>$^{32}$Ge</td>
<td>Ge</td>
<td>9.6</td>
</tr>
</tbody>
</table>
Table III. Target thicknesses for $^7$Li ions.

<table>
<thead>
<tr>
<th>Element</th>
<th>Material</th>
<th>Thickness ($\mu g/cm^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{20}$Ca</td>
<td>CaCl</td>
<td>1.6</td>
</tr>
<tr>
<td>$^{26}$Fe</td>
<td>Fe</td>
<td>2.5</td>
</tr>
<tr>
<td>$^{28}$Ni</td>
<td>Ni</td>
<td>2.9</td>
</tr>
<tr>
<td>$^{29}$Cu</td>
<td>Cu</td>
<td>3.6</td>
</tr>
<tr>
<td>$^{32}$Ge</td>
<td>Ge</td>
<td>6.0</td>
</tr>
</tbody>
</table>
does not evaporate well, thus a compound of zinc phosphide was used instead. Calcium suffers from the same problem; hence, calcium chloride was used. Further, the carbon K-shell x-ray is very near the calcium L-shell x-rays. To alleviate this difficulty, calcium chloride was evaporated onto a self-supporting nickel foil.

Since the targets were very thin, impurities in the target foil, especially sodium and silicon, became a concern. The self-supporting carbon substrate was obtained from a commercial manufacturer, who arc-evaporated carbon onto a glass slide that had been treated with a parting agent. The parting agent will dissolve in a liquid solution, freeing the carbon from the glass slide and allowing the foil to be transferred to an aluminum frame. The parting agent and the liquid used to dissolve this agent have been considered to be the major source of impurities. When evaporated in this manner, the carbon foil is a chemically active surface, which readily adsorbs impurities.

To reduce the impurity level, a procedure described by Weathers et al. was followed. The parting agent was dissolved in deionized water at ~50°C, freeing the carbon foil. The foils were then cleaned using a 1:100 acetic acid solution in a four minute ultrasonic bath. The foil was then transferred to a fresh acetic acid solution, where the ultrasonic bath was repeated. The foil was then transferred to deionized water, from which it was placed
onto a frame. To improve the survival rate of the foils, they were first treated with collodion. The collodion evaporated when exposed to the beam, leaving a clean carbon foil.

The effectiveness of this cleaning process was analyzed by particle induced x-ray emission (PIXE). Blank carbon foils that had been floated in deionized water were compared to foils that had been cleaned with the procedure described above. Figure 7 shows the results of this cleaning procedure. As can be seen, this procedure reduced the concentration of light element impurities.
Figure 7. Comparison of light element concentrations for cleaned and uncleaned blank carbon foils.
CHAPTER IV

ANALYSIS

The x-ray production cross sections were calculated in two ways. Where possible, the x rays were accumulated simultaneously with Rutherford scattered particles. Then, the x-ray cross section was related to the theoretical Rutherford cross section. When this method was not possible, the thickness of the target and the integrated charge were used to determine the x-ray production cross section.

For lower energy ions, the experimental cross section was calculated from the formula

\[ \sigma_x = \frac{Y_x t_p \sigma_B(\theta) \Delta \Omega}{TY_R \epsilon} \]  

where \( Y_x \) is the yield of measured x rays, \( Y_R \) is the yield of scattered particles, \( t_p \) is a detector dead time correction, \( \sigma_B(\theta) \) is the modified Rutherford differential cross section, \( \Delta \Omega \) is the solid angle subtended by the particle detector, \( \epsilon \) is the absolute detector efficiency, and \( T \) is a self-attenuation coefficient given by equation III.3. The Rutherford cross section includes a screening correction by Andersen et al.\textsuperscript{92} given as
\[ \sigma_R(\theta) = \sigma_R(\theta) \left( \frac{1}{1 + V_1/E_{cm}} \right), \]  

where \( E_{cm} \) is the center-of-mass energy for the incident ion, and \( V_1 \) is given as

\[ V_1 = 48.73 eV \frac{Z_1 Z_2}{{(Z_1^{2/3} + Z_2^{2/3})}^{3/2}}. \]

Unfortunately, elastically scattered particles do not always follow the Rutherford formula. If the energy of the ion is high enough, then it may pass close enough to the target nucleus for nuclear forces to become important. In this case, large resonances in the elastic scattering cross section may be several times that calculated by the Rutherford formula. At these high energies, use of the Rutherford cross section for x-ray normalization is inadequate.

Bozoian et al.\(^93\) have determined a formula that estimates the ion energy at which large deviations (greater than 6\%) occur. This formula, which calculates the center-of-mass energy, is

\[ E_{cm} = \frac{Z_1 Z_2 e^2}{2 r_{\text{min}}} \left[ 1 + \frac{1}{\sin(\Theta/2)} \right], \]

The collision distance, \( r_{\text{min}} \), is given by

\[ r_{\text{min}} = -\frac{Z_1 Z_2 e^2}{2 U_{\infty}} \left[ \ln \left( \frac{Z_1 Z_2 e^2}{2 U_{\infty}} \right) \right]. \]
where \( U \) is a measure of the internuclear energy taken to be 300 MeV and \( r_0 \) is 1.3 fm. For hydrogen on iron at 135°, equation (IV.4) gives a laboratory energy of 2.7 MeV. For helium on iron at 173°, this formula calculates a laboratory energy of 6.8 MeV. The x-ray production cross section could not be calculated from equation (IV.1), for ion energies above these thresholds.

At higher ion energy, the x-ray production cross section was calculated from

\[
\sigma_x = \frac{Y_x t_d}{T N_0 N_1 \epsilon},
\]

where \( N_0 \) is the target thickness in atom/cm\(^2\) and \( N_1 \) is the number of incident ions. The target thickness was obtained from Rutherford backscattering measurement and calculation at lower ion energies. The number of incident ions was found from the total integrated charge. Due to the extra errors involved in charge collection and target thickness determination, this method had a higher uncertainty than the low energy method (equations IV.4 and IV.5).

A typical x-ray spectrum is displayed in figure 8. The x-ray yields were obtained by a fitting routine applied to the experimental data. This routine was the Gupix analysis program of Maxwell et al. This program performs a linear background subtraction by employing a top hat filter for each peak within the spectrum. The filtered data is then
Figure 8. Typical x-ray spectrum. The copper target was bombarded with 2.5 MeV protons. The peak at channel 45 (0.0 keV) is a pulse processor induced noise peak.
X-Ray Energy (keV)

0.0  0.5  1.0  1.5  2.0

Counts

Carbon $K_{\alpha} = 282$ ev
Oxygen $K_{\alpha} = 523$ ev
Copper $L_{\alpha} = 928$ ev
Aluminum $K_{\alpha} = 1487$ ev
fit with gaussian peaks by a Marquardt nonlinear fitting method. This program has been tested by the analysis of PIXE spectra obtained from standard targets.\textsuperscript{95}

Errors involved in the low energy formula entered from statistical uncertainty, fitting uncertainty, and uncertainties in the measurement of the particle detector solid angle and the x-ray detector efficiency. The statistical uncertainty was kept below 2\% for all measurements. The fitting uncertainty was never above 5\% and rarely above 3\%. The measurement of the solid angle was known to 3\%, due primarily to the uncertainty in the activity of the standards used. The efficiency of the x-ray detector had a 12\% uncertainty as discussed previously. The total uncertainty was 14\%.

The high energy formula also had the above uncertainties, plus additional uncertainties involved with the target thickness and charge collection. The target thickness had a 6\% to 7\% uncertainty. The charge collection was accurate to 5\%. The total uncertainty when this method was employed was 17\% to 18\%.
CHAPTER V

RESULTS

In this chapter, the results of the measurements are presented and compared to the first Born and ECPSSR theories. Also presented, where available, are the results of previous investigators. The data are presented as a function of energy according to each ion: hydrogen, helium and lithium. Following, the same results are presented as a function of the velocity of the ion.

The two theories predict results for ionization cross sections, not x-ray production cross sections. In order to make comparison with experiment, the value calculated by these theories must be converted into x-ray production cross sections. This is done, for subshell \textit{i}, by multiplying the ionization cross section by the effective L-subshell fluorescence yield;

\[ \sigma_{L_i \gamma}^{\text{theo}} = v_{L_i} \sigma_{L_i I}^{\text{theo}}. \]  
\[ \text{V.1} \]

The effective fluorescence yields were obtained from the single-hole subshell fluorescence yields:

\[ v_{L_1} = \omega_1 + \omega_2 f_{12} + \omega_3 (f_{13} f_{12} f_{23}), \]  
\[ \text{V.2a} \]

\[ v_{L_{11}} = \omega_2 + \omega_3 f_{23}, \]  
\[ \text{V.2b} \]
The fluorescence yields, $\omega_i$, and the Coster-Kronig yields, $f_{ij}$, are from the single-vacancy values of Krause. Since the resolution of the x-ray detector could not separate the individual x-ray peaks, only total cross sections are compared. The theoretical total x-ray production cross sections are obtained by summing the three subshell x-ray production cross sections.

Hydrogen

The total L-shell x-ray production cross sections of $^{26}\text{Fe}$, $^{28}\text{Ni}$, $^{29}\text{Cu}$, $^{30}\text{Zn}$, $^{31}\text{Ga}$, and $^{32}\text{Ge}$ for hydrogen ions are presented in table IV, along with the value for the first Born and ECPSSR theories. Figures 9 through 14 graphically display this data as a function of incident ion energy.

Figures 9-11 present the results for protons on germanium, gallium and zinc. The results agree well with both theories; except for 0.5 MeV and 0.75 MeV, where both theories slightly overpredict the measurements. The results of Button et al. and Duggan et al. agree with the germanium data in the energy range investigated. The results of Button et al. are from 25% to 30% below the data for gallium and zinc in the energy range 1.0 to 2.4 MeV. The more recent investigations agree with the gallium and zinc data.
Figure 12 presents the data for copper, along with several previous results. The two theories agree well with each other and with the data for energies above 2.0 MeV. The data falls to 20% below the ECPSSR theory and 35% below the first Born theory for energies less than 2.0 MeV. The data of Khan et al. is for the L subshell only, and thus falls well below the data. The measurements of Button et al. are total cross sections, yet still are 33% below the present data. The more recent data of Duggan et al. and Orlic et al. are in much better agreement with this work.

The data for nickel are shown in figure 13. The data are in good agreement with both theories, except for a slight overprediction by the first Born theory below 2.0 MeV. The data of Duggan et al. are in good agreement with the measurements, while the data of Orlic et al. are slightly above the data.

The results for iron are presented in figure 14. No previous work could be found in this energy range. The data agree very well with both the first Born and ECPSSR theories, except at 0.5 MeV where the first Born theory overpredicts the results by 20%.

In general, the data for protons agree well with the ECPSSR and the first Born theories, except for a slight overprediction at low proton energy. The two theories give very close predictions, only 15% difference in extreme cases. The uncertainty in the measurements is such that the
Table IV. Total L-shell x-ray production cross section by protons (barns).

<table>
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<th>Energy (MeV)</th>
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<th>ECPSSR</th>
</tr>
</thead>
<tbody>
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<td>870 (\pm)130</td>
<td>1310</td>
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<tr>
<td>1.0</td>
<td>1470 (\pm)160</td>
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<td>1650</td>
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<td>1960 (\pm)220</td>
<td>2240</td>
<td>2160</td>
</tr>
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<td>2.0</td>
<td>2250 (\pm)250</td>
<td>2470</td>
<td>2420</td>
</tr>
<tr>
<td>2.5</td>
<td>2410 (\pm)270</td>
<td>2540</td>
<td>2530</td>
</tr>
<tr>
<td>3.0</td>
<td>2470 (\pm)280</td>
<td>2560</td>
<td>2560</td>
</tr>
<tr>
<td>3.5</td>
<td>2460 (\pm)280</td>
<td>2530</td>
<td>2540</td>
</tr>
<tr>
<td>4.0</td>
<td>2460 (\pm)280</td>
<td>2480</td>
<td>2500</td>
</tr>
<tr>
<td>4.5</td>
<td>2430 (\pm)270</td>
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<td>2440</td>
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Table IV (cont). Total L-shell x-ray production cross section by protons (barns).

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<th>ECPSSR</th>
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<td>1280 ±140</td>
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<td>2240</td>
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<td>2550 ±280</td>
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<td>2560</td>
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<td>2700 ±410</td>
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<td>2620</td>
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Table IV (cont). Total L-shell x-ray production cross section by protons (barns).

Zinc

<table>
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<td>2660</td>
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Table IV (cont). Total L-shell x-ray production cross section by protons (barns).

Copper

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<th>ECPSSR</th>
</tr>
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<td>1010 ±110</td>
<td>1540</td>
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<td>1620 ±290</td>
<td>2220</td>
<td>2020</td>
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</tr>
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<td>3190</td>
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<td>3170 ±450</td>
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<td>2500 ±290</td>
<td>2470</td>
<td>2480</td>
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<tr>
<td>5.0</td>
<td>2720 ±410</td>
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Table IV (cont). Total L-shell x-ray production cross section by protons (barns).

Nickel

<table>
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<th>ECPSSR</th>
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<td>0.75</td>
<td>1850 ±200</td>
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<td>1.0</td>
<td>2470 ±270</td>
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<td>2640 ±290</td>
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<td>3190 ±350</td>
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Table IV (cont). Total L-shell x-ray production cross section by protons (barns).

<table>
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<th>Energy (MeV)</th>
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<td>3210</td>
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<td>3200 ±360</td>
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</tr>
<tr>
<td>5.0</td>
<td>2430 ±370</td>
<td>2470</td>
<td>2510</td>
</tr>
</tbody>
</table>
Figure 9. Total L-shell x-ray production cross section for germanium by protons.
Cross Section (b)

Proton Energy (MeV)

- - First Born
- ECPSSR
- Button et al. (1979)
- Duggan et al. (1985)
- Marble et al. (1989)
- This Work

_32 Ge_
Figure 10. Total L-shell x-ray production cross section for gallium by protons.
First Born
ECPSSR
Button et al. (1979)
Orlić et al. (1989)
This Work
Figure 11. Total L-shell x-ray production cross section for zinc by protons.
First Born
ECPSSR
Button et al. (1979)
Pethukov et al. (1980)
This Work

Proton Energy (MeV)

Cross Section (b)

$^{30}\text{Zn}$
Figure 12. Total L-shell x-ray production cross section for copper by protons. The data for Khan et al. are for the L_3 subshell only.
$^{29}\text{Cu}$

Cross Section (b)

Proton Energy (MeV)

First Born
ECPSSR
Khan et al. (1966)
Button et al. (1979)
Pethukov et al. (1980)
Duggan et al. (1985)
Orlic et al. (1989)
Marble et al. (1989)
This Work
Figure 13. Total L-shell x-ray production cross section for nickel by protons.
First Born
ECPSSR
Pethukov et al. (1980)
Duggan et al. (1985)
Orlic et al. (1989)
This Work
Figure 14. Total L-shell x-ray production cross section for iron by protons.
data cannot distinguish between the two theories. The data matches well with the more recent measurements; however, older data sets tend to fall below the results of this investigation.

**Helium**

The results for helium ions on $^{26}$Fe, $^{28}$Ni, $^{29}$Cu, $^{30}$Zn, $^{31}$Ga, and $^{32}$Ge are presented in table II, along with the value for the first Born and ECPSSR theories. The data are also presented in figures 15 to 20 as a function of the incident helium energy.

The results for helium on germanium are presented in figure 15, along with previous work of Button et al.\textsuperscript{74} and Lapicki et al.\textsuperscript{77} The data falls slightly below the ECPSSR theory at energies of 1.0 MeV and above. The first Born theory greatly overpredicts the data at all energies, however. The first Born theory is 1.5 times the measurements at 8 MeV, and it is a factor of 4 higher at 0.5 MeV. The data also falls slightly below the results of previous investigators.

Figures 16 and 17 show the results for gallium and zinc. While the ECPSSR theory is within experimental uncertainties of the data for energies greater than 2.5 MeV, it is up to 25% higher than the data in the energy range 1.5 to 2.5 MeV. The theory again matches the data below 1.0 MeV. The first Born theory again greatly overpredicts the
data. At 0.5 MeV, the theory is approximately five times greater than the data. The results of Button et al.\textsuperscript{76} agree very well with this work.

The results for copper are presented in figure 18. The data agree very well with the ECPSSR theory for all energies measured. The first Born overpredicts the data, from 20\% at 8.0 MeV to a factor of four at 0.5 MeV. The data of Button et al. fall below the data, while the results of Lapicki et al.\textsuperscript{76} match the data fairly well.

The results for nickel are presented in figure 19. The ECPSSR again fits the data very well. There is a 25\% overprediction from 1.0 to 2.0 MeV, however. The first Born again seriously overpredicts the data. The results of Lapicki et al.\textsuperscript{76} are in good agreement at energies above 2.0 MeV, but are much greater than these results below this energy.

Figure 20 presents the results for helium on iron. The ECPSSR theory falls within experimental uncertainty at energies above 3.0 MeV or below 1 MeV. In the intermediate energies, the theory is up to 30\% above the data. The first Born theory falls well above the data, except at the highest energies.

The results for helium tend to favor the ECPSSR theory over the first Born, especially at lower energy. The ECPSSR theory falls within experimental uncertainties at all energies except within the band 1.0 to 2.5 MeV for Ge, Ga,
Table V. Total L-shell x-ray production cross section by helium ions (barns).

<table>
<thead>
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<th>Energy (MeV)</th>
<th>Experiment</th>
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Table V (cont). Total L-shell x-ray production cross section by helium ions (barns).

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<th>Energy (MeV)</th>
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<th>ECPSSR</th>
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Table V (cont). Total L-shell x-ray production cross section by helium ions (barns).

Zinc

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Table V (cont). Total L-shell x-ray production cross section by helium ions (barns).

Copper

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Table V (cont). Total L-shell x-ray production cross section by helium ions (barns).

**Nickel**

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<th>ECPSSR</th>
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Table V (cont). Total L-shell x-ray production cross section by helium ions (barns).

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<th>ECPSSR</th>
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<tr>
<td>8.0</td>
<td>14900 ±1800</td>
<td>14700</td>
<td>13800</td>
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</table>
Figure 15. Total L-shell x-ray production cross section for germanium by helium.
This Work

first Born

ECPSSR

Button et al. (1979)

Lapicki et al. (1986)

This Work

Helium Energy (MeV)

Cross Section (b)

$^{32}\text{Ge}$
Figure 16. Total L-shell x-ray production cross section for gallium by helium.
$3_{1}Ga$

Cross Section (b)

0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0
Helium Energy (MeV)

- - first Born
ECPSSR

Button et al. (1979)
This Work
Figure 17. Total L-shell x-ray production cross section for zinc by helium.
$30\text{Zn}$

- - first Born
--- ECPSSR
○ Button et al. (1979)
■ This Work
Figure 18. Total L-shell x-ray production cross section for copper by helium.
First Born
ECPSSR
Button et al. (1979)
Lapicki et al. (1986)
This Work
Figure 19. Total L-shell x-ray production cross section for nickel by helium.
$^{28}\text{Ni}$

Cross Section (b)

Helium Energy (MeV)

- first Born
- ECPSSR
- Lapicki et al. (1986)
- This Work
Figure 20. Total L-shell x-ray production cross section for iron by helium.
Zn, and Fe. In this region for these elements, the theory slightly overpredicts the data. Except for germanium, the first Born theory agrees with the data at high energy, slightly overpredict the data at intermediate energies, and is several times greater than the data at the lowest energies.

Lithium

The L-shell x-ray production cross sections for lithium ions on $^{20}$Ca, $^{26}$Fe, $^{28}$Ni, $^{29}$Cu, and $^{32}$Ge are presented in table VI, along with the values for the first Born and ECPSSR theories. Figures 21 through 25 graphically present this data as a function of incident ion energy.

The results for lithium on germanium, copper, and nickel are presented in figures 21 through 23. For each of these elements, the first Born theory greatly overpredicts the data, by a factor of two greater than the data at 4.5 MeV to a factor of four at 0.75 MeV. The ECPSSR theory, while significantly closer than the first Born theory, also overpredicts the data at 2.0 to 4.5 MeV. The theory matches well with the data at 1.0 MeV and below.

Figure 24 shows the data x-ray cross sections of iron for lithium ions. The ECPSSR theory is within the experimental uncertainty for all data points. The first Born theory still overpredicts the data, by factors of 2 to 3.
Table VI. Total L-shell x-ray production cross section by Li$^+$ ions (barns).

<table>
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<tr>
<th>Energy (MeV)</th>
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</tr>
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Table VI (cont). Total L-shell x-ray production cross section by Li⁺ ions (barns).

Copper

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<th>ECPSSR</th>
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Table VI (cont). Total L-shell x-ray production cross section by Li$^+$ ions (barns).

<table>
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Table VI (cont). Total L-shell x-ray production cross section by Li$^+$ ions (barns).

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<th>ECPSSR</th>
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Table VI (cont). Total L-shell x-ray production cross section by Li$^+$ ions (barns).

**Calcium**

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<th>ECPSSR</th>
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<td>2220 ±400</td>
<td>7180</td>
<td>3120</td>
</tr>
<tr>
<td>2.0</td>
<td>2710 ±400</td>
<td>8530</td>
<td>4550</td>
</tr>
<tr>
<td>2.5</td>
<td>3790 ±560</td>
<td>9410</td>
<td>5720</td>
</tr>
<tr>
<td>3.0</td>
<td>3960 ±710</td>
<td>9900</td>
<td>6590</td>
</tr>
<tr>
<td>3.5</td>
<td>4500 ±810</td>
<td>10200</td>
<td>7220</td>
</tr>
<tr>
<td>4.0</td>
<td>4612 ±830</td>
<td>10200</td>
<td>7610</td>
</tr>
<tr>
<td>4.5</td>
<td>4960 ±890</td>
<td>10100</td>
<td>7930</td>
</tr>
</tbody>
</table>
Figure 21. Total L-shell x-ray production cross section for germanium by Li⁺ ions.
Cross Section (b)

\[ 10^0 \quad 10^1 \quad 10^2 \quad 10^3 \quad 10^4 \]

Lithium Energy (MeV)

\[ 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 10 \]

- - First Born
ECPSSR
This Work

\[ ^{32}\text{Ge} \]
Figure 22. Total L-shell x-ray production cross section for copper by Li⁺ ions.
Figure 23. Total L-shell x-ray production cross section for nickel by Li$^+$ ions.
$^{28}$Ni

Cross Section (b)

Lithium Energy (MeV)

- First Born
- ECPSSR
- This Work
Figure 24. Total L-shell x-ray production cross section for iron by Li$^+$ ions.
Figure 25. Total L-shell x-ray production cross section for calcium by Li⁺ ions.
Cross Section (b)

Lithium Energy (MeV)

- - First Born
- - ECPSSR
- - This Work

20Ca
The data for calcium is presented in figure 25. The first Born theory is still very high, a factor of 2 to 6 above the data. The ECPSSR theory is closer to the data. This theory overpredicts the measurements by 30% to 45% in the energy range 2.0 to 4.5 MeV. At 1 MeV the data matches the ECPSSR theory. The overprediction could be due to the chemical compound used to fabricate the target, since the chemical environment can alter the fluorescence yield.\(^9\)

For lithium ions, the ECPSSR theory is a significant improvement over the first Born theory. Yet, the ECPSSR theory tends to over-predict the data from 2.0 to 4.5 MeV. Only for iron does the theory match the data well.

**Cross Section Ratios**

In order to take a closer look at the data in the low energy regime, figures 26-31 present the ratio of the experimental cross section to both the first Born theory and the ECPSSR theory. This data is presented as a function of the scaled ion velocity, \(v_i/v_{2\ell}\), where \(v_{2\ell}\) is the electron velocity as calculated by the Bohr model.

Figure 26 presents the ratio of experiment to theory for germanium. The first Born theory shows a dramatic overprediction of the data when the velocity ratio 0.50 for hydrogen and 0.75 for helium. X-ray production cross sections for lithium ions, at even lower velocity ratios, fall well below the first Born theory. The ECPSSR is much
closer to the data at low ion velocity. However, it overpredicts the data by 20% to 35% in the velocity range 0.45 to 0.12. The ratio of the experiment to the ECPSSR theory shows a minimum at a velocity ratio of ~0.2. At very low velocity, the ratio of experiment to ECPSSR crosses 1.0, and continues to increase.

Figures 27 and 28 display the experimental to theoretical ratios for gallium and zinc. For gallium, the ratio for the first Born theory falls below 0.8 at velocities of 0.42 for hydrogen and 0.56 for helium. These values are 0.45 and 0.51 for zinc. The ECPSSR theory again is much better than the first Born. However, the data falls to 25% below the ECPSSR theory in the velocity region 0.35 to 0.25.

The experimental to theoretical ratios for copper are shown in figure 29. The first Born ratios follow the familiar trend, falling below 0.8 at an ion velocity of 0.5. The ECPSSR ratios for helium are 25% to 30% above hydrogen and lithium at equal velocities, a discrepancy not seen with other elements. The ECPSSR ratio for hydrogen is within experimental uncertainty, except at the lowest velocity measured (0.38). The helium data matches the ECPSSR theory very well. The lithium data exhibits the crossover behavior, having a value of 1.45 at a velocity of .084.

The experimental to theoretical ratios for nickel are presented in figure 30. The first Born ratio falls below
0.8 at a velocity of 0.52. The ECPSSR theory matches the data very well for velocities above 0.40. However, the data falls 25% below the theory at a velocity of 0.2. The lowest velocity measured, 0.087, is at a ECPSSR ratio of 1.6.

Figure 31 displays the experimental to theoretical ratio for iron. The first Born theory matches the hydrogen data well, but the helium falls below 0.8 at a velocity of 0.65. The ECPSSR is in good agreement with the data for velocities above 0.43. For velocities from 0.26 to 0.33, the ECPSSR theory is at least 25% above the data. At the lowest velocities, the data lies above the ECPSSR theory.
Figure 26. Ratio of the experimental cross section to the theoretical cross section for germanium. Open symbols represent the first Born theory, and closed symbols represent the ECPSSR theory. The graphs are a function of the ion velocity over the electron velocity.
Figure 27. Ratio of the experimental cross section to the theoretical cross section for gallium. Open symbols represent the first Born theory, and closed symbols represent the ECPSSR theory. The graphs are a function of the ion velocity over the electron velocity.
Figure 28. Ratio of the experimental cross section to the theoretical cross section for zinc. Open symbols represent the first Born theory, and closed symbols represent the ECPSSR theory. The graphs are a function of the ion velocity over the electron velocity.
Figure 29. Ratio of the experimental cross section to the theoretical cross section for copper. Open symbols represent the first Born theory, and closed symbols represent the ECPSSR theory. The graphs are a function of the ion velocity over the electron velocity.
Figure 30. Ratio of the experimental cross section to the theoretical cross section for nickel. Open symbols represent the first Born theory, and closed symbols represent the ECPSSR theory. The graphs are a function of the ion velocity over the electron velocity.
Figure 31. Ratio of the experimental cross section to the theoretical cross section for iron. Open symbols represent the first Born theory, and closed symbols represent the ECPSSR theory. The graphs are a function of the ion velocity over the electron velocity.
CHAPTER VI

CONCLUSION

Total L-shell x-ray production cross sections have been measured for $^{20}$Ca, $^{26}$Fe, $^{28}$Ni, $^{29}$Cu, $^{30}$Zn, $^{31}$Ga, and $^{32}$Ge by 0.5 to 5.0 MeV protons, 0.5 to 8.0 MeV helium ions, and 0.75 to 4.5 MeV lithium ions. The data have been compared to both the first Born and the ECPSSR theories. The data have also been compared to the results of previous investigators, where experimental data was available. The data in this report are in best agreement with the more recent measurements.

The first Born theory fails to predict the measurements at low ion velocity. The data fall below a 20% discrepancy at a velocity ratio of -0.55. The ECPSSR theory does succeed at extending the velocity regime in which the Born calculations may be applied. This theory matches the data very well for velocity ratios above 0.40. However, the ECPSSR theory also overpredicts the data by ~25% in the velocity region 0.25 to 0.35. A crossover behavior is observed for velocities less than 0.10, with the data falling above the ECPSSR theory.

In general, the ECPSSR theory is an improvement over the first Born theory, especially at low ion velocity. It
is seen to fail at the lowest ion velocities measured. In this region, velocity of the ion is much less than the velocity of the electron. Thus Pauli excitation from quasi-molecular production, an effect not considered in the ECPSSR theory, will have a significant contribution to the total ionization cross section. This limits the velocity regime in which the ECPSSR theory may be expected to successfully predict the data.

The depression in the cross section for the velocity region from 0.25 to 0.35 is most likely due to the increased binding correction. For velocities slightly above the region where quasi-molecular orbits began to form, large perturbations may be expected in the electron's orbit due to the presence of the ion. The first order calculation of the increased binding energy is insufficient for such gross changes in the wave function.
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