Inner Shell Atomic Processes in Highly Charged Argon EBIT Plasma Relevant to Astrophysics

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INNER SHELL ATOMIC PROCESSES IN HIGHLY CHARGED ARGON
EBIT PLASMA RELEVANT TO ASTROPHYSICS

A Dissertation
Presented to
the Graduate School of
Clemson University

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy
Physics

by
Amy Christina Gall
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Accepted by:
Dr. Endre Takacs, Committee Chair
Dr. Chad Sosolik
Dr. Marco Ajello
Dr. Randall Smith
Abstract

Astrophysics is a broad and dynamic field that has led to an ever increasing number of incredible discoveries. Just in the past decade or so astrophysicists have detected gravitational waves (and the electromagnetic counterpart) from a neutron star merger, imaged a black hole for the first time, discovered thousands of new planets orbiting stars, and have shown that the expansion of the Universe is accelerating. Many of these discoveries come from new facilities with advanced technologies, an increase in computational capabilities, and creative new analytical techniques. These continued improvements have led to higher quality data that often reveals that our understanding of the processes responsible for the observations is far from complete. It is the field of laboratory astrophysics (experimental and theoretical) that aims to advance our understanding of the underlying processes for more reliable interpretations of astrophysical observations.

With this motivation in mind, this work first describes the electron beam ion trap (EBIT), a facility well suited for systematic atomic studies. The EBIT has a nearly monoenergetic electron beam and allows for the injection of a variety of species, including astrophysically relevant elements such as Fe or Ar. Since ions are present almost everywhere in the Universe, and are responsible for much of the measured emission, it is important to note that the tunable electron beam energy can reach up to about 30 keV and is capable of producing basically all charge states of astrophysically relevant elements. The narrow electron beam energy profile allows the user to select the charge state and to an extent the excited state, and is well suited for systematic studies. The EBIT contains a series of electrodes used to manipulate the electron beam and electrostatically trap the ions. The
space charge of the electron beam and shape of the trapping electrodes work to radially trap ions. Observation ports are located radially around the trap and are oriented perpendicular to the direction of the electron beam.

The non-thermal uni-directional electron beam interacts with stationary ions in the trap. This setup leads to non-statistically populated magnetic sublevels that produce polarized and anisotropic emission, and provides a unique opportunity to study magnetic sublevels which are typically inaccessible in spectroscopic observations. In the second part of this work we take advantage of this capability of the EBIT and report the measurement of the linear polarization of He-like and Li-like Ar transitions. Measurements were taken with two Johann-type crystal spectrometers in different orientations corresponding to the dispersion plane parallel and perpendicular to the electron beam direction. The Li-like transitions result from the resonant dielectronic recombination process while the He-like transitions are produced from electron impact excitation. Our results show a strong positive polarization of the $w$, $j$, $k$, and $q$ transitions (in notation of Gabriel [45]), and a negative polarization of the $a$, $x$, $y$, and $z$ lines.

Since the polarization depends on the magnetic sublevel specific direct excitation or dielectronic capture cross-sections, our results can be used to benchmark different methods used to calculate these cross-sections. In this work we compare measurements with polarization values calculated using the density matrix formalism. For dielectronic recombination, the Flexible Atomic Code (FAC) [55] was used to produce the atomic data ($Q_d$ values, autoionization energies, and cross-sections) required to calculate the polarization and produce the synthetic spectra. Since measurements were taken at the resonance energy, cascade effects were ignored. For transitions resulting from direct excitation the collisional-radiative model NOMAD [96] was used to solve the system of steady-state rate equations for the magnetic sublevel populations, and included excitation up to $n = 5$. For both direct excitation and dielectronic recombination the theoretical predictions agree well with measured values.

The final part of this work was motivated by an exciting 2014 study [26] that re-
ported a possible dark matter signature at 3.55 keV - 3.57 keV in the stacked spectra of galaxy clusters. To help rule out possible atomic origins suggested by the authors, we measured Ar emission from $1s^22l - 1s2l3l$ satellite transitions near 3.6 keV x-ray energy. X-rays were measured simultaneously with a high count-rate, high-purity Ge detector and a high energy-resolution Johann-type crystal spectrometer. The collisional-radiative model NOMAD was used to create synthetic spectra for comparison with both our EBIT measurements and with spectra produced with the AtomDB database [43] and the Astrophysical Plasma Emission Code (APEC) [117] used in the 2014 work. Excellent agreement was found between the NOMAD and EBIT spectra at each electron beam energy, providing a high level of confidence in the atomic data used. Comparison of the NOMAD and APEC spectra revealed a number of missing lines at 3.56 keV, 3.62 keV, 3.64 keV, and 3.66 keV in the APEC spectra. These features are primarily due to Be-like Ar DR data missing in the database. At an electron temperature of $T_e = 1.72$ keV, the inclusion of $1s2l'2l''$ and $1s2l'3l''$ data in AtomDB increased the total flux in the 3.5 keV to 3.66 keV energy band by a factor of 2. While important, this extra emission is not enough to fully explain the unidentified line found in the galaxy cluster spectra [48] leaving the possibility open for dark matter related origin.
Dedication

This work is dedicated to my mother Belle who gives the best pep talks and is an inspiration to me, my brother Tony who I will forever be in competition with, my father Steve who reminds me to let loose and enjoy life, and my grandmother Kay who is always there when I need someone to talk to. Most of all I dedicate this to my partner and best friend Deighton, who has always encouraged and supported me.
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Chapter 1

Introduction

X-rays can be classified as high-energy electromagnetic radiation with a wavelength range of about 0.01 nm to 10 nm. X-rays were officially discovered by German scientist Wilhelm Röntgen in 1895, while experimenting with a Crookes tube. A Crookes tube is basically a glass tube partially evacuated to about \(10^{-5}\) Torr pressure containing a cathode and anode electrode. When a voltage is placed on the electrodes, the electric field accelerates any charged particles in the tube, and electrons collide with gas particles, ionizing them and creating more electrons. If a high enough voltage is applied, the electrons can produce bremsstrahlung, or “braking radiation”, as they collide with the anode or glass, or electrons may excite an inner-shell bound electron, producing x-rays during radiative stabilization.

While using a Crookes tube covered with black cardboard, Röntgen noticed that a fluorescent barium platinocyanide screen located about 1 m away in the laboratory was glowing. This indicated that some unknown (x) and invisible rays were passing through the cardboard. Röntgen spent weeks in his lab investigating the rays and noticed that they did not reflect or refract like visible light. Röntgen also recognized the medical applications after photographing the bones in his wife’s hand in x-rays. The discovery was followed by great enthusiasm and interest from physics and medical communities.

In 1917, Charles Glover Barkla won the Nobel Prize in Physics for his work on x-rays. In 1906, he investigated the scattering of x-rays and showed that elements have a
characteristic x-ray line spectra. He also discovered the polarization of x-rays, indicating that x-rays are similar to ordinary light [44]. In 1912, Max von Laue, Paul Knipping, and Walter Friedrich were the first to observe the diffraction of x-rays from crystals. Max von Laue was awarded the Nobel Prize in Physics in 1914 for the discovery.

While advancements in the understanding, production, and detection of x-rays were ongoing in physics, it was not obvious that x-rays are ubiquitous in the cosmos because x-rays are absorbed in the Earth’s atmosphere. X-ray astronomy would have to wait for technology that allowed measurements to be taken at high altitudes. This began with interest in short wave communications for the U.S. Navy, which led to studies of the Earth’s ionosphere. At the Naval Research Laboratory (NRL) around 1929, Edward Hulburt proposed a program to study the upper atmosphere in x-ray and EUV regions using a rocket. Then, in 1948 a team led by Herbert Friedman used German V-2 rockets to observe x-rays from the Sun [72].

In 1962 Riccardo Giacconi, Herb Gursky, Bruno Rossi, and Frank Paolini observed the first x-rays from cosmic sources using an Aerobee 150 rocket. While they observed x-rays coming from every direction, they noticed one bright source in particular, later named Scorpius X-1, now known to be a neutron star in a binary system [49]. Giacconi would go on to be one of the leaders in x-ray astronomy and in 2002 was awarded a share of the Nobel Prize in Physics “for pioneering contributions to astrophysics, which have led to the discovery of cosmic X-ray sources”.

In 1970, the first x-ray satellite Uhuru (Swahili word for “freedom”) was launched. The payload included two proportional counters, sensitive to x-rays in the 2 keV to 20 keV range. From Uhuru and the multiple x-ray satellites launched since then, energetic x-ray sources have been discovered all across the sky and include supernova remnants, active galactic nuclei, x-ray binaries, galaxy clusters, and x-ray transients. Fig. 1.1 shows an image released in 2003 of x-ray sources observed with the Chandra x-ray telescope. The observing area is about 3/5 the size of the full moon. There are over 500 objects in the image, mostly supermassive black holes at the center of galaxies, demonstrating the abundance of x-ray
sources in the sky.

Since astrophysical objects cannot be directly probed, astrophysicists rely on spectroscopy to understand the inherent and extrinsic properties of matter. Astrophysical sources span a range of densities and temperatures with ions making up the majority of the observed matter in the cosmos. For highly energetic plasmas where electron-ion collisions dominate the ionization process, the plasma typically contains highly charged ions which emit in the x-ray energy band. Therefore, analysis of x-ray spectra from these objects can provide physical information such as elemental abundance, temperature, velocity, and density of the emitting plasma. However, interpretation of the x-ray spectra requires an accurate understanding of the underlying atomic physics.

The need to improve our understanding of atomic physics has led to numerous laboratory and theoretical efforts. Many of the experimental techniques allow electrons or photons to interact with ions and atoms, and closely replicates the conditions of astrophysical sources. Experimental facilities include electron beam ion trap (EBITs) where ions are electrostatically trapped and interact with a controllable electron beam, ion storage rings where ions are magnetically confined for long periods of time, and advanced light sources where photons can interact with ions. Like in astrophysics, the plasmas produced in these laboratories vary in temperature and densities.

These facilities can be used to produce accurate atomic data such as transition wavelengths, branching ratios, and rates from processes such as electron impact excitation and ionization, and recombination. Though these processes have been studied for many years now, there are still gaps in our understanding. In these cases, measurements can allow us to verify models and sometimes distinguish between different theoretical approaches. Many of the relevant issues and atomic data needs have been highlighted in recent reports such as [116, 15, 71].

The motivation behind our work is to contribute experimental data to this effort, leading to increased reliability of spectral interpretations of astrophysical sources. In this work we demonstrate the capabilities of an electron beam ion trap, with plasma conditions
The Chandra Deep Field North image (left) was made by observing an area of the sky three-fifths the size of the full moon for 23 days. It is the most sensitive or "deepest" x-ray exposure ever made. The faintest sources produced only one X-ray photon every 4 days.
comparable to the solar corona, to produce a clean, almost single species environment, perfect for systematic atomic studies. This work is broken up into 3 primary sections. After providing a brief description of the atomic physics required, the details of the electron beam ion traps at the National Institute of Standards and Technology (NIST) and at the Smithsonian Astrophysical Observatory (SAO) are discussed. This includes a basic description of the design and operation of the device, injection methods, and an overview of the detectors and spectrometers used for this work. Then in Chapters 4 and 5 we discuss x-ray measurements of highly charged Ar ions.

In Chapter 4 we present linear polarization measurements relevant for reliable interpretation of spectra from non-thermal plasma sources. First a theoretical description of polarization is formulated for the He- and Li-like Ar transitions of interest. Then the experimental details, analysis, and results are presented. Measurements are finally compared with theoretical results calculated in the photon density matrix formalism.

In Chapter 5 we present a study of the dielectronic resonance (DR) process in He-like Ar. The measurements were motivated by an unidentified feature found in the stacked spectrum of galaxy clusters, which may or may not have atomic origins. We discuss our experimental setup, measurements, and analysis. Measured spectra are then used to verify the atomic data used in a collisional-radiative model. Finally we are able to compare our spectra with those produced with APEC (the model used for the galaxy clusters), and rule out Ar DR emission as the sole source of the unidentified line.

Finally in Chapter 6, we summarize our work and results. This is followed by additional analysis details and relevant publications included in the Appendices.


Chapter 2

Atomic Physics

This chapter provides a brief overview of the notation and atomic physics processes relevant for this work. A more in depth discussion can be found in Gall (2017) [47] or in text such as [34, 42, 91].

2.1 Introduction

The observed spectrum from an emitting source fundamentally depends on the atoms or ions present and the atomic processes occurring in the plasma. Therefore both the atomic structure and these processes must be understood to interpret spectra. Spectroscopy can be traced back to the 17th century when Isaac Newton used a prism to study white light from the sun. Later, Joseph von Fraunhofer developed the diffraction grating and in 1814 discovered hundreds of dark lines in the solar spectrum. These lines were not understood at the time and it was not until about 1859, when Gustav Kirchhoff and Robert Bunsen systematically studied the emission spectra from highly pure samples and began to associate spectral patterns with specific elements, that these dark lines were understood to be signatures of the elemental composition of the Sun.

In 1885 Johann Balmer discovered an empirical formula that described the wavelengths of n→2 electron transitions in hydrogen (n is the principal quantum number and
in this case \( n > 2 \). Following this, in 1888 Johannes Robert Rydberg formulated a more general empirical equation (the Rydberg formula) that explained all of the observed lines in the hydrogen emission spectra. In 1913 Niels Bohr developed a theoretical model suggesting that electrons travel in discrete, stable orbits around a heavy stationary nucleus without radiating energy. He calculated the size of the orbits by assuming that the orbital angular momentum of the orbiting electron is equal to an integer multiple (\( n \)) of \( h \), where \( n \) is again the principle quantum number. Given the discrete orbits, Bohr was able to calculate the discrete energy of each orbit, called the energy level. Finally Bohr explained that the electron could jump between orbits, emitting or absorbing radiation equal to the difference in energy levels. This allowed him to reproduce the Rydberg formula theoretically. From Bohr’s theory, the radius and energy of the allowed orbits are (generalized beyond hydrogen by including \( Z \)):

\[
\begin{align*}
  r &= \frac{n^2 \hbar^2}{Z \left( \frac{e^2}{4\pi\epsilon_0} \right) m_e} \\
  E &= -\frac{Z^2 e^2}{8\pi\epsilon_0 a_0 n^2} \approx -13.6 Z^2 \frac{eV}{n^2}
\end{align*}
\]

where \( Z \) is the atomic number, \( a_0=\frac{\hbar^2}{(\frac{e^2}{4\pi\epsilon_0}) m_e} \) is the Bohr radius (the smallest orbit in hydrogen), \( \epsilon_0 \) is the permittivity of free space, and \( e \) and \( m_e \) are the charge and mass of an electron, respectively. Using the energy equation for hydrogen, the energy of a photon emitted during an electron orbit jump is given by:

\[
E = E_i - E_f = R_E \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)
\]

where \( R_E \) is the Rydberg energy. These equations assume that only one electron is orbiting the nucleus; therefore this works to explain the lines from hydrogen, but fails to accurately predict the wavelength of emission from many electron systems.

Around this same time period, H.G.J. Moseley noticed that for heavy atoms, the
frequency of the emission is proportional to the atomic number \((\sqrt{f} \propto Z)\). This observation led to a more accurate formula describing electron transitions. The new equation takes into account the non-transitioning electrons that act to partially screen the nuclear charge. For example, for \(n = 2 \rightarrow 1\) transitions, the empirical equation is [42]:

\[
\frac{1}{\lambda} = R \left\{ \frac{(Z - \sigma_K)^2}{l^2} - \frac{(Z - \sigma_L)^2}{2^2} \right\}
\]

(2.4)

Where \(\sigma_K\) and \(\sigma_L\) are the screening factors, and \(R\) is the Rydberg constant. This shows that for high \(Z\), Moseley’s observation is recovered.

