Electron Impact Ionization of Highly Charged Lithiumlike Ions

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(Ph.D. Thesis)

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Electron Impact Ionization of Highly Charged Lithiumlike Ions

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Abstract

Electron impact ionization cross sections can provide valuable information about the charge-state and power balance of highly charged ions in laboratory and astrophysical plasmas. In the present work, a novel technique based on x-ray measurements has been used to infer the ionization cross section of highly charged lithiumlike ions on the Livermore electron beam ion trap. In particular, a correspondence is established between an observed x ray and an ionization event. The measurements are made at one energy corresponding to approximately 2.3 times the threshold energy for ionization of lithiumlike ions. The technique is applied to the transition metals between Z=22 (titanium, Ti$^{19+}$) and Z=26 (iron, Fe$^{22+}$) and to Z=56 (barium, Ba$^{53+}$). The results for the transition metals, which have an estimated 17-33% uncertainty, are in good overall agreement with a relativistic distorted-wave calculation. However, less good agreement is found for barium, which has a larger uncertainty. Methods for properly accounting for the polarization in the x-ray intensities and for inferring the charge-state abundances from x-ray observations, which were developed for the ionization measurements, as well as an x-ray model that assists in the proper interpretation of the data are also presented.
To my parents, Alice and the late Calvin Wong, and to my family
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Chapter 1

Introduction

1.1 Ionization of Highly Charged Ions

Electron impact ionization is one of the fundamental collision processes that influences the evolution of both laboratory and astrophysical plasmas. Plasma properties such as the power balance, line radiation, and charge-state distributions depend on the values of ionization cross sections and rates [1, 2, 3]. To predict and interpret these properties accurate knowledge of ionization cross sections and rates is needed. Because of the lack of data scaling laws are commonly used for ionization cross sections in modeling programs [4]. These formulations are believed to be accurate to only within a factor of 2 [2]. Measurements of ionization are needed to test these approximations that are frequently used in plasma models and to provide data to test fundamental theories.

There is a particular need for ionization data in fusion research. Ionization data is important, for example, for inferring the radial transport of impurity ions such as Ti, Cr, and Fe in tokamaks from spectral observations and for determining the power balance. High concentrations of these transition metal impurities (Z=22-28), which occur due to sputtering of vacuum wall and limiter material, are detrimental in that they cool the plasma by emitting line radiation. Isler et al. [5] was the first to determine that im-
purity concentrations as small as 0.1% in tokamaks can account for 40-80% of the radiated power. They can also trigger instabilities and disruptions of current flow.

The data on electron impact ionization pertinent to fusion has come from primarily two experimental techniques. The crossed electron-ion beam method and plasma spectroscopy experiments. Absolute ionization cross sections have been measured using the crossed beam technique. These experiments have small uncertainties, typically 8-10%, and cross sections have been measured for Ti, Cr, and Fe ions up to +15 \([6, 7, 8]\). The plasma spectroscopy method is another approach to measuring ionization. This technique is used to determine ionization rates, i.e., the product of the cross section and the electron velocity averaged over the Maxwellian velocity distribution. Although this technique has been used to measure rates in Ti and Fe for charge-states up to +21 \([9, 10]\) in tokamaks, it is model dependent. In particular, this method finds a set of ionization and recombination rates that best describes the observed spectra. In addition, it is somewhat circular in that theoretical ionization and recombination rates are adjusted iteratively to least squares fit the data. The accuracy of these ionization rates is estimated to be only 20-40%.

Because of their crucial role in laboratory and astrophysical plasma research, there is clearly a need for accurate ionization cross section measurements for highly charged transition metal ions, which has not yet been met with the current experimental methods. The purpose of this thesis is to provide such data. This is accomplished by using a novel x-ray technique to study electron-impact ionization on an Electron Beam Ion Trap (EBIT). The ionization cross sections that were measured are for highly charged lithium-like ions, in particular for the process

\[
1s^2 2s + e^- \rightarrow 1s^2 + 2e^-.
\]

This is done for the ions Ti\(^{19+}\), V\(^{20+}\), Cr\(^{21+}\), Mn\(^{22+}\), Fe\(^{23+}\), and Ba\(^{53+}\) \((Z=22-26,56)\).
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1.2 The Physics of Lithiumlike Ions

1.2.1 Atomic Structure

The ground state of a lithiumlike ion represents a configuration with one electron outside a heliumlike closed shell:

$$1s^2 2s.$$ 

Excited states are formed by excitation of an electron from the 2s level to a 2p level ($\Delta n=0$ transitions), 1s to a 2s or 2p level ($\Delta n=1$ transitions), and 1s or 2s to levels with even higher principal quantum number. In this thesis, where we use a spectroscopic technique for measuring ionization cross sections, we will be concerned with excited states of the type $1s^2 2s 2p$ that are separated from the ground state via $\Delta n=1$ transitions.

Excited states in lithiumlike ions are also formed by the process of dielectronic recombination of heliumlike ions. Dielectronic recombination is a resonance process in which an incoming electron excites an electron in the ion and itself becomes bound forming a doubly excited state. The excited state may decay by autoionization (Auger decay), the inverse process of dielectronic recombination. However, if the state decays radiatively, the electron remains with the ion, and the recombination process is completed. Dielectronic recombination on heliumlike ions can be represented by:

$$1s^2 + e^- \rightarrow 1s 2l' 2l'' \rightarrow 1s^2 2l + h\nu.$$ 

This process also results in lithiumlike $\Delta n=1$ transitions. We will use the Auger notation to label the resonances; the KLL resonances, for example, have an intermediate state in which an electron is captured into the L shell, and a bound electron is excited from the K shell to the L shell.

For the highly charged lithiumlike transition metal ions Ti, V, Cr, Mn, and Fe ($Z=22-26$) relativistic effects become important [11], and intermediate coupling (IC) is used to describe the excited states, i.e., a coupling
scheme between L-S and j-j coupling. In intermediate coupling the electrostatic interaction between electrons (L-S) and the spin-orbit interaction (j-j) are treated on an equal basis [12]. For lithiumlike excited states this is approximately the case for ions with nuclear charge Z \geq 14 [13]. In this scheme the excited states are designated by either the L-S or j-j notation. In the L-S notation the interaction between the individual orbital angular momenta \( l_i \) and spin angular momenta \( s_i \) of each electron are strong, and they combine to give resultant \( L \) and \( S \) values, where \( L = |l_1 - l_2|, ..., |l_1 + l_2| \) and \( S = |s_1 - s_2|, ..., |s_1 + s_2| \). The resultant \( L \) and \( S \) values then combine to yield the value total angular momentum \( J \), where \( J = |L - S|, ..., |L + S| \).

Using this coupling scheme lithiumlike excited states are designated by the notation \( 2S+1LJ \) where \( L \) and \( S \) are the resultant angular momentum of the \((1s2l)\) core and the \( 2l' \) electron.

However, for lithiumlike ions with an atomic number as high as barium (Z=56) j-j coupling is used to describe the states because the spin-orbit interaction is more important than the electrostatic interaction between electrons [14]. In this scheme the orbital angular momentum \( l \) and the spin angular momentum \( s = 1/2 \) of each electron are coupled to give the total angular momentum \( j = |l \pm s| \). The values of \( j \) then combine to yield the value of total angular momentum \( J \). Using this coupling scheme lithiumlike excited states are designated by the notation \( (j_1,j_2)J \), where \( j_1 \) is the angular momentum of the \((1s2l)\) core, \( j_2 \) is the angular momentum of the \(2l'\) electron, and the total angular momentum \( J \) is given by \( J = |j_1 - j_2|, ..., |j_1 + j_2| \).

The energy level differences due to electrostatic differences between electrons that have the same principal quantum number \( n \) but different orbital angular quantum number \( l \) scale as [15]:

\[
\Delta E(l) = E_{nl_1} - E_{nl_2} \sim Z_{\text{eff}}. \tag{1.1}
\]

where \( Z_{\text{eff}} \) is equal to the nuclear charge minus the effective screening of the electrons [16]. The energy level differences due to the fine structure splitting
is given by [17]:

$$\Delta E(j) = E_{nj} - E_{n^2} = \frac{\alpha^2 Z_{\text{eff}}^4}{n^3(i+1)} E_{Ry} \sim Z_{\text{eff}}^4.$$  \hspace{1cm} (1.2)

where the equality is for hydrogenic ions and $E_{Ry} \approx 13.6$ eV is the ionization energy of hydrogen. An example of this x-ray transition energy scaling will be shown later for the case when $Z$ increases from 26 (Fe) to 56 (Ba).

### 1.2.2 Forbidden versus Allowed Transitions

The excited lithium-like ions, which are produced by the process of direct excitation or dielectronic recombination, decay in $\Delta n=1$ transitions to the ground state observable in the x-ray region. Following the selection rules for transitions between two eigenstates in $j,j$ coupling [18] we expect to observe allowed electric dipole ($E1$) transitions. In these types of transitions parity changes, and the total angular momentum $J$ changes by $\Delta J = 0, \pm 1$ with the restriction that $J=0 \rightarrow J=0$ transitions are forbidden [19]. For highly charged ions we expect to observe forbidden or higher multipole transitions. The next higher transitions are [20]: the electric quadrupole ($E2$), for which parity remains fixed and $\Delta J = 0, \pm 1, \pm 2$; the magnetic dipole ($M1$), for which parity remains fixed and $\Delta J = 0, \pm 1$; and the magnetic quadrupole ($M2$), for which parity changes and $\Delta J = 0, \pm 1, \pm 2$.

### 1.3 Previous Experimental Techniques

In recent years there has been much progress in the experimental studies of highly charged ions. Particle accelerators and new ion sources such as the electron cyclotron ion source (ECR) [21] and electron beam ion source (EBIS) [22] have made measurements of multiply-charged ions possible. In addition, tokamaks are capable of high electron temperatures and confinement times making studies of highly charged ions possible. In this section
we will discuss three alternative methods of determining ionization cross sections and rates, which employ the different experimental apparatuses listed above.

1.3.1 Beam Experiments

The crossed electron-ion beam method has provided the most accurate and detailed information of electron impact ionization of ions of fusion interest. Absolute ionization cross sections of ions have been measured since 1961, when Dolder et al. originated the technique [23]. Subsequently, ionization cross sections for Ti, Cr, and Fe with charge states up to +15 have been measured using an ECR ion source [6, 7, 8]. The results this method provides are highly accurate with typical uncertainties of 8-10%, and the cross sections are obtained as a function of beam energy. Moreover, the crossed beam technique provides the highest energy resolution and is the only method in which indirect, near threshold processes such as excitation-autoionization and resonance excitation followed by double autoionization have been studied [24].

The method consists of crossing a collimated beam of ions of known charge state with a monoenergetic beam of electrons at an angle $\theta$. The resultant ions are then analyzed magnetically or electrostatically and collected by Faraday cups. The cross section as a function of electron beam energy is determined by the currents and velocities of the particles and the beam overlap of the electrons and the ions. The electron beam energy so far is limited to $\leq 1.5$ keV.

In accelerator based beam experiments, where a beam of ions collides with a gaseous [25] or a crystal target [26], charge states up to $O^{7+}$ and $U^{91+}$ have been measured, respectively. In the rest frame of the projectile ion the target acts as the electron beam, e.g., the electron-ion interaction energy is 222 keV for the U experiment. In the particular case of the crystal channeling experiment, the crystal is rotated until collisions of the U ions of known charge state with the Si crystal nuclei are distant. The ions, therefore,
only interact with the electrons of the Si (110) crystal plane. Once the U ions of known charge state have channeled through the Si (110) plane, they are magnetically analyzed and detected with a position sensitive proportional counter. The electron density is determined from the radiative capture of electrons by the channeled ions. U ions that have captured an electron are also seen in the charge-state spectra. The electron density is believed to be a major source of uncertainty in this measurement. The ionization cross sections inferred using this method are estimated to be accurate to only a factor of 2.

1.3.2 Plasma Spectroscopy

The plasma spectroscopy technique is based on modeling the x-ray spectra from a well diagnosed plasma in theta-pinches [27] and tokamaks [28]. Ionization rates, i.e. the product of the cross section and the electron velocity averaged over the Maxwellian electron velocity distribution, are inferred. In theta-pinches the time evolved line emission of x rays from impurity ions in different ionization stages is recorded following the initial compression of the plasma. Concurrently, the electron temperature and density are measured. These two parameters are used as input for a program, which models the time history of the x-ray lines. The simulation is done iteratively by varying the ionization and recombination rates until the modeled data best fits the experimental data. The major limitation of the measurements from theta-pinches is that because of low electron temperatures, typically a few hundred eV, only ions of relatively low charge state such as Ti$^{8+}$ can be studied [29].

On the other hand, in high temperature devices such as tokamaks one takes advantage of a magnetohydrodynamic (MHD) instability, which is linked to variations in the electron temperature while the electron density is essentially constant, to measure ionization rates. This instability causes a sawtooth-like modulation of the x-ray intensity and is therefore dubbed the sawtooth instability [30]. The modulation of the x-ray emission is then mod-
eled with the rate coefficients (ionization and recombination) as adjustable parameters until the calculation best matches the experimental data. Ionization rates for Ar, Ti, and Fe have been inferred for charge states up to $+15$, $+19$, and $+21$ [9, 10, 31], respectively.

Although this technique has thus far provided the highest charge-state measurements of ionization of the transition metals, it has disadvantages. The method is model dependent and relies on approximate formulas for ionization and recombination. It measures many rates at once and the details are washed out in the least squares fit. In addition, ionization rates are balanced by recombination rates, which compensate for each other, e.g., if one rate is multiplied by 2 the other must also be multiplied by 2. Therefore, this is only a relative rate measurement. The method is also dependent on electron temperature and density measurements, and the uncertainties in measurements of these quantities translates into uncertainties in the ionization rates. Furthermore, a sensitivity study of the ionization rates determined from the tokamak measurements show the rates accurate to only 20-40%.

### 1.3.3 Trapped-Ion Method

The trapped ion method consists of trapping ions in an electric and/or magnetic field and ionizing them with an electron beam. The cross section for successive ionization to higher charge states is determined from extracting and analyzing the ions as a function of the time the ions spend in the trap. *The ions are analysed using a mass spectrometer or a time of flight analysis.*

The best experiments using this technique has been the work of Donets and Ovsyannikov [32]. They varied the trapping time of ions in an EBIS and measured the time history of the charge-state distribution for Ar up to $+21$, Kr up to $+33$, and Xe up to $+47$ [32]. The ionization cross sections are determined using a similar modeling and fitting procedure used in the plasma spectroscopy technique in which the ionization cross sections are fit parameters. Ionization from the ground state is the only fit parameter and
other processes such as multiple ionization, charge exchange, recombination, and ion losses from the trap are neglected. Despite the simplicity of the model, the results are in good agreement with crossed beam data where comparison is possible. The uncertainties range from 10-20%; however, for heavier ions ignoring multiple ionization may cause the uncertainties to be much larger.

1.4 Theoretical Approaches

The complete theoretical solution to the electron impact ionization of an atom or ion is a very complex problem and has not been done. In general, one must solve the long range Coulomb three-body problem with a final state of two electrons in the continuum. However, several classical, semi-classical, quantum, and semi-empirical approximations exist to calculate these cross sections.

1.4.1 Classical and Semi-Classical Methods

Thomson in 1912 [33] made the first attempt to solve the problem of electron impact ionization of atoms. He determined a total ionization cross section by using energy conservation in the collision between an incident electron and a target electron assumed at rest. The total ionization cross section at a collision energy $E$ is:

$$
\sigma(E) = 4\pi^2 a_0^2 \frac{E_{Ry}}{E_b} \frac{q_i}{E} \left(1 - \frac{E_b}{E}\right),
$$

where $a_0 = 0.529 \, \text{Å}$ (Bohr radius), $E_{Ry} = 13.6 \, \text{eV}$, and $q_i =$ number of equivalent electrons of a shell with binding energy $E_b$. The major shortcoming of the theory is the incorrect high energy dependence of Eq. (1.3). Bethe in 1930 [34] derived the correct dependence at high energy using the first quantum calculation. The ionization cross section behaves like:

$$
\sigma \sim A \frac{\ln(x)}{x} + \frac{B}{x},
$$

(1.4)
where $x = E/E_0$ is the reduced energy, and $A$ and $B$ are constants.

Despite the inadequacy of the classical theory for ionization of atoms at high energy, the theory has been extended to ions because of its simplicity. Binary Encounter Approximations (BEA) include the Coulomb effect of the target ion on the incident electron, i.e., when the electron is close to ion, it accelerates toward the ion. Gryziński in 1959 [35] improved the approximation by removing the constraint that the target electrons are at rest before the collision. He assumed that the target electrons had a distribution of initial velocities. Burgess in 1963 [36, 37] made a further modification by adding quantum features such as electron exchange and interference. This method was known as the exchange-classical (EC) approximation.

Another classical approach was proposed by Alder in 1956 [38], which is based on the impact parameter method (IP) of treating collisions. In this approximation the many body effects are accounted for, and the binary collision process is removed. The correct high energy behavior is reproduced in this theory.

Lastly, the exchange-classical impact parameter (ECIP) [36, 37] method uses the advantages of the (EC) and the (IP) approaches and includes quantum features in computing ionization. The (EC) approach is used for electron collisions close to the ion ($r < R_0$). In this region electron exchange at the target ion and interference between outgoing electrons is accounted for. For ($r > R_0$) the impact parameter approximation is used and the correct high energy dependence is preserved. The main difficulty in this technique is choosing a suitable cutoff impact parameter $R_0$.

1.4.2 Quantum Methods

Bethe in 1930 [34] performed the first quantum calculation using the Born approximation. In this formulation the incident and outgoing electron wavefunctions are plane waves. The plane waves are expanded in terms of spherical Bessel functions. The electron-electron and electron-nucleus interactions
CHAPTER 1. INTRODUCTION

are treated as perturbations. The ionization cross section is determined from the square of the matrix element of the perturbation terms and the initial and final plane waves using Fermi's golden rule [39]. The results of the Born approximation are good at high energies or for fast collisions, i.e., the speed of the incident electron compared to the orbital velocity of the target electron. At low energies the cross sections are underestimated, particularly for highly charged ions.

The quantum mechanical approach, which is used the most in calculating ionization cross sections is the Coulomb-Born approximation. This technique is a modification of the Born approximation in which the ionizing and ejected electron wave functions are described by Coulomb waves instead of plane waves. In this case the electron-ion interaction term $-Ze^2/r_e$ is more important than the electron-electron term $\sum_j e^2/r_{ej}$, where $Z$ is the nuclear charge of the target atom or ion, $e$ is the charge of the electron, $r_e$ is the distance between the projectile electron and the target nucleus, and $r_{ej}$ is the inter-electron distance between the projectile electron and all the bound target electrons. The cross section is determined by the square of the matrix element of the electron-electron perturbation term interacting with the final and initial Coulomb wave functions again using Fermi's golden rule [39]. A variant of the Coulomb-Born approximation with exchange is the infinite $Z$ or scaled hydrogenic approximation. In this case a change in the radial scale of the many-electron Hamiltonian gives an unperturbed Hamiltonian equivalent to the hydrogenic case plus an electron-electron perturbation term times $1/Z$. Sampson, Golden, and Moores [40, 41] have applied this approximation to the ionization of the orbitals 1s through 4f. The method is inadequate when the target potential has a large influence on the Coulomb waves, i.e., in slow collisions.

A further modification of the Coulomb-Born method is the distorted-wave approximation, which accounts for the screening of the target ion by bound electrons. In this approach distorted waves replace the Coulomb waves when the ionizing electron is close to the target ion. Younger has success-
fully applied this technique to obtain cross sections for the ionization of highly charged hydrogen-, helium-, lithium-, and sodiumlike ions [42, 43, 44]. Zhang et al. extended this approximation using a rapid relativistic distorted wave formulation [45, 46]. In this method the Dirac equation replaces the Schrödinger equation, and the distorted waves are expansions of the Dirac spinors.

In order to account for indirect effects near threshold such as inner-shell excitation followed by autoionization the closed-coupling/Coulomb-Born or R-matrix method [47] is used. In this approach one must solve a set of coupled integrodifferential equations to determine the wavefunctions. The incident electron and the target ion form a compound intermediate state. This is an example of a slow collision. By selecting suitable target configurations it is possible to include such effects as those of excitation-autoionization in the calculated ionization cross sections.

1.4.3 Semi-Empirical Methods

In order to provide reasonably accurate estimates of ionization cross sections for a wide variety of elements, charge states, and energies for plasma modeling semi-empirical formulas have been proposed. The most widely used is the Lotz formula [48, 49, 50]:

$$\sigma(E) = \sum_{i=1}^{3} a_i q_i \ln \left( \frac{E}{E_b} \right) \left( 1 - b_i \exp \left[ -c_i (E/E_b - 1) \right] \right),$$  \hspace{1cm} (1.5)

where $E$ is the energy of the electron impact, $q_i$ is number of equivalent electrons in the $i$-th subshell with binding energy $E_b$. The coefficients $a_i$, $b_i$, and $c_i$ are tabulated constants, which have been fitted to best reproduce the existing experimental ionization data. The Lotz formula is based in part on Coulomb-Born calculations for hydrogenic ions and has the correct high energy dependence. The error in the formula is estimated to be less than $\pm40\%$ for ions where indirect processes are not important. The ionization cross sections predicted reflect only direct contributions. For ions in charge states
it is customary to set \( b_i = c_i = 0 \) and \( a_i = 4.5 \times 10^{-14} \text{ cm}^2\text{eV}^2 \), which gives the usual one-parameter Lotz formula.

A similar formula has been proposed by Burgess and Chidichimo [51] to account for indirect process near threshold such as inner-shell excitation-autoionization. Their formula is:

\[
\sigma(E) = C \sum_j q_j (E_{Ry}/E_j)^2 (E_j/E) \ln(E/E_j) W(E/E_j) \pi a_0^2, \tag{1.6}
\]

where \( E_{Ry} = 13.6 \text{ eV} \), \( a_0 = 0.529 \text{ Å (Bohr radius)} \), \( W(E/E_j) = 0 \) for \( E \leq E_j \) and \( W(E/E_j) = \ln(E/E_j)^n E_j/E \) for \( E > E_j \), \( n \approx 1 \), \( C = 2.30 \) is an empirical constant, \( E_j \) is the ionization or excitation energy of the \( j^{th} \) shell or subshell, and \( q_j \) = occupation number of \( j^{th} \) shell or subshell. The function \( W(E/E_j) \) assures the correct threshold behavior and approach unity at very high energies, thus preserving the asymptotic Bethe energy dependence. The constant \( C \) is determined empirically from a fit to all the available cross section data.

Excitation-autoionization is included in the same manner as direct ionization, except that the lowest excitation threshold energy is used for \( E_j \). Thus, the direct and indirect contributions can be separated. The Burgess-Chidichimo formula gives reasonable predictions for the cross section and is an improvement over the Lotz formula since a much larger data base was used.

### 1.5 Short Overview of This Work and Organization of Thesis

In this thesis we report on ionization measurements of highly charged lithium-like titanium (\( Z=22 \)), vanadium (\( Z=23 \)), chromium (\( Z=24 \)), manganese (\( Z=25 \)), iron (\( Z=26 \)), and barium (\( Z=56 \)) ions made on an electron-beam ion trap (EBIT). The measurements were made using a novel technique that relies on the observations of x rays. The technique thus contrasts with those based on particles, commonly used in accelerator, ECR ion source, and EBIS...
CHAPTER 1. INTRODUCTION

Based experiments. EBIT is a tool for studying the x rays of highly charged ions, presently up to U$^{89+}$ [52, 53, 54], and the technique developed in this thesis, in principle, allows us to measure the ionization cross section of any of these lithium-like ions. These charge states are much higher than those currently available with either the crossed beam or the plasma spectroscopy approaches. Moreover, EBIT has the advantage of measuring electron-ion collision cross sections rather than rates. In the current set of measurements of ionization the electron beam energy is a factor of two to three times higher than the beam energy of the crossed beam experiments. The uncertainties in this technique are on the order of the best plasma spectroscopy measurements.

The instrumentation with which the measurements have been carried out is described in Chapter 2 together with a brief description and overview of EBIT. The x-ray measurements were performed using a solid-state germanium (Ge) detector and a high resolution Bragg crystal spectrometer. The solid-state detector provides x-ray information over a wide range of energies 1-100 keV in our measurements of bare, hydrogen-like, helium-like, lithium-like, and beryllium-like ions, while the crystal spectrometer resolves the individual components of the broad solid-state detector peaks in the range from 4-7 keV of the same ions except the bare charge state.

In Chapter 3 we show an example of how the linear polarization of the x rays from EBIT resulting from the excitation of the ions by an electron beam affects the line ratio measurements and how we account for it. This is important for the ionization measurements because the x-ray intensities measured by the solid-state detector and crystal spectrometer are affected by polarization. In particular, we present a measurement of the ratio of the unpolarized Ly-$\alpha_2$ (2$p_{1/2} \rightarrow 1s_{1/2}$) transition relative to the polarized Ly-$\alpha_1$ (2$p_{3/2} \rightarrow 1s_{3/2}$) transition in hydrogen-like iron. There are two effects (1) polarization causes the angular distribution of the x rays to be non-isotropic and (2) the crystal spectrometer acts as a polarizer that preferentially reflects one component of the polarization.
A comprehensive study of how we determine the charge-state balance of the ions from x-ray observations is presented in Chapter 4. Understanding how the charge-state abundances are inferred from the x-ray measurements is crucial because later in the chapter on determining ionization cross sections these same techniques are used. Here we also present a comparison of the ionization balance from the x-ray measurements with a model calculation and with the ions extracted out of the trap.

We present the ionization measurements using two techniques in Chapter 5. In the first technique we infer cross sections from x-ray measurements using a solid-state germanium (Ge) detector and normalize to the theoretical radiative recombination\(^1\) cross section onto lithiumlike ions. In the second approach ionization cross sections are determined from high resolution crystal spectrometer measurements and are normalized to theoretically and experimentally determined values of the direct excitation cross section of the lithiumlike line \(q\) \(1s^2s(3S)2p \ ^2P_{3/2} \rightarrow 1s^22s \ ^2S_{1/2}\). The experimental measurement of the cross section of line \(q\) is in turn also normalized to the radiative recombination cross section onto lithiumlike ions. As a subsection to the description of the technique, we also demonstrate the method of determining the excitation cross section of the other heliumlike and lithiumlike direct excitation lines present in the spectrum. In the analysis we modeled the charge-state balance in the trap and the resulting x-ray spectra. The comparison between the experimental and the modeled x-ray spectra is important because the model is used to properly interpret the ionization balance during the experiment and to infer the effect of charge-exchange recombination of the ions with background gases in EBIT.

In Chapter 6 we present the results of the ionization and direct excitation cross sections and compare the results to theoretical values. We also discuss the uncertainties in the measurements. Furthermore, the advantages and disadvantages are discussed for the techniques.

\(^1\)X rays resulting from the capture of a beam electron with an ion.
A summary and suggestions for future research are presented in Chapter 7.
Chapter 2

Experimental Arrangement

2.1 Introduction

In this chapter we discuss the spectroscopic equipment used to make the measurements that are presented in this thesis, and we give a brief description and overview of the operation of the electron beam ion trap (EBIT).

The standard x-ray detection equipment on EBIT consists of solid-state germanium (Ge) or lithium-drifted silicon Si(Li) detectors and high resolution Bragg crystal spectrometers. Solid-state detectors measure radiation over a wide range of energies (1-100 keV) and are used to diagnose what elements and charge-states are present in the trap. In addition, we use these detectors to tune EBIT by maximizing the x-ray count-rate due to a particular ion charge state. For example, when injecting the transition metals ($Z=22-26$) we set the electron beam energy to the heliumlike KLL dielectronic recombination resonance and adjust the ion injection and trap voltages to optimize the transition metal dielectronic recombination x-ray count-rate relative to that of the barium x rays; barium is an impurity emitted by the electron gun. The detectors are calibrated to the x-ray energies of known radioactive sources.

By contrast, the Bragg crystal spectrometers are used to examine the fine details of the broad peaks seen in the solid-state detectors. In partic-
ular, we are interested in the high resolution spectra between 4 and 7 keV which contain the 2→1 spectra of the transition metals titanium, vanadium, manganese, vanadium, and iron (Z=22-26). The line ratios of Kα spectra of these ions are also used for inferring the charge-state balance. In order to measure these x-rays we employ a flat-crystal Bragg spectrometer, which is enclosed in vacuum, and a helium-filled Bragg spectrometer that is in the von Hámos geometry [55]. The von Hámos spectrometer will be described in more detail in Section 2.5

### 2.2 Description of EBIT

In this thesis, we describe measurements made on an electron beam ion trap (EBIT). EBIT is used to produce and trap very highly charged ions (up to U$^{99+}$) for x-ray measurements [52, 53, 54]. It has been used to obtain measurements of transition energies [56, 57, 58, 59] and electron ion cross sections for excitation [60, 61], dielectronic recombination [62, 63, 64], and ionization [65, 66]. More recently, it has been used as a source of highly charged ions [67, 68] for ion-surface interaction measurements.

A schematic of EBIT is shown in Fig. 2.1. Low-charge ions are introduced into the trap by injection from the MeVVA ion source [69] or by injecting gas through one of the side ports. An electron beam ≤ 240 mA compressed to a diameter of roughly 70 µm by a 3-Tesla magnetic field successively ionizes the ions to the desired charge state. The ions are trapped radially by the electrostatic potential of the electron beam and axially by two end drift tubes, which are biased positive with respect to the center drift tube, as shown in Fig. 2.2. The trapping region contains, typically, 40,000 ions. The ion density is about $10^9$ cm$^{-3}$, while the electron density is approximately $10^{12}$ cm$^{-3}$. Thus, the trap operates in a low-collisional regime where collisional excitation rates are much smaller than radiative decay rates, and essentially all ions exist in the ground level. Therefore, the population of metastable ions is negligible under most circumstances. Furthermore, in this regime the
distribution of atoms among the various ionization stages is determined by the balance between the ionization and recombination rates.

A feature that improves the performance of EBIT is the use of light-ion cooling to minimize heavy-ion losses [70, 71]. Low-Z gases such as nitrogen are introduced into EBIT for this purpose. Collisions between fully stripped nitrogen (N$^7+$) and, for example, neonlike gold (Au$^{69+}$) reduce the kinetic energy of the heavy ions. Therefore, as the light ions leave the trap they carry away heat and prevent the build up of ion temperatures sufficient to allow heavy ions to escape. For example, neonlike gold would be trapped for only a few seconds without cooling. However, trapping times of up to 4 hours were observed with light-ion cooling [70].

Another important feature of EBIT is the ability to produce ions at one electron energy and to probe these ions at another. This is accomplished by switching the electron beam accelerating voltage (5 kV/msec) from one value to another and back. This feature has allowed us, for example, to perform ionization measurements [65, 66], which form the basis of this thesis.

2.3 EBIT Operation

The EBIT voltages and data acquisition are controlled and run by IBM-type AT computers. The two computers use a CAMAC interface and are controlled by programs written in the C programming language.

The control program, as shown in Fig. 2.3, allows the user to change the drift tube high voltage (electron beam accelerating voltage), axial trap potential (to trap, inject, or dump ions), the MeVVA extraction voltage (to inject ions), and the anode voltage (electron beam current) in milliseconds depending on the response time of the power supply. It also sends trigger pulses to the data acquisition modules in order to acquire x-rays at different portions of the timing cycle. The voltages are controlled by an analog signal, and a summing module allows us to add several voltages together such as the DT (drift tube) 1-3 voltages. Each voltage can also be turned on and off
CHAPTER 2. EXPERIMENTAL ARRANGEMENT

Figure 2.1: Schematic of EBIT and the x-ray detection apparatus.
Figure 2.2: Schematic of three drift tubes. The expanded region of drift tube 2 shows that the ions (circles) are bound radially by the electron beam (straight lines) and longitudinally by voltages applied to the end drift tubes 1 and 3.
by a digital timing signal. If the value is one, the power supply is on, and if the value is zero, the output is turned off. The digital signal rate is set by the user, and 1 or 2 milliseconds is a typical clock period.

The data acquisition system on EBIT can store data from up to four x-ray detectors. The user can view data from the current run or past runs without interrupting the data acquisition. The data is stored in two multichannel analyzers (LeCroy 3001 qVt's charge, voltage, and time) and two analog to digital converters (LeCroy 3512 ADC's). The output of the ADC's are fed through a data router (LeCroy 3587) into a histogramming memory (LeCroy 3588). The data router allows the ADC to store information from different parts of the timing cycle in 15 separate spectra. This feature is important in our ionization measurements where we produce ions at one electron energy and probe these ions at another.

2.4 X-Ray Instrumentation

EBIT was specifically designed for the observation of x rays and x rays are viewed through 127-μm beryllium windows at 90° to the electron beam, as shown in Fig. 2.1. To detect the x rays we use solid-state germanium (Ge) and lithium drifted silicon Si(Li) detectors, as well as Bragg crystal spectrometers. Solid-state detectors provide a highly efficient way for x-ray observation because of their near 100% quantum efficiency. This is important for EBIT as the number of photons is smaller than from plasma or beam-foil sources. Another advantage is their wide energy coverage from 1-100 keV with a resolution of $\Delta E/E \approx 200$ eV. In Fig. 2.4(a) we show a spectrum of heliumlike iron obtained with a Si(Li) detector at a beam energy of 12 keV. The largest feature in the spectrum is the peak due to $n=2\rightarrow 1$ direct excitation transitions, e.g. of the process:

$$1s^2 + e^- \rightarrow 1s2\ell + e^- \rightarrow 1s^2 + \nu + e^-.$$
CHAPTER 2. EXPERIMENTAL ARRANGEMENT

Clock period = 2.0 ms; Total period = 4.5960 sec

Figure 2.3: Timing pattern for EBIT control program. The pattern determines whether a voltage is on (upper line) or off (lower line). The portions of the cycle under the loops are repeated the number of times indicated. A typical timing cycle consists of the following: The ions are dumped (DT 1-3 Dump is negative to expel ions) and the electron beam (anode) and electron accelerating voltage (DT Ionization) are turned off. In the interval between loops, the MeVVA is fired (MeVVA Trigger) and a new supply of ions is introduced into the trap. In the second loop the accelerating voltage is alternated between two values (DT Ionization and DT Probe). Data acquisition pulses (DAQ Start 1 and 2 and qVt Gate) activate the detectors during the second loop where the voltages are being switched.
It also shows 3→1 and 4→1 transitions. The peaks situated at energies above the beam energy are x rays due to radiative capture of beam electrons. For example, the photons given off in the radiative recombination (RR) onto the n=2 levels in heliumlike ions are due to:

$$1s^2 + e^- \rightarrow 1s^22\ell + h\nu.$$  

The energy of the photon is the sum of the beam energy and the binding energy of the newly formed ion.

Crystal spectrometers provide much higher spectral resolution than solid-state detectors. Their counting efficiency, however, is greatly reduced because of low crystal reflectivities. Figures 2.4(b) and (c) show spectra obtained with EBIT's flat crystal and von Hámos [55] spectrometers. The flat crystal spectrometer provides a resolution of $\lambda/\Delta\lambda \leq 1000$. The von Hámos [55] spectrometer has a resolution of $\lambda/\Delta\lambda \leq 4500$ and because of the curved crystal geometry has a high relative counting efficiency. The von Hámos spectrometer has become the spectrometer of choice for x-ray measurements in the wavelength region $\lambda \leq 3$ Å. Both spectrometers employ position-sensitive, gas-filled proportional counters.

2.5 von Hámos Spectrometer

In order to measure high resolution x-ray spectra in the energy region between 4.0 ≤ $E$ ≤ 12 keV a helium-filled, von Hámos type [72], Bragg-crystal spectrometer is used on EBIT [55]. For the measurements presented in this thesis, the instrument was setup to measure the n=2→1 spectrum of hydrogenlike, heliumlike, lithiumlike, and berylliumlike Ti, V, Cr, Mn, and Fe in the energy range between 4.7 ≤ $E$ ≤ 7 keV.

The spectrometer is matched to the unique characteristics of the EBIT line source, and it has become the spectrometer of choice for many high resolution spectral measurements. It has about five times higher throughput and three times better resolving power than the flat-crystal spectrometer.
Figure 2.4: X-ray emission from EBIT of iron ions at 12 keV: (a) Broadband spectrum ($\Delta E/E \approx 200$ eV) from a solid-state detector showing bound-bound and free-bound emission; (b) survey spectrum ($\Delta E/E \approx 10$ eV) from a flat-crystal spectrometer; (c) high-resolution spectrum of heliumlike iron ($\Delta E/E \approx 1.7$ eV) from a von Hámos spectrometer.
The focussing properties of the von Hámos geometry are shown in Fig. 2.5. A crystal that is cylindrically bent about an axis in the horizontal plane diffracts x rays with wavelength $\lambda$ according to Bragg's law:

$$\lambda = \frac{2d}{n}\sin \theta. \quad (2.1)$$

where $d$ is the lattice spacing of the crystal, $n$ is the order of diffraction, and $\theta$ is the Bragg angle. The x rays form a monochromatic image of a line source at different positions along its axis of curvature. The photons are measured by setting up the spectrometer such that the distance $D$ between the crystal and detector (and between crystal and source) equals

$$D = \frac{R}{\sin \theta}, \quad (2.2)$$

where $R$ is the radius of curvature of the crystal.

The resolving power $\lambda/\Delta \lambda$ or resolution of a spectrometer is the ability to distinguish between two photons whose wavelengths are close together. Several factors affect the resolving power of the von Hámos spectrometer. The height of the source, the spatial resolution of the position-sensitive detector, and the width of the source all limit the resolution of the spectrometer. The height of the source limits the resolving power to:

$$\frac{\lambda}{\Delta \lambda} = \frac{2R^2}{h^2 \sin^2 \theta}. \quad (2.3)$$

where $R$ is the radius of curvature of the crystal, $h$ is the height of the source, and $\theta$ is the Bragg angle. The inaccuracy of the position-sensitive proportional counter (≤ 250 μm) results in a resolving power of:

$$\frac{\lambda}{\Delta \lambda} = \frac{2R}{\Delta w \cos \theta}. \quad (2.4)$$

where $\Delta w$ is the detector resolution. Finally, the source width, which is approximately 70 μm, similarly, limits the resolution to:

$$\frac{\lambda}{\Delta \lambda} = \frac{2R}{\Delta s \cos \theta}. \quad (2.5)$$
Figure 2.5: Focussing geometry of a von Hémos-type spectrometer. Monochromatic x rays from a line source (EBIT) are imaged by a cylindrically bent crystal onto a position-sensitive proportional counter.
where $\Delta s$ is the source width. We note that using a crystal with a larger radius of curvature increases the resolution in all three cases, discussed above.

The layout of the spectrometer is shown in Fig. 2.6. The crystal and position-sensitive proportional counter are both mounted on aluminum platforms, which must be leveled with respect to EBIT. Since the energy of the x rays of interest (4-7 keV) are strongly attenuated by air, the enclosed volume of the spectrometer is filled with helium during experiments. For our measurements we used LiF(200) crystals with $2d = 4.028$ Å bent to radii of curvature of 30 and 75 cm. The Bragg angles ranged from approximately 40.7° for Ti to 26.8° for Fe. The nominal resolving power is $\lambda/\Delta\lambda \approx 2700$ for the 30 cm radius of curvature crystal and 7000 for the 75 cm radius crystal. These values are largely the result of aberrations caused by the finite detector resolution given by Eq. (2.4). Measured values of the resolving power are typically $\lambda/\Delta\lambda \approx 1500$ and 4500 for 30 and 75 cm radii of curvature crystals, respectively and appear related to the quality of the particular crystal, the quality of its curvature, and the ion temperature.

The crystals, which are 50 x 120 x 0.25 mm$^3$ in size, are attached to aluminum blocks with the correct radius of curvature using melted wax. A precision large diamond optics lathe machined the aluminum blocks. A quartz pusher with a matching radius of curvature was placed on top of the crystal and the aluminum block until the wax solidified.

The proportional counter used in the spectrometer was designed and built by Källne [73] et al. The signal induced in a helical delay-line cathode provides position information. A mixture of 70% xenon and 30% methane at 16-psi overpressure is employed as the working gas. This detector was chosen for the spectrometer because of its good position resolution ($\leq 250$ μm) and its large active area (11 x 3 cm$^2$). Since the source is imaged on to the detector in the von Hámos geometry, the detector must be as high as the source to capture all the Bragg-diffracted x rays.
Figure 2.6: Layout of the von Hámos spectrometer in the horizontal plane of EBIT. The electron beam direction is out of the page.
Chapter 3

X-ray Polarization

3.1 Introduction

In Chapter 3 we will demonstrate how linear polarization of the x rays in EBIT affects the x-ray intensities used to infer ionization cross sections. The excitation of the ions by an electron beam introduces a preferred direction. This leads to selective population of magnetic sublevels in the excited upper levels and, thus, to emission of polarized, anisotropic radiation. This has two effects on the x rays we measure: (1) since we measure x rays at 90° to the electron beam our solid-state detectors and spectrometers are sensitive to the angular distribution of the x rays, and (2) our crystal spectrometer acts as a polarimeter, which preferentially detects x rays polarized perpendicular to the plane of dispersion.

In this chapter we present a line ratio measurement of the unpolarized Ly-α₂ (2p₁/₂ → 1s₁/₂) transition relative to the polarized Ly-α₁ (2p₃/₂ → 1s₁/₂) transition in hydrogenlike iron in EBIT. Evidence for the polarization of line radiation in EBIT was given recently by Henderson et al. [74], who observed the n=2→1 direct-excitation transitions of heliumlike scandium (Z=21). We will show that observations of B, i.e. the ratio of Ly-α₂ and Ly-α₁, result in values smaller than the theoretically predicted value without polarization. We demonstrate how polarization affects this measurement.
The same techniques will be used later to adjust for polarization of the x-rays in the charge-state balance and ionization measurements.

3.2 Polarization Effects

Before presenting the experiment we will discuss the angular distribution and reflectivity adjustments needed to account for the polarization of the line radiation observed from EBIT. These adjustments are required for any x-ray line ratio measurements using the high resolution crystal spectrometer. Whereas, only the angular portion of this adjustment is needed for the Ge detector measurements.

For electric dipole (E1) radiation, i.e., the primary type we study in this thesis, the expression for the x-ray intensity at 90°, \( I(90°) \), and the average over the \( 4\pi \) solid angle, \( \langle I \rangle \), is [75]

\[
I(90°) = \frac{3}{3 - P} \langle I \rangle. \tag{3.1}
\]

\( P \) is defined as the linear polarization and is given by

\[
P = \frac{I_\parallel - I_\perp}{I_\parallel + I_\perp}, \tag{3.2}
\]

where \( I_\parallel \) and \( I_\perp \) are the intensities of the x-ray emission components with electric field vectors parallel and perpendicular electron beam, respectively, and

\[
I_\parallel + I_\perp = I(90°). \tag{3.3}
\]

The x-ray intensity \( I^{\text{meas}} \) measured with our crystal spectrometer is

\[
I^{\text{meas}} = R_\parallel I_\parallel + R_\perp I_\perp, \tag{3.4}
\]

where \( R_\parallel \) and \( R_\perp \) are the integrated reflectivities of the crystal for x rays polarized parallel and perpendicular to the electron beam, which were provided by Gullikson [76].
Combining Eqs. (3.1)-(3.4), the intensity ratio we measure for two electric dipole x-ray lines is related to their 4π average by the expression

\[
\frac{I_1}{I_2} = \frac{W_1(I_1)}{W_2(I_2)},
\]

where we define \( W \) to be

\[
\frac{W_1}{W_2} = \frac{R_1(P)A_1(P)}{R_2(P)A_2(P)} = \frac{(1 + P_1) + \frac{R_1}{R_2}(1 - P_1)}{(1 + P_2) + \frac{R_1}{R_2}(1 - P_2)} \left( \frac{3 - P_2}{3 - P_1} \right),
\]

The terms \( R(P) \) and \( A(P) \) represent the reflectivity and angular distribution terms, respectively.

For the LiF(200) crystals we use in our measurements, \( R(P) \), which is a function of x-ray energy, varies from 0.115 for x-rays at 4.714 keV to 0.606 for x-rays at 6.986 keV. This is the approximate range of the Ti-Fe photons we observe with the crystal spectrometer. Therefore, positive polarization enhances and negative polarization decreases the intensity of an x-ray line relative to an unpolarized line (\( P=0 \)).

### 3.3 Experiment

The x rays generated by the electron-ion collisions are recorded with EBIT's curved crystal Bragg spectrometer in the von Hámos geometry [55]. In our experiment we used a LiF(200) crystal with a lattice spacing of 2\( d = 4.027 \) Å. The crystal was bent to a radius of curvature of 30 cm. The resolving power of the setup is \( \Delta \lambda / \lambda \approx 1500 \). The spectrometer was set to a nominal Bragg angle of 26.8° which corresponds to a wavelength of 1.81 Å. The total wavelength covered was 1.77 Å < \( \lambda < 1.88 \) Å which contains the hydrogen-like transitions Ly-\( \alpha_1 \) (2p\( 3/2 \)→1s\( 1/2 \)) at 1.7780 Å and Ly-\( \alpha_2 \) (2p\( 1/2 \)→1s\( 1/2 \)) at 1.7834 Å [77]. A typical x-ray spectrum taken with the electron beam energy set to 15 keV is shown in Fig. 3.1. The Ly-\( \alpha_2 \) intensity has a contribution from an M1 (2s\( 1/2 \)→1s\( 1/2 \)) transition, which cannot be resolved from
the Ly-α₂ x ray. The separation between the two transitions in iron is 0.03 eV. The 2s₁/₂ upper level decays 10% of the time by M₁ (magnetic dipole) radiation and 90% of the time by two photon decays [78]. Therefore, the M₁ transition results in a x ray which blends with and adds to the effective intensity of Ly-α₂.

We have measured Ly-α₂ and Ly-α₁ in iron as a function of electron beam energy for energies near the excitation threshold of Ly-α₁ at 7.1 keV to 18 keV. The measurements for energies from 10 to 18 keV were made in steady-state at one beam energy, and recording a spectrum of approximately 250 counts in Ly-α₂ and 500 counts in Ly-α₁ typically lasted 50 min. However, the measurements made below 8.828 keV, which is the ionization potential for producing hydrogenlike iron, are made by taking advantage of EBIT’s ability to alternate the electron beam accelerating voltage (5 kV/ms) from one value to another and back. This feature allows us to create the ionization balance at, e.g., 15 keV and to probe the hydrogenlike transitions at energies below 8.828 keV. These spectra took roughly 6 hours each to acquire. The excitation energies of Ly-α₂ and Ly-α₁ in iron are 6.962 keV and 6.973 keV, respectively.

We compare the experimental intensities of Ly-α₂ and Ly-α₁ with those predicted at 90° to the electron beam direction. For Ly-α₂ and Ly-α₁, the predicted x-ray intensities are:

\[
I_{\text{Ly-α₂}} = \frac{j_e}{e} (\sigma_{\text{Ly-α₂}} + 0.1\sigma_{\text{M₁}}) n_H W_{\text{Ly-α₂}} G_2, \quad \text{(3.7)}
\]

\[
I_{\text{Ly-α₁}} = \frac{j_e}{e} \sigma_{\text{Ly-α₁}} n_H W_{\text{Ly-α₁}} G_2, \quad \text{(3.8)}
\]

where \(j_e\) is the effective current density, \(e\) is the charge of the electron, \(\sigma_{\text{Ly-α₂}}\), \(\sigma_{\text{M₁}}\), and \(\sigma_{\text{Ly-α₁}}\) are excitation cross sections calculated with the distorted-wave code of Zhang [79], \(n_H\) is the number densities of ground-state hydrogenlike ions, and \(G_2\) is the solid angle subtended by the spectrometer. \(W\), which we derived in the last section, accounts for the angular distribution of the x rays, their linear polarization, and the reflectivity of the LiF(200)
Figure 3.1: Direct excitation x-ray spectrum of iron measured with a Bragg crystal spectrometer at an electron beam energy of 15 keV showing Ly-$\alpha_1$ and Ly-$\alpha_2$. 
crystal. $P=0$ for Ly-$\alpha_2$ plus the M1 contribution ($J=1/2\rightarrow 1/2$ transitions), thus $W_{\text{Ly-}\alpha_2} = 1.606$. The polarization for Ly-$\alpha_1$ is given by:

$$P = \frac{3(N_{1/2} - N_{3/2})}{3N_{3/2} + 5N_{1/2}},$$

(3.9)

where $N_{1/2}$ and $N_{3/2}$ are the magnetic sublevel populations also calculated using the code of Zhang [79]. This formula was derived by Inal and Dubau [80] for ions excited by an electron beam. It was derived for the lithium-like line \(q\) (1s2s(3S)2p \(2P_{3/2} \rightarrow 1s^22s \ 2S_{1/2}\)), which is analogous to Ly-$\alpha_1$ for hydrogen-like ions, for X rays observed at 90° to the electron beam. Line \(q\) and Ly-$\alpha_1$ are both E1 (electric dipole), $J=3/2\rightarrow 1/2$ transitions. Because the magnetic sublevel populations are energy dependent, the theoretical value $P$ for Ly-$\alpha_1$ varies from 0.363 near the excitation threshold of the Ly-$\alpha$ lines at 7.025 keV to 0.250 at 20 keV; the corresponding variation of $W_{\text{Ly-}\alpha_1}$ is from 1.99 to 1.86.

### 3.4 Results

The observed value of $B$, which is the ratio of Ly-$\alpha_2$ to Ly-$\alpha_1$, is shown in Fig. 3.2. The results are compared with theoretical calculations of $B$ which includes contributions with and without the M1 transition. The results show that the value of $B$ clearly deviates from the predicted value without polarization. The positive polarization of Ly-$\alpha_1$ enhances the intensity relative to Ly-$\alpha_2$ resulting in a smaller value of $B$. We also plot how $B$ changes when the reflectivity of the crystal, $R_\lambda$, is varied between upper (0.675) and lower (0.525) limits. The value we use in the calculations is 0.606.

This measurement has an important application to plasma diagnostics and astrophysics. In particular, Laming [81] has suggested that previous solar flare observations of $B$ in Mg$^{11+}$ by Sylwester et al. [82] who reported a value as low as 0.38 and by McWhirter and MacNeice [83] who reported 0.35 to be the result of the excitation of the ions by electrons in a beam. Therefore,
our measurement shows the feasibility of using the Ly-$\alpha_2$ to Ly-$\alpha_1$ ratio as a diagnostic to detect non-Maxwellian electron velocity distributions.

3.5 Conclusion

The results of this line ratio measurement shows that we need to account for the effects of polarization in our x ray measurements. This will be important in the following chapters because the dielectronic recombination, radiative recombination, as well as the direct excitation x rays we observe to infer ionization cross sections are highly polarized, from +0.60 to -0.75. This results in significant enhancements and reductions in relative line intensities that must be accounted for. The x-ray intensities measured with the solid-state detector will be adjusted by the angular distribution factor $A(P)$, while the transitions measured with the crystal spectrometer will be modified by $W = R(P)A(P)$ which includes a correction due to the reflectivity of the crystal in addition to that resulting from the angular distribution.
Figure 3.2: Dependence of ratio of Ly-α₂ to Ly-α₁ known as $B$ with beam energy. The circles represent the measurement. The error bars are purely statistical. Also shown are the theoretical predictions with no polarization and the M₁ contribution (dashed line), with polarization and no M₁ contribution (dot-dashed line), and with polarization and the M₁ contribution (solid line). We also show how $B$ changes if the reflectivity is varied between upper and lower bounds.
Chapter 4

X-ray Ionization Balance Measurements

4.1 Introduction

The ionization cross section measurements are dependent on an accurate determination of the relative ion charge-state abundances in the trap. In this chapter we focus on a set of x-ray measurements to infer the charge-state abundances of bare, hydrogenlike, heliumlike, lithiumlike, and berylliumlike iron in EBIT. The techniques presented here are important because we employ the same methods in Chapter 5 to infer the ionization cross sections. The x-ray ionization balance is determined in two ways: (1) by observing radiative recombination photons with a solid-state germanium detector, and (2) by observing line radiation with the von Hámos Bragg crystal spectrometer. In addition, the results are compared to an ionization balance model of the trap and to the extracted ions from the trap.

The method for inferring the charge-state balance consists of measuring the intensity ratios of x-ray emission lines and normalizing to their theoretical cross sections for excitation. In particular we made measurements of radiative recombination and direct excitation x-rays at beam energies between 10 and 18 keV for iron. 10 keV is just above the ionization potential to produce
bare ions (9.278 keV) in iron, therefore we produce appreciable numbers of the hydrogenlike and heliumlike charge states. The ratio of the bare and hydrogenlike abundances is determined from K-shell radiative recombination (RR) lines and is accurate to \( \approx 3\% \). The hydrogenlike, heliumlike, lithiumlike, and berylliumlike ratios are determined from \( n=2\rightarrow1 \) lines and are believed to be accurate to \( \approx 15\% \).

### 4.2 Experiment

In this experiment the x rays were detected with a solid-state germanium detector, as well as a curved-crystal Bragg spectrometer in the von Hámos geometry [55]. For the iron measurements we used a LiF(200) crystal with a lattice spacing of \( 2d=4.027 \) Å bent to a radius of curvature of 30 cm. The resolving power of the crystal spectrometer is \( \lambda/\Delta \lambda \approx 1500 \).

The germanium detector allows us to observe both the \( n=2\rightarrow1 \) x rays and x rays from radiative recombination, as shown in Fig. 4.1. The \( n=2\rightarrow1 \) x rays stem from impact excitation of the hydrogen-, helium-, lithium-, and beryllium-like charge states of iron present in the trap, while the recombination x rays result from the radiative capture of beam electrons by the ions. The energy of the recombination x rays is the sum of the electron kinetic energy and the binding energy of the state into which it is captured. The K-shell binding energy of hydrogenlike iron (9278 eV) differs by 450 eV from that of heliumlike iron, and x rays from radiative recombination onto the bare and hydrogenlike charge states are well resolved with the germanium detector whose resolution is \( \Delta E/E(\text{FWHM}) = 200 \) eV. This can be used to get the relative abundance of bare and hydrogenlike ions. By contrast, the differences in the L-shell binding energies of different ionization states is smaller than the resolution of the detector, and the x rays from \( n=2 \) radiative recombination onto bare, hydrogenlike, heliumlike, lithiumlike, and berylliumlike ions cannot be resolved. As a result, the peak due to radiative recombination into the \( n=2 \) shell shown in Fig. 4.1 is a blend of x rays from
capture into all the ionization stages with an open L shell and cannot easily be fitted to determine the ionization balance.

In order to determine the abundance of hydrogenlike ions and ions with a filled K shell, we use the von Hámos spectrometer [55] to resolve n=2→1 transitions. The spectrometer was set to a nominal Bragg angle of 26.8°, which corresponds to a wavelength of 1.81 Å. The total range covered was 1.77 Å < λ < 1.38 Å, which includes the hydrogenlike transitions Ly-α₁ (2p₃/₂→1s) at 1.7780 Å and Ly-α₂ (2p₁/₂→1s) at 1.7834 Å [77], the heliumlike transitions w (1s²p¹P₁→1s²¹S₀) at 1.8505 Å, x (1s²p³P₂→1s²¹S₀) at 1.8555 Å, y (1s²p³P₁→1s²¹S₀) at 1.8595 Å, and z (1s²s³S₁→1s²¹S₀) at 1.8682 Å [84], the lithiumlike transitions q (1s²s²²P₃/₂→1s²²S₁/₂) and r (1s²s²²P₁/₂→1s²²S₁/₂), and the berylliumlike transition β (1s²s²²P₁→1s³²S₁₀), as shown in Fig. 4.2.

We determine the relative bare and hydrogenlike abundances from the radiative recombination x rays observed with the solid-state Ge detector, and the relative hydrogenlike, heliumlike, lithiumlike, and berylliumlike ratios are determined from the n=2→1 direct excitation line ratios from the von Hámos crystal spectrometer.

4.3 Radiative Recombination

The determination of the relative ionization balance from radiative recombination x rays requires that the ionization potential of adjacent charge states be well separated compared to the resolution of the detector. This is the case for the bare and hydrogenlike charge states of iron measured with a solid-state germanium detector. Radiative recombination onto hydrogenlike ions can be displayed schematically as:

\[ 1s + e^- \rightarrow 1s^2 + h\nu. \]

Furthermore, recombination x rays are the only spectroscopic way of determining the number of bare ions in a trap as bare ions do not emit photons
Figure 4.1: X-ray spectrum of iron taken with a Ge detector at an electron beam energy of 15 keV. The dominant feature is the peak from the n=2→1 hydrogenlike, heliumlike, lithiumlike, and berylliumlike x rays. The smaller peaks, shown in the enlarged area, are x rays from radiative recombination onto the n=1 2, and 3 shells.
Figure 4.2: K x-ray spectrum of iron taken with the von Hámos crystal spectrometer at an electron beam energy of 15 keV. The marked lines are identified in the text.
by any other means.

For the case of RR onto the K-shell of bare and hydrogenlike iron, the observed x-ray intensities at 90° to the beam direction are given by:

\[ J_B = \frac{j_e}{e} \sigma_B n_B, \]  

\[ J_H = \frac{j_e}{e} \sigma_H n_H, \]

where \( j_e \) is the effective current density of the electron beam, \( e \) is the charge of the electron, \( \sigma_B \) and \( \sigma_H \) are the radiative recombination cross sections calculated using the relativistic formulation described by Scofield [85], which accounts for the angular distribution of emitted photons at 90°, and \( n_B \) and \( n_H \) are the numbers of bare and hydrogenlike iron ions in the trap. The effective current density includes the electron-ion overlap factor, which is the fraction of time that each ion spends within the electron beam. The overlap factor is a function of the ion charge, the ion temperature, and the electron beam space charge. It is usually \( \geq 0.5 \) but is not well known. For bare to berylliumlike iron ions \( j_e \) is calculated to differ by 2%. In what follows we neglect this small difference. Dividing (4.1) and (4.2) and solving for \( \sigma_B/\sigma_H \), we obtain:

\[ \frac{n_B}{n_H} = \frac{J_B \sigma_H}{J_H \sigma_B}, \]

The observed radiative recombination x-ray intensities \( J_B \) and \( J_H \) are obtained from the solid-state detector spectra by fitting the K-shell recombination peaks with a line shape that includes the detector resolution and the electron beam energy spread.

The Fe\textsuperscript{26+}/Fe\textsuperscript{25+} ratio, determined from radiative recombination, has the highest accuracy among the present x-ray measurements because of the high detection efficiency of the solid-state detector. For example, the time for each run (approximately 50 min.) is sufficient to acquire 40,000 radiative recombination events making the statistical uncertainty small. In addition, the calculated radiative recombination cross sections are believed to be correct.
to within 3%. This is substantiated by a large body of cross section measurements for the inverse process of photoionization, to which the calculations can be compared at similar electron and photon energies [86].

4.4 Direct Excitation

We employ the von Håmos crystal spectrometer to resolve the \( n=2\rightarrow1 \) x rays into the individual charge-state components. The primary lines we observe, \( \text{Ly-}\alpha_1, \omega, \eta, \) and \( \beta, \) are all dipole-allowed (E1) transitions, and they are the dominant transitions of their respective charge states. Consequently, the ion abundances in the trap can be determined from the line ratios of these x rays. Furthermore, they are populated purely by direct excitation and have essentially no contribution from cascades due to excitation from higher lying levels.

For direct excitation, the x-ray intensities observed at 90° to the electron beam direction for \( \text{Ly-}\alpha_1 \) and \( \omega \) are:

\[
I_{\text{Ly-}\alpha_1} = \frac{je}{e} \sigma_{\text{Ly-}\alpha_1} n_H W_{\text{Ly-}\alpha_1}, \quad (4.4)
\]

\[
I_{\omega} = \frac{je}{e} \sigma_{\omega} n_{\text{He}} W_{\omega}, \quad (4.5)
\]

where \( \sigma_{\text{Ly-}\alpha_1} \) and \( \sigma_{\omega} \) are the excitation cross sections calculated with the relativistic distorted-wave code of Zhang et al. [79], \( n_H \) and \( n_{\text{He}} \) are the ion numbers of hydrogenlike and heliumlike iron, and \( W_{\text{Ly-}\alpha_1} \) and \( W_{\omega} \) account for the angular distribution of the x rays, their linear polarization, and the reflectivity of the LiF(200) crystal. The x-ray angular distributions and polarizations were also obtained from the code of Zhang et al. [79]. Dividing (4.4) and (4.5) and solving for \( n_H/n_{\text{He}} \), we obtain:

\[
\frac{n_H}{n_{\text{He}}} = \frac{I_{\text{Ly-}\alpha_1}}{I_{\omega}} \frac{\sigma_{\omega} W_{\omega}}{\sigma_{\text{Ly-}\alpha_1} W_{\text{Ly-}\alpha_1}}, \quad (4.6)
\]

Similar expressions are obtained for \( n_{\text{Li}}/n_{\text{He}} \) and \( n_{\text{Be}}/n_{\text{He}} \) except that the excitation cross sections of the lithiumlike line \( \eta \) and the berylliumlike line \( \beta \)
must be multiplied by the fluorescence yield. The fluorescence yield is smaller than one because inner-shell excited lithiumlike and berylliumlike ions also decay by Auger emission. We use the fluorescence yield values calculated using the methods of Chen [87] for lines \( q \) and \( \beta \).

The \( \text{Fe}^{25+}/\text{Fe}^{24+} \) measurement, which is determined from the intensities of Ly-\( \alpha_1 \) and \( w \), had the highest accuracy among the crystal spectrometer measurements because the two transitions are the brightest in the observed K\( \alpha \) spectra. The \( \text{Fe}^{23+}/\text{Fe}^{24+} \) and \( \text{Fe}^{22+}/\text{Fe}^{24+} \) ratios depend on crystal spectrometer x-ray measurements of \( q/w \) and \( \beta/w \). Very few lithiumlike or berylliumlike ions are present at the beam energies covered in the measurement, so these intensities are smaller and the inferred ratios have a larger statistical uncertainty.

The uncertainty of the x-ray measurements also depends on systematic errors in the calculations of the cross sections, the fluorescence yields, polarization, and the crystal reflectivity. For example, while the theoretical radiative recombination cross sections are believed to be correct within 3%, the theoretical excitation cross sections for lines Ly-\( \alpha_1 \), Ly-\( \alpha_2 \), \( w \), \( q \), and \( \beta \) are believed to be correct to 10%. In addition, for the lithiumlike line \( q \) and line \( r \) there is a 0.2% and 6% and difference, respectively, in the values calculated for the fluorescence yield using the code of Chen [87] and by Vainshtein and Safronova [88].

4.5 Results and Discussion

We recorded x-ray spectra for fixed electron beam energies from 10 to 18 keV. At these energies the predominant charge states are \( \text{Fe}^{25+}, \text{Fe}^{24+} \), and \( \text{Fe}^{24+} \) because the ionization potential of lithiumlike iron is 2.046 keV. The fractional abundances measured as a function of beam energy are shown in Fig. 4.3. The berylliumlike charge state is not shown because its population fraction is less than 0.01 of the total.

Penetrante et al. [89] have developed an ionization balance model for
Figure 4.3: Fractional ion abundance determined from x-ray observations and a model calculation. The triangles, diamonds, squares, and circles refer to Fe$^{26+}$, Fe$^{25+}$, Fe$^{24+}$, and Fe$^{23+}$, respectively. The solid curves represent the results from a model calculation with an assumed oxygen background density of 1.05 x 10$^7$ cm$^{-3}$. Fe$^{22+}$ is not shown; its abundance is less than 0.01. The statistical error bars are on the order of the size of the points.
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EBIT that includes the processes of electron impact ionization, radiative recombination, and charge exchange recombination from neutral background gases. The ion temperature is also calculated as part of the model.

Figure 4.3 plots the charge balance predicted with the model described by Penetrante et al. [89] for different beam energies, assuming an oxygen background density of $1.05 \times 10^7$ cm$^{-3}$. For the present data set charge exchange recombination is greater than radiative recombination, and the neutral density in the model was chosen to provide the best fit to the measured ionization balance. Comparing the predictions with the measurements we find good agreement. Differences are apparent only for the lithiumlike fraction and can be attributed to the measurement uncertainty.

4.6 Comparison with Extracted Ions

The x-ray ionization balance inferred by looking at photons emitted by ions in the trap was also compared to the charge-state abundance of the ions extracted from the trap. Following the measurements of the x rays, the electron beam was turned off and the ions were extracted through the top of EBIT, as indicated in Fig. 4.4. The ions were bent by an electrostatic bender, focussed by einzel lenses, collimated, magnetically analyzed, and detected by an electron multiplier. A typical extracted ion spectrum is shown in Fig. 4.5 where the current of the analyzing magnet was stepped from 42 to 49 A in increments of 0.033 A. Each datum represents the sum of three extraction cycles, where a cycle consists of ion injection, ionization to the desired charge state, x-ray data acquisition, and extraction of the ions.

The relative charge-state balance from the extracted ions is straightforward although we have to correct for isotope effects and dead time in the counting electronics. In Fig. 4.5 the peak due to the bare $^{54}\text{Fe}^{26+}$ (5.82%) isotope is clearly seen. The peak from the bare $^{56}\text{Fe}^{26+}$ (91.66%) isotope also contains a contribution from $^{54}\text{Fe}^{25+}$, which blends with $^{56}\text{Fe}^{26+}$ due to their nearly identical charge to mass ratios. Similarly, each subsequent $^{56}\text{Fe}$ peak
Figure 4.4: Schematic of EBIT and the ion extraction system.
Figure 4.5: Spectrum of extracted iron ions following 15 keV electron impact. Also marked are peaks from oxygen which is a background gas in EBIT.
has a small contribution from $^{54}\text{Fe}$ of the next lower charge state. We take into account the $^{54}\text{Fe}$ isotope contribution to peaks from $^{56}\text{Fe}$ by subtracting the portion of $^{54}\text{Fe}$ from each of the $^{56}\text{Fe}$ peaks. The $^{57}\text{Fe}$ isotope (2.19%) does not affect the $^{56}\text{Fe}$ peaks due to the difference in their charge to mass ratios. We neglect the contribution of the $^{58}\text{Fe}$ isotope (0.33%) to the $^{56}\text{Fe}$ peaks because it has an extremely small isotopic abundance. The dead time is calculated by comparing the measured peak isotopic ratios (peak rate) of bare $^{54}\text{Fe}^{26+}/^{56}\text{Fe}^{28+}$ with the known isotopic ratio. The number of counts (count rate) for each ion extraction datum is then adjusted for the dead time in the particle detection electronics. After the dead time and isotope contributions are accounted for, the charge-state ratios are simply the integrated peak areas of $^{56}\text{Fe}$.

The comparison between the x-ray and extracted ion charge-state balance is shown in Fig. 4.6 (a)-(b) and Fig. 4.7(a)-(b). The Fe$^{26+}$/Fe$^{28+}$ and Fe$^{25+}$/Fe$^{24+}$ ion extraction ratios in Figs. 4.6(a) and (b) have the highest statistical certainty amongst the extracted ion measurements due to the fact that the peaks associated with these charge states had the largest number of counts as seen in Fig. 4.5. As in the x-ray measurements, the Fe$^{23+}$/Fe$^{24+}$ and Fe$^{22+}$/Fe$^{24+}$ ion extraction ratios in Figs. 4.7 (a) and (b) have a higher uncertainty because there was only a small amount of these charge states present in the scans. Nevertheless, the statistical uncertainty with the ion extraction measurements generally is lower than the x rays. On the other hand, the variation among the ion extractor results from different scans is large; we find variations are as large as 32%. This implies that the extraction efficiency for different charge states, and thus the accuracy of the ion extraction data, depends on processes in the trap and the extraction system that affect our measurements.

Possible sources of error in the ion extraction data include variation in the total number of ions entering the trap per injection, blends with background gases that have similar charge to mass ratios as iron, and charge exchange (CX) recombination which occurs along the 3.25 m transfer path from the
Figure 4.6: Dependence of the relative charge-state balance of (a) Bare/Hydrogenlike and (b) Hydrogenlike/Heliumlike iron on beam energy. The circles with the dot-dashed line represent the x-ray charge balance and the triangles with the solid line represent the extracted ion charge balance. Typical statistical error bars from the x-ray and ion extraction measurements are shown for the 13 keV data. The deviation between three runs for the x-ray and ion extraction measurements is shown for the 15 keV data.
Figure 4.7: Dependence of the relative charge-state balance of (a) Lithiumlike/Heliumlike and (b) Berylliumlike/Heliumlike iron on beam energy. The circles with the dot-dashed line represent the x-ray charge balance and the triangles with the solid line represent the extracted ion charge balance. Typical statistical error bars from the x-ray and ion extraction measurements are shown for the 13 keV data. The deviation between three runs for the x-ray and ion extraction measurements is shown for the 15 keV data.
A comparison of the x-ray and ion extraction data shows that, although the charge-state ratios determined by the two techniques show the same trends, the ion extractor consistently exhibits a higher charge-state balance than the x rays. In some cases such as in Figs. 4.6 (a) and (b) they disagree by as much as 50%. We believe that this result can be explained by noting that the extraction data is very sensitive to the setting the extractor voltages. A different setting might favor the extraction of different charge states. Also, there is a large variation from run to run, possibly due to space charge effects in the extractor data, which affects how the ions are bound to the electron beam, that can alter the results.

The data at 15 keV was compared to results from the charge-balance model of Penetrante et al. [89]. The measured x-ray and ion-extraction charge balance from the 15 keV data is shown in Fig. 4.8 where the sum of all the charge states is normalized to one. The computed relative charge-state balance is shown in Fig. 4.9 as a function of the oxygen background gas pressure. Comparing the computation with the x-ray charge balance, we find agreement for a pressure of roughly $4 \times 10^{-10}$ torr ($1.05 \times 10^7$ cm$^{-3}$) of oxygen; comparing with the ion extractor data we find agreement for a pressure of approximately $2 \times 10^{-10}$ torr ($0.502 \times 10^7$ cm$^{-3}$). Therefore, the calculation implies a corresponding background pressure for the x rays which is twice that for the ion extractor.

Although the uncertainties discussed above may cause the disagreement, another possible explanation for the discrepancy is that the x-ray and ion charge-state balances are determined from different regions of the trap. The x rays are measured from the central 1 cm of the trapping region, and correspond only to ions that intersect the electron beam. Whereas, the ions are extracted through a hole in the top drift tube, and ions from, possibly, a different trapping region are flushed out. However, we believe the discrepancy results from the dependence of the extraction efficiency of the different
4.7 Conclusion

We have developed an accurate method based on x-ray measurements for determining the ionization balance of an electron beam ion trap. The method will be used in Chapter 5 in the determination of the ionization cross sections for lithiumlike titanium, vanadium, chromium, manganese, and iron ($Z=22-26$). In particular, we will be interested in inferring the relative heliumlike, lithiumlike, and berylliumlike charge-state abundances from line ratio measurements of the $2p\rightarrow1s$ transitions. Furthermore, this technique can be extended beyond the K-shell to infer the relative abundances of L-shell and M-shell ions. For example, the high resolution crystal spectrometer can be used to determine the charge-state balance of L-shell nitrogenlike, oxygenlike, fluorinelike, and neonlike barium ($Z=56$) from $3d\rightarrow2p$ direct excitation transitions [57]. Similarly, M-shell ironlike, cobaltlike, and nickellike uranium ($Z=92$) can be determined from $4f\rightarrow3d$ transitions [90].
Figure 4.8: Relative iron charge-state balance determined from x-rays and ion extractor data at 15 keV. The sum of all the charge states is normalized to one.
Figure 4.9: Relative iron charge-state calculated as a function of oxygen background gas pressure for a beam energy of 15 keV and a beam current of 148 mA. The vertical line represents the charge-state balance inferred from the x rays.
Chapter 5

Ionization of Lithiumlike Ions

5.1 Introduction

In this chapter we present electron impact ionization measurements using two variations of a novel x-ray technique. The measurement technique is based upon correlating ionization events with the observation of dielectronic recombination x rays. In particular, we observe $\Delta n=1$ transitions following dielectronic recombination on the KLL resonance for heliumlike ions and show that there is almost a one to one correspondence between dielectronic recombination and ionization. In the first method ionization cross sections of lithiumlike titanium, vanadium, chromium, manganese, iron and barium ($Z=22-26,56$) are inferred using measurements from the solid-state Ge detector and are normalized to the cross section for radiative recombination onto lithiumlike ions. In the second approach, cross sections for ionization of lithiumlike (Ti, V, Cr, Mn, and Fe) are determined from measurements using the von Hámos Bragg crystal spectrometer. These measurements are normalized to the direct excitation cross section of the lithiumlike line $q (1s2s(3S)2p^2P_{3/2} \rightarrow 1s^22s^2S_{1/2})$. We use both theoretically and experimentally determined excitation cross sections for line $q$ to infer the ionization cross sections. The experimental cross sections of line $q$ are also normalized to the cross section for radiative recombination onto lithiumlike ions.
CHAPTER 5. IONIZATION OF LITHIUMLIKE IONS

The analysis of the ionization measurements includes modeling the charge-state abundances in the trap and a detailed comparison of the observed x-ray spectra with the results from a spectral model. This comparison is important because we use these models to adjust the charge-state balance inferred from our measurements and to account for the charge-exchange recombination of the ions with the neutral background atoms present in the trap.

The chapter is organized as follows. First, we will discuss the technique for determining ionization cross sections using the solid-state Ge detector and the crystal spectrometer. As a subsection, we discuss the method of inferring excitation cross sections from the data. In Section 5.3 we will show spectra and describe the experiment. We also describe the analysis using the charge-state balance and the x-ray models.

5.2 Description of Technique

The measurement scheme is based on a steady-state balance between the processes of dielectronic recombination and ionization. Steady state is achieved when the charge-state abundances, which are determined from the individual recombination and ionization rates in the plasma, are not changing in time. The scheme is illustrated in Fig. 5.1. In this approximation, we have neglected radiative recombination and charge exchange recombination of heliumlike to lithiumlike ions, which we assume are small. Therefore, with the electron beam energy set to the KLL dielectronic resonance energy for heliumlike ions, the abundance ratio of the heliumlike and lithiumlike charge states is equal to the ratio of the cross sections for ionization and dielectronic recombination. As a result, an x ray emitted during dielectronic recombination indicates that an ionization event has occurred, and we determine the ionization cross section by counting the n=2→1 dielectronic recombination x rays. We are able to establish this steady-state balance because the KLL dielectronic recombination energy of heliumlike ions is greater than the ionization energy of lithiumlike ions. For example, for iron the heliumlike
KLL resonances occur at energies from 4.54-4.76 keV, while the lithiumlike ionization energy is only 2.046 keV. A similar steady-state scheme was used recently to measure the dielectronic recombination cross section of Ar\textsuperscript{16+} on an electron beam ion source (EBIS) \cite{91, 92}. The two experiments, however, are very different. The EBIS group measured dielectronic recombination by extracting the ions, counting the electron energy dependent yields of heliumlike and lithiumlike argon ions, and normalizing to the theoretical ionization cross section of lithiumlike argon. On the otherhand, we measure ionization by counting dielectronic recombination x rays and normalizing to theoretical radiative recombination or excitation cross sections.

The general rate equation for the density of heliumlike ions, which includes the processes of radiative recombination and charge-exchange recombination with residual gas atoms in EBIT, is given by:

\[
\frac{dn_{\text{He}}}{dt} = \frac{je}{e} (\sigma_i n_{\text{Li}} - \sigma_{\text{DR}n_{\text{He}}} - \sigma_{\text{RR}n_{\text{He}}}) - n_0 v_0 \sigma_{\text{ex}} n_{\text{He}},
\]

(5.1)

where \( j_e \) is the effective current density, \( e \) is the charge of the electron, \( \sigma_i \) is the cross section for ionization of a lithiumlike ion, \( \sigma_{\text{DR}} \) and \( \sigma_{\text{RR}} \) the total capture cross sections for dielectronic and radiative recombination onto the heliumlike ion, and \( \sigma_{\text{ex}} \) the cross section for charge-exchange recombination with neutral background gases. The number densities of ground-state heliumlike and lithiumlike ions are \( n_{\text{He}} \) and \( n_{\text{Li}} \), \( n_0 \) is the density of neutral background atoms, and \( v_0 \) is the relative velocity of the neutrals and ions. The density of hydrogenlike ions plays no role in Eq. (5.1) because the electron beam energies in the measurements are always below the ionization threshold energy to produce hydrogenlike ions. In steady-state, \( \frac{dn_{\text{He}}}{dt}=0 \), so we can express \( \sigma_i \) as:

\[
\sigma_i = \frac{n_{\text{He}}}{n_{\text{Li}}} \left( \sigma_{\text{DR}} + \sigma_{\text{RR}} + \frac{e n_0 v_0}{j_e} \sigma_{\text{ex}} \right).
\]

(5.2)

In the next two subsections we discuss how we determine ionization cross sections from Ge detector and crystal spectrometer x-ray measurements using
Figure 5.1: Steady-state measurement scheme for lithium-like ions. By counting the $n=2\rightarrow 1$ x rays given off in the dielectronic recombination of heliumlike ions, the ionization cross section can be measured. $E_{\text{DR}}$ and $E_{\text{ion}}$ represent the dielectronic recombination energy for heliumlike ions and ionization energy of lithiumlike ions. The arrows labeled DR, x-ray, and ion represent the dielectronic capture of a heliumlike ion to a doubly excited lithiumlike state, the x ray emitted following dielectronic recombination, and the ionization of lithiumlike ions, respectively.
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Eq. (5.2) as the starting basis. Finally, in the third subsection we describe how to infer direct excitation cross sections of the lithiumlike line \( \eta \) from the data, relative to radiative recombination, in order to normalize the high resolution measurements. This procedure can be generalized to infer the excitation cross sections of the associated heliumlike and lithiumlike \( n=2 \rightarrow 1 \) direct excitation lines observed in our data.

5.2.1 Ge Detector Measurements

In the first approach we determine the ionization cross section of lithiumlike titanium, vanadium, chromium, manganese, iron, and barium (\( Z=22-26,56 \)) from x-ray observations using the solid-state Ge detector. The relative heliumlike and lithiumlike ion densities in Eq. (5.2) are inferred by measuring the x-ray intensities of dielectronic recombination onto heliumlike ions and radiative recombination onto lithiumlike ions, respectively. They are expressed as:

\[
J_{DR}^{Ge} = \frac{j_e}{e} \sigma_{DR} n_{He} A_1 G_1,
\]

\[
J_{RR}^{Li} = \frac{j_e}{e} \sigma_{RR} n_{Li} G_1,
\]

where \( \sigma_{RR}^{Li} \) is the radiative recombination cross section onto lithiumlike ions at 90° (the angular distribution has been folded in), and \( A_1 \) represents the angular distribution factor of the dielectronic recombination x rays. \( G_1 \) is the solid angle subtended by the Ge detector. Substituting these into Eq. (5.2) for \( n_{He}, n_{Li} \), we get:

\[
\sigma_i = \frac{J_{DR}^{Ge} \sigma_{RR}^{Li}}{J_{RR}^{Li} A_1} \left( 1 + \frac{\sigma_{RR}}{\sigma_{DR}} + \frac{\epsilon_{\eta} u_0 \sigma_{ce}}{j_e \sigma_{DR}} \right).
\]

However, the x rays we measure from \( n=2 \) radiative recombination onto heliumlike, lithiumlike, and berylliumlike ions are unresolved. Therefore, we must determine the fraction of the total that are due to recombination onto
lithiumlike ions. $I_{RR}^{Li}$ can be expressed as:

$$I_{RR}^{Li} = I_{RR}^{tot} \left( \frac{n_{He} \sigma_{RR}^{He} + n_{Li} \sigma_{RR}^{Li} + n_{Be} \sigma_{RR}^{Be}}{n_{He} \sigma_{RR}^{He}} \right),$$

(5.6)

where $I_{RR}^{tot}$ is the total number of radiative recombination photons onto the $n=2$ shell at 90°, $\sigma_{RR}^{He}$ and $\sigma_{RR}^{Be}$ are the radiative recombination cross sections at 90° onto the heliumlike ($n_{He}$) and berylliumlike ($n_{Be}$) charge states, respectively. The term in parenthesis on the rightside of Eq. (5.6) represents the fraction of the radiative recombination x rays due to the lithiumlike charge state. Substituting Eq. (5.6) into Eq. (5.5) we get:

$$\sigma_i = \frac{I_{DR}^{Ge}}{I_{RR}^{tot}} \left( 1 + \frac{\sigma_{RR}^{He} n_{He}}{\sigma_{RR}^{Li} n_{Li}} + \frac{\sigma_{RR}^{Be} n_{Be}}{\sigma_{RR}^{Li} n_{Li}} \right) \sigma_{RR}^{Li} \left( 1 + \frac{\sigma_{RR} \sigma_{cx}}{\sigma_{DR} \sigma_{ei}} \right)$$

(5.7)

The ionization cross section in Eq. (5.7) is evaluated using the measured values of $I_{DR}^{Ge}$ and $I_{RR}^{tot}$. We use theoretical radiative recombination cross sections calculated with the methods described by Scofield [85], which accounts for the angular distribution of emitted photons at 90°. The relative charge-state abundances $n_{He}/n_{Li}$ and $n_{Be}/n_{Li}$ are determined from direct excitation line ratio measurements, similar those described in Chapter 4, of $I_{He}/I_{Li}$ and $I_{Be}/I_{Li}$, respectively, for the Ti-Fe ionization measurements. These x rays were monitored with the crystal spectrometer at the same time the radiative recombination photons onto the $n=2$ shell were being acquired with the Ge detector. Alternatively, for the barium ionization measurements we fitted the $n=2$ radiative recombination peak to infer the relative charge-state balance. The dielectronic recombination cross sections are calculated by the method of Chen [93], and the charge-exchange recombination term is determined from the charge-state balance and x-ray models, which will be described in Sections 5.3.2 and 5.3.3. The measurement is normalized to the radiative recombination cross section onto lithiumlike ions [85]. The radiative recombination code has been compared to measurements of photoionization, the inverse process of radiative recombination, at photon energies similar to the present experiments. The agreement is within a few percent [86].
Since $\sigma_{\text{DR}}$ and the dielectronic recombination rate are very large at the resonance energies used in the Ti-Fe measurements, the second to the last (radiative recombination) and the last (charge-exchange recombination) terms in Eq. (5.7) are $\ll 1$. For example, for iron at 4.64 keV the theoretical ratio of the radiative recombination [85] and the dielectronic recombination [93] cross sections is 0.012, and the charge-exchange term inferred from the comparison of the steady-state data in Fig. 5.10(b) with the x-ray model in Fig. 5.11, discussed below, is 0.016. However, for the barium measurements we will show that radiative and charge-exchange recombination are not small compared to dielectronic recombination.

We adjust $I_{\text{DR}}^{\text{Ge}}$ for the angular distribution of the dielectronic recombination x rays and for the contribution due to lithiumlike to berylliumlike dielectronic satellites. Since the energy of the transition metal ionization measurements is always close to the energy of the heliumlike dielectronic satellites $j$ and $k$, we set $A_1 = 1.22$, which is the average of the angular distribution correction for these satellites. For barium, we made measurements close to the dielectronic recombination of satellites $o$ and $p$, $r$, and $e$ and $s$, and the corresponding factors of $A_1$ were 1.0, 1.0, and 1.23, respectively. On the other hand, for the runs in which the dielectronic recombination of lithiumlike ions occurs, $I_{\text{DR}}^{\text{Ge}}$ is multiplied by the fraction of the heliumlike dielectronic recombination x rays relative to the total as measured by the crystal spectrometer. This fraction is never smaller than 74% for the Ti-Fe measurements. For barium, we were careful to stay away from any lithiumlike dielectronic recombination resonances, and this factor is always 1.0.

The Ti-Fe measurements of $I_{\text{DR}}^{\text{Ge}}$ and $I_{\text{RR}}^{\text{tot}}$ are also affected by absorption of the x rays by the beryllium window on the detector and on EBIT and also by the small air gap between EBIT and the solid-state detector. We correct the measurements for the absorption of the x rays by the 5 mil Ge detector and the 7 mil EBIT beryllium windows. We also have to adjust these x rays for absorption by the 1 inch of air, which also absorbs x rays as a function of energy. The largest absorption occurred for the Ti data, where the ratio of
the dielectronic and recombination radiative x rays was attenuated by 23%.
The 32 keV barium x rays were unaffected by the beryllium windows or the
air gap.

5.2.2 High Resolution Technique

In this modification of the measurement scheme we follow the same procedure
outlined above for Ti, V, Cr, Mn, and Fe. However, we determine lithium­
like ionization cross sections by counting the dielectronic recombination x
rays recorded with the crystal spectrometer and normalizing to the excita­
tion cross section of the lithiumlike line \( q \) \( (1s2s^2 \! \! ^3S_1 2p^2 \! \! ^2P_{3/2} \rightarrow 1s^22s^2 \! \! ^2S_{1/2}) \) produced with the same ions. We normalize the measurements in two ways:
(1) by using theoretically calculated cross sections for \( q \) and (2) by inferring
the excitation cross section of line \( q \) relative to radiative recombination x
rays onto the \( n=2 \) levels in lithiumlike ions.

The technique has the same starting point as in Eq. (5.2). The x-ray
intensities of dielectronic recombination onto heliumlike ions and direct ex­
citation of the lithiumlike line \( q \) as measured by the von Hámos crystal spec­
trometer measured at 90° to the electron beam are expressed as:

\[
I_{DR} = \frac{j_e}{e} \sigma_{DR} n_{He} W_{DR} G_2, \tag{5.8}
\]

\[
I_q = \frac{j_e}{e} \beta_r \sigma_q n_{Li} W_q G_2, \tag{5.9}
\]

where \( \sigma_q \) is the excitation cross section of the lithiumlike line \( q \), and \( \beta_r \) is
the radiative branching ratio of line \( q \). \( G_2 \) is the solid angle subtended by
the spectrometer. \( W \) accounts for the angular distribution of the x rays,
the linear polarization of the x rays, and the reflectivity of the analyzing
crystal, which was discussed in Chapter 3. We use the theoretical values for
polarization of the dielectronic recombination x rays calculated by Inal and
Dubau [94].
Substituting Eq. (5.8) and Eq. (5.9) into Eq. (5.2) for \(n_{\text{He}}\) and \(n_{\text{Li}}\), we get:

\[
\sigma_i = \frac{J_{\text{DR}} \beta_i \sigma_q W_q}{I_q W_{\text{DR}}} \left( 1 + \frac{\sigma_{\text{RR}} + \epsilon \sigma_{\text{L}}}{\sigma_{\text{DR}}} \right).
\] (5.10)

The ionization cross section in Eq. (5.10) is evaluated using the measured values of \(J_{\text{DR}}\) and \(I_q\). We use radiative branching ratios calculated using the methods of Chen [87]. We normalize the measurement either to theoretical excitation cross sections of line \(q\) determined from the distorted-wave code of Zhang, Sampson, and Clark [79] or to experimental values. The procedure for determining the experimental excitation cross sections from our measurements will be described in the next subsection. The radiative recombination cross sections are calculated with the methods described by Scofield [85], and the dielectronic recombination cross sections are calculated by the method of Chen [93]. The charge-exchange cross section term will be evaluated using our models, which will be discussed later. For the transition metal ion measurements, \(\sigma_{\text{DR}}\) and the dielectronic recombination rate are very large at the resonance energies used, similar to the Ge detector measurements, and, consequently, the second and third terms in Eq. (5.10) are \(\ll 1\).

### 5.2.3 Direct Excitation

In this subsection we present the technique for inferring the electron impact excitation cross sections for the heliumlike transitions \(w, x, y,\) and \(z\) and the lithiumlike transitions \(q, r, t, u,\) and \(v\) for titanium, vanadium, chromium, manganese, and iron. The cross sections for \(q\) will be used to normalize the ionization cross sections determined from the high resolution method. The measurements were made at approximately 100 eV above the threshold for the excitation of line \(w\), where no other processes but electron impact excitation contribute to the excitation of the lines. The technique is similar to the one used by Marrs et al. [60] who measured the electron impact excitation of transitions in neonlike barium. The data we analyze are similar to the Fe
data in Fig. 5.10(a) and (b) where the charge-state abundances are 95% helium-like and 5% lithium-like (the “low lithium-like” case), and the Fe data in Fig. 5.4(a) and (b) where the charge-state abundances are 34% helium-like, 63% lithium-like, and 3% beryllium-like (the “high lithium-like” case).

5.2.3.1 Experimental Technique

We determine the excitation cross section of these transitions in three steps. First, we determine the excitation cross sections of the four helium-like lines from the low-lithium-like data. Then, we use these experimentally determined cross sections to infer the excitation cross section of the lithium-like line \( q \) from the high-lithium-like data. Finally, the cross sections of the remaining lithium-like satellite lines are inferred relative to the experimental cross section of line \( q \). The technique is based on summing the intensity of the \( n=2 \rightarrow 1 \) direct excitation photons measured with the crystal spectrometer and relating the sum to their combined intensity observed with a solid-state Ge detector. The individual cross sections are determined from the fraction of the transition to the sum of all the transitions as measured by the crystal spectrometer and the solid-state Ge detector. The helium-like lines are normalized to the \( n=2 \) radiative recombination cross section onto helium-like ions, while the lithium-like lines are normalized to the radiative recombination cross section onto lithium-like ions. The radiative recombination x rays are measured with the Ge detector.

First, we present the example of determining the excitation cross section of the helium-like line \( \omega \) for the low lithium-like case. The corresponding cross sections for the helium-like lines \( x, y, \) and \( z \) are determined in a similar manner. For direct excitation the sum of all the \( n=2 \rightarrow 1 \) x rays measured at 90° with the Ge detector is:

\[
\sum I_{\text{Ge}}^{90°} = \frac{j_e}{e} [\sigma_w n_{He} + \sigma_x n_{He} + \sigma_y n_{He} + \sigma_z n_{He} + \beta_q \sigma_q n_{Li}] G_1, \quad (5.11)
\]

where \( j_e \) is the effective current density of the electron beam, \( e \) is the charge of the electron, \( \sigma_w, \sigma_x, \sigma_y, \sigma_z, \) and \( \sigma_q \) are the excitation cross section of lines \( \omega, \)
CHAPTER 5. IONIZATION OF LITHIUMLIKE IONS

x, y, z and q, respectively, \( n_{\text{He}} \) and \( n_{\text{Li}} \) are the number density of heliumlike and lithiumlike ions, \( \beta_q \) is the radiative branching ratio for line q, and \( G_1 \) is the solid angle subtended by the solid-state Ge detector. In the case where the other lithiumlike or berylliumlike lines are seen, such as in Fig. 5.4(b), Eq. (5.11) is expanded to include terms from these transitions. The angular distribution factors \( A(P) \) has not been accounted for here because we want to equate these x-rays with those seen by the crystal spectrometer at 90°. It will be accounted for in the last step.

The x rays corresponding to radiative recombination, observed at 90°, onto the n=2 shell of heliumlike ions is:

\[
I_{\text{RR}}^{\text{He}}(90°) = \frac{j_e}{e} \sigma_{\text{He}}^{\text{RR}} n_{\text{He}} G_1,
\]

where \( \sigma_{\text{He}} \) is the sum of the radiative recombination cross sections onto heliumlike ions calculated using the relativistic formulation described by Scofield [85], which accounts for the angular distribution of emitted photons at 90°.

However, the solid-state detector cannot resolve the individual charge-state components of radiative recombination onto the n=2 shell. Consequently, we must determine the fraction of the total that are due to recombination onto heliumlike ions before we can determine \( \sigma_w \). \( I_{\text{RR}}^{\text{He}} \) can be expressed as:

\[
I_{\text{RR}}^{\text{He}}(90°) = I_{\text{RR}}^{\text{tot}}(90°) \left( \frac{n_{\text{He}} \sigma_{\text{He}}^{\text{RR}}}{n_{\text{He}} \sigma_{\text{He}}^{\text{RR}} + n_{\text{Li}} \sigma_{\text{Li}}^{\text{RR}} + n_{\text{Be}} \sigma_{\text{Be}}^{\text{RR}}} \right),
\]

where \( I_{\text{RR}}^{\text{tot}}(90°) \) is the total number of radiative recombination photons onto the n=2 shell at 90°, \( \sigma_{\text{Li}}^{\text{RR}} \) and \( \sigma_{\text{Be}}^{\text{RR}} \) are the radiative recombination cross sections at 90° onto the lithiumlike \( n_{\text{Li}} \) and berylliumlike \( n_{\text{Be}} \) charge states, respectively. The term in parenthesis on the rightside of Eq. (5.13) represents the fraction of the radiative recombination x rays due to the heliumlike charge state.

The individual line \( w \) as seen on the crystal spectrometer at 90° is:

\[
I_w^{\text{cr}}(90°) = \frac{j_e}{e} \sigma_w R_w n_{\text{He}} G_2.
\]
Again, the angular distribution $A(P)$ will be accounted for later. The sum of the $n=2\rightarrow 1$ X rays as measured by the crystal spectrometer at $90^\circ$ is:

$$I_{DE}^c(90^\circ) = \sum_i I_i^c(90^\circ) = \frac{j_e}{e} [\sigma_w R_w n_{He} + \sigma_x R_x n_{He} + \sigma_y R_y n_{He} + \sigma_z R_z n_{He} + \beta_q q R_q n_{Li}],$$

(5.15)

where the sum over $i$ consists of lines $w$, $x$, $y$, $z$, and $q$, and $R$ is the reflectivity portion of the crystal adjustment as we have described in Chapter 3. The angular distribution $A(P)$ will be added later. $G_2$ is the solid angle subtended by the crystal spectrometer. Combining Equations (5.11), (5.14), and (5.15), which relates the individual intensity of line $w$ to the total of all the $n=2\rightarrow 1$ transitions as observed with the crystal spectrometer and the Ge detector, we get:

$$\frac{I_w^c(90^\circ)/R_w}{\sum_i[I_i^c(90^\circ)/R_i]} \sum_i I_{DE}^c(90^\circ)/G_1 = \frac{j_e}{e} \sigma_w n_{He}.$$  

(5.16)

Dividing Eq. (5.16) by Eq. (5.12) and solving for $\sigma_w$ we obtain:

$$\sigma_w = \frac{I_w^c(90^\circ)/R_w}{\sum_i[I_i^c(90^\circ)/R_i]} \frac{\sum I_{DE}^c(90^\circ)}{G_1} \sigma_{He}.$$  

(5.17)

Substituting Eq. (5.13) into Eq. (5.17) we get:

$$\sigma_w = \frac{I_w^c(90^\circ)/R_w}{\sum_i[I_i^c(90^\circ)/R_i]} \frac{\sum I_{DE}^c(90^\circ)}{G_1} \sigma_{He} \left( 1 + \frac{\sigma_{Li}^{He} n_{Li}}{\sigma_{He} n_{He}} + \frac{\sigma_{Be}^{He} n_{Be}}{\sigma_{He} n_{He}} \right).$$  

(5.18)

The relative charge-state abundances $n_{Li}/n_{He}$ and $n_{Be}/n_{He}$ are determined from line ratio measurements of $I_q/I_w$ and $I_{q}/I_w$, respectively and theoretical excitation cross sections and branching ratios as described in Chapter 4. These terms are negligible for the low-lithiumlike case.

In determining the electron impact excitation cross sections of the heliumlike and lithiumlike lines from our measurements we need to account for the polarization and angular distribution as we discussed in Chapter 3. Calculations of the magnetic sublevels populations including cascades using the relativistic distorted-wave code of Sampson, Zhang and Clark [79] show that
the polarization of \( w, x, y, z, \) and \( q \) are +60\%, -52\%, -19\%, -7\%, and +34\%, respectively, at an energy approximately 100 eV above the threshold for \( w \). The polarization at an electron beam energy of 6.8 keV and x-ray energies of all the direct excitation transitions for iron are given in Table 5.1.

Table 5.1: Fe\(^{24+}\), Fe\(^{23+}\), and Fe\(^{22+}\) direct excitation data. Key letters are from Gabriel \cite{95}. \( E_{x \, \text{ray}} \) is the x-ray transition energy in keV, and \( P \) is the polarization of the x rays at an electron beam energy of 6.8 keV.

<table>
<thead>
<tr>
<th>Transitions</th>
<th>Key</th>
<th>( E_{x , \text{ray}} )</th>
<th>( P )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 1s^2 1P\rightarrow 1s^2 1S_0 )</td>
<td>( w )</td>
<td>6.6700</td>
<td>0.60</td>
</tr>
<tr>
<td>( 1s^2 3P\rightarrow 1s^2 1S_0 )</td>
<td>( x )</td>
<td>6.6818</td>
<td>-0.52</td>
</tr>
<tr>
<td>( 1s^2(1S)2p^2 2P_{3/2} \rightarrow 1s^2 2s^2 2S_{1/2} )</td>
<td>( t )</td>
<td>6.6766</td>
<td>0.00</td>
</tr>
<tr>
<td>( 1s^2 3P\rightarrow 1s^2 1S_0 )</td>
<td>( y )</td>
<td>6.6667</td>
<td>-0.19</td>
</tr>
<tr>
<td>( 1s^2(3S)2p^2 2P_{3/2} \rightarrow 1s^2 2s^2 2S_{1/2} )</td>
<td>( q )</td>
<td>6.6624</td>
<td>0.34</td>
</tr>
<tr>
<td>( 1s^2(3S)2p^2 2P_{1/2} \rightarrow 1s^2 2s^2 2S_{1/2} )</td>
<td>( r )</td>
<td>6.6522</td>
<td>0.00</td>
</tr>
<tr>
<td>( 1s^2 3S_1 \rightarrow 1s^2 1S_0 )</td>
<td>( z )</td>
<td>6.6356</td>
<td>-0.074</td>
</tr>
<tr>
<td>( 1s^2(3S)2p^1 1P\rightarrow 1s^2 2s^2 1S_0 )</td>
<td>( \beta )</td>
<td>6.6300</td>
<td>0.60</td>
</tr>
<tr>
<td>( 1s^2(3S)2p^4 3P_{3/2} \rightarrow 1s^2 2s^2 2S_{1/2} )</td>
<td>( u )</td>
<td>6.6164</td>
<td>-0.31</td>
</tr>
<tr>
<td>( 1s^2(3S)2p^4 3P_{3/2} \rightarrow 1s^2 2s^2 2S_{1/2} )</td>
<td>( v )</td>
<td>6.6115</td>
<td>0.00</td>
</tr>
</tbody>
</table>

\( ^a \)Values from Zhang, Sampson, and Clark, Ref. \cite{79} normalized to to \( w \) of Ref. \cite{84}.

\( ^b \)Calculated using the formulas given by Inal and Dubau, Ref. \cite{80} with the magnetic sublevel calculations of R... \cite{79}.

In order to obtain the total cross section, \( \sigma_{w}^{4\pi} \), we divide the excitation cross section at 90° by the angular factor \( A(P) \), discussed in Chapter 3:

\[
\sigma_{w}^{4\pi} = \frac{\sigma_{w}}{A(P)} = \sigma_{w} \frac{3 - P}{3}.
\]

Once the excitation cross sections for \( w, x, y, \) and \( z \) are determined for the low-lithiumlike case, we use these cross sections to determine the
excitation cross section of the lithiumlike line \( q \) from the high-lithiumlike data. We follow a similar procedure, which is outline above, except that the measurements are normalized to the radiative recombination cross section onto lithiumlike ions. The final expression for the excitation cross section of line \( q \) is:

\[
\sigma_q = \frac{I_q^{Cr}(90^\circ)/\beta_q R_q A_q \sum I_{DE}^q(90^\circ) / R_i \cdot I_{RR}^{tot}(90^\circ) \cdot \sigma_{Li}^{RR}}{\sum I_i^{Cr}(90^\circ)/R_i \cdot I_{RR}^{tot}(90^\circ) \cdot \sigma_{Li}^{RR}} \left( 1 + \frac{\sigma_{He}^{He} n_{He}^{He}}{\sigma_{RR}^{He} n_{Li}^{He}} + \frac{\sigma_{Be}^{Be} n_{Be}^{Be}}{\sigma_{RR}^{Be} n_{Li}^{Be}} \right),
\]

where \( I_q^{Cr}(90^\circ) \) is the intensity of line \( q \) as measured with the crystal spectrometer, and \( \beta, R, \) and \( A \) are the appropriate radiative branching ratio, reflectivity factor and angular distribution factor, respectively. We substitute the following expressions for \( n_{He}, n_{Li}, \) and \( n_{Be} \) into Eq. (5.30):

\[
n_{He} = \frac{I_w/(R_w A_w) + I_x/(R_x A_x) + I_y/(R_y A_y) + I_z/(R_z A_z)}{\frac{I_q}{\sigma_q + \sigma_x + \sigma_y + \sigma_z}},
\]

\[
n_{Li} = \frac{I_q/(R_q A_q)}{\beta_q \sigma_q},
\]

\[
n_{Be} = \frac{I_{Ry}/(R_{Ry} A_{Ry})}{\beta_{Ry} \sigma_{Ry}},
\]

where \( I \) represents the intensity of the lines from the high-lithiumlike data. We use the experimentally determined cross sections for \( \sigma_w, \sigma_x, \sigma_y, \) and \( \sigma_z, \) and the theoretically determined cross sections for \( \sigma_{Ry} \) [79]. We determined that the charge-state fraction due to berylliumlike ions is about 3%, while the fraction due to boronlike, carbonlike, and higher charge states is less than 1%. We define \( \kappa \):

\[
\kappa = \frac{\sum I_{DE}^q(90^\circ)}{\sum I_i^{Cr}(90^\circ)/R_i \cdot I_{RR}^{tot}(90^\circ)}. \quad (5.24)
\]

Then, solving for \( \sigma_q \), we obtain:

\[
\sigma_q = \frac{\kappa I_q^{Cr} \sigma_{Li}^{RR} / R_q A_q \beta_q}{1 - \kappa \sigma_{He}^{He} I_w/R_w A_w + I_x/R_x A_x + I_y/R_y A_y + I_z/R_z A_z + \frac{\kappa I_{Ry}^{Be} \sigma_{Ry}^{Be} / R_{Ry} A_{Ry} \beta_{Ry}}{\sigma_w + \sigma_x + \sigma_y + \sigma_z}}, \quad (5.25)
\]
Finally, we determine the cross sections of the other lithiumlike lines relative to $\sigma_q$. For example for line $r$:

$$\sigma_r = \frac{I_r^{Cr} \beta_q A_q R_q}{I_q^{Cr} \beta_r A_r R_r} \sigma_q,$$

(5.26)

where $I_r^{Cr}$ is measured from the crystal data for the high lithiumlike data. The cross sections for $t$, $u$, and $v$ are calculated similarly.

### 5.3 Ionization Cross Section Experiment

The ionization measurements are performed by taking advantage of EBIT's ability to rapidly alternate the electron beam energy from one value to another. First, we establish the steady-state charge-state balance with the electron beam energy set to the KLL dielectronic recombination resonance. This is where we measure the dielectronic recombination x rays, which are related to ionization events. Then, we change the electron beam energy to a value away from the KLL resonance for a short period of time to measure the relative charge-state abundances from radiative recombination photons onto the $n=2$ shell and from the direct excitation x rays $w$, $q$, and $\beta$. We minimize this time so that the steady-state ionization balance established on the dielectronic recombination resonance is perturbed as little as possible. We will show later that the ionization varies and this is accounted for using the charge-state balance model in section 5.3.2.

The energy resolution of the electron beam is approximately 40 eV FWHM, which is more than the separation of individual dielectronic resonances. Thus, setting the beam to a given energy results in the excitation of several dielectronic satellite lines. Table 5.2 gives the Auger energies and resonance strengths ($\mathcal{S}$) for recombination onto the corresponding upper levels for the heliumlike KLL dielectronic recombination resonances of iron. The table also includes the radiative branching ratios of the upper levels and the resulting x-ray transitions given by their key labels [95]. For the heliumlike KLL di-
electronic resonances there are 16 upper levels and 22 x-ray transitions. We
do not list the upper level 1s2s2p 4P3/2, which cannot decay by an E1 tran­
sition but decays by an E2 transition. The capture rate for this level is large
but the dielectronic recombination is small. The table is ordered in terms of
E_{Auger}, which is the dielectronic recombination energy (E_{DR}) or the electron
beam energy used in the experiments. Therefore, satellites o and p are the
first dielectronic recombination x rays to appear at E_{beam}\approx4.553\text{ keV}; while
j and k appear at the higher energy E_{beam}\approx4.660\text{ keV}. For example, dielec­
tronic recombination onto the first upper level results in the x-ray transition
o 50.3\% and p 49.7\% of the time. For the transition elements we set the beam
energy to be near E_{Auger} of satellites j and k where the beam samples the
largest resonance strengths. Table 5.3 shows the KLL dielectronic satellite
transitions of iron, key labels, x-ray energies (E_{x\text{ ray}}), and polarization (P).
The polarization of the dielectronic recombination x rays was calculated by
Inal and Dubau [94].

5.3.1 Lithiumlike Ti, V, Cr, Mn, and Fe Measure­
ments
The x rays from the transition metal experiments are monitored with a solid-
state Ge detector and a curved crystal Bragg spectrometer in the von Hámos
geometry [55]. The crystal spectrometer employs a LiF(200) crystal with a
lattice spacing of 2d = 4.027 Å. The crystal was bent to a radius of curvature
of 30 cm for chromium, manganese, and iron and 75 cm for titanium and
vanadium. The resolving power of the setup is \lambda/\Delta\lambda \approx 1500 for the 30 cm
crystal and \lambda/\Delta\lambda \approx 4000 for the 75 cm crystal. For the case of iron, which
we will discuss in this subsection, the spectrometer was set to a nominal
Bragg angle of 26.8°, which corresponds to a wavelength of 1.81 Å. The total
wavelength covered was 1.77 Å < \lambda < 1.88 Å which includes the heliumlike
transitions w (1s2p 1P1 \rightarrow 1s^2 1S_0) at 1.8505 Å, x (1s2p 3P_2 \rightarrow 1s^2 1S_0) at
1.8555 Å, y (1s2p 3P_1 \rightarrow 1s^2 1S_0) at 1.8595 Å, and z (1s2s 3S_1 \rightarrow 1s^2 1S_0)
Table 5.2: Fe\textsuperscript{23+} KLL dielectronic recombination data. $E_{\text{Auger}}$ is the Auger or dielectronic recombination energy in keV, and $S$ is the resonance strength in $10^{-21}$ cm\textsuperscript{2}\cdot eV for dielectronic recombination into the upper levels. The upper levels decay with the radiative branching ratios ($\beta_r$) to x-ray transitions denoted by their key letter from Gabriel [95].

<table>
<thead>
<tr>
<th>Upper Level</th>
<th>$E_{\text{Auger}}$</th>
<th>$S$</th>
<th>$\beta_r$</th>
<th>Key</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1s2s^2, ^2S_{1/2}$</td>
<td>4.5534</td>
<td>15.63</td>
<td>0.503</td>
<td>$o$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.497</td>
<td>$p$</td>
</tr>
<tr>
<td>$1s2s(3S)2p, ^4P_{1/2}$</td>
<td>4.5663</td>
<td>0.0621</td>
<td>1.000</td>
<td>$v$</td>
</tr>
<tr>
<td>$1s2s(3S)2p, ^4P_{3/2}$</td>
<td>4.5701</td>
<td>0.3279</td>
<td>1.000</td>
<td>$u$</td>
</tr>
<tr>
<td>$1s2s(3S)2p, ^2P_{1/2}$</td>
<td>4.6049</td>
<td>43.40</td>
<td>1.000</td>
<td>$r$</td>
</tr>
<tr>
<td>$1s2s(3S)2p, ^2P_{3/2}$</td>
<td>4.6153</td>
<td>2.739</td>
<td>1.000</td>
<td>$q$</td>
</tr>
<tr>
<td>$1s2p^2, ^4P_{1/2}$</td>
<td>4.6246</td>
<td>0.2017</td>
<td>0.006</td>
<td>$h$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.994</td>
<td>$i$</td>
</tr>
<tr>
<td>$1s2s(1S)2p, ^2P_{1/2}$</td>
<td>4.6312</td>
<td>50.66</td>
<td>1.000</td>
<td>$t$</td>
</tr>
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<td>$1s2p^2, ^4P_{3/2}$</td>
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<td>0.8565</td>
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<td></td>
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<td></td>
<td>0.004</td>
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<td>$1s2s(1S)2p, ^2P_{3/2}$</td>
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<td>$1s2p^2, ^2D_{3/2}$</td>
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<td></td>
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<td>$k$</td>
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<td>$1s2p^2, ^2P_{1/2}$</td>
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<td>1.751</td>
<td>0.236</td>
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<td></td>
<td></td>
<td>0.764</td>
<td>$d$</td>
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<tr>
<td>$1s2p^2, ^2D_{5/2}$</td>
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<td>255.9</td>
<td>1.000</td>
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<td>64.19</td>
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<td></td>
<td></td>
<td>0.011</td>
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<td>$1s2p^2, ^2S_{1/2}$</td>
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<td></td>
<td></td>
<td></td>
<td>0.048</td>
<td>$n$</td>
</tr>
</tbody>
</table>

\textsuperscript{a}Calculated using the methods of Chen Ref. [87].
\textsuperscript{b}Calculated using the methods of Chen Ref. [93].
Table 5.3: Fe$^{23+}$ n=2 dielectronic satellite data. Key letters are from Gabriel [95]. $E_{x\text{ ray}}$ is the x-ray transition energy in keV, and P is the polarization of the x rays.

<table>
<thead>
<tr>
<th>Transitions</th>
<th>Key</th>
<th>$E_{x\text{ ray}}$</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s2p$^2$ 2P$<em>{3/2}$→1s$^2$2p $^3$P$</em>{3/2}$</td>
<td>a</td>
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<td>-0.75</td>
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<tr>
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<td>c</td>
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<td>0.00</td>
</tr>
<tr>
<td>1s2p$^2$ 2P$<em>{1/2}$→1s$^2$2p $^3$P$</em>{1/2}$</td>
<td>d</td>
<td>6.6554</td>
<td>0.00</td>
</tr>
<tr>
<td>1s2p$^2$ 4P$<em>{5/2}$→1s$^2$2p $^3$P$</em>{3/2}$</td>
<td>e</td>
<td>6.6199</td>
<td>0.50</td>
</tr>
<tr>
<td>1s2p$^2$ 4P$<em>{3/2}$→1s$^2$2p $^3$P$</em>{3/2}$</td>
<td>f</td>
<td>6.6138</td>
<td>-0.75</td>
</tr>
<tr>
<td>1s2p$^2$ 4P$<em>{3/2}$→1s$^2$2p $^3$P$</em>{1/2}$</td>
<td>g</td>
<td>6.6298</td>
<td>0.60</td>
</tr>
<tr>
<td>1s2p$^2$ 4P$<em>{1/2}$→1s$^2$2p $^3$P$</em>{3/2}$</td>
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<tr>
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<td>q</td>
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<tr>
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<td>s</td>
<td>6.6788</td>
<td>0.60</td>
</tr>
<tr>
<td>1s2s$^2$(1S)2p $^3$P$<em>{1/2}$→1s$^2$2s $^2$S$</em>{1/2}$</td>
<td>t</td>
<td>6.6768</td>
<td>0.00</td>
</tr>
<tr>
<td>1s2s$^2$(3S)2p $^3$P$<em>{3/2}$→1s$^2$2s $^2$S$</em>{1/2}$</td>
<td>u</td>
<td>6.6157</td>
<td>0.60</td>
</tr>
<tr>
<td>1s2s$^2$(3S)2p $^3$P$<em>{1/2}$→1s$^2$2s $^2$S$</em>{1/2}$</td>
<td>v</td>
<td>6.6120</td>
<td>0.00</td>
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</tbody>
</table>

*Calculated using the methods of Chen Ref. [87].

$b$Inal and Dubau, Ref. [94].
CHAPTER 5. IONIZATION OF LITHIUMLIKE IONS

at 1.8682 Å [84], as well as the lithiumlike satellite lines.

A typical x-ray spectrum taken with the electron beam energy set to the iron KLL dielectronic resonance is given in Figure 5.2(a) for the Ge detector. Fig. 5.2(b) shows the corresponding spectrum recorded with the crystal spectrometer. The spectrum shows the lithiumlike dielectronic recombination satellite lines $e \left(1s^2p^2 4P_{5/2} \rightarrow 1s^22p^2 2P_{3/2}\right)$, $j \left(1s^2p^2 2D_{5/2} \rightarrow 1s^22p^2 2P_{3/2}\right)$, $k \left(1s^2p^2 2D_{3/2} \rightarrow 1s^22p^2 2P_{1/2}\right)$, and a blend of $s \left(1s^2s(1S)2p^2 2P_{3/2} \rightarrow 1s^22s 2S_{1/2}\right)$ and $t \left(1s^2s(1S)2p^2 2P_{1/2} \rightarrow 1s^22s 2S_{1/2}\right)$. These spectra are used to provide a count of the number of ionization events from the dielectronic recombination x rays. An x-ray spectrum, which is acquired when the electron beam energy is changed for 6 ms away from the KLL resonance and set to a value, where direct excitation is the only excitation mechanism, is shown in Fig. 5.4(a) for the Ge detector. We observe both the $n=2\rightarrow 1$ x rays and x rays from radiative recombination onto the $n=2$ shell. Fig. 5.4(b) shows the corresponding spectrum recorded with the crystal spectrometer. The heliumlike transitions $w$, $x$, $y$, and $z$, the lithiumlike transitions $t$, $q$, $r \left(1s2s(3S)2p 2P_{1/2} \rightarrow 1s^22s 2S_{1/2}\right)$, $u \left(1s2s2p 4P_{3/2} \rightarrow 1s^22s 2S_{1/2}\right)$, and $v \left(1s2s2p 4P_{1/2} \rightarrow 1s^22s 2S_{1/2}\right)$, and the berylliumlike transition $\beta \left(1s2s^22p^1P_1 \rightarrow 1s^22s^2 1S_0\right)$ are identified in the figure. The purpose of these spectra is to provide information on the relative charge-state abundances from the radiative recombination onto the $n=2$ shell and the direct excitation x rays. Figures 5.3 and 5.5 give the results of an x-ray model, which we describe later. We note that the electron beam energy of the model is different from the experimental energy. This is due to the space charge of the electron beam or, simply, this is the result of the electrons in the center of the hollow drift tubes feeling a different accelerating potential than the actual voltage we apply to the drift tubes. In what follows the electron beam energies we discuss will have the space charge subtracted out.

The first step in the experiment is to determine the electron beam energy at which to probe the steady-state ionization balance when the beam energy
Figure 5.2: Dielectronic recombination x-ray spectrum of iron (a) measured at an electron beam energy of 4.86 keV with a solid-state Ge detector and (b) measured at an electron beam energy of 4.86 keV with a Bragg crystal spectrometer. The marked lines are identified in the text.
Figure 5.3: Dielectronic recombination x-ray spectrum of iron modeled at an electron beam energy of 4.64 keV with an electron beam width of 40 eV (FWHM). The additional marked lines are identified in the Section 5.3.3.
Figure 5.4: Direct excitation x-ray spectrum of iron (a) measured at an electron beam energy of 7.0 keV with a solid-state Ge detector and (b) measured at an electron beam energy of 7.0 keV with a Bragg crystal spectrometer. The marked lines are identified in the text.
Figure 5.5: Direct excitation x-ray spectrum of iron modeled at an electron beam energy of 6.8 keV with an electron beam width of 40 eV (FWHM). The marked lines are identified in the text.
is switched away from the KLL dielectronic resonance. The choice of energy is important because we want to be above threshold for the direct excitation of the $n=2\rightarrow1$ heliumlike x rays $w$, $x$, $y$, and $z$ and away from any resonances, which enhances these lines. This is done by performing a scan of $w$, $x$, $y$, and $z$ near their excitation threshold as shown in Fig. 5.6 for iron. We observe that $w$ and $y$ appear to be present below their respective excitation thresholds, whereas $x$ and $z$ are not. What is observed are not the apparent heliumlike lines but dielectronic recombination satellite lines produced by dielectronic recombination onto high $n$ Rydberg levels, i.e. of the process:

$$1s^2 + e^- \rightarrow 1s2pn\ell, n \gg 2.$$ 

The levels decay radiatively,

$$1s2pn\ell \rightarrow 1s^2n\ell + h\nu,$$

by emitting a photon whose energy differs only sightly from that of the heliumlike lines $w$ and $y$. Lines $w$ and $y$ have these high-$n$ satellites because they are electric dipole allowed (E1), while $x$ (M2) and $z$ (M1) do not because they are forbidden. In addition, above threshold processes such as the KMM resonances enhance lines $w$, $x$, $y$, and $z$. This process can be expressed as:

$$1s^2 + e^- \rightarrow 1s3\ell3\ell' \rightarrow 1s2\ell + e^-.$$ 

Since we infer the ionization balance from measurements of $I_w/I_y$, it is important that line $w$ is populated solely by direct excitation. Consequently, we choose the energy to be above the excitation threshold of $x$ and $z$ and below the KMM resonances.

The ionization experiment was performed by alternating the electron beam energy between two values and recording separate spectra with the Ge detector and the crystal spectrometer. Initially, the electron beam energy was set to the KLL resonance, situated at electron energies between 4.54 and 4.76 keV in iron, for a period of 24 ms; this establishes the steady-state
Figure 5.6: Relative intensities of the triplet lines in Fe$^{24+}$ as a function of electron beam energy. The intensities are normalized to the intensity of $w$. $E_{th}$ denotes the threshold energy for direct electron-impact excitation.
condition. We then probe the charge-state balance for 6 ms at 6.8 keV, which is above the direct excitation threshold for the $n=2\rightarrow 1$ x-ray transitions in order to measure lines $\omega$, $q$, and $\beta$. This is the beam energy we determined from the threshold scan. Concurrently, the radiative recombination photons onto the $n=2$ shell are recorded during this portion of the cycle at 6.8 keV. The data is divided into 15 2-ms bins. The dielectronic recombination x rays are summed from the last 4 ms of the 24 ms on the KLL resonance as shown in Fig. 5.2(a) and (b). The first 20 ms on this portion of the cycle allows the charge states to reach steady-state. The direct excitation spectrum is acquired during the last 4 ms of the 6 ms at 6.8 keV as shown in Fig. 5.4(a) and (b). We omit the first 2-ms time group, acquired while the beam energy is changed to the direct excitation energy, in order to allow the drift tube voltage to reach a steady value of 6.8 keV.

We made ionization measurements on the KLL resonance of iron at beam energies of 4.62 to 4.68 keV, titanium at 3.31 to 3.35 keV, vanadium at 3.61 to 3.66 keV, chromium at 3.95 to 4.00 keV, and manganese at 4.28 to 4.35 keV in 10-eV steps. Examples of the dielectronic recombination spectra for Ti, V, Cr, and Mn are shown in Fig. 5.7(a)-(b) and Fig. 5.8(a)-(b). For determining ionization cross sections we analyze and average the measurements taken at these energies.

5.3.2 Analysis

The scheme provides the most accurate results for electron beam energies near the dielectronic resonance energy of satellites $j$ and $k$ listed above for Ti-Fe where the dielectronic resonance strength is largest. For energies below this range, dielectronic recombination is weak, and radiative and charge-exchange recombination have large relative contributions. For energies above this range, beam electrons sample dielectronic resonances in lithiumlike ions, and transitions in berylliumlike ions begin to appear in the spectrum; at the same time the heliumlike dielectronic satellites become weaker, and, again,
Figure 5.7: Dielectronic recombination x-ray spectrum of (a) titanium at 3.31 keV and (b) vanadium at 3.61 keV taken using the 75-cm crystal. The marked lines are identified in the text.
Figure 5.8: Dielectronic recombination x-ray spectrum of (a) chromium at 3.95 keV and (b) manganese at 4.28 keV taken using the 30-cm crystal. The marked lines are identified in the text.
the scheme provides less accurate results because dielectronic recombination is weaker relative to radiative and charge-exchange recombination. For example, charge-exchange recombination is difficult to account for because we do not know the exact background neutral gas density in EBIT, and its contribution must be estimated. In addition, if radiative recombination is large this introduces a background, which must be subtracted from the dielectronic recombination x rays, as we will show later in the lithiumlike barium measurements. Therefore, if the dielectronic recombination rate is much stronger than the radiative and charge-exchange recombination rates, then we can treat these processes as perturbations, and their contributions are small.

We determined from a model of the ionization balance in EBIT that the lithiumlike iron charge-state established during the 24-ms dielectronic recombination phase of the measurement cycle was significantly reionized during the 6-ms probing time at 6.8 keV. This causes the steady-state lithiumlike ion density, inferred from the direct excitation measurement of line \( q \) at 6.8 keV, to be underestimated. The modeled charge-state abundances are shown in Fig. 5.9 for a cycle of 24 ms at the dielectronic energy of 4.64 keV, which is a value close to the resonance energy of satellites \( j \) and \( k \), and 6 ms at the direct excitation beam energy of 6.8 keV. The model assumes an electron beam FWHM of 40 eV and uses heliumlike and lithiumlike dielectronic recombination cross sections calculated by the method of Chen [93], the Lotz formula [49] is used for ionization, and scaling formulas by Kim and Pratt [96] and by Janev, Belić, and Bransden [97] are used for radiative recombination and charge-exchange recombination, respectively. The time it takes the ion density to fall to \( 1/e \) of its original value at an electron beam energy of 4.64 keV and a beam current of 148 mA are 5.4 ms for dielectronic recombination onto heliumlike iron, 8 ms for ionization of lithiumlike iron, 465 ms for radiative recombination onto the heliumlike state, and 338 ms for charge exchange recombination between heliumlike iron and the surrounding background gas assumed to be hydrogen at a density of \( 1.1 \times 10^7 \text{ cm}^{-3} \).
Figure 5.9: The computed relative charge-state balance of iron as a function of time. The computer model includes contributions from dielectronic recombination, ionization, radiative recombination, and charge-exchange recombination. The cycle remains at 4.64 keV for 24 ms, switching to 6.8 keV for 6 ms.
Because significant reionization takes place during the 6 ms at 6.8 keV, the lithiumlike abundance is reduced compared to the amount present at the end of the dielectronic recombination part of the measurement cycle. This can be corrected by a normalization factor. Specifically, for the Ge detector measurements the radiative recombination measurement onto the n=2 shell $R_{\text{RR}}^{\text{tot}}$ is multiplied by the fraction of the radiative recombination x rays due to the lithiumlike ions computed average for the last 4 ms of the 24 ms on the KLL resonance and the last 4 ms of the 6 ms on the direct excitation portion of the cycle. For the high resolution measurements the direct excitation measurement of the lithiumlike line $q$ is multiplied by the computed average ratio of the integrated lithiumlike abundance for the last 4 ms of the 24 ms on the KLL resonance and the last 4 ms of the 6 ms on the direct excitation portion of the cycle. Table 5.4 gives the normalization factors for the solid-state (Ge) detector measurements and for the von Hamos (VH) crystal spectrometer measurements for iron at beam energies of 4.62-4.68 keV assuming the surrounding background gas to be hydrogen at a density of $1.1 \times 10^7$ cm$^{-3}$. We explain how we determine this density in the next subsection.

We performed a sensitivity study of how the normalization factors varied as the input model parameters were varied. For example, a background gas density 5 times larger and 5 times smaller translates into a 3% uncertainty in the normalization factors. Similarly, a change in the electron beam width from 40 eV to 60 eV results in a 3.6% change in the normalization factors.

Therefore, since the the normalization factors are relatively insensitive to variations in the model parameters, we are confident this adjustment of the data to be valid.

### 5.3.3 X-ray Model

The charge-state abundances of heliumlike, lithiumlike, and berylliumlike iron from our ionization balance model were then combined with calculated
Table 5.4: Fe normalization factors for the ionization measurements using the solid-state (Ge) detector measurements and for the von Hámos (VH) crystal spectrometer measurements at electron beam energies ($E_{\text{beam}}$) of 4.62-4.68 keV. We assume the surrounding background gas to be hydrogen at a density of $1.1 \times 10^7$ cm$^{-3}$.

<table>
<thead>
<tr>
<th>$E_{\text{beam}}$</th>
<th>Ge $^a$</th>
<th>VH $^b$</th>
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<tr>
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</tr>
<tr>
<td>4.68</td>
<td>1.154</td>
<td>1.107</td>
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</tbody>
</table>

$^a$Calculated from the ratio of $\frac{n_{\text{Li}^8}}{n_{\text{H}^q} + n_{\text{Li}^6} + n_{\text{Li}^3}}$ predicted from the dielectronic recombination and the direct excitation portions of the cycle.

$^b$Calculated from the ratio of $n_{\text{Li}^8}$ predicted from the dielectronic recombination and the direct excitation portions of the cycle.
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x-ray rates, energies, and cross sections of dielectronic recombination [87, 93] and of direct excitation [79] to generate synthetic x-ray spectra which could be compared directly with the measured spectra. The predicted iron x-ray spectrum for dielectronic recombination corresponding to the experimental conditions in Fig. 5.2(b) is shown in Fig. 5.3. The peak labeled s,t contains 33% of satellite s and 67% of satellite t. The model spectrum also shows the lithiumlike satellites l (1s2p2 2P1/2 → 1s2p2 2P3/2), r (1s2s2p 2P1/2 → 1s2p 2S1/2), and a (1s2p2 2P3/2 → 1s2p 2P3/2), which are unresolved in by the spectrometer. The small peaks labeled 7 and 2 are the contributions from the berylliumlike satellites (1s2s2p1/2 2P3/2) → (1s2s2p3/2) and (1s2s2p1/2) → (1s2s2s)0, respectively. A synthetic iron spectrum corresponding to direct excitation at 6.8 keV is shown in Fig. 5.5. A comparison between the synthetic and experimental spectra shows good agreement. This agreement is obtained with only one free parameter in the x-ray model, namely, the charge exchange contribution, as discussed below.

With our x-ray model we can also estimate the effect of charge-exchange recombination. Typically, during an experiment we take a steady-state x-ray spectrum at one energy as shown in Fig. 5.10(a) and (b) for iron at 6.8 keV. We obtain steady-state conditions when the time rate of change of the charge-state abundances, which are determined from the individual recombination and ionization rates in the plasma, is zero. This is the same electron beam energy that was determined from our threshold scan and used in the direct excitation portion of the ionization measurement. The energy is chosen to be above the excitation threshold of lines w, x, y, and z and away from any resonances that would enhance these transitions. It is also below the ionization potential of heliumlike iron which is at 8.828 keV and above that of lithiumlike iron at 2.046 keV. Therefore, in steady-state at this beam energy, ionization of the lithiumlike state is balanced by radiative recombination and charge-exchange recombination onto the heliumlike state, as shown in Eq. (5.1) without the dielectronic recombination term. The intensity ratio \( I_w/I_q \) in the steady-state spectrum tells us the ratio of heliumlike to liti-
umlike ions. Since ionization and radiative recombination are known from calculations in the x-ray model, the only unknown is the charge exchange recombination term. Consequently, the hydrogen or equivalent neutral density in the x-ray model is adjusted until the predicted heliumlike to lithiumlike ratio matches the measured ratio. The result of the calculation is used to account for the charge-exchange recombination term in Eq. (5.10). The result of the modeled direct excitation x-ray spectrum is shown in Fig. 5.11. The neutral density that provides a match to the observed ionization balance is $1.1 \times 10^7$ cm$^{-3}$ of H$_2$ or equivalent. The charge exchange term we infer from the x-ray model is 1.33 times larger than the radiative recombination term. The ionization cross sections we measure are relatively insensitive to changes in the background neutral density. For example, increasing or decreasing the density by 5 results in a 2% change in the ionization cross sections.

### 5.3.4 Lithiumlike Barium Measurements

For the lithiumlike barium ($Z=56$) measurements we follow the procedure outlined above for the Ge detector measurements. We used the solid-state Ge detector. We did not use the von Hámos crystal spectrometer to measure dielectronic recombination and direct excitation x rays because the efficiency of the gas-filled detector is extremely low (<5%) for the 32 keV barium x rays, and because of the $Z^4$ scaling of the separation of the energy levels not all of the dielectronic recombination x-rays would be detected due to the limited spectral range of the spectrometer. The experiment was performed by alternating the electron beam between the KLL resonances of barium ($E_{beam} = 21.8-22.5$ keV) and below the dielectronic resonances ($E_{beam} = 21.2$ keV) in order to probe the charge-state balance by measuring radiative recombination x rays. Since the crystal spectrometer was not available to infer the ionization balance, we fit the n=2 radiative recombination peak in the solid-state Ge detector to infer the relative charge-state abundances. The barium ionization measurements were made near the dielectronic resonance
Figure 5.19: Steady-state direct excitation x-ray spectrum of iron (a) measured at an electron beam energy of 7.0 keV with a solid-state Ge detector and (b) measured at an electron beam energy of 7.0 keV with a Bragg crystal spectrometer.
Figure 5.11: Steady-state direct excitation x-ray spectrum of iron modeled at an electron beam energy of 6.8 keV with an electron beam width of 40 eV (FWHM).
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energy of satellites \( o \) and \( p, \tau, \) and \( e \) and \( s \). At these energies dielectronic recombination is weaker relative to radiative and charge-exchange recombination. Therefore, we must subtract a radiative recombination background from the dielectronic recombination x rays and account for charge-exchange recombination. The KLL resonance energies were chosen so that there was no contribution from dielectronic recombination onto lithiumlike ions. The resulting berylliumlike x rays would blend with the heliumlike dielectronic recombination photons, and it is difficult to subtract them out of the low-resolution Ge detector data.

The dielectronic recombination and radiative recombination x rays are measured with a solid-state germanium detector. Typical results are shown in Fig. 5.12 for the dielectronic recombination x rays and in Fig. 5.13 for radiative recombination x-ray data for barium. We were careful to excite only heliumlike dielectronic recombination transitions and omitted data taken when lithiumlike dielectronic recombination x rays were present.

The results of the fine-structure splitting, which causes the energy level differences of transitions between electron configurations with different total angular momentum \( j \) to be split as \( \sim Z^4 \), is seen when comparing Fig. 5.2 and Fig. 5.12. For Fe (\( Z=26 \)) a crystal spectrometer is needed to resolve dielectronic transitions \( e \) and \( s \) (\( \Delta E \approx 59 \) eV); while for Ba (\( Z=56 \)) the Ge detector is able to resolve the transitions (\( \Delta E \approx 541 \) eV).

The sequence in which the spectra were taken is as follows: (1) We allow the barium to ionize to the heliumlike charge state and to reach steady-state at the electron beam energy equal to the dielectronic recombination resonance energy, \( E_{\text{beam}}=E_{\text{DR}} \). (2) We change the electron beam energy away from the dielectronic recombination resonance \( E_{\text{beam}}\neq E_{\text{DR}} \) and measure radiative recombination x rays onto heliumlike, lithiumlike, and berylliumlike barium for 20 ms, Fig. 5.13. Note that this time is short compared to the theoretical ionization time of 200 ms for changing the charge balance. From this we determine the relative abundance of heliumlike, lithiumlike, and berylliumlike barium ions. (3) Finally, we switch the beam energy back to the
Figure 5.12: Dielectronic recombination (DR) x-ray spectrum, $E_{\text{beam}}=22.4$ keV. The $n=2\rightarrow 1$ feature contains a contribution from x rays due to radiative recombination onto the $n=2$ shell of barium (hatched area). Peak 1 is due to transition $e [(1s2p)1^2P_{3/2}]s_{3/2}\rightarrow 1s^22p_{3/2}$; Peak 2 is due to transition $s [(1s2s)0^2P_{3/2}]s_{3/2}\rightarrow 1s^22s$. 
Figure 5.13: Radiative recombination (RR) x-ray spectrum, \( E_{\text{beam}} = 21.2 \text{ keV} \). The radiative recombination x rays onto the \( n=2 \) shell are fitted to determine a charge balance. The solid and dashed lines represent the relative theoretical cross sections of radiative recombination onto the different charge states.
CHAPTER 5. IONIZATION OF LITHIUMLIKE IONS

dielectronic recombination resonance $E_{\text{beam}} = E_{\text{DR}}$ and measure the dielectronic recombination x rays, Fig 5.12. This period takes 40 ms which is long compared to theoretical dielectronic recombination time of 14 ms.

The radiative recombination x-ray signal, $J_{\text{RR}}^m$, shown in Fig. 5.13, contains contributions from heliumlike, lithiumlike, and berylliumlike ions. The relative heliumlike, lithiumlike, and berylliumlike densities are determined from a fit of the radiative recombination data with known radiative recombination cross sections and photoionization energies. A 100-eV detector resolution (gaussian width) is assumed in the fitting procedure.

The background present to the left of the dielectronic recombination peaks in Fig. 5.12 and the n=2 radiative recombination peaks in Fig. 5.13 is due to radiative recombination onto the lower n=2 charge states of barium such as boronlike, carbonlike, nitrogenlike, oxygenlike, and fluorineline. We have determined that only radiative recombination onto boronlike barium produces x rays that would introduce a background under the important dielectronic and radiative recombination peaks in the ionization measurement. The uncertainty associated with this background will be included in uncertainty in the radiative recombination fitting procedure.

Because $\sigma_{\text{DR}} \gg \sigma_{\text{RR}}$, the dielectronic recombination x-ray signal in Fig. 5.12 is more intense than the radiative recombination signal in Fig. 5.13. $J_{\text{DR}}^m$, however, has contributions from x rays due to radiative recombination onto heliumlike, lithiumlike, and berylliumlike ions due to the fact that at $E_{\text{beam}} = E_{\text{DR}}$ the dielectronic recombination x rays and radiative recombination x rays appear in the same energy region. Because $E_{\text{beam}}$ (Fig. 5.13) is approximately equal to $E_{\text{beam}}$ (Fig. 5.12), radiative recombination is approximately the same in both spectra. Thus, we can determine $J_{\text{DR}}^m$ in Eq. (5.7) by subtracting the measured $J_{\text{RR}}^m$ signal in Fig. 5.13 from the measured $J_{\text{DR}}^m$ signal in Fig. 5.12. We checked the validity of this approach by comparing the x-ray signal of radiative recombination onto the n=3 shell, which is seen in both the dielectronic recombination and radiative recombination x-ray spectra, and verified that they are equal.
Substituting the experimental quantities into the expression in Eq. (5.7) we obtain:

\[
\sigma_i = \frac{I_{\text{DR}}^0 - I_{\text{RR}}^0}{I_{\text{RR}}^0} \left( 1 + \frac{\sigma_{\text{He}}^\text{He} n_{\text{He}}}{\sigma_{\text{RR}}^\text{He} n_{\text{Li}}} + \frac{\sigma_{\text{Be}}^\text{Be} n_{\text{Be}}}{\sigma_{\text{RR}}^\text{Be} n_{\text{Li}}} \right) \frac{\sigma_{\text{Li}}^\text{Li}}{A_i} \left( 1 + \frac{\sigma_{\text{DR}}}{\sigma_{\text{RR}} + \frac{e\eta_0 v_0}{j_e} \sigma_{\text{ex}}} \right)
\]

Thus, we can determine \(\sigma_i\) from a measurement of \(I_{\text{DR}}\) and \(I_{\text{RR}}^0\) by normalizing to \(\sigma_{\text{RR}}^\text{He}\). The relative charge-state abundances \(n_{\text{He}}/n_{\text{Li}}\) and \(n_{\text{Be}}/n_{\text{Li}}\) are determined from the fit of the radiative recombination spectrum. The values of \(A_i\) are 1.0, 1.0 and 1.23 for the measurements made near the dielectronic resonance energy of satellites \(\sigma\) and \(p\), \(r\), and \(e\) and \(s\), respectively, unlike for the measurements of the transition metals discussed in Section 5.3.2. We have determined from the charge-state balance model that no adjustment is needed for the reionization of lithiumlike barium when \(E_{\text{beam}}\) is away from the KLL resonance. However, since the barium \(\sigma_{\text{DR}}\)'s and the dielectronic recombination rates are weaker relative to those of the Ti-Fe measurements, the second to the last (radiative recombination) and the last (charge-exchange recombination) terms in Eq. (5.27) are large compare to 1. For example, for barium at 22.4 keV the theoretical ratio of the radiative recombination [85] and the dielectronic recombination [93] cross sections is 0.276, and the charge exchange term inferred from the comparison of the x-ray spectra observed on the resonance and off the resonance, discussed below, is 0.223. Therefore, we must account for these processes in the barium ionization measurements.

In order to determine the effect of charge-exchange recombination, we measured the x-ray signal at energies away from the dielectronic recombination resonance. In this regime ionization is approximately balanced by charge exchange and radiative recombination. Knowing radiative recombination we can infer charge-exchange recombination. Since radiative recombination does not change as a function of electron beam energy, we can use this to correct the dielectronic recombination data.
5.4 Conclusion

In this chapter we have developed the technique used for determining ionization cross sections from Ge detector and crystal spectrometer x-ray measurements. We also describe the method for inferring excitation cross sections, which support the ionization measurements. In addition, the x-ray data was compared to synthetic x-ray spectra calculated using an ionization balance model. This comparison is important because it assists in the proper interpretation of our data. In the next chapter we will show the results and discuss the uncertainties in the measurements.
Chapter 6

Results

6.1 Introduction

In this chapter we give the results of the excitation and ionization measurements from the Ge detector and the crystal spectrometer. We also discuss the uncertainties in the measurements. In addition, we discuss the advantages and disadvantages of the two ways we determine ionization cross sections.

6.2 Excitation Results

Tables 6.1 and 6.2 lists the experimentally determined electron-impact excitation cross sections of the four heliumlike transitions and values calculated by Zhang, Sampson, and Clark [79] for the low-lithiumlike case. These measurements were made in steady-state at one electron beam energy, and the primary charge state present was the heliumlike state. Table 6.3 lists the uncertainties for line $\omega$, which had the largest amount of counts among the four heliumlike lines and the lowest uncertainty. The largest uncertainty among the remaining heliumlike transitions is 15.4%. The total uncertainty was calculated from the quadrature sum of all the individual components except for the uncertainty of the radiative recombination cross section, which was added linearly. In the case of the 75-cm crystal measurements of Ti and V
we determined from a crystal scan that there is an additional 6% systematic uncertainty in the uniformity of the crystal response. The 30-cm measurements had a negligible uncertainty in the uniformity of the crystal response. The values for the heliumlike lines take into account radiative cascades and the hyperfine decay of the $^3P_0$ level. Radiative cascades strongly affect the $^3S_1$ level. For example, in iron branching ratios calculated by Lin, Johnson, and Dalgarno [98] show that 18.3% of the $^3P_2$ level decays to the $^3S_1$ level, thereby increasing line $z$. In addition, the $^3P_0$ level is forbidden to radiatively decay to the $^1S_0$ ground state in iron (cf. Fig. 6.1), chromium, and titanium, (even Z) whose most abundant isotopes have no nuclear magnetic moment. It instead decays to the $^3S_1$ level and further increases the intensity of line $z$. However, the manganese and vanadium (odd Z) nuclei have a finite magnetic moment, and the $^3P_0$ level decays directly to the ground state because of the hyperfine interaction. The energy of the $^3P_0$ is within 2.6 and 3.4 eV of the $^3P_1$ level in vanadium and manganese, respectively, and the result is an apparent enhancement of the intensity of $y$. Consequently, the theoretical cross section of $y$ and the $^3P_0$ level are added. The effect of the hyperfine interaction is seen in the difference between the effective excitation cross sections of $y$ and $z$ for even (Ti, Cr, and Fe) and odd (V and Mn) nuclei.

Tables 6.4 and 6.5 list the experimentally determined excitation cross sections of the lithiumlike satellite transitions and values calculated by Zhang, Sampson, and Clark [79] for the high-lithiumlike case. For these measurements we established a high-lithiumlike charge-state fraction at an electron beam energy corresponding to the KLL resonance and switched the energy to measure the direct excitation transitions. The vanadium data was omitted because of a contamination of the data evidenced by enhanced background levels in both the Ge detector direct excitation and radiative recombination spectra that could not be accounted for in the analysis. Table 6.6 lists the uncertainties for line $q$. The cross sections of the other transitions are measured relative to $q$. We calculated the total uncertainty from the quadrature sum of all the individual sources except for the uncertainty of the radiative
Table 6.1: Electron impact excitation cross sections of K x-ray transitions $w$ and $x$ in heliumlike ions in units of $10^{-22}$ cm$^2$ for the low-lithiumlike case. These measurements were made in steady-state at one electron beam energy, which is listed, where the heliumlike state was the dominant charge state. Theoretical values have been calculated with the relativistic distorted-wave code of Zhang, Sampson, and Clark [79] and take into account radiative cascade contributions discussed in the text. The experimental values are accurate to within 15.4%. The electron-ion interaction energies are known to within 100 eV.

<table>
<thead>
<tr>
<th>Element</th>
<th>Energy (keV)</th>
<th>$w$</th>
<th>$x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti$^{20+}$</td>
<td>4.9</td>
<td>7.61 ± 1.11</td>
<td>7.63</td>
</tr>
<tr>
<td>V$^{21+}$</td>
<td>5.3</td>
<td>4.72 ± 0.59</td>
<td>6.28</td>
</tr>
<tr>
<td>Cr$^{22+}$</td>
<td>5.8</td>
<td>5.30 ± 0.53</td>
<td>5.27</td>
</tr>
<tr>
<td>Mn$^{23+}$</td>
<td>6.3</td>
<td>3.80 ± 0.31</td>
<td>4.44</td>
</tr>
<tr>
<td>Fe$^{24+}$</td>
<td>6.8</td>
<td>3.17 ± 0.24</td>
<td>3.72</td>
</tr>
</tbody>
</table>

Table 6.2: Electron impact excitation cross sections of K x-ray transitions $y$ and $z$ in heliumlike ions in units of $10^{-22}$ cm$^2$ for the low-lithiumlike case. These measurements were made in steady-state at one electron beam energy, which is listed, where the heliumlike state was the dominant charge state. Theoretical values have been calculated with the relativistic distorted-wave code of Zhang, Sampson, and Clark [79] and take into account radiative cascade contributions discussed in the text. The experimental values are accurate to within 15.4%. The electron-ion interaction energies are known to within 100 eV.

<table>
<thead>
<tr>
<th>Element</th>
<th>Energy (keV)</th>
<th>$y$</th>
<th>$z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti$^{20+}$</td>
<td>4.9</td>
<td>2.71 ± 0.41</td>
<td>2.39</td>
</tr>
<tr>
<td>V$^{21+}$</td>
<td>5.3</td>
<td>2.72 ± 0.34</td>
<td>2.73</td>
</tr>
<tr>
<td>Cr$^{22+}$</td>
<td>5.8</td>
<td>2.04 ± 0.24</td>
<td>1.79</td>
</tr>
<tr>
<td>Mn$^{23+}$</td>
<td>6.3</td>
<td>2.06 ± 0.19</td>
<td>2.01</td>
</tr>
<tr>
<td>Fe$^{24+}$</td>
<td>6.8</td>
<td>1.32 ± 0.12</td>
<td>1.38</td>
</tr>
</tbody>
</table>
Figure 6.1: Energy level diagram of Kα x rays from helium-like Fe$^{34+}$ iron ions. Radiative transitions are labeled in the notation of Gabriel [95]. Level 1s2s$^1S_0$ decays via two photons. Level 1s2p$^3P_0$ decays to the ground level via the hyperfine interaction. Level 1s2p$^3P_2$ decays 18.3% of the time to level 1s2s$^3S_1$. 
CHAPTER 6. RESULTS

Table 6.3: Uncertainties (%) for the excitation cross sections of the heliumlike line \( u \).

<table>
<thead>
<tr>
<th>Source</th>
<th>Ti(^{2+})</th>
<th>V(^{2+})</th>
<th>Cr(^{2+})</th>
<th>Mn(^{2+})</th>
<th>Fe(^{2+})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Counting statistics</td>
<td>2.0</td>
<td>1.3</td>
<td>2.9</td>
<td>2.5</td>
<td>2.6</td>
</tr>
<tr>
<td>Be window and air transmission</td>
<td>9.5</td>
<td>6.8</td>
<td>6.0</td>
<td>4.0</td>
<td>3.2</td>
</tr>
<tr>
<td>Spectrometer response ((W))</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Crystal response linearity</td>
<td>6.0</td>
<td>6.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Radiative recombination cross section</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
</tr>
<tr>
<td>Total uncertainty</td>
<td>14.6</td>
<td>12.4</td>
<td>10.0</td>
<td>8.1</td>
<td>7.6</td>
</tr>
</tbody>
</table>

recombination cross section, which was added linearly. The largest individual source of error came from the experimental excitation cross sections of the four heliumlike lines, which are used in the calculation of cross section for line \( q \) (cf. Eq. 5.25)

6.3 Ionization Results

The results for ionization of lithiumlike ions at average electron energies near the dielectronic resonance energy of satellites \( j \) and \( k \) are given in Table 6.7, except for barium where the measurements are made near the energies of satellites \( o \) and \( p \), \( r \), \( e \) and \( s \), respectively. These energies correspond to approximately 2.3 times the threshold energy for ionization of lithiumlike ions. The vanadium measurements from the Ge detector data were omitted because an unknown impurity was present in the trap during these measurements that precluded a determination of the ionization cross section. However, we were able to infer an ionization cross section from the vanadium high resolution data that was normalized to theoretical cross sections of line \( q \). The results are graphically displayed for the transition metals in Fig. 6.2, Fig. 6.3, and Fig. 6.4 for the solid-state and crystal spectrometer measurements, respectively. We estimate a 17-33% total uncertainty for the
CHAPTER 6. RESULTS

Table 6.4: Electron impact excitation cross sections of K x-ray transitions in lithiumlike ions in units of $10^{-22}$ cm$^2$ for the high-lithiumlike case. These measurements were made by preferentially populating the lithiumlike state at the KLL resonance and, then, probing these transitions at the energies listed. Theoretical values have been calculated with the relativistic distorted-wave code of Zhang, Sampson, and Clark [79]. The experimental values are accurate to within 26.9%. The electron-ion interaction energies are known to within 100 eV.

<table>
<thead>
<tr>
<th>Element</th>
<th>Energy (keV)</th>
<th>( \varphi ) (expt)</th>
<th>( \varphi ) (theo)</th>
<th>( r ) (expt)</th>
<th>( r ) (theo)</th>
<th>( t ) (expt)</th>
<th>( t ) (theo)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti$^{19+}$</td>
<td>4.9</td>
<td>4.64 ± 1.06</td>
<td>4.88</td>
<td>2.18 ± 0.54</td>
<td>2.03</td>
<td>1.00 ± 0.27</td>
<td>1.21</td>
</tr>
<tr>
<td>Cr$^{21+}$</td>
<td>5.8</td>
<td>2.29 ± 0.36</td>
<td>3.44</td>
<td>1.09 ± 0.20</td>
<td>1.36</td>
<td>0.65 ± 0.13</td>
<td>0.93</td>
</tr>
<tr>
<td>Mn$^{22+}$</td>
<td>6.3</td>
<td>3.39 ± 0.50</td>
<td>2.93</td>
<td>1.29 ± 0.24</td>
<td>1.13</td>
<td>1.44 ± 0.27</td>
<td>0.82</td>
</tr>
<tr>
<td>Fe$^{23+}$</td>
<td>6.8</td>
<td>2.41 ± 0.33</td>
<td>2.49</td>
<td>1.06 ± 0.18</td>
<td>0.94</td>
<td>0.74 ± 0.13</td>
<td>0.72</td>
</tr>
</tbody>
</table>

Table 6.5: Electron impact excitation cross sections of K x-ray transitions in lithiumlike ions in units of $10^{-22}$ cm$^2$ for the high-lithiumlike case. These measurements were made by preferentially populating the lithiumlike state at the KLL resonance and, then, probing these transitions at the energies listed. For Cr the brackets represent the blend of satellites \( u \) and \( v \). Theoretical values have been calculated with the relativistic distorted-wave code of Zhang, Sampson, and Clark [79]. The experimental values are accurate to within 25.8%. The electron-ion interaction energies are known to within 100 eV.

<table>
<thead>
<tr>
<th>Element</th>
<th>Energy (keV)</th>
<th>( u ) (expt)</th>
<th>( u ) (theo)</th>
<th>( v ) (expt)</th>
<th>( v ) (theo)</th>
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<tbody>
<tr>
<td>Ti$^{19+}$</td>
<td>4.9</td>
<td>2.29 ± 0.58</td>
<td>1.47</td>
<td>0.97 ± 0.25</td>
<td>0.73</td>
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<tr>
<td>Cr$^{21+}$</td>
<td>5.8</td>
<td>(1.09 ± 0.20)</td>
<td>(1.61)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mn$^{22+}$</td>
<td>6.3</td>
<td>1.60 ± 0.29</td>
<td>0.93</td>
<td>0.43 ± 0.09</td>
<td>0.45</td>
</tr>
<tr>
<td>Fe$^{23+}$</td>
<td>6.8</td>
<td>0.77 ± 0.13</td>
<td>0.81</td>
<td>0.39 ± 0.07</td>
<td>0.39</td>
</tr>
</tbody>
</table>
Table 6.6: Uncertainties (%) for the excitation cross sections of the lithium-like line $\ell$.

<table>
<thead>
<tr>
<th>Source</th>
<th>Ti$^{20+}$</th>
<th>Cr$^{22+}$</th>
<th>Mn$^{23+}$</th>
<th>Fe$^{23+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Counting statistics</td>
<td>3.5</td>
<td>3.7</td>
<td>4.4</td>
<td>3.5</td>
</tr>
<tr>
<td>Be window and air transmission</td>
<td>9.5</td>
<td>6.0</td>
<td>4.0</td>
<td>3.2</td>
</tr>
<tr>
<td>Spectrometer response ($W$)</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Crystal response linearity</td>
<td>6.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Radiative branching ratio</td>
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<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
</tr>
<tr>
<td>Experimental $\sigma_w, \sigma_x, \sigma_y, \sigma_z$</td>
<td>14.6</td>
<td>9.8</td>
<td>8.0</td>
<td>7.4</td>
</tr>
<tr>
<td>Radiative recombination cross section</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
</tr>
<tr>
<td>Total uncertainty</td>
<td>22.8</td>
<td>15.6</td>
<td>14.8</td>
<td>13.8</td>
</tr>
</tbody>
</table>

transition metal ionization measurements, which is the quadrature sum of the statistical uncertainty and the estimated systematic uncertainties. The individual sources of uncertainty are listed in Table 6.8 for the solid-state Ge detector measurements, Table 6.9 for the high resolution von Hámos spectrometer measurements, normalized to theoretical cross sections of line $\ell$, and Table 6.10 for the von Hámos spectrometer measurements, normalized to the experimental cross sections of line $\ell$. We calculated the total uncertainty from the quadrature sum of all the individual sources except for the uncertainty of the radiative recombination and theoretical and experimental excitation cross sections used to normalize the different measurements, which were added linearly. The largest source of uncertainty in the solid-state detector measurements was in the determination of the fraction of the total $n=2$ radiative recombination photons from lithium-like ions. This fraction was determined from the crystal spectrometer line ratio measurements for the transition metal ions and from the fit of the radiative recombination peak for barium. Because of the low resolution of the Ge detector there is a large uncertainty in the determination of the charge balance from the fit of the barium radiative recombination data. The error bars for barium are,
therefore, calculated assuming maximum possible variations in the charge states $n_{He}, n_{Li},$ and $n_{Be}$. For example, the limits are calculated by assuming that $n_{Li} = 100\%$, even though this assumption is unphysical. The largest uncertainties in the high resolution von Hamos spectrometer measurements was in the determination of the theoretical and experimental excitation cross section of the lithiumlike line $q$.

Table 6.7: Electron impact ionization cross section of lithiumlike ions in units of $10^{-21}$ cm$^2$. The energy listed is an average of several measurements close to the dielectronic resonance energy of satellites $j$ and $k$, except for barium. Ge represents the measurements made with the solid-state detector. VH($q_{\text{theo}}$) and VH($q_{\text{expt}}$) represent the measurements made using the high resolution spectrometer that are normalized to the theoretical and experimental values of the excitation cross section of line $q$, respectively.

<table>
<thead>
<tr>
<th>Element</th>
<th>Energy (keV)</th>
<th>Ge</th>
<th>VH($q_{\text{theo}}$)</th>
<th>VH($q_{\text{expt}}$)</th>
<th>Z&amp;S*</th>
<th>Lotzb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti$^{19+}$</td>
<td>3.33</td>
<td>6.67 ± 1.73</td>
<td>6.98 ± 1.38</td>
<td>6.64 ± 2.16</td>
<td>7.81</td>
<td>8.04</td>
</tr>
<tr>
<td>V$^{20+}$</td>
<td>3.64</td>
<td>5.58 ± 1.07</td>
<td>4.88 ± 0.83</td>
<td>3.25 ± 0.74</td>
<td>5.35</td>
<td>5.50</td>
</tr>
<tr>
<td>Cr$^{21+}$</td>
<td>3.97</td>
<td>4.44 ± 1.07</td>
<td>4.82 ± 0.71</td>
<td>4.77 ± 1.03</td>
<td>4.44</td>
<td>4.61</td>
</tr>
<tr>
<td>Mn$^{22+}$</td>
<td>4.31</td>
<td>3.70 ± 0.87</td>
<td>4.22 ± 0.71</td>
<td>3.96 ± 0.85</td>
<td>3.80</td>
<td>3.89</td>
</tr>
<tr>
<td>Fe$^{23+}$</td>
<td>4.66</td>
<td>3.27 ± 0.75</td>
<td>4.09 ± 0.72</td>
<td>3.96 ± 0.85</td>
<td>3.80</td>
<td>3.89</td>
</tr>
<tr>
<td>Ba$^{31+}$</td>
<td>21.83c</td>
<td>0.36 ± 0.28</td>
<td></td>
<td>0.143</td>
<td>0.142</td>
<td></td>
</tr>
<tr>
<td>Ba$^{32+}$</td>
<td>21.97d</td>
<td>0.38 ± 0.23</td>
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<td>0.143</td>
<td>0.142</td>
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</tr>
<tr>
<td>Ba$^{32+}$</td>
<td>21.44e</td>
<td>0.36 ± 0.24</td>
<td></td>
<td>0.143</td>
<td>0.142</td>
<td></td>
</tr>
</tbody>
</table>

*aH. L. Zhang and D. H. Sampson. Ref. [45].
*bW. Lotz, Ref. [49].
*cThe energy listed is an average of several measurements close to the dielectronic resonance energy of satellites $o$ and $p$.
*dThe energy listed is an average of several measurements close to the dielectronic resonance energy of satellite $r$.
*eThe energy listed is an average of several measurements close to the dielectronic resonance energy of satellites $e$ and $s$. 
Figure 6.2: Measurement of the electron impact ionization cross section of lithiumlike ions using the solid-state Ge detector versus atomic number. The measurements were made at an energy corresponding to 2.3 times the threshold energy for ionization of lithiumlike ions. The solid curve represents results from the relativistic distorted-wave calculation.
Figure 6.3: Measurement of the electron impact ionization cross section of lithiumlike ions using the crystal spectrometer normalized to the theoretical cross section of line $q$, calculated with the relativistic distorted-wave code of Zhang, Sampson, and Clark [79], versus atomic number. The measurements were made at an energy corresponding to 2.3 times the threshold energy for ionization of lithiumlike ions. The solid curve represents results from the relativistic distorted-wave calculation.
Figure 6.4: Measurement of the electron impact ionization cross section of lithiumlike ions using the crystal spectrometer normalized to the experimental cross section of line $q$, determined for the high lithiumlike case, versus atomic number. The measurements were made at an energy corresponding to 2.3 times the threshold energy for ionization of lithiumlike ions. The solid curve represents results from the relativistic distorted-wave calculation.
Table 6.8: Uncertainties (%) for the solid-state Ge detector measurements. The fraction of $I_{RR}^{tot}$ from lithiumlike ions was determined from crystal spectrometer line ratios for Ti, Cr, Mn, and Fe, while for Ba the fraction was determined from a fit of the radiative recombination peak.

<table>
<thead>
<tr>
<th>Source</th>
<th>$\text{Ti}^{19+}$</th>
<th>$\text{Cr}^{21+}$</th>
<th>$\text{Mn}^{22+}$</th>
<th>$\text{Fe}^{23+}$</th>
<th>$\text{Ba}^{23+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Counting statistics</td>
<td>0.6</td>
<td>0.5</td>
<td>0.2</td>
<td>0.3</td>
<td>0.0</td>
</tr>
<tr>
<td>Be window and air transmission</td>
<td>9.5</td>
<td>6.0</td>
<td>4.0</td>
<td>3.2</td>
<td>9.5</td>
</tr>
<tr>
<td>Model adjustment of $I_{RR}^{tot}$</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Fraction of $I_{RR}^{tot}$ from lithiumlike ions</td>
<td>21.0</td>
<td>20.0</td>
<td>20.0</td>
<td>20.0</td>
<td>20.0</td>
</tr>
<tr>
<td>Radiative recombination cross section</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
</tr>
<tr>
<td>Background in radiative recombination</td>
<td></td>
<td></td>
<td></td>
<td>20.0</td>
<td></td>
</tr>
<tr>
<td>Total uncertainty</td>
<td>26.0</td>
<td>24.0</td>
<td>23.5</td>
<td>23.0</td>
<td>66.0</td>
</tr>
</tbody>
</table>

Table 6.9: Uncertainties (%) for the high resolution von Hámos spectrometer measurements, normalized to theoretical excitation cross sections for line $q$.

<table>
<thead>
<tr>
<th>Source</th>
<th>$\text{Ti}^{19+}$</th>
<th>$\text{V}^{20+}$</th>
<th>$\text{Cr}^{21+}$</th>
<th>$\text{Mn}^{22+}$</th>
<th>$\text{Fe}^{23+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Counting statistics</td>
<td>3.8</td>
<td>2.3</td>
<td>2.5</td>
<td>1.4</td>
<td>3.7</td>
</tr>
<tr>
<td>Spectrometer response ($W$)</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Radiative branching ratio</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
</tr>
<tr>
<td>Model adjustment of $I_q$</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Crystal response linearity</td>
<td>6.0</td>
<td>6.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Excitation cross section</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
</tr>
<tr>
<td>Total uncertainty</td>
<td>19.7</td>
<td>19.2</td>
<td>17.1</td>
<td>16.8</td>
<td>17.6</td>
</tr>
</tbody>
</table>
Table 6.10: Uncertainties (%) for the high resolution von Hámos spectrometer measurements, normalized to experimental excitation cross sections for line $q$.

<table>
<thead>
<tr>
<th>Source</th>
<th>$\text{Ti}^{19+}$</th>
<th>$\text{Cr}^{21+}$</th>
<th>$\text{Mn}^{22+}$</th>
<th>$\text{Fe}^{23+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Counting statistics</td>
<td>3.8</td>
<td>2.5</td>
<td>1.4</td>
<td>3.7</td>
</tr>
<tr>
<td>Spectrometer response ($W$)</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Radiative branching ratio</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
</tr>
<tr>
<td>Model adjustment of $I_q$</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Crystal response linearity</td>
<td>6.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Excitation cross section</td>
<td>22.8</td>
<td>15.6</td>
<td>14.8</td>
<td>13.8</td>
</tr>
<tr>
<td>Total uncertainty</td>
<td>32.5</td>
<td>22.7</td>
<td>21.6</td>
<td>21.4</td>
</tr>
</tbody>
</table>

The results of our measurements are compared to theoretical values calculated using the relativistic distorted-wave code of Zhang and Sampson [45] and to the semi-empirical Lotz formula [49]. The Ti, V, Cr, Mn, and Fe measurements are within 20% of the distorted-wave results, except for the Cr high resolution measurement, normalized to the experimental excitation cross section of line $q$, which was within 40% of the distorted-wave results. The barium results are approximately 2.5 times larger than theory. The accuracy of these transition metal ionization cross sections is on the order of the best tokamak ionization rate experiments for highly charged Ti and Fe ions where the rates are believed to be accurate to within 20-40% [9, 10]. There has been no previous ionization measurements for highly charged barium ions.

In the discussion that follows we will discuss the advantages and disadvantages of the two techniques for measuring ionization cross sections. The first method, which consisted of the Ge detector measurements, is the most fundamental approach. These measurements had the best statistics, no reflectivity correction, and were normalized to theoretical radiative recombination cross sections, which are known to within 3%. On the other hand, the high reso-
lution technique adds a further level of complexity. The measurements have less statistics, rely on calculated reflectivities and radiative branching ratios, and are normalized to excitation cross sections, which are not believed to be as well known as radiative recombination. In particular, the high resolution measurements are normalized to theoretical excitation cross sections of the lithiumlike line $q$, which are believed to be accurate to only 10%, while those measurements normalized to the experimental cross sections of line $q$ have the uncertainty in the cross section measurement of $q$ plus the uncertainty propagated from the independent determination of the excitation cross sections of the heliumlike lines $w$, $z$, $y$, and $z$. An alternative approach would be to determine the excitation cross section of line $q$ from these data by normalizing to the experimentally inferred ionization cross sections.

The disadvantages of the Ge detector measurements involve the importance of resolution. For the elements we studied the Ge detector cannot distinguish between individual charge-states in the $n=2$ radiative recombination peak. We have attempted to fit the radiative recombination peak; however, this procedure had a large uncertainty as evidenced by the barium ionization measurements. Furthermore, the Ge detector cannot resolve the heliumlike dielectronic recombination x rays from those of the lithiumlike charge state. For the transition metal ionization measurements the high resolution data provides complementary information to that of the Ge detector by distinguishing between the individual charge states in the direct excitation-radiative recombination spectra and providing information as to the contribution of the lithiumlike dielectronic satellites to the heliumlike dielectronic recombination spectra.

6.4 Conclusion

We have measured the ionization cross section of lithiumlike Ti, V, Cr, Mn, Fe, and Ba at the KLL resonance energy. These cross sections represent the highest known charge-state ionization measurements of these ions to date.
The measurements were made relative to the radiative recombination cross section of lithiumlike ions, which are believed to be correct to within a few percent, and to the theoretical and experimental excitation cross section of line \( q \). The largest errors in the Ge detector measurements came from inferring a charge-state balance from the direct excitation line ratio measurements and normalizing to their theoretically calculated cross sections, which are believed to be correct to within 10%. The largest errors in the high resolution crystal spectrometer measurements resulted from the corresponding theoretically and experimentally inferred cross sections for the lithiumlike line \( q \). The results for Ti, V, Cr, Mn, and Fe agree within the error bars with distorted-wave calculations of Zhang and Sampson [45] with the exception of one Cr measurement. The results for Ba, which has a large uncertainty, are higher than theory.
Chapter 7

Summary and Future Research

In this thesis we have attempted to advance the understanding of the ionization of highly charged ions. The measurements were performed on an electron beam ion trap (EBIT) using a technique based on equating a dielectronic recombination photon with an ionization event. In the first part of the thesis we developed the skills necessary to infer the ionization cross sections from the x-ray measurements. We demonstrated how polarization affects the observed x-ray intensities, and we presented an example by making a measurement of the relative intensities of Ly-α₂ and Ly-α₁ of iron. In addition, we showed how accurate relative charge-state abundances can be determined from x-ray observations. In the second part we presented the methods for inferring ionization cross sections from Ge detector and crystal spectrometer measurements. We investigated the dependence of the lithiumlike ionization cross section as a function of Z for the elements of titanium (Z=22), vanadium (Z=23), chromium (Z=24), manganese (Z=25), iron (Z=26), and barium (Z=56) at approximately 2.3 times the threshold energy for ionization of lithiumlike ions. An essential part of the analysis of this data consisted of the modeling of the charge-state abundances and the corresponding x-ray spectra. This modeling gave important insight as to how the charge-state abundances varied as the electron beam energy was alternated between the dielectronic recombination resonances to values away from any resonance and
back again. The x-ray model was also used to account for the contribution of charge-exchange recombination of neutral background gas atoms in EBIT with the highly charged ions in the data.

The ionization cross sections we determine have important applications for understanding high temperature laboratory and astrophysical plasmas. They are important, for example, for determining the charge-state balance and are required for proper interpretation of spectra in plasmas. Accurate ionization cross sections are also needed for inferring the diffusive and convective transport of transition metal impurity ions in tokamaks and for determining the power balance. Furthermore, the ionization cross section measurements are important for testing current theoretical calculations. The measurements have been compared to the results from a recent theoretical distorted-wave calculation. The comparison shows excellent agreement overall. The Ti, V, Cr, Mn, and Fe ionization cross sections agree with the theory within the experimental error bars, except for the least accurate Cr measurement. The Ba results were consistently larger than theory, but have a large experimental uncertainty.

We have studied many atomic processes in this thesis such as ionization, dielectronic recombination, direct excitation, and radiative recombination. For the ionization measurements presented these cross sections are interrelated, i.e., ionization cross sections were dependent on the radiative recombination and direct excitation cross sections and formed a self-consistent picture. We have developed the skills needed to study each of these processes separately. In the future with the advent of Super-EBIT, currently operational up to 80 keV (and proposed to ultimately operate up to 250 keV), higher charge states and higher energy cross sections can be studied. For example, if we can properly fit the n=2 radiative recombination x-rays in the solid-state Ge detector, our technique can be extended to measure ionization cross sections for higher Z lithiumlike ions up to $U^{89+}$. Such a fit should be possible because of the $Z^4$ scaling of the separation of the energy levels.
Bibliography