2.2 Atomic Structure

2.2.1 Electron Configuration

Throughout this work we will use various notations to represent energy levels. To understand the notations, we start by describing the basic arrangement of electrons in an atomic system. Three quantum numbers, \(n\), \(l\), and \(m_l\) are required to define an atomic orbital. The principal integer quantum number, \(n\), represents shells, where traditionally \(n=1, 2, 3, 4...\) etc. are referred to as K, L, M, N...etc. Based on this nomenclature, K-shell transitions are defined as transitions into the \(n=1\) shell and \(K\alpha\) and \(K\beta\) describe \(n=2 \rightarrow 1\) and \(n=3 \rightarrow 1\) transitions, respectively. The orbital quantum number, \(l\), is an integer that can range from 0 to \(n-1\) and represents sub-shells within the \(n\) shell. For example, the \(n=1\) shell only has an \(l=0\) sub-shell, while \(n=2\) shell, can have 2 sub-shells representing \(l=0\) and \(l=1\). The angular momentum quantum number \(l=0, 1, 2, 3, 4...\) etc. is often referred to by alphabetic characters s, p, d, f, g, h...etc. This quantum number also defines the shape of the orbital. The magnetic quantum number, \(m_l\), is an integer that can range from 0, \(\pm 1,\ldots,\pm l\) in steps of 1, and further divides \(nl\) orbitals into sub-orbitals. The magnetic quantum number \(m_l\) describes the projection of \(l\) onto a specified axis and defines the orientation of the shape of the subshell.

The intrinsic angular momentum of the electron, \(s\), is equal to \(1/2\), and has a
projection of $m_s = \pm 1/2$. Since electrons are particles with a half-integer spin (fermions), according to the Pauli exclusion principle, two electrons cannot occupy the same quantum state within a quantum system simultaneously. This means that two electrons cannot have the same set of quantum numbers. Because of this, each atomic shell can only contain $2n^2$ electrons, for example the n=1 shell (l=0, $m_l=0$, $s = \pm 1/2$) can contain 2 electrons, while the n = 2 shell can have 8. Then using the Aufbau principle, which states that orbitals are filled in the order of increasing n+l, we can understand the ground state electron configurations of the elements. For example, carbon atoms have a configuration of 1s$^2$2s$^2$2p$^2$, meaning there are 2 electrons in the n=1 shell (s sub-shell) and 4 electrons in the n=2 shell, 2 in the s sub-shell and 2 in the p sub-shell. This method is simple but does not provide all of the information about the atom or ion required to describe the energy. For this we also need to know how the electrons couple to each other.

To understand the primary coupling schemes used, we first need to understand the interactions occurring between atomic particles. We know a stationary charge produces an electric field, but from special relativity we also know an observer in a moving frame will experience an electric and magnetic field due to the charge. As a result, an orbiting electron will experience a magnetic field, proportional to the orbital angular momentum l. The magnetic moment due to the intrinsic spin of the electron can interact with the orbital field, called the spin-orbit interaction. In addition to this, when more than one electron is present in an atom or ion, the charged particles will interact through mutual repulsion.

For light (Z < 30) systems, the electrostatic interaction between electrons is much greater than the spin-orbit interaction and the LS or Russell-Saunders coupling scheme describes the atoms. In the LS scheme, due to the dominance of the electrostatic repulsion between the electrons their orbital angular momenta couple together to form an overall total orbital angular momentum $L$ and the individual electron spins also couple to each other to form the total S. The $L$ total orbital angular momentum of the system is given by the sum of individual orbital angular momenta $l_i$: $L = \sum_i l_i$, and the total spin is similarly defined as: $S = \sum_i s_i$. The total $L$ and $S$ then couple together to form a total angular momentum J.
with values ranging from \(|L - S|\) to \(|L + S|\) in steps of 1. For LS coupling, the term, \(2^{S+1}L\), and level notations \(2^{S+1}L_J\) describe the total angular momentum quantum numbers. The energy levels are then defined by the configuration and the term symbol. An example given by \(3d^7(^4F)4s4p(^3P)\text{ }^6F_{9/2}\) shows that the 7 electrons in the d sub-shell couple and give the \(^4F\) term, while the 4s and 4p electrons couple to give the \(^3P\) term. The two terms then couple to give the \(^6F\) (which is one of nine possible terms) \([130]\).

For higher Z elements the electron-nucleus interaction increases, the velocity of the electrons becomes relativistic, and the spin-orbit interaction becomes stronger than the electron-electron interaction. Under these conditions, the jj coupling scheme is used, where l and s couple for each electron and the total angular momentum for each electron is: \(j = l + s\). The total angular momenta of each electron then couple to give a total angular momentum of the system \(J = \sum_j j_i\). This scheme also includes a configuration/term notation that is given by \((n_1l_1j_1 \ldots )_j(n_2l_2j_2 \ldots )_j\), where \(n, l, j,\) and \(J\) are the quantum numbers and \(N\) is the number of electrons in a particular sub-level. For example \(\left(6p_{\frac{7}{2}}^26p_{\frac{5}{2}}^1\right)_{\frac{3}{2}}\) shows that there are 2 electrons in the 2p sub-level with \(j = 1/2\) and one electron in the 2p sub-level with \(j = 3/2\). The \(j\) then couple to give a total \(J=3/2\) for this level.

While the two schemes discussed here are widely used, there are other coupling schemes that are sometimes more appropriate. These are described in works such as \([34]\), and some instructive examples can be found on the NIST website \([130]\).

### 2.2.2 Schrödinger Equation

The empirical formulas and simple Bohr model described in the introduction were able to provide an intuitive description and reproduce the features from hydrogen, but they failed to provide an accurate theory for multi-electron atoms. We now know that a quantum mechanical treatment is required, where electrons are no longer considered to be in stable orbits, but are described by the probability of being in a particular region around the nucleus at a particular time. The Schrödinger equation represents the quantum mechanical
analogue of the classical conservation of total energy. For example, the Schrödinger equation for an electron in a spherically-symmetric potential is (e.g. hydrogen atom):

\[
\left\{ -\frac{\hbar^2}{2m_e} \nabla^2 + V(r) \right\} \psi = E\psi \tag{2.5}
\]

where \( \psi \) is the wavefunction, \( E \) is the energy, \( V(r) \) is the potential, and \( \nabla^2 \) is the Laplacian. The expression in the brackets is called the Hamiltonian and first term on the left represents the kinetic energy while \( V(r) \) is the attractive Coulomb potential between the electron and the nucleus. The solution for the hydrogen atom, described in text such as [42, 91], gives energy eigenvalues equal to those derived by Bohr, and the wavefunctions can be used to find expectation values of the physical quantities describing the electron.

Atomic systems containing more than one electron become complex and an analytic solution for the state functions might no longer exists. Following [71], for multi-electrons systems the Schrödinger (or its relativistic counterpart the Dirac) equation can be expressed as:

\[
\left\{ \sum_i h_i + \sum_{i<j} V_{ij}^{e-e} \right\} \psi = E\psi \tag{2.6}
\]

where \( h_i \) are the single electron Hamiltonians containing the kinetic energy and attractive electron-nucleus potential, and \( V_{ij}^{e-e} \) are the electron-electron interaction potentials, including the two-electron Coulomb repulsion operator.

While there are a number of methods used to tackle the multi-electron atom problem, one of the simplest treatments uses an analogy to the hydrogen atom. This method replaces the electron-electron repulsion term with a local central potential \( (\sum_{ij} V_{ij}^{e-e} \sim V_i(r)) \). The atomic state function \( \psi \) can then be expressed as a product of wavefunctions of the single electron Hamiltonians \( \phi_i \), where: \( \{ h_i + V_i(r)\} \phi_i = \epsilon_i \phi_i \) and \( i = 1...N \) (N is the number of electrons) [71]. Various forms of the effective potential can be considered as described in [34].

Other methods used for the muti-electron atom include the Hartree-Fock method that follows the prescription of the variational principle (or multi-configuration Hartree-Fock
when considering more than one configuration), and the many-body perturbation theory which writes the Hamiltonian as a sum of a zero-order Hamiltonian and a perturbation term: \( H = H_0 + H_{\text{pert}} \), where \( H_0 = \sum_i (h_i + V_i(r)) \) and \( H_{\text{pert}} = \sum_{i>j} V_{ij}^{e-e} - \sum_i V_i(r) \) [71]. Overviews of the available procedures, and details can be found in text such as [91].

In the next section we will consider processes that involve the interaction of continuum (non-bound) electrons and ions. In this case the state function includes the free electron orbitals, and the state function of the bound target electrons [71]. The free electron wavefunctions are found by solving the Schrödinger equation with a Hamiltonian including the kinetic energy of the free electron, and the potential describing the electron-electron and electron-nuclear interactions. There are also a variety of approximations used to treat processes that include the continuum. The approximations are also described in detail in text such as [91], and a nice summary is provided in [71].

### 2.3 Atomic Processes in Plasmas

The temperature of a system or plasma is often discussed in the context of describing its properties. Generally we can relate the kinetic temperature to the particle kinetic energy (KE): \( \frac{1}{2}mv^2 = \frac{3}{2}kT \). This works well in an EBIT where the electron beam energy is almost mono-energetic, however in many astrophysical and laboratory plasma sources the electrons have a range of energies so it doesn’t make sense to define the temperature in terms of a single particle. Instead we typically define an average KE over a specified distribution of particle velocities [91]. In many plasma sources the particles typically follow a Maxwellian speed distribution:

\[
    f(v) = \frac{4}{\sqrt{\pi}} \left( \frac{m}{2kT} \right)^{3/2} v^2 \exp \left( \frac{-mv^2}{2kT} \right)
\]

From this distribution a temperature can be found that best describes the distribution of kinetic energies of the system. In this section when discussing the energy of the free electron, we can consider this to be either a single value (as with the EBIT) or a range of
values (as in typical astrophysical plasmas).

Using the simplified Bohr model, we can picture electrons orbiting in well defined atomic orbitals, labeled by the principle quantum number, where electrons may jump from one orbital to another if radiation is absorbed or emitted. If an atom or ion interacts with an incoming photon of sufficient energy, it may become ionized or excited. If the energy of the photon is greater than the ionization energy of the bound electron, then the atom may lose an electron and become ionized. The energy of the ionized electron ($\epsilon$) will be equal to the initial photon energy ($h\nu$) minus the ionization energy (IE): $\epsilon = h\nu - \text{IE}$. This process, called photoionization (PI), can be represented by the equation:

$$X + h\nu \rightarrow X^+ + e^- (\epsilon)$$

(2.8)

where $X$ is the initial ion or atom, $h\nu$ represents the photon with frequency $\nu$, $X^+$ represents the ion or atom with one higher charge and $e^- (\epsilon)$ is the free electron with energy $\epsilon$. The inverse process of PI, called radiative recombination (RR), occurs when a free electron is captured into a bound state of an ion. The RR process can be described by:

$$X^+ + e^- (E_e) \rightarrow X + h\nu$$

(2.9)

where the photon energy is equal to the energy of the free electron ($E_e$) plus the binding energy. The RR and PI process are shown, using a simplified model, in Fig. 2.1. In both cases the charge state of the ion changes, therefore the atomic structure changes.

An atom or ion may also become ionized through electron impact ionization. This process can occur if the energy of the free electron ($E_{e1}$) is greater than the ionization energy (IE) of the bound electron. The energy of the free electron ($E'_{e1}$) after this process will be equal to original energy ($E_{e1}$) minus the sum of the energy of the ionized electron energy ($E_{e2}$) and the binding energy. The equation describing this process is:

$$X^{+n} + e^- (E_{e1}) \leftrightarrow X^{+(n+1)} + e^- (E'_{e1}) + e^- (E_{e2})$$

(2.10)
Figure 2.1: Top.) Simple cartoon of radiative recombination process. Bottom.) Photoionization process.
where \( X^{+n} \) is the initial ion with charge +n, \( e^- (E_{e1}) \) is the free electron with energy \( E_{e1} \), \( X^{+(n+1)} \) is the ion with one additional charge due to the removed electron, \( e^- (E'_{e1}) \) is the free electron with energy \( E'_{e1} \), and \( e^- (E_{e2}) \) is the ionized electron with energy \( E_{e2} \). This process also changes the charge state of the atom or ion and is depicted in Fig. 2.2. The reverse process is three-body recombination and involves the collision and recombination of the two free electrons and the ion.

If an atom or ion is in a radiation field, photons with energy \( (h\nu) \) near the transition energy may be absorbed and excite a bound electron from an initial state \( i \) to an excited state \( j \) in a process called photo-excitation. Once the lifetime of the transition has been exceeded, the excited electron will radiatively decay, emitting one (or more) photons in the reverse process. This process is shown in Fig. 2.3 and described by:

\[
X_i^{+n} + h\nu_{ij} \leftrightarrow X_j^{+n}
\]  (2.11)
Figure 2.3: top.) Photo-excitation process. bottom.) Spontaneous decay process.

where $X_i^{+n}$ is an ion with charge $+n$ in state $i$, $h\nu_{ij}$ is a photon with energy near the transition energy, and $X_j^{+n}$ is the excited ion in state $j$. This process preserves the charge of the ion.

Electron impact excitation is similar to photo-excitation in that it preserves the charge state and leaves the ion in an excited state. In this case however, a free electron with energy $E_{e1}$ may excite a bound electron. Once excited, the ion then spontaneously decays and emits a photon (or multiple photons) equal to the transition energy. The final energy of the free electron $E_{e1}'$ is equal to the initial energy $E_{e1}$ minus the excitation energy. This process is shown in Fig. 2.4 and is described as:

$$X_i^{+n} + e^-(E_{e1}) \rightarrow X_j^{+n} + e^-(E_{e1}') \quad (2.12)$$

where $X_i^{+n}$ is an ion in state $i$ with positive charge $n$, $e^-(E_{e1})$ is a free electron with energy $= E_{e1}$, $X_j^{+n}$ is an ion in an excited state $j$, and $e^-(E_{e1}')$ is the free electron with energy $E_{e1}'$. 

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Dielectronic recombination (DR) is a two-step resonant process by which a free electron is captured into a bound state of an ion while simultaneously exciting an inner shell electron. To complete the DR process one of the excited electrons then spontaneously decays, producing one (or multiple) photons. This is followed by the decay of the second electron. The DR process can be described by (see Fig. 2.5):

$$X^{+n} + e^- \rightarrow (X^{+n-1})^{**} \rightarrow X^{+n-1} + h\nu$$

(2.13)

where $e^-$ represent the free electron, $X^{(+n)}$ is an ion with positive charge (+n), $(X^{(+n-1)})^{(**)}$ is the recombined ion with charge (+n-1) in the doubly excited state, $X^{(+n-1)}$ the stabilized ion, and $h\nu$ is the emitted photon energy.

After the first step of the DR process, the ion is in a doubly excited state. At this point, the DR process may proceed or the reverse process may occur where one of the excited electrons spontaneously decays and the energy ionizes the second electron. This radiationless process leaves the ion in its original charge state as shown in Fig. 2.5, and is
The DR process is often described using an inverse Auger notation (Auger electron emission by autoionization is the inverse process of DR) given by three letters representing the principle quantum numbers of the electron orbitals involved \( n \). The first letter represents the initial \( n \) of the bound electron, the second letter is the principle quantum number of the excited electron, and the third letter is the principle quantum number of the capture site. As an example of DR, the two step KLL DR process in He-like Ar is depicted in Fig. 2.5. The resonant nature of the DR process emerges from the required energy matching of the free electron \( (E_e) \) plus binding energy \( (E_b) \) with the excitation energy \( (E_2) \). The photon emitted from the \( n=2-1 \) transition in Li-like Ar \( (Ar^{15+}) \), is slightly lower in energy than the analogous transition in the He-like \( (Ar^{16+}) \) charge state, and is thusly termed a satellite. The energy difference is attributed to the so called spectator electron that somewhat shields the nuclear charge. The satellite energy approaches the He-like transition energy threshold as the principle quantum number \( n \) of the spectator electron increases.

\[
e^- + X^{+n} \rightarrow (X^{+n-1})^{**} \rightarrow X^{+n} + e^- \tag{2.14}
\]
2.3.1 Plasma Emission Modeling

The collisional-radiative model NOMAD [96] was used in much of this work to model the EBIT plasma. Traditionally the charge state balance of EBIT plasmas had been calculated by modeling each ion as one state with no internal structure and used approximate formulas to describe the atomic processes [92]. However, the NOMAD code includes more accurate descriptions of the processes and charge stages. The code works by solving the system of time dependent rate equations described in [96] as:

\[
\frac{d\tilde{N}}{dt} = \tilde{A}(N_i, N_e, f_e, t)\tilde{N}(t) + \tilde{S}(t)
\]  

(2.15)

where here \(\tilde{N}\) is the vector of atomic state populations, \(\tilde{A}(N_i, N_e, f_e, t)\) is the rate matrix, and \(\tilde{S}(t)\) is the source function. The rate matrix generally depends on ion density \(N_i(t)\), electron density \(N_e(t)\) (which can have contributions from background and ionization), and electron-energy distribution function (EEDF) \(f_e(E, t)\). For this discussion we ignore the source function. For the EBIT we typically assume the EEDF has a Gaussian profile with a full-width at half maximum (FWHM) of 40 eV (see Chapter 4).

As a simple example, we can look at the rate equation of a singly charged ion experiencing ionization, recombination, and charge-exchange. This can be expressed as:

\[
\frac{dn_1}{dt} = -R_{1i}n_1 + R_{2r}n_2 - R_{CX}^1n_1 + R_{CX}^2n_2 - R_{1r}^1n_1
\]  

(2.16)

where \(n_q\) is the number density of ions with charge \(q\), \(R_{CX}^q\) is the charge exchange rate between an ion of charge \(q\) and neutral or low charge states, and \(R_{1i}^q\) and \(R_{1r}^q\) are the rate of ionization and recombination for the ion with charge \(q\), respectively. The population density will change due to the atomic processes. For example, recombination of the \(q=1\) ions will change the charge state to \(q=0\), removing them from the population, while recombination of ion with \(q=2\) will be added to the \(q=1\) ion population.

The NOMAD model includes processes such as spontaneous decay, electron-impact (EI) excitation, EI de-excitation, EI ionization, recombination (including three-body, radia-
tive and dielectronic), autoionization and dielectronic capture, charge exchange (between ions and neutrals and between ions and ions), and laser photopumping. NOMAD uses atomic data from external sources to solve the system of differential rate equations, and for this work atomic data including the atomic structure, transition probabilities, and collisional cross-section data was calculated with the Flexible Atomic Code (FAC). FAC, described in detail in [55], uses the Dirac Coulomb Hamiltonian and a modified Dirac-Fock-Slater central potential, and uses the jj coupling scheme described in previous sections.

For this work we allow the plasma to reach steady-state, so NOMAD solves the time independent equations. The charge exchange rate $R_{CX}$ generally depends on the density of neutrals, the charge-exchange cross section and the relative velocity of the neutrals and ions: $R_{CX} = \langle \sigma_{CX} v_r N_o \rangle$, which is averaged over the energy distribution of neutral and ions. To simplify the equation, we instead use $R_{CX} = \sigma_{CX} \tilde{v}_r N_0$, where $\tilde{v}_r$ is the effective average velocity [92]. Since neither $N_0$ or $\tilde{v}_r$ are known, we use the product as a free parameter. Then using $\sigma_{CX}$, such as the approximate $\sigma_{CX} \approx z \times 10^{-15} cm^2$, the free parameter can be varied until an agreement with the experimental spectra is reached. In the end NOMAD provides the level populations, line intensities, and the charge state balance.
Chapter 3

Electron Beam Ion Trap

3.1 Introduction

The inception of the electron beam ion trap (EBIT) can be traced back to the 1960s when the modern electron beam ion source (EBIS) was designed by Donets [36, 37]. This familiar design proposed using a dense mono-energetic electron beam to create (through electron impact ionization) and radially trap (using the space charge of the beam) highly charged ions. Since EBIS devices were designed to produce ions for injection into accelerator facilities, early iterations looked for ways to produce ever higher charge states and ways to increase the ion yield. This lead to new developments, such as techniques for increasing the electron beam density and cooling the ions heated by elastic collisions with energetic electrons (see [38] for a historical review of EBISs). The results from the first EBIS model (IEL-1), which included a Pierce-type electron gun, 5 drift tubes, and an electron beam capable of up to 2 keV energy and 40 mA current, were published in 1969 [37]. Measurements showed the production of $N^{7+}$ and $Au^{19+}$ and caught the attention of scientists all around the world.

Starting in the 1970’s at the Lawrence Livermore National Laboratory (LLNL), the cold war era Project Excalibur was attempting to create an x-ray laser as part of a ballistic missile defense initiative program. This later became part of President Reagan’s proposed
missile defense program called the Strategic Defense Initiative (SDI), later nicknamed “Star Wars” as the program relied on futuristic technology such as space based lasers and particle beam weapons that had yet to be developed [123]. The concept for Excalibur was that x-ray lasers could be packaged with a nuclear device, so that x-rays released from the detonation could be focused and aimed at target missiles [127]. While the funding for Excalibur was drastically cut by the end of the 1980’s and x-ray laser’s were never successfully developed as a ballistic missile defense, x-ray laser research continued at LLNL in a scientific capacity. The research into x-ray lasers required a better understanding of the atomic physics of highly charged ions (HCIs) as the hosts of proposed lasing transitions and scientist often had to travel to external research facilities such as UNILAC at GSI Darmstadt to measure line positions and intensities to test atomic theories [86].

Donets’ modern EBIS caught the attention of LLNL scientist as an alternative to the large and expensive experimental facilities [86], and in 1988 Mort Levine, in collaboration with Ross Marrs created the first EBIT. Building on the principles and techniques developed by the early EBIS community, the EBIT is notably different in that it was designed specifically for the spectroscopic studies of atomic processes of HCIs rather than as an ion source [79]. While it is still technically an EBIS, it has a much smaller trapping drift tube (3 cm), and it contains view ports around the trap region that allow for spectroscopic observations. Adding these ports required changing the single long solenoid used in an EBIS to two Helmholtz coils that are placed above and below the small trapping drift tube. While the smaller trapping region makes this device a less efficient ion source, it reduces instabilities, which allows for longer trapping times, the production of higher charge states, and makes the device much smaller overall.

After the original LLNL EBIT was built in 1988 [79], a number of new EBIT facilities, each with their own modified version specific to their research interest, emerged. This included super-EBIT designs, which are capable of producing any charge state of any element of the periodic table (see e.g. Marrs (1994) [81], where the LLNL super-EBIT was used to produce bare uranium ions). While many of the new EBITs are custom made construc-
tions, there are commercially available devices as well. Over the years these included for example the “refrigerated” EBIT designed by Physics & Technology, LLC (P&T) [82] and a number of room temperature and superconducting EBIT/EBIS designs sold by Dreebit, GmbH [39]. The P&T refrigerated (dry cryogenic) EBIT includes a closed cycle cryocooler that allows the system to be cooled below 4 K without the use of cryogens. To the best of my knowledge P&T only produced two units, one purchased by the Smithsonian Astrophysical Observatory (SAO) [113] and the second was commissioned by Stockholm University [27] and later re-designed/optimized by the group at Stockholm [61, 103].

Measurements described in this thesis were performed at the NIST EBIT facility; therefore the design and operational parameters of that device and the spectrometers used for this work will be described in section 3.2. Part of my time as a graduate student was also spent at the SAO EBIT facility, so the current status of that EBIT and a summary of the work performed there is described in section 3.5. Finally we note that Clemson University (CU) has a relatively new EBIT facility. The superconducting CU-EBIT/S, purchased from Dreebit GmbH, operates with a closed cycle cryocooler and was designed primarily as an EBIS. Some of the works from the CU-EBIT facility include: [118, 111, 76].

3.2 Design and Theory of Operation

Mort Levine, one of the creators of the original EBIT, also helped design the NIST EBIT. The design of the original and NIST EBIT are similar with a few exceptions including the addition of field penetrators, to drain electrons trapped by stray fields, and a few design modifications made to some of the electrodes (see [53] and [40] for a historical introduction to the NIST EBIT project). Figure 3.1 shows a scaled sketch of the EBIT from Levine (1988) [79]. The simplified sketch shows the vertical orientation of the small about 1 m tall device.

The EBIT produces an almost mono-energetic electron beam that travels from the electron gun at the bottom of the device, through the trap (drift tubes) in the middle,
and finally ends up making contact with the collector at the top. The electron beam is compressed by a superconducting magnet as it travels from the electron gun to the trap. The magnet structure includes two Helmholtz coils surrounding the drift tubes, producing a nearly uniform field in the trap. The magnet includes observation ports around the trap. Neutral or low charge state ions are injected into the trap where they interact with the electron beam and become ionized through electron impact ionization. The ions are electrostatically trapped in the axial direction and radially trapped by the space charge of the electron beam (discussed below).

The cross section view in Fig. 3.1 highlights the cryogenic environment required for the superconducting magnet (SCM). The room temperature vacuum vessel encloses a liquid nitrogen ($\text{LN}_2$) temperature (77 K) shell that acts as a thermal shield for the 4 K SCM and drift tube region. The cryogenic temperatures also improve the ultra high vacuum level ($\sim 10^{-10}$ Torr), provided by turbo and ion pumps, as gases condense on the cold surfaces.

The detailed cross section drawing of the NIST EBIT, edited from [53], is shown in Fig. 3.2, where the overall height is about 1 m. This design drawing is more comprehensive and shows the geometry of the drift tube assembly, collector (with $\text{LN}_2$ cooling channels), and to-scale distances between elements. The control of the EBIT can be understood by breaking the series of internal electrodes up into three main sub-assemblies including: the electron gun, the drift tube, and the collector. A schematic of the electrodes was provided in the *First Results from the EBIT at NIST* by J.D. Gillaspy [50] and is shown in Fig. 3.3.

### 3.2.1 Drift Tube Assembly

The drift tube assembly consist of 4 electrodes: the lower, middle, and upper drift tubes, and a shield electrode that surrounds them. The three drift tube power supplies are electrically floated on top of the high voltage of the shield that in turn is capable of reaching up to 30 kV voltages. For these experiments, the 3 cm middle drift tube voltage was placed to zero (equal to the shield voltage), while the lower and upper drift tubes were placed at +500 V and +260 V above the shield voltage, respectively, during the 5 s trapping/charge
Figure 3.1: Schematic of original EBIT from Levine (1988) [79].
Figure 3.2: Cross section of NIST EBIT from [53].
Figure 3.3: Schematic of EBIT electrodes from [50].
breeding period. During measurements the trap was dumped for 10 ms every 5 s to remove any build up of contaminants, such as barium from the electron gun. During the dumping period, the middle drift tube voltage was raised above the upper drift tube voltage to +400 V (but still below the lower drift tube voltage). This pushes the ions out of the trap while ensuring they do not travel down towards the electron gun.

A computer aided design (CAD) model of the SAO drift tube assembly (similar to the NIST assembly, but in a horizontal orientation) is shown in Fig. 3.5. The center drift tube, shown in blue, has a constant inner diameter and contains axial slits that allow for injection of neutrals and spectroscopic examination of the trapped plasma (surrounding shield electrode also has slits). The SCM surrounding the drift tubes produces a magnetic field of 2.7 T and compresses the electron beam to \( \sim 35 \mu m \) (discussed below). The potential placed on the middle drift tube determines the electron beam energy in the trap from the expression \( E = qV \); however the potential from the electron beam must also be taken into account when calculating the electron beam energy at in the trap.

To calculate the space charge, we first approximate the electron beam to be an infinite line charge \( \lambda \) (charge per length), and use Gauss’s law:

\[
\oint_S \mathbf{E} \cdot d\mathbf{a} = \frac{Q_{\text{enc}}}{\epsilon_0}
\]

(3.1)

where \( Q_{\text{enc}} \) is the total charge enclosed within the surface, \( \epsilon_0 \) is the free space permittivity, \( \mathbf{E} \) is the electric field vector and \( d\mathbf{a} \) is the infinitesimal surface vector element.

Using a cylindrical surface to surround the infinite line charge, this simplifies to:

\[
E(2\pi rl) = \frac{\lambda l}{\epsilon_0} \hat{r} \rightarrow E = \frac{\lambda}{2\pi r\epsilon_0} \hat{r}
\]

(3.2)

and if the surface is inside of the line charge this changes to:

\[
E(2\pi rl) = \frac{\lambda l \left( \frac{2l^2}{l^2} \right)}{\left( \frac{2l^2}{l^2} \right)\epsilon_0} \hat{r} \rightarrow E = \frac{\lambda r}{2\pi r^2 \epsilon_0} \hat{r}
\]

(3.3)
where \( r \) is the radius of the Gaussian surface, and \( r_e \) is the radius of the electron beam. Integrating to find the \( V \), the potential outside of the electron beam is given as:

\[
V_{\text{out}} - V_{0_{\text{out}}} = \frac{\lambda}{2\pi \varepsilon_0} \ln \left( \frac{r}{r_e} \right) \tag{3.4}
\]

where \( V_{\text{out}} \) is the potential outside of the electron beam, and \( V_{0_{\text{out}}} \) is a constant.

Inside of the electron beam, the potential is:

\[
V_{\text{in}} - V_{0_{\text{in}}} = \frac{\lambda}{4\pi \varepsilon_0} \left( \frac{r^2}{r^2_e} \right) \tag{3.5}
\]

where \( V_{\text{in}} \) is the potential inside of the electron beam radius, and again \( V_{0_{\text{in}}} \) is a constant. Setting the potential \( V_{\text{in}} \) equal to zero at \( r=0 \) inside of the electron beam, \( V_{0_{\text{in}}} \) becomes zero. Then, at the electron beam radius \( V_{\text{out}} = V_{\text{in}} \), so \( V_{0_{\text{out}}} = \frac{\lambda}{4\pi \varepsilon_0} \). The potential outside of the electron beam then becomes:

\[
V_{\text{out}} = \frac{\lambda}{4\pi \varepsilon_0} + \frac{\lambda}{2\pi \varepsilon_0} \ln \left( \frac{r}{r_e} \right) \tag{3.6}
\]

Finally using the relation \( \lambda = \frac{I}{v} \), where \( I \) is the electron beam current and \( v \) is the electron velocity, and the electron kinetic energy \( E = \frac{1}{2}mv^2 \), the potential can be expressed as:

\[
V_{\text{out}} = \frac{I}{4\pi \varepsilon_0 \sqrt{\frac{2E}{m}}} + \frac{I}{2\pi \varepsilon_0 \sqrt{\frac{2E}{m}}} \ln \left( \frac{r}{r_e} \right) \tag{3.7}
\]

where \( E \) is the electron beam energy. The potential calculated at the drift tube inner diameter is called the space charge \( V_{sc} \). Using an electron beam radius of 35 \( \mu \)m, and radius of the middle drift tube = 5 mm, the space charge is shown for a range of electron beam energies in Fig. 3.4. This shows that the space charge can be high at low electron beam energies; however the electron beam current is typically set lower at lower beam energies. The space charge calculation does not take into account the neutralization that results from the positive ion charges in the trap. Typically to estimate the total space charge (including
neutralization), theoretical and experimental spectra are compared where resonances, such as from dielectronic recombination, occur as a function of the electron-beam energy. As an example, a KLM DR resonance in Li-like Ar occurred at an experimental beam energy of 2795 eV (with 60 mA electron beam current and calculated from the potential difference between the middle drift tube and the cathode), however the theoretical value was 2730 eV. The calculated space charge potential is 203 eV, indicating that there must have been a neutralization of $\sim 32\%$ of the total charge of the electrons in the trap region, so the total energy was 65 eV lower than the potential set on the middle drift tube.

Going back to Fig. 3.5, we see that the upper and lower drift tubes, shown as a salmon color, have a tapered inner diameter. This results in a changing space charge. At the larger inner diameter, towards the outside of the drift tubes, the space charge increases, decreasing the electron beam energy. This acts as additional axial trapping potential that
3.2.2 Electron Gun Assembly

The commercially available electron gun, with Pierce geometry, includes a 3 mm diameter curved “M” type (tungsten and barium oxide) cathode, a focusing electrode, and an anode. The electron gun is capable of producing electron beam currents up to 0.15 A. An image of early LLNL electron gun simulations, taken from a NIST EBIT laboratory notebook, is shown in Fig. 3.6. Equipped with the same or similar electron gun, the figure shows electrons emitted from the curved filament/cathode surface. The negative voltage placed on the specially shaped focus electrode produces a transverse force that overcomes the space charge repulsion of the electrons to create a converging beam. A positive voltage placed on the anode attracts the electrons and sets the electron beam current. The electron gun sits in a copper plated steel plate that aids in shaping the magnetic field lines near the electron gun [50]. This “snout” plate was made of iron on the original EBIT, and is made of copper in the SAO EBIT. An image of the SAO EBIT electron gun (identical to the one at NIST) and snout plate is shown in Fig. 3.7. The electron gun is surrounded by a bucking coil, with its magnetic field opposing that produced by the SCM, to minimize the field...
in the electron gun region. The bucking magnet is actively cooled using a non-corrosive, electrically isolating fluid.

If the magnetic field surrounding the electron gun is zero, and if the temperature of the cathode is ignored, the electron beam radius can be described by the Brillouin formula:

\[ r_b = \frac{150}{B} \sqrt{\frac{I_e}{E_e}} \]  

(3.8)

where \( B \) is the magnetic field at the trap, \( I_e \) is the electron beam current, and \( E_e \) is the electron beam energy at the trap. Since we know that the cathode electrons have a temperature, the electron beam radius can be better estimated using the Herrmann theory [60], where the radius of a circle through which 80% of the beam passes is given by:

\[ r_h = r_b \sqrt{\frac{1}{2} + \frac{1}{2} \sqrt{1 + 4 \left( \frac{8 kT r_c^2}{m n^2 r_b^2 B^2} + \frac{B_c^2 r_c^4}{B^2 r_b^4} \right)}} \]  

(3.9)

where \( B_c \) is the magnetic field at the cathode, \( kT \) is the electron temperature at the cathode, \( r_c \) is the cathode radius, \( m \) is the mass of an electron, and \( \eta \) is the electron charge to mass ratio. Using this equation to plot the Herrmann radius as a function of the cathode magnetic field, Fig. 3.8 shows that the smallest radius occurs at a magnetic field of zero, and the radius is relatively unaffected for \( B_c < \sim 5 \) G. For this calculation, the following values were used as an estimate: \( E_e = 5 \) keV, \( I_e = 130 \) mA, \( T = 1400 \) K, \( B = 2.7 \) T, and \( r_c = 1.5 \) mm.

To estimate the Herrmann radius sensitivity to electron beam energy and current, Figs. 3.9 and 3.10 show the radius as a function of energy and current, respectively. For these calculations the magnetic field at the cathode was assumed to be zero. These figures show that the radius is relatively insensitive to the electron beam energy and current. Over the range of electron beam currents (50 - 150 mA) the radius only increased by \( \sim 2 \) \( \mu \)m for 1 keV electron beam energy, and only by \( \sim 0.1 \) \( \mu \)m for 20 keV. Similarly over the typical electron beam energies, the radius changes by less than \( \sim 1 \) \( \mu \)m. This demonstrates the importance of the magnetic field near the cathode and why great efforts are taken to reduce
Currently the snout electrode is tied to the anode on both the NIST and SAO EBITs, although they could technically be separated later to improve the performance. The electron gun is currently referenced to ground (both NIST and SAO); however the electron gun assembly is electrically isolated from all other ground reference components, making it possible to float the assembly to a negative voltage to increase the electron beam energy capabilities.

3.2.3 Collector Assembly

The collector assembly consist of a copper suppressor, collector, and extractor electrode. An electromagnet surrounds the collector and is designed to oppose the magnetic field produced by the SCM. This spreads the electron beam radially out to contact the collector. As electrons travel up from the drift tube region to the collector, they first pass the suppressor electrode. This electrode is negatively biased relative to the collector and deflects secondary electrons, created from contact of the electron beam with the collector,
Figure 3.7: Pierce geometry electron gun currently housed in SAO and NIST EBITs.

Figure 3.8: Herrmann radius as a function of magnetic field at the cathode
Figure 3.9: Herrmann radius as a function of electron beam energy

Figure 3.10: Herrmann radius as a function of electron beam current
away from the trap and back towards the collector. The voltage placed on the extractor electrode attracts the positive ions (for extraction) and simultaneously deflects electrons. The collector assembly, biased at +2 kV with respect to the potential of the cathode, collects a high current of electrons producing a dissipating power and as a result a large heat load. To deal with this, the collector assembly is cooled with LN$_2$ to 77 K (and in the SAO EBIT cooled to -20 ° with an electrically isolating fluid). It is difficult to resolve the NIST collector assembly in Fig. 3.2, so the CAD model of the SAO EBIT collector assembly is shown in Fig. 3.11. The model shows the electrodes mentioned, but is not showing the electromagnet that surrounds the collector. The NIST EBIT collector assembly is currently referenced to ground; however, like the electron gun, it is electrically isolated from other components so that it could be floated in the future.

There is one additional electrode, called the transition electrode, that is not really part of the three main sub-assemblies mentioned. The transition electrode includes a small aperture placed in the cold shield that separates room and cryogenic temperature regions of the EBIT. This electrode is designed to guide the electrons from the room temperature electron gun through the thermal shield and to the cryogenic temperature trap.

3.2.4 Typical Operation

The EBIT operates at ultra high vacuum levels, therefore the vacuum chamber is constantly pumped to maintain the vacuum. The pressure is monitored at various places in the EBIT including the electron gun and beam line regions. The SCM needs to maintain a temperature below the material’s critical temperature to have a zero resistance and produce a maximum magnetic field. The critical temperature for niobium-titanium, the material of the SAO EBIT SCM, is 10 K. Therefore the best way to reach this temperature is with liquid He, with a boiling point of around 4 K. The NIST EBIT consumes about 3.5 L of liquid helium per hour during measurements, so the SCM not actively cooled while the EBIT is idle.

Prior to any NIST EBIT experiment, the 4 K section of the EBIT is first filled with
LN₂ to pre-cool the region. The resistance of the superconducting magnet is monitored, and once the magnet reaches 77 K the resistance reads 5.5 Ω. After a few days, the LN₂ is allowed to boil off (or it is blown out with room temperature nitrogen gas) and liquid helium is transferred from an external dewar to the pre-cooled 4 K section of the EBIT. Once the magnet reaches 0 Ω resistance and become superconducting the magnet current is slowly ramped up to 147.8 A to produce a 2.7 T magnetic field inside the coils.

The electron gun filament is slowly ramped to 6.3 V producing a current of about 0.487 A. Equating the electrical power to the radiative power, this give a temperature of roughly 1400 K at the cathode. The electron gun anode setting determines the electron beam current, but care must be taken to ensure the electron beam is aligned and not making contact with any of the electrodes. While slowly increasing the the anode voltage, the beam is tuned and the current on the collector is monitored (lack of current indicates the electrons are going elsewhere). The voltages placed on the transition, suppressor and focus electrodes
are tuned along with the bucking coil current to minimize the current reading on the snout (the best diagnostic of beam tuning) [50]. The NIST EBIT electronics have a built in safety precaution, where a snout current above 80 $\mu$A shuts off the anode. The snout current is typically less than 20 $\mu$A when ideally tuned [50]. In some cases the use of shim coils, located around the trap and outside of the vacuum chamber, are needed to properly tune the electron beam. These are not required at the NIST EBIT, which is likely attributed to excellent alignment of the electrodes [50].

Typical operating parameters (used during the experiments described in our work) is shown in Fig. 3.12, where the gas injection pressure is recorded with no gas injected, and the recorded SCM resistance is after $LN_2$ boil off and prior to liquid helium fill. The gas injection chamber pressure is noted before filling it with injector gases.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam Line Pressure (Torr)</td>
<td>1.44E-09</td>
</tr>
<tr>
<td>E-Gun Pressure (Torr)</td>
<td>1.40E-10</td>
</tr>
<tr>
<td>Crystal Spectrometer (Torr)</td>
<td>2.60E-03</td>
</tr>
<tr>
<td>Gas Injection Pressure (Torr)</td>
<td>4.34E-09</td>
</tr>
<tr>
<td>Super Magnet Resistance (Ohm)</td>
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</tr>
<tr>
<td>Focus (V)</td>
<td>-8.39</td>
</tr>
<tr>
<td>Suppressor (V)</td>
<td>620</td>
</tr>
<tr>
<td>Extractor (V)</td>
<td>-2180</td>
</tr>
<tr>
<td>Transition (V)</td>
<td>5.36</td>
</tr>
<tr>
<td>Filament (V)</td>
<td>6.3</td>
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<td>0.482</td>
</tr>
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<td>Upper Drift Tube (V)</td>
<td>260</td>
</tr>
<tr>
<td>Lower Drift Tube (V)</td>
<td>500</td>
</tr>
<tr>
<td>Middle Drift Tube (V)</td>
<td>400</td>
</tr>
<tr>
<td>Collector Magnet Voltage (V)</td>
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</tr>
<tr>
<td>Collector Magnet Current (A)</td>
<td>0.5478</td>
</tr>
<tr>
<td>SC Magnet Current (A)</td>
<td>147.7</td>
</tr>
<tr>
<td>Bucking Coil Voltage (V)</td>
<td>0.53709</td>
</tr>
<tr>
<td>Snout (mA)</td>
<td>&lt; 15</td>
</tr>
<tr>
<td>Collector Voltage (kv)</td>
<td>2</td>
</tr>
</tbody>
</table>

Figure 3.12: Typical NIST EBIT settings.
3.3 Neutral Atom and Ion Injection

The NIST EBIT contains two primary methods of injecting neutral atoms, or low charge state ions into the trap. These include a neutral gas injection system and a Metal Vapor Vacuum Arc (MeVVA) ion source. The gas injection system is attached to one of the radial observation ports surrounding the trap region. A schematic of the differentially pumped ballistic gas injection system was provided by [41] and is shown in Fig. 3.13 with a photo of the system installed on the NIST EBIT. The gas reservoir is a 6 way mini conflat cross that has a pressure gauge, pump, and 3 needle valves attached. One of the needle valves is connected to a gas manifold, which is separately pumped, containing gasses such as Ar, Kr, Ne, N$_2$, and CO$_2$. Additional gases can be easily added to the manifold or added directly onto one of the other needle valves connected to the gas reservoir. Since the injected species are neutral, they can be directly injected into the middle drift tube/trap without being affected by the magnetic field.

The typical gas injection pressure used for our work, measured at the gas reservoir (P1) is around 2.5 x 10$^{-5}$ Torr. This pressure is typically adjusted while monitoring the x-ray signal to maximize the count rate. As discussed in works such as [41], the gas injection pressure can alter the charge state balance. An increased pressure introduces more neutral atoms which, through processes such as charge exchange recombination, produce lower charge state ions. For example, Fahy et al. noticed a 40% increase in the number density of Xe$^{24+}$ ions relative to Xe$^{23+}$ when using a gas injection pressure of 9.1 x 10$^{-6}$ as opposed to 6.4 x 10$^{-3}$ Torr. It is important to note however that the pressure in the trap region of the EBIT in both cases remains lower than 10$^{-9}$ Torr as the EBIT and gas injection system are separated by a small aperture and the EBIT, with its cryogenic temperatures and lower base pressure, pumps more efficiently. Figs 3.13 and 3.14 give a rough estimate of the pressures in each section of the gas injection system. For a gas reservoir pressure of about 3 x 10$^{-4}$ Torr, the pressure in section 2 is about 10$^{-6}$ Torr, and as previously mentioned, the pressure in the EBIT, P$_b$ is about 10$^{-9}$ Torr. The pressure differences, combined with
the series of nozzles and apertures, shown in Fig. 3.13, produce a well collimated beam of atoms directed directly into the trap region of the EBIT.

The MeVVA was not used for our work, and has been described extensively in previous works such as [62]. Briefly, the MeVVA at NIST sits on top of the vertically oriented NIST EBIT, as also shown in Fig. 3.1. The NIST MeVVA is an upgrade to previous MeVVA designs and removes the need for cooling fluids or moving parts in vacuum. The design includes one common anode and 8, selectable, 1-2 mm diameter cathode rods that can be manually chosen from a control panel. These include elements such as W, Nd, Os, Fe, Pr, Ir, among other metals. The cathodes rest on the sides of a channeled quartz anode insulator, while the anode grid rest on top of an insulator element (see Fig. 3.15). The tip of the cathode is about 0.508 mm from the anode grid.

The cathode and anode are electrically isolated from the EBIT and floated to a positive bias voltage of about 10 kV. During operation, a high voltage pulse sent to the cathode jumps from the tip of the cathode to the anode along the quartz insulator. Ions produced in this discharge travel towards the EBIT-grounded extractor grid, where they continue to travel down the EBIT along the magnetic field lines. When the MeVVA fires, the potential in the EBIT trap region is quickly (for about 1 ms) changed to match that of the MeVVA by setting the shield electrode to about +9.6 kV and the middle drift tube to +0.4 kV. This allows the ions to easily travel down into the trap. Once the ions reach the trap, the middle drift tube voltage is quickly lowered to 0 kV to trap the ions followed by lowering the shield voltage to match the desired electron beam energy.

3.4 Spectrometers and Detectors

The NIST EBIT facility currently includes a flat-field grazing-incidence EUV spectrometer, a Johann-type geometry crystal spectrometer, a high purity Ge (HPGe) detector, and traditionally an x-ray microcalorimeter.

The EUV spectrometer was optimized specifically for the NIST EBIT source and
Figure 3.13: top) Photo of NIST EBIT gas injection system. bottom.) Schematic and caption of the NIST gas injection system from [41].
Figure 3.14: Print out from J.D. Gillaspy of recorded pressures in the first nozzle section (P2) vs. recorded pressure in the gas reservoir (P1) section for various elements (see Fig. 3.13 for reference).

Figure 3.15: MeVVA vacuum assembly, design from [62].
covers a 4 nm to 40 nm wavelength range \cite{20} with a resolving power $\frac{\lambda}{\Delta \lambda}$ of about 400. EUV light coming from the EBIT is collected by a gold coated spherical mirror and constrained by a bilaterally adjustable entrance slit. If the vacuum in the spectrometer is a concern, a 0.1 $\mu$m zirconium window (supported by a nickle mesh) can be introduced to separate the EUV and EBIT vacuum. The dispersion element is a gold-coated-concave reflection grating that allows wavelength separated EUV photons be detected by a $LN_2$ cooled CCD camera.

CCD detectors contain an array of Si pixels. The array and pixel size can vary depending on the design specifications and the manufacturer. The EUV CCD has 2048 x 512 array with 13.5 $\mu$m x 13.5 $\mu$m pixel size. Upon absorbing a photon, the Si semiconducting material excites bound valence band electrons into the free flowing conduction band. This creates “holes” in the valence band and photoelectrons in the conduction band. The free charges are collected electrostatically for each pixel until the exposure time is over. The collected charge can be read out as amplified voltage that is converted into a digital number, termed an analog-to-digital unit or ADU. Knowing that it takes about 3.66 eV to create an electron-hole pair in Si, the output ADU can be used to determine the energy of the incoming photon assuming that its full energy is absorbed by the pixel through a series of atomic cascade events. The CCD chip pixels this way can be considered as energy dispersion detectors, and can detect individual x-ray photons (see Chapter 4 for a relevant example).

As previously mentioned the EUV CCD is actively cooled with $LN_2$. This is done to reduce thermal energy which may excite electrons and produce electronic noise signal (see text such as Howell’s handbook of CCD astronomy \cite{63} for additional theoretical details and examples). The NIST EUV spectrometer with its CCD detector has been a powerful workhorse device used to produce atomic data for many years now (see e.g. \cite{115, 41, 73, 87, 92, 51}). Additional details of the design and setup of the EUV spectrometer can be found in Blagojevi\'et al. \cite{20} and many of the works cited.

The broadband, high count-rate HPGe detector has a similar operating principle as a single pixel of the CCD chip with an energy resolution of about 135 eV at 5.9 keV x-ray energy, but a lot larger collection area of about 10 mm$^2$. This detector is often used
to quickly diagnose the EBIT plasma in real time. Parameters, such as the gas injection pressure or MeVVA trap voltage matching, are tuned until the HPGe line intensity of interest is maximized. The Ge semiconductor crystal indeed works in a similar manner as the CCD pixels, meaning the incoming photon produces electron hole pairs in the \( LN_\text{2} \) cooled crystal that are electrostatically collected. Each photon hit takes some time to be processed, so any new photon hit that occurs during that time (called the dead time) is ignored. The voltage pulse-height of the signal is proportional to the photon energy, and it takes about 2.96 eV to produce an electron-hole pair in the Ge crystal. A 340 nm thin aluminum-coated polymer window separates the EBIT and detector vacuums. This window has almost a 100% transmission for x-ray energies above 2 keV, while energies below about 0.5 keV are almost entirely absorbed.

The Johann-type crystal spectrometer is the primary device used for this work. The design of this device was described in detail in Brennan et al. (1989) [22] and has also been discussed in Gall (2017) [47], but some of the details are included here.

Spectrometers typically consist of an entrance slit, lenses (or mirror), a dispersion element, and a detector. Since lenses and mirrors are difficult to design for x-rays, x-ray spectrometers typically only include a slit, a crystal, and a detector [66]. In the case of the EBIT source (slit like in nature), the use of a slit is not required. In this work we used a spectrometer that consist of a \(-75^\circ\text{C}\) cooled CCD camera with a 2048 x 2048 pixel array (13.5 \( \mu \text{m} \) pixel size), a crystal bender (used to create Johann geometry, discussed below), and an energy selector [22]. The low transmittance of x-rays through air require the spectrometer to be placed in vacuum. At NIST, the spectrometer vacuum (\( \sim 4x10^{-7} \) Torr) is separated from the EBIT by a 230 \( \mu \text{m} \) thick beryllium window. Using a filter transmission calculator [77], results shown in Fig. 3.17, we see that the higher energy photons have almost 100% transmission, while x-rays below 2 keV are totally or partially absorbed by the Be window.

To understand how the x-ray spectrometer works, we can consider a simple crystal consisting of planes of atoms that are spaced a distance \( d \) apart (see Fig. 3.16). In general
an x-ray incoming at an angle $\theta$ will be scattered in all directions; however, under certain conditions the scattered x-rays will constructively interfere and diffraction will occur. These conditions are that i.) the incident and scattered angles are equal and ii.) the x-rays scattered from different planes are in phase. Condition ii requires that the path length difference ($CB + DB = 2CB$ in Fig. 3.16) equals an integer number ($n$) of wavelengths ($\lambda$). Then from the geometry we find that the extra length traveled is $2AB\sin(\theta)$ which equals $2d\sin(\theta)$. Condition ii then gives us Bragg’s law:

$$2d\sin(\theta_B) = n\lambda$$  \hspace{1cm} (3.10)

where $\theta_B$, is called the Bragg angle, and $n$ is the order of reflection. As the x-rays travel into the crystal, the wavelength (Bragg angle) may change slightly due to the index of refraction $n_r = \frac{\lambda}{\lambda'} = 1 - \delta$. A more exact expression of Bragg’s law is then: $n\lambda = 2d\sin(\theta_B)\left[1 - \left(\frac{2d}{n}\right)^2 \frac{\delta}{\lambda^2}\right]$, where $\frac{\delta}{\lambda^2}$ is a refractive index correction. Typically this correction is negligible, so we ignore it for this discussion.

The ideal case (Eqn. 3.10) shows that radiation with wavelength $\lambda$ (proportional to energy through $E = \frac{hc}{\lambda}$) in first order is reflected only at the Bragg angle $\theta_B$. In the case of real crystals, incident radiation of wavelength $\lambda$ can be reflected not only at the Bragg angle, but also within a narrow range of angles around the Bragg angle [4]. Since the Bragg angle is proportional to the wavelength, this also means that radiation incident at the Bragg angle can be reflected within a small wavelength range centered on $\lambda$. The curve describing the reflectivity of the crystal over this range of angles is called the rocking curve (also called Darwin curve or reflectivity curve).

As the x-ray enters the crystal it mostly reflected in the first 1-2 layers of the crystal. As it travels deeper into the crystal it has a chance to be transmitted or reflected (also absorbed) at each atomic plane. The Darwin model describes the total reflected radiation by including contributions to the interference from each layer [2]. From this model, the
width of the rocking curve (centered on the Bragg angle), is given as [4]:

$$\Delta \theta = \frac{r_e \lambda^2}{\pi V_{uc}} F \frac{(1 + |\cos(2\theta_B)|)}{2\sin(2\theta_B)}$$  \hspace{1cm} (3.11)

where $r_e$ is the electron radius, $\theta_B$ is the Bragg angle, $F$ is the structure factor of the unit cell and $V_{uc}$ is its volume. This equation shows that the width of the possible reflected angles depends of the crystal structure, and the wavelength of the incident radiation. In Chapter 4, we will see that the width also depends on the polarization of the radiation (Fig. 4.7). An example of a rocking curve for a flat crystal, from [4], is shown in Fig. 3.18.

While the flat crystal case is easily understood, the efficiency is low compared to that of a bent crystal [66]. For the Johann-type geometry used in this work, the crystal is bent to a radius of $2R$, where $R$ is the radius of the focusing circle (Rowland circle). The Rowland circle touches the bent crystal at the center of the crystal (see Fig. 3.19). This geometry has the advantage that x-rays with the same wavelength scattered by different parts of the crystal will be almost completely focused onto the Rowland circle, regardless of the position of the source [66]. The shape of the rocking curve however changes as we consider curved crystals, where atomic planes may no longer be parallel (see Fig. 4.7).

According to Bragg’s law, and as shown in Fig. 3.19, x-rays of different wavelengths are reflected and focused at different points on the Rowland circle. Therefore, the detector
Figure 3.17: Transmission of Be filter as a function of photon energy. Online calculator: 
http://henke.lbl.gov/optical_constants/

Figure 3.18: Figure of rocking curve calculated for flat crystal (and caption) from [4].
would need to be moved along the circle to detect different lines. Keeping the detector on the Rowland circle then requires the detector to crystal distance, given as \( L = 2R \sin(\theta) \) where \( R \) is the radius of the Rowland circle, to change. Since the energy resolution is proportional to the crystal to detector distance [22], the energy resolution then varies with the wavelength as the crystal to detector distance changes. To avoid this issue, the tunable spectrometer at NIST has an energy selector that defines the angle of incidence of the x-rays and rotates the crystal and CCD accordingly (holding the crystal to detector distance constant). Because the crystal to detector distance \( (L) \) is held constant, the detector may be moved off the Rowland circle. To account for this, the crystal bender changes the radius of curvature to focus x-rays onto the detector (changes the Rowland circle to be at the detector position). This is shown in Fig. 3.20 from [22], where the geometry for two different energies are shown. This figure shows the stationary source inside of the Rowland circles. While changing \( \theta \), the crystal to detector distance stays the same, so the crystal is bent to create a new Rowland circle \( (R) \) to keep x-rays focused on the detector.

The source position and size affects both the collection efficiency and bandwidth (range of wavelengths that can be reflected) [22]. From Barnsley et al. [7], the bandwidth \( (\Delta \theta) \) can be expressed as:

\[
\Delta \theta = \frac{W \sin(\theta)}{b} - \frac{W}{r} - \frac{x}{b} 
\]

where \( r \) is the radius of the bent crystal, \( b \) is the distance from the crystal to the source, \( \theta \) is the Bragg angle, \( W \) is the crystal width, and \( x \) is the spatial extent of the source. This could also be expressed in terms of wavelength \( (\Delta \lambda) \) or position \( (\Delta x) \). If the detector size is smaller than the allowable reflected wavelength range, then the spectrum is limited by the detector size rather than the crystal bandwidth. For this work, the bandwidth is typically about 120 eV.

From Bragg’s law, the instrumental broadening can be expressed in terms of \( \lambda, \theta, \)
Figure 3.19: Sketch of Johann geometry from [7].

Figure 3.20: Sketch of the tunable spectrometer at two different energies from [22].
or x (position/pixel) as:

\[
cot(\theta) \Delta \theta = \cot(\theta) \frac{\Delta x}{L} = \frac{\Delta \lambda}{\lambda}
\]  

(3.13)

where Barnsley et al. [7] show that the instrumental broadening (\(\Delta \theta\) (instr)) is a function of the crystal broadening (rocking curve), broadening due to the size of the detector pixels, aberrations due to the Johann geometry (crystal width and height), alignment of the detector on the Rowland circle (only touches at one point), and source size. For our work, we found that the NIST spectrometer has an energy resolution (FWHM) of about 1.4 eV at 3.5 keV x-ray energy.

3.5 SAO EBIT

As previously mentioned, the EBIT at the Smithsonian Astrophysical Observatory (SAO) was commissioned from Physics & Technology, LLC, in Livermore CA. A photo of the original EBIT setup at SAO is shown in Fig. 3.21. The design is updated from the original by Levine et al. [79] in that it has a horizontal orientation, does not require liquid cryogens, and has a compact configuration. One of the advantages of this design is its potential portability. For example, in 2011 the SAO EBIT was used at the Argonne National Laboratory and combined with the Advanced Photon Source to search for emission from highly charged Kr driven by photoionization [113].

The cross-section of the EBIT CAD model is shown in Fig. 3.22 with the major components labeled. The SUMITOMO cryocooler of the SAO EBIT includes a helium refrigerator that operates on the Gifford-McMahon cycle. The cold stages of system are used to cool the SCM to 4 K and the thermal shield, separating the room temperature vacuum vessel from the SCM, to around 50 K. An additional cryocooler is attached to the thermal shield (near the collector) for additional cooling. The bucking coil surrounding the electron gun (and outside of the vacuum) is cooled by a glycol-water mixture chilled to -20°C, and the collector and collector coil were originally cooled by a silicone oil cooling liquid chilled to -20°C.
Figure 3.21: Picture of the Original configuration of the SAO EBIT (photo from Dr. Eric Silver).
In 2015, the SAO EBIT experienced a leak in the collector cooling lines that coated interior vacuum components with a silicone oil. The cooling lines inside the vacuum were attached to the collector by a metal braze, which was the source of the leak (see Fig. 3.23). Later that year the EBIT was disassembled and the components were cleaned with an aggressive cleaning agent (Hexane). Starting in 2016, I worked with a team led by Dr. Eric Silver to systematically reassemble and test the EBIT. During this process we have encountered a number of issues that have required the re-design and creation of a number of components. These issues and solutions are summarized below.

After failed attempts to repair (re-braze) the collector cooling line connections, a new collector was designed. Fig. 3.24 shows the tip of the collector where the cooling lines connect. This shows that the previous collector design used flexible bent threaded rods with nylon washers to isolate the collector from the suppressor support. This design allows the tip of the collector to easily move, which could lead to potential alignment issues, especially
when placed in a horizontal orientation. To avoid this, a new insulator support bracket consisting of a solid insulating material with heli-coil inserts was created. The new collector design also includes the addition of a suppressor electrode (missing from the original design), suppressor insulator rings, and new TIG welded (instead of brazed) cooling line connections (see Fig. 3.24).

Since the oil leak was so devastating to the EBIT system, a new coolant was selected. The fluid had to fulfill the following requirements: 1.) must have a high resistivity so it can go from ground potential up to 20 kV, 2.) it should remove 1 W to 300 W of heat from the copper electrode, 3.) it must not freeze at low temperatures, 4.) it should not corrode the copper collector electrode, and 5.) it must not leave a residue in the case of a leak. Based on this criteria, a Fluorinert FC-770 fluid and a Thermo Scientific, Merlin M75 chiller was selected. Fluorinert has a pour point of -127 °C, thermal conductivity of 0.063 W m⁻¹ °C⁻¹, an electrical resistivity of >3 x 10¹⁴ ohm cm, and it evaporates in air without leaving a residue.

After assembling and cleaning the new collector assembly, the EBIT was reassembled and vacuum tested piece by piece to ensure each component was not contaminated and leak free. Since it can take weeks to fully pump (degassing components) and cool down the EBIT, this process was extremely time consuming and often required repeated pump downs as a result of failed leak checks followed by numerous replacements of copper gaskets. Optical alignment of the components also proved to be difficult as the EBIT’s horizontal configuration requires the magnet/drift tube assembly to sit on top of the cryocooler cold head, limiting the available range of motion. To add to this difficulty, the cold head contracts when cooled; therefore alignment at room temperature had to take into account the contraction of components at cryogenic temperatures. After making minor alterations of the thermal shield’s middle plate to allow for additional rotation of the magnet, the drift tubes were successfully aligned to the center of the vacuum chamber. Finally, with the system completely reassembled and aligned, we were able to achieve a vacuum level on the order of 10⁻¹⁰ Torr and a SCM temperature below 4 K.
Vacuum chamber with new end flanges.

Collector assembly

Braze (source of leak)

Disassembled EBIT Components

Figure 3.23: Pictures of disassembled EBIT.
Next the electron gun was activated by grounding the focus electrode and slowly ramping the filament voltage to about 6.3 V and the anode to about 2 mA. From our test, we were able to verify that the electron gun is still operational after the contamination event and able to produce a current.

The SCM is capable of producing a 3T magnetic field at a current of 62.5 A (coil constant = 409 Gauss/A), and the Nb-Ti coils have a critical temperature of around 10 K. During the first magnet test, the SCM temperature read 3.5 K and the current was slowly ramped at a rate of 0.01 A/s. The magnet quenched at around 3.0 A. To understand the thermal environment of the magnet, Fig. 3.25 (left) shows a picture looking into the EBIT from the collector end of the device (collector removed). Magnet wires run from the power supply to the vacuum chamber where there are thick copper feed-throughs that connect to thinner, bent copper rods inside of the vacuum (shown on right side of photo). These copper rods are attached to larger copper blocks (in center of photo) that attach to the thermal shield (gold colored) to help produce a smooth thermal gradient from the 4 K magnet to the room temperature feed-through. The copper rod has a high current running through
Figure 3.25: left.) Original SCM magnet connections inside of EBIT. right.) Updated copper block design and replaced polyimide sheet with higher thermal conductivity.
Figure 3.26: Pictures of showing magnet thermal environment. Top.) Picture of EBIT cryocooler outside of EBIT. Bottom.) left, shows the magnet assembly; right, shows where the magnet makes contact with the cold head; bottom right shows the cryocooler cold head inside of the EBIT chamber.
Figure 3.27: Left.) Old cold head adaptor that contact magnet. Right.) New adaptor.

it, so the copper blocks are electrically isolated from the thermal shield with a Kapton sheet. The copper blocks then connect to a copper braid leading to the high temperature superconducting leads (green rods on the left). Fig. 3.26 shows the magnet assembly, and how it connections to the cryocooler. The cold head of the cryocooler has a small copper adapter that sits on top with a tapped hole that allows the magnet to be connected with a screw.

To test if the magnet quenched due to a heat load from the collector (not actively cooled at the time), the collector was removed and the magnet was tested again. Still it quenched around 3.8 A. Next the Kapton sheet, separating the copper blocks from the thermal shield, was replace with Kapton MT$^+$ (still a polyimide film, but with a thermal conductivity of 0.8 W/mK vs. 0.12 W/mK of the original film). In addition to these changes, the copper blocks were modified. As shown in Fig. 3.25 (left picture) the copper braid makes minimal contact with the copper blocks. A new copper block was designed to increase the area of contact, shown in the right of the figure. With these improvements, the magnet current reached 8 A before quenching. Next the Kapton film on the magnet
was also replaced with Kapton Mt⁺, and all of the magnet contacts were tightened (may have loosened during alignment). With these improvements the magnet reached the normal operating current of 30 A. With the current at normal operating conditions, the collector (cooled to -20°C) was reinstalled and the magnet was tested again. This time it quenched at 24 A.

To test the remaining electronics and alignment, we re-conditioned the electron gun and ramped the magnet to 15A. The electrodes and magnets (bucking coil, collector coil) were turned on and adjusted until the current on the anode was minimized and a current was seen on the collector (an indication that electrons are making it through the entire EBIT). We were successfully able to see about 2 mA of current on the collector, verifying that the EBIT is operational.

While we were able to operate the EBIT at low magnetic fields and currents, there
were still obviously thermal issues causing the magnet to quench below the standard operating current. Fig. 3.26 (bottom) shows that the area of contact between the magnet and the cold head adaptor is very small (basically a thin ring). To improve this, a new cold head adaptor was designed to increase the area of contact. This new design, shown in Fig. 3.27 (right), increases the contact with the magnet by extending out further longitudinally and by fitting into the recessed hole in the magnet (see Fig. 3.26). The contact in this hole will be further improved by adding a thin gold foil to ensure contact between the adaptor and the magnet body.

Since the heat load from the collector also seemed to be affecting the SCM, an additional thermal barrier was designed. This design included a thin cup that attaches to the gold thermal shield and shields the majority of the 4 K section (magnet/drift tubes) from the warmer collector to reduce the radiative heating. Installing these new components required disassembling the entire EBIT again. The new components have been installed and the system was pumped down again. The new magnet tests are currently under way and upon completion the full EBIT operation will be tested. At this stage a solid-state x-ray detector will be installed to look for signal from trapped highly charged ions. The plan is to have a fully operational and tested EBIT device available for laboratory astrophysics studies at SAO within the next year.
Chapter 4

Linear Polarization of Emission from Highly Charged Ar Ions

4.1 Introduction

Since astrophysical plasmas exist at large distances from Earth it is not feasible to locally probe these sources for information about their environmental conditions. Physical properties such as density, elemental abundance, and temperature are commonly extracted using spectral analysis. The interplay between the collisional excitation of ions that depend on the plasma conditions and their de-excitation processes affect the line intensities of spectral lines and, therefore, can be used for diagnosis. As a particular example, the relative strength of lines in the He-α series (the resonance $1s^2 1S - 1s2p \,^1P$ (w), intercombination $1s^2 1S - 1s2p \,^3P$ (x,y), and forbidden $1s^2 1S - 1s2s \,^3S$ (z) lines) are commonly used to determine the temperature and densities of plasmas (e.g. [46, 114]). Dielectronic Recombination (DR) satellite lines are another good example for probing physical properties of plasmas. Since DR occurs at electron energies below the direct excitation threshold of the parent line (as explained in DR theory section), the ratio of unblended satellite lines to strong DE lines samples different regions of the electron energy distribution and is a good diagnostic of plasma temperature (see e.g. [10, 101, 19, 45, 19]).
Spectral observations need to be compared with theoretical models to determine physical properties of plasmas. The analysis of spectra often requires reliable knowledge of the ionization balance, which can only be achieved by including reliable atomic data in the models [100]. This has been demonstrated in studies such as by Savin and Laming [102], where uncertainties in DR rate coefficients led to inferred relative abundances in the solar upper atmosphere that were off by a factor of 2-5 from those inferred using more accurate data. The need for high quality DR data has led to increasingly accurate calculations (e.g. [24, 5]) and to a number of electron beam ion trap (EBIT) and storage ring experiments (see e.g. [100, 126, 13, 1]). The ongoing effort to produce accurate DR data and test of theory will continue as experimental and theoretical methods become increasingly sophisticated and as high-resolution X-ray satellites, such as the X-ray Imaging and Spectroscopy Mission (XRISM), demand more from astrophysical models such as the CHIANTI package [35] and the astrophysical plasma emission code (APEC) [117].

EBITs, commonly used in laboratory astrophysics investigations (see e.g. [52, 23, 107]), are well suited for systematic atomic studies due to the variety of accessible elements and its tunable quasi mono-energetic electron beam that allows for a degree of charge state and excitation selectivity. These devices are used to produce atomic data such as measured wavelengths [29, 78], atomic lifetimes [105], emission cross sections following charge exchange [121, 88], cross sections from electron impact excitation (EIE) [30] and ionization [128], and DR cross sections [83, 74]. EBITs may also be used in tandem with collisional-radiative models for line identification studies [95, 94, 115].

Because the emission produced in an EBIT originates from ions excited by a unidirectional electron beam, the emitted radiation can be anisotropic and polarized [89]. Since the angle of observation and the degree of polarization may alter the observed line intensities [119, 14], it is crucial to take these effects into account when analyzing spectral features. The linear polarization produced in anisotropic sources such as EBITs, and natural sources such as solar flares where beams of electrons travel along magnetic field lines, originates from non-statistically populated magnetic sublevels, where the sublevels are pop-
ulated from processes such as electron impact excitation (EIE) or recombination (radiative or dielectronic). Therefore, to understand the emitted line intensity ratios, sublevel specific differential analysis may be required.

The controlled and relatively simple plasma environment created by EBITs (compared with astrophysical environments) is ideal for polarization studies needed to benchmark various theoretical approaches used to calculate differential cross sections. This has lead to a number of EBIT investigations of linear polarization following EIE. These include studies of: He-like Sc [58], He-like and Li-like Fe [14, 11], Ne-like Ba [119], He-like Ti [9], H-like Ti [85], He-like Mg [17], Ne-like and F-like Fe [31], He and Li-like S [99], H-like Ti [85], He-like Mg [17], Ne-like and F-like Fe [31], He and Li-like S [99], H-like Fe and Ar [98], and Ni-like W [32]. However, EBIT polarization measurements focused on DR transitions only include studies of highly charged Xe [70], Kr [108], and Fe [106].

As argon is an important element often found in astrophysical plasmas, we carried out the first measurements of linear polarization of the $1s2p^2(^1D)^2D_{5/2} \rightarrow 1s^22p_{3/2}^2P_{3/2}^0$ (j), in the notation of [45]), $1s2p^2(^1D)^2D_{3/2} \rightarrow 1s^22p_{1/2}^2P_{1/2}^0$ (k), $1s2p^2(^3P)^2P_{3/2} \rightarrow 1s^22p_{3/2}^2P_{3/2}^0$ (a), $1s2s2p(^3P)^2P_{1/2}^0 \rightarrow 1s^22s^2S_{1/2}^0$ (r), $1s2s2p(^3P)^2P_{3/2}^0 \rightarrow 1s^22s^2S_{1/2}^0$ (q), and the blended $1s2s2p(^1P)^2P_{1/2}^0 \rightarrow 1s^22s^2S_{1/2}^0$ and $1s2s2p(^1P)^2P_{3/2}^0 \rightarrow 1s^22s^2S_{1/2}^0$ (t/s) lines of Li-like Ar, that are satellite transitions of the w, x, y and z lines originating from He-like Ar. Our measurements are intended to improve the quality of atomic data that will be produced from anisotropic laboratory plasmas, and also to benchmark theories used to interpret spectra from anisotropic astrophysical plasma sources.

In the sections that follow, a physical description of the polarization of electromagnetic waves is first formed. This is followed by a discussion of how polarization and anisotropic emission may affect measurements of atomic line spectra and how we may adjust theoretical calculations (which may not take these effects into account). We then give a brief overview of a few techniques used to measure polarization and provide a description of the experimental setup used for our work. A detailed description of our analysis and results are then presented. Finally a brief theoretical description is given, followed by a comparison of our experimental and theoretical results.
4.2 Developing a Description for Polarized Emission from EBIT Plasmas

The light emitted from an atomic electron transition can be considered as a transverse (electromagnetic) wave traveling through space (or through the ultra-high vacuum environment of the EBIT). The transverse nature requires that the direction of a.) propagation, b.) the electric field vector \( \mathbf{E} \), and c.) the magnetic field vector \( \mathbf{B} \) are all perpendicular to each other as shown in Fig. 4.1.

The polarization of a transverse electromagnetic wave (EM) is a property that describes the geometrical orientation of the field oscillations. More specifically, polarization is traditionally defined as the direction of the \( \mathbf{E} \). If the electric field is broken up into two plane wave components (ex. x and y components, as shown in Fig. 4.2), and if the two component waves are in phase, \( \mathbf{E} \) oscillates in a fixed plane (see Fig.4.2). In this case, the wave is said to be linearly polarized. If the two components are not in phase, then \( \mathbf{E} \) will form a helix as the wave propagates, and will trace out an ellipse in the x/y plane. This is referred to as elliptically polarized light. In the special case where the two component magnitudes are equal and the phase difference is 90 degrees, the electric field vector traces out a circle in the x/y plane and is said to be circularly polarized (see Fig.4.3). (See text such as [84] for a complete description).
Figure 4.2: Depiction of linear Polarization. Electric field plane wave components Ex and Ey shown along with $\mathbf{E}$. Due to the phase matching of the component waves, $\mathbf{E}$ oscillates in only one direction. Right panels shows $\mathbf{E}$ as the wave propagates. Image source: http://kestrel.nmt.edu/ mce/Polarization
Figure 4.3: Depiction of circular Polarization. Electric field plane wave components Ex and Ey (90 degrees out of phase) shown along with $\mathbf{E}$ (arrow). $\mathbf{E}$ traces out a circle in the x/y plane as the wave propagates. Image source: http://kestrel.nmt.edu/ mce/Polarization
4.2.1 Emission Measured at 90°

The polarization, magnetic quantum number M, and direction of observation are all defined with respect to a quantization axis. Defining the z-axis as our quantization axis (in EBIT experiments commonly chosen as the direction of the electron beam) our measurements were taken at 90° with respect to this direction. Since the propagation direction of the emitted electromagnetic waves is always perpendicular to $E$, photons moving in the direction of our detector (let us say the x direction) can only have their electric field components $E$ in the $(z,y)$ plane of this coordinate system. Based on this concept, the total observed intensity can be decomposed into $I_{\parallel}$ and $I_{\perp}$ components as measured photon intensities with their respective electric field vectors parallel and perpendicular to the z-axis, namely the electron beam direction (see Fig. 4.4).

The intensity measured at 90°, is then:

$$I(90°) = I_{\parallel} + I_{\perp} \quad (4.1)$$

In general terms, the formula describing the angular dependence of the intensity of dipole radiation propagating in all directions was given in [89] as:

$$I(\theta) = \langle I \rangle \frac{3(1 - P \cos^2(\theta))}{3 - P} \quad (4.2)$$

where $\langle I \rangle$ is the 4$\pi$ average intensity, $\theta$ is the angle between the quantization axis (direction of the electron beam in our case) and the direction of propagation of the emitted photon, and the degree of linear polarization ($P$) is defined as:

$$P = \frac{I_{\parallel} - I_{\perp}}{I_{\parallel} + I_{\perp}} \quad (4.3)$$

Combining Eqns. 4.2 and 4.3 and plugging in 90° for the angle of observation, we find the relationship between the 4$\pi$ average intensity and the intensity observed at 90° as:
Figure 4.4: a.) Depiction of a wave traveling in the x direction and polarized parallel to the z-direction ($I_\perp$). b.) Depiction of wave traveling in the x direction and polarized perpendicular to z-direction ($I_\parallel$).
\[ I(90^\circ) = \langle I \rangle \frac{3}{3-P} \] (4.4)

The factor \( \left( \frac{3}{3-P} \right) \) that we can obtain this way has been used in previous studies such as [52] to correct theoretical predictions, that do not account for polarization and angle of observation, for accurate comparison with experimental EBIT measurements. Alternatively, Eqn. 4.2 also shows that if measurements could be taken at the so-called “magic angle” of 55°, then the measured intensity would be equal to the 4\( \pi \) average intensity.

By combining Eqns. 4.1, 4.3, and 4.4, the 4\( \pi \) average intensity and polarization values may be used to find the two polarization components:

\[ I_\perp = \frac{3}{2} \langle I \rangle \frac{(1-P)}{(3-P)} \] (4.5)

\[ I_\parallel = \frac{3}{2} \langle I \rangle \frac{(1+P)}{(3-P)} \] (4.6)

As we will see in later sections, the polarization components are required when comparing theoretical calculations with measurements taken with a polarization sensitive device, such as a crystal spectrometer.

Furthermore, following the procedure of Shlyaptseva [110], \( \langle I \rangle \) can be written in terms of the intensity factor \( Q_d \) [124], the electron energy distribution function \( f(E) \), and the autoionization energy \( E_{AI} \), and 4.5 and 4.6 becomes

\[ I_\perp = \frac{3}{2} Q_d e^{\exp \left[ -\left( \frac{E_b - E_{AI}}{\Delta E} \right)^2 \right] \frac{(1-P)}{(3-P)}} \] (4.7)

\[ I_\parallel = \frac{3}{2} Q_d e^{\exp \left[ -\left( \frac{E_b - E_{AI}}{\Delta E} \right)^2 \right] \frac{(1+P)}{(3-P)}} \] (4.8)

where, as discussed later, the electron energy distribution can be characterized by a Gaussian function with a central electron beam energy \( E_b \) and \( \Delta E \) (proportional to the FWHM, in
this experiment around 40 eV).

In our case the theoretical polarization (P) values used in the Eqns. 4.7 and 4.8, were calculated using the photon density matrix formalism (see e.g. [69, 21, 110, 6, 109]). The density matrix ($\rho$) describes the excited atomic ensemble and is a useful formalism to determine the angular distribution of the polarization of light emitted from excited atomic sublevels [68]. For an axially symmetric system (and choosing the quantization axis as the axis of the electron beam) the density matrix is diagonal with the diagonal elements proportional to the cross section for excitation of the magnetic sublevel M ($\sigma(M)$) [68]:

$$\langle JM | \rho | JM \rangle = \sigma(M) \quad (4.9)$$

In Eqn. 4.9, J and M represent the total angular momentum and magnetic quantum numbers respectively. Works by Inal & Dubau [68] and Blum [21], provide extensive details in deriving the polarization from the density matrix. For the cylindrically symmetric system, such as with the EBIT, their analysis shows that excited atomic ensembles only produce linearly polarized light (i.e. no circular polarization), which can be expressed as:

$$P(\theta) = \frac{W_\parallel(\theta) - W_\perp(\theta)}{W_\parallel(\theta) + W_\perp(\theta)} \quad (4.10)$$

where $W_\parallel(\theta)$ and $W_\perp(\theta)$ are the intensity distribution functions for light linearly polarized parallel and perpendicular to the quantization axis. They can be expressed as (see [14]):

$$W_\parallel(\theta) = \sum_{k=even} A_{kq} G^k \left[ P_k(cos(\theta)) + \Lambda(\kappa) f_k P_k^2(cos(\theta)) \right] \quad (4.11)$$

and

$$W_\perp(\theta) = \sum_{k=even} A_{kq} G^k \left[ P_k(cos(\theta)) - \Lambda(\kappa) f_k P_k^2(cos(\theta)) \right] \quad (4.12)$$

where again $\theta$ is the angle between the direction of the electron beam and the direction of propagation of the emitted photon ($\theta = 90^\circ$ in our case), $P_k$ and $P_k^2$ are the Legendre and associated Legendre polynomials, $A_{kq}$ is the alignment parameter, $G^k$ is the
structure function, and $f_k$ is a coefficient. $\Lambda(\kappa)=1$ for electric and -1 for magnetic multipole transitions.

The alignment parameter $A_{kq}$ in this formalism plays a central role in determining the anisotropy of the system and is given by:

$$A_{kq} = \rho_{kq}(\alpha_{id}J_{id})$$  \hspace{1cm} (4.13)

Here $\rho_{kq}$ is the statistical tensor with rank $k$ and component $q$ [109]. Its components can generally range from $-k \leq q \leq k$ and include magnetic sublevel specific cross-sections of populating atomic levels. Due to the symmetry of the system, according to Blum only even rank $k$ values with $q=0$ survive [21] and the alignment parameter takes the form of:

$$A_{k0} = \sqrt{2J_{id} + 1}\sqrt{2k + 1}\sigma(\alpha_{id}J_{id}M_{id})\Sigma_{M_{id}}(-1)^{J_{id}-M_{id}}\begin{pmatrix} J_{id} & J_{id} & k \\ M_{id} & -M_{id} & 0 \end{pmatrix}$$  \hspace{1cm} (4.14)

$J$, $M$, and $\alpha$ again denote the total angular momentum, its corresponding magnetic component, and all other quantum numbers required to describe the state, respectively, $\begin{pmatrix} J_{id} & J_{id} & k \\ M_{id} & -M_{id} & 0 \end{pmatrix}$ is the Wigner 3-J symbol [34] (proportional to Clebsch-Gordon coefficients), and $\sigma(\alpha_{id}J_{id}M_{id})$ is the cross section of populating the sub-state with magnetic quantum number $M$, via e.g. the dielectronic capture or the electron impact excitation process. For the dielectronic recombination process specifically, the initial state of the ion (prior to $e^-$ capture), the intermediate doubly excited state, and the final state (after photon emission) are characterized by subscripts $i$, $id$, and $f$, respectively. For the direct excitation process, $id$ represents the initial excited state, and $f$ is the final state after radiative stabilization.

The structure function $G^k$, which describes the angular momentum coupling between
the intermediate doubly excited and the final states is expressed as:

\[
G^k(\alpha_{id}J_{id}, \alpha_fJ_f) = (-1)^{1+J_{id}+J_f} \begin{pmatrix} L & L & k \\ 1 & -1 & 0 \end{pmatrix} \begin{pmatrix} L & L & k \\ J_{id} & J_{id} & J_f \end{pmatrix} \frac{(2L+1)\sqrt{(2k+1)(2J_{id}+1)}}{(2J_{id}+1)}
\]

where the quantity in curly brackets denotes the Wigner 6j-symbol \([34]\), and \(L\) denotes the order of the multipole operator (for E1 and M1 transitions, \(L=1\) and for M2 transitions \(L=2\)). The coefficient \(f_k\) is:

\[
f_k = -\frac{(k-1)!}{(k+2)!} \begin{pmatrix} L & L & k \\ 1 & 1 & -2 \end{pmatrix}
\]

(4.16)

From the properties of the Wigner 3-J symbol in Eqns. 4.14 and 4.15, the values of \(k\) are restricted [34]. Specifically, if \(k > 2J_{id}\), \(A_{k0}=0\) and if \(k > 2L\), \(G^k=0\) [68]. Most of the DR transitions of interest (see Table 4.1) have \(2J_{id} < 4\), so only \(A_{00}\) and \(A_{20}\) terms are present. The \(j\) line which has a \(2J_{id}=5\), is an electric dipole transition; therefore \(L=1\) and terms higher than \(G^2\) are zero. This means that only \(G^0(\alpha_{id}J_{id}, \alpha_fJ_f)\), \(G^2(\alpha_{id}J_{id}, \alpha_fJ_f)\), \(A_{00}\) and \(A_{20}\) terms will contribute to the calculation of the polarization for the DR transitions listed in Table 4.1.

The monopole term \((A_{00})\) is a constant related to the total dielectronic capture (or EIE) cross section \((\sigma(\alpha_{id}J_{id}))\):

\[
A_{00} = \frac{\sigma(\alpha_{id}J_{id})}{\sqrt{2J_{id}+1}}
\]

(4.17)

where \(\sigma(\alpha_{id}J_{id}) = \sum_M \sigma(\alpha_{id}J_{id}M_{id})\). Combining Eqn. 4.14 and 4.17, the \(A_{20} \)
(normalized to $A_{00}$) alignment parameter can be written as:

$$A_{20} = \frac{\sqrt{2J_{id} + 1}}{\sigma(\alpha_{id}J_{id})} \sum_{M_{id}} (-1)^{J_{id} - M_{id}} \langle J_{id}M_{id}J_{id} - M_{id}|20\rangle \sigma(\alpha_{id}J_{id}M_{id}) \sigma(\alpha_{id}J_{id}M_{id}) (4.18)$$

where $\langle J_{id}M_{id}J_{id} - M_{id}|20\rangle$ represents the Clebsch-Gordan coefficient. The structure function $G^0 = 1$ and $G^2$ is given as:

$$G^2(\alpha_{id}J_{id}, \alpha_fJ_f) = (-1)^{(1+J_{id}+J_f)} \begin{pmatrix} 1 & 1 & 2 \\ J_{id} & J_{id} & J_f \end{pmatrix} \sqrt{\frac{3(2J_{id} + 1)}{2}} (4.19)$$

The remaining 00 and 20 terms describing electric dipole transitions observed at 90° are calculated to be: $f_0 = 0$, $f_2 = -1/2$, $P_0(0) = -1/2$, $P_0(0) = 1$, $P_0^2(0) = 0$, $P_2^2(0) = 3$, and using the normalized alignment parameter, $A_{00}G^0(\alpha_{id}J_{id}, \alpha_fJ_f) = 1$. Inserting these into 4.11 and 4.12, the intensity distribution functions for electric dipole transitions are:

$$W_{\parallel}(90°) = 1 - 2G^2(\alpha_{id}J_{id}, \alpha_fJ_f)A_{20} (4.20)$$

and

$$W_{\perp}(90°) = 1 + G^2(\alpha_{id}J_{id}, \alpha_fJ_f)A_{20} (4.21)$$

Plugging these expressions into Eqn. 4.10, the linear polarization of E1 transitions observed at 90° is:

$$P = \frac{W_{\parallel}(90°) - W_{\perp}(90°)}{W_{\parallel}(90°) + W_{\perp}(90°)} = -\frac{3G^2(\alpha_{id}J_{id}, \alpha_fJ_f)A_{20}}{2 - G^2(\alpha_{id}J_{id}, \alpha_fJ_f)A_{20}} (4.22)$$

Eqns. 4.20 - 4.22, highlight the special case of $J_{id} = 1/2$. In this case, from earlier arguments, $k > 1$ makes $A_{k0} = 0$, so there are no $k=2$ terms, and as shown previously the $k=0$ terms are equal to one. In this case $W_{\parallel}(90°) = 1 = W_{\perp}(90°)$ and $P=0$. Based on this the previously mentioned $r$, $t$, $m$, and $n$ Li-like satellite lines (see Table 4.1) are expected to be isotropic and unpolarized.

For the He-like lines $w$ and $x$, both with $J_i = 1$ and $J_f = 0$, the alignment parameter
and structure function \((A_{20}, \text{and} G^2)\) are:

\[
A_{20} = \frac{1}{\sqrt{2\sigma(\alpha_{id}J_{id})}} \left[ \sigma(-1) - 2\sigma(0) + \sigma(1) \right]
\]

(4.23)

and

\[
G^2(\alpha_{id}J_{id}, \alpha_fJ_f) = \frac{1}{\sqrt{2}}
\]

(4.24)

giving a polarization of:

\[
P(90^\circ) = \frac{-3\sigma(-1) - 2\sigma(0) + \sigma(1)}{2\sigma(-1) + 2\sigma(0) + \sigma(1)}
\]

(4.25)

This expression can finally be simplified to:

\[
P(90^\circ) = \frac{-\sigma(-1) - 2\sigma(0) + \sigma(1)}{\sigma(-1) + 2\sigma(0) + \sigma(1)}
\]

(4.26)

The same procedure can be followed for the other DR transitions. For example, the \(k, q,\) and \(s\) lines have \(J_{id}=3/2\) and \(J_f=1/2,\) producing \(A_{20}\) and \(G^2\) values of:

\[
A_{20} = \frac{1}{\sigma(\alpha_{id}J_{id})} \left[ \sigma(3/2) - \sigma(1/2) - \sigma(-1/2) + \sigma(-3/2) \right]
\]

(4.27)

and

\[
G^2(\alpha_{id}J_{id}, \alpha_fJ_f) = \frac{1}{2}
\]

(4.28)

This leads to a polarization of:

\[
P(90^\circ) = \frac{-3\sigma(3/2) - \sigma(1/2) - \sigma(-1/2) + \sigma(-3/2)}{3\sigma(3/2) + 5\sigma(1/2) + 5\sigma(-1/2) + 3\sigma(-3/2)}
\]

(4.29)

The \(z\) line is an M1 transition, so all terms are the same as in the cases above except \(\Lambda(\kappa) = -1.\) The \(x\) line \((1s^2 \, 1S_0 - 1s2p \, ^3P_2)\) is an M2 magnetic quadrupole transition and has \(2J_{id} = 4\) so \(k\) can be 0, 2 and 4, \(\Lambda(\kappa) = -1,\) and \(L = 2.\) Although the \(x\) line has
contributions from \( k = 4 \) term, Vogel showed [125] that the \( k = 4 \) term is much smaller than the \( k = 2 \) term; therefore the \( x \) line follows the same angular dependence as \( E1 \) transitions.

The theoretical description of polarization formulated so far, shows that polarization depends on the sub-level specific cross-sections of the excited ion. In this description, only one process has been considered to directly populate the upper level of the transition in question (i.e \( E1 \) or \( DR \) capture). This assumption is valid when the electron beam energy is tuned such that excitation above the transition threshold (or \( DR \) capture to a higher lying state) cannot occur. However, in the case when the upper level is also populated through cascades, the alignment parameter has to be modified to include alignment information from the contributing states. The effects can be taken into account by multiplying the alignment parameter of the higher energy states by their coupling coefficients also named the de-orientation factor (described e.g. in [14]):

\[
A_{k0}(J_{f'}) = \sum_{i'} A_{k0}(J_{i'}) U_{k}(J_{i'}, J_{f'}, L) f_{i'}
\]  

(4.30)

where subscripts \( i' \) and \( f' \) represent the initial and final state of the cascade transition, respectively, \( f_{i'} \) represents the fraction of the population received from \( i' \), \( A_{k0}(J_{i'}) \) is the alignment parameter of the initial state \( i' \), and \( U_{k}(J_{i'}, J_{f'}, L) \) is the de-orientation factor, given in [14] as:

\[
U_{k}(J_{i'}, J_{f'}, L) = (-1)^{J_{i'}J_{f'}+k+L} \sqrt{(2J_{i'}+1)(2J_{f'}+1)} \begin{pmatrix} J_{i'} & J_{f'} & k \\ J_{f'} & J_{f'} & L \end{pmatrix}
\]  

(4.31)

Applying these factors, for example the modified alignment parameter of the \( \text{He-like level} \ 1s2s \ ^3S_1 \) (which is the upper level of the \( z \) transition that has zero polarization when populated directly by \( E1 \) from the ground state) can be non-zero and, can be expressed
as:

\[ A_{20}(^3S_1) = \frac{\sum_{i'} A_{20}(J_{i'}) U_2(J_{i'}, J_{i'}, 1) \beta_{i'} \sigma_{i'}}{\sum_{i'} \sigma_{i'}} \]  

(4.32)

Here \( \beta_{i'} \) is the branching ratio, and \( \sigma_{i'} \) are the excitation cross sections of the respective levels \( i' \).

### 4.3 Methods of Measuring Linear Polarization

The intensity emitted from the EBIT plasma at 90° relative to the electron beam (quantization) axis was given by Eqn. 4.1. This generally represents the total intensity measured, however when detectors such as crystal spectrometers are used to disperse the emitted x-rays, the polarization sensitivity of the device must be considered in the analysis. Crystal spectrometers generally reflect the parallel and perpendicular polarization intensity components unequally, and the expression for the measured intensity is:

\[ I_{observed} = R_{\parallel} I_{\parallel} + R_{\perp} I_{\perp} \]  

(4.33)

where \( I_{observed} \) is the measured intensity, and \( R_{\parallel} \) and \( R_{\perp} \) are the integrated crystal reflectivities for x-rays polarized parallel and perpendicular to the plane of dispersion of the crystal respectively. As described below, the polarization sensitivity can be exploited in a number of ways such that the components \( I_{\parallel} \) and \( I_{\perp} \) can be determined from measured intensities. The measured polarization then follows from 4.3.

It is important to note that the reference frames being used to describe \( I_{\parallel, \perp} \) and \( R_{\parallel, \perp} \) are different. The intensities \( (I_{\parallel, \perp}) \) are defined with respect to the stationary quantization \( (z\text{-axis}) \), whereas the reflectivities \( (R_{\parallel, \perp}) \) are defined relative to the plane of incidence/dispersion of the crystal (see Fig. 4.5), which may be rotated as the Bragg-angle of the crystal is set for a certain wavelength transition. Typically in EBIT polarization experiments, the plane of dispersion of the crystal is oriented either parallel or perpendicular.
The light is linearly polarized perpendicular to the plane of incidence; therefore, $R_\perp$ describes the reflectivity of the light in this case.

The light is linearly polarized parallel to the plane of incidence; therefore, $R_\parallel$ describes the reflectivity of the light in this case.

Figure 4.5: a.) Showing a wave polarized perpendicular to the plane of dispersion. b.) Showing a wave polarized parallel to the plane of dispersion.
ular to the electron beam (see Fig. 4.6). This means that 1. the effective source size is different for the two orientations (discussed later) and 2. the relationship between the \( R \) and \( I \) will be different for the two orientations. While \( I_{\parallel} \) represents intensities with electric field vectors parallel to the electron beam direction, its polarization will be parallel to the plane of dispersion when the spectrometer is in the “vertical orientation”, but perpendicular to the plane of dispersion when the spectrometer is in the “horizontal orientation”. (This notation assumes a vertically oriented electron beam, such as the one of the NIST EBIT.) Given these geometrical definitions, the equations for the intensities observed with a horizontally and vertically oriented crystal are:

\[
I_{\text{vertical}} = RI_{\parallel} + I_{\perp}
\]

\[
I_{\text{horizontal}} = I_{\parallel} + RI_{\perp}
\]

(4.34) (4.35)

where \( R = \frac{R_{\parallel}}{R_{\perp}} \) and \( R_{\text{max}} = 1 \). These equations show that both spectrometers preferentially reflect x-rays polarized perpendicular to the dispersion plane. However, due to the different orientations, the vertical spectrometer preferentially reflect x-rays polarized perpendicular to the the electron beam, while horizontal spectrometer preferentially reflects x-rays polarized parallel to the electron beam direction.

Reflectivity values can be found in sources such as [59] or they may be calculated using X-ray Oriented Program (XOP) software where they are typically defined using the traditional \( R_s \) (s from the German word senkrecht, meaning perpendicular) and \( R_p \) (p for parallel, which is the same in German) to the plane of incidence notation. Note on notation: \( R_s = R_{\sigma} = R_{\perp} \) and \( R_p = R_{\pi} = R_{\parallel} \). Values for \( R \) may also be roughly estimated by \( R = |\cos^m(2\theta)| \), where \( 1 \leq m \leq 2 \), and \( \theta \) is the Bragg angle. The limits of \( m \) correspond to perfect (\( m=1 \)) and mosaic (\( m=2 \)) crystals. From this equation, we see that if the Bragg angle is close to 45°, \( R \) is zero and the crystals act as perfect polarizers.

For the Si(111) crystal used in our experiment, XOP was used to calculate the
Figure 4.6: top.) Orientation of the crystal’s plane of dispersion relative to the electron beam in the horizontal orientation. bottom.) Orientation of the crystal’s plane of dispersion relative to the electron beam in the vertical orientation.
diffraction line profile (rocking curve) (Fig. 4.7) for a number of photon energies of interest. The s and p curves in Fig. 4.7 show the intensity of diffracted light as a function of $(\Theta - \Theta_{Bc})$ (microradians), where $\Theta$ is the incident angle of a monochromatic x-ray photon (3318 eV in the example used in Fig. 4.7), and $\Theta_{Bc}$ is the nominal Bragg angle for the given wavelength. The curves are asymmetric due to the bending of the crystal in Johann-type crystal spectrometers, because the atomic planes are no longer parallel to each other. The widths of the curves depend on the atomic structure of the crystal, the wavelength of the incident light, and obviously the polarization [4]. This shows that when the radiation is polarized parallel to the dispersion plane, the scattering amplitude is reduced, and the wave penetrates deeper into the crystal [2]. As expected the intensity is highest near the nominal Bragg angle. A further description of crystal spectrometers can be found in the spectrometer instrumentation section of this work.
To obtain the reflectivity value for a particular photon energy, we integrate over the diffraction line profile. This gives the value for $R_s$, $R_p$ ($R_{\perp}$, $R_{\parallel}$), from which we can find $R = \frac{R_p}{R_s} = \frac{R_{\parallel}}{R_{\perp}}$. Our calculated R values for Si(111) are shown in Fig. 4.8 as a function of energy (related to the Bragg angle through Bragg’s law, $2dsin(\theta) = n\lambda$) along with values from [59]. Figure 4.8 shows that while our calculations agree with [59], we have produced a number of additional data points. Typically line energies fall between data points given by [59], so R values used in the past were found by fitting a line to the two nearest calculated data points. Therefore, the additional data points that we have calculated (most of which are near our measured lines), increases the accuracy of the R values used for each line. Figure 4.8 also shows that certain energies have an R value close to 0. As previously mentioned, this corresponds to a Bragg angle close to 45°, and in this case the crystal acts as a perfect polarizer reflecting only one polarization component depending on the orientation of the dispersion plane (expressed in Eqns. 4.36 and 4.37). This simplifying feature was exploited in a number of measurements including [58, 14, 119].

$$I_{\text{horizontal}} = I_{\parallel} \quad (4.36)$$

$$I_{\text{vertical}} = I_{\perp} \quad (4.37)$$

There are a few techniques used to measure polarization. From Eqn. 4.3 it is obvious that if the polarization components ($I_{\parallel}$ and $I_{\perp}$) can be measured, then P is easily calculated. The case of a 45° Bragg angle hints at a way to measure these components. In the next sections, we demonstrate how the single and double crystal techniques are used to measure the linear polarization of emission produced in an EBIT.

### 4.3.1 The One Detector Method

Following the notation of [19], we may express the measured intensities from the crystal spectrometers in terms of factors $\Omega$ (representing the geometry with solid angle of
Figure 4.8: Calculated reflectivity as a function of energy (Bragg angle) for a Si(111) crystal.

acceptance) and \( \eta \) (representing the detection efficiency).

\[
I_{\text{observed}} = \Omega \eta \left[ R_{\parallel} I_{\parallel} + R_{\perp} I_{\perp} \right]
\]  

(4.38)

In Eqns. 4.5 and 4.6 we showed the relationship between the \( 4\pi \) averaged intensity and the intensities polarized parallel and perpendicular to the electron beam. By combining Eqns. 4.5 and 4.6 with Eqn. 4.38, the observed intensities may be expressed in terms of the \( 4\pi \) averaged intensity.

\[
I_{\text{observed}} = \Omega \eta^3 \frac{3}{2} \langle I \rangle \left[ \frac{(1 + P)}{(3 - P)} R_{\parallel} + \frac{(1 - P)}{(3 - P)} R_{\perp} \right]
\]  

(4.39)

When looking at the ratio of two lines (1 and 2) measured with a single crystal spectrometer, we get:

\[
\frac{I_{\text{obs}1}}{I_{\text{obs}2}} = \frac{\langle I_1 \rangle \left[ (1 + P_1)R_{\parallel}^1 + (1 - P_1)R_{\perp}^1 \right]}{\langle I_2 \rangle \left[ (1 + P_2)R_{\parallel}^2 + (1 - P_2)R_{\perp}^2 \right]} \frac{3 - P_2}{3 - P_1}
\]  

(4.40)
Defining the spectrometer response factor as:

\[
G_{\text{line1}}^{\text{line2}} = \frac{(1 + P_1)R_1^\parallel + (1 - P_1)R_1^\perp}{(1 + P_2)R_2^\parallel + (1 - P_2)R_2^\perp} (3 - P_2) (3 - P_1)
\]

(4.41)

a simplified equation for the ratio of lines can be expressed as:

\[
\frac{I_{\text{obs1}}}{I_{\text{obs2}}} = \frac{\langle I_1 \rangle}{\langle I_2 \rangle} G_{\text{line1}}^{\text{line2}}
\]

(4.42)

Eqn. 4.42 has been used in studies such as [85], where \(\langle I \rangle\) values calculated with the HULLAC (Hebrew University Lawrence Livermore Atomic Code) based on the parametric-potential theoretical method for atomic structure and collisional rate calculations and were combined with measured intensities (\(I_{\text{obs}}\)) to obtain P values. This method has the advantage of only requiring one detector, but it also relies on theoretically calculated values and requires that one of the lines has a known or zero polarization.

### 4.3.2 The Two Detector Method

Traditionally EBIT polarization studies have utilized two crystal spectrometers. Some of these investigations have had both spectrometers in the horizontal orientation but used two different crystals [14], while others placed one spectrometer in the horizontal orientation and the second in the vertical orientation [119]. For our work, crystal spectrometers were placed at horizontal and vertical orientations with the same crystal used in both spectrometers. If the notation of [19] is again used, the observed intensities for the horizontally and vertically oriented spectrometers are:

\[
I_{\text{vert}} = \Omega_v \eta_v [R I_\parallel + I_\perp]
\]

(4.43)

\[
I_{\text{hor}} = \Omega_h \eta_h [I_\parallel + R I_\perp]
\]

(4.44)
The spectrometers used in this work were normalized to each other using an unpolarized \((I_\perp = I_\parallel)\) line. Since the same crystal was used (same \(R\) value) for both spectrometers, the ratio of intensities for this line gives the ratio of geometrical factors and efficiency.

\[
\frac{I_{\text{hor}}}{I_{\text{vert}}} = \frac{\Omega_h \eta_h}{\Omega_v \eta_v} = N \tag{4.45}
\]

By multiplying \(I_{\text{vert}}\) by the normalization factor \((N)\), the vertical intensity can be expressed in terms of the horizontal efficiency:

\[
NI_{\text{vert}} = N\Omega_v \eta_v \left[RI_\parallel + I_\perp\right] = \frac{\Omega_h \eta_h}{\Omega_v \eta_v} \Omega_v \eta_v \left[RI_\parallel + I_\perp\right] = \Omega_h \eta_h \left[RI_\parallel + I_\perp\right] \tag{4.46}
\]

Combining the equations for the measured intensities for the two spectrometers (Eqns.4.44, 4.46) with the polarization equation (4.3), the final expression for the measured polarization of a spectral line is:

\[
P = \frac{(1 + R) \left(\frac{I_{\text{hor}}}{\Omega_h \eta_h} - N\frac{I_{\text{vert}}}{\Omega_v \eta_v}\right)}{(1 - R) \left(\frac{I_{\text{hor}}}{\Omega_h \eta_h} + N\frac{I_{\text{vert}}}{\Omega_v \eta_v}\right)} = \frac{(1 + R) \left(I_{\text{hor}} - NI_{\text{vert}}\right)}{(1 - R) \left(I_{\text{hor}} + NI_{\text{vert}}\right)} \tag{4.47}
\]

As seen in Eqn. 4.47, by normalizing the vertical spectrometer to the horizontal, the efficiencies and geometrical factors drop out. It should be noted that if different crystals (different \(R\) values) are used, Eqn. 4.45 does not simplify to the ratio of efficiency and geometrical factors. When two different crystals are used, it is common to instead use the ratio of two lines in the same spectra. For example in [9], Si(110) and Si(111) crystals were used (both in the horizontal orientation). The line intensity ratios in this case can be expressed as:

\[
\frac{I_1^a}{I_2^b} = \frac{\Omega_1 \eta_1 \left(I_{a\parallel}^1 + R_1 I_{a\perp}^1\right)}{\Omega_2 \eta_2 \left(I_{a\parallel}^2 + R_2 I_{a\perp}^2\right)} = \frac{\left(I_{a\parallel}^1 + R_1 I_{a\perp}^1\right)}{\left(I_{b\parallel}^1 + R_1 I_{b\perp}^1\right)} \tag{4.48}
\]

\[
\frac{I_2^a}{I_2^b} = \frac{\Omega_2 \eta_2 \left(I_{a\parallel}^2 + R_2 I_{a\perp}^2\right)}{\Omega_2 \eta_2 \left(I_{b\parallel}^2 + R_2 I_{b\perp}^2\right)} = \frac{\left(I_{a\parallel}^2 + R_2 I_{a\perp}^2\right)}{\left(I_{b\parallel}^2 + R_2 I_{b\perp}^2\right)} \tag{4.49}
\]

where \(a\) and \(b\) represent the two lines and 1 and 2 represent spectrometer 1 and 2 respectively.
(i.e. $I^1_a$ represents the intensity of line a in spectrometer 1 and $I^2_b$ is intensity of line b in spectrometer 2). Then combining Eqn. 4.3 with Eqns. 4.48 and 4.49, the measured polarization can be expressed in terms of the line ratios:

$$P_a = \frac{\frac{I^1_a}{I^1_b} \left( 1 + R_1 \frac{1-P_{b1}}{1+P_{b1}} \right) (R_2 + 1) - \frac{I^2_a}{I^2_b} \left( 1 + R_2 \frac{1-P_{b2}}{1+P_{b2}} \right) (R_1 + 1)}{\frac{I^1_a}{I^1_b} \left( 1 + R_1 \frac{1-P_{b1}}{1+P_{b1}} \right) (R_2 - 1) - \frac{I^2_a}{I^2_b} \left( 1 + R_2 \frac{1-P_{b2}}{1+P_{b2}} \right) (R_1 - 1)}$$

(4.50)

Eqn. 4.50 shows that using the ratio of two lines removes any differences in the detector responses and expresses the polarization of one line in terms of the polarization of a second line. Therefore, this method works if one of the lines has a zero polarization or a well known polarization. This method also assumes that $R$ is constant over the energy region spanned by the two lines, adding to the total uncertainty.

4.4 Measurement Setup

4.4.1 Setup for He-like Measurements

Measurements were taken at the electron beam ion trap (EBIT) facility at the National Institute of Standards and Technology (NIST). The EBIT and detectors have been described in detail in previous sections of this work, so many detail are omitted in this discussion.

Measurements were taken simultaneously with two Johann-type crystal spectrometers (able to resolve features less than 2 eV apart at 3 keV x-ray energy) and a high count-rate, high-purity Ge (HPGe) detector (130 eV energy resolution at 3 keV x-ray energy). The HPGe was used as a diagnostics of the ideal EBIT plasma conditions with the maximum detector signal found by optimizing the EBIT operating parameters and the Ar gas injection pressure. The drift tube voltage cycle consisted of a 5 s “cooking” time and a 10 ms “dumping” period. During cooking, a higher voltage is placed on the upper (+250 V) and lower drift tubes (+500 V), trapping the ions electrostatically in the axial direction. During the dump cycle, the middle drift tube voltage is raised above the upper drift tube to
+400 V to displace any buildup of trapped contaminates, such as barium emitted from the cathode surface of the electron gun. All measurements described in this work were taken in a steady-state mode, where the electron beam energy and current remain constant during measurements. In addition to improving the signal to noise, this mode allows the charge state balance to reach steady-state.

The two crystal spectrometers (one in the horizontal and one in the vertical orientation, and both housing cylindrically bent Si(111) single crystals) use x-ray CCD detectors to record the diffracted x-rays. The spectrometers were first set to detect the He-like Ar (He-α) lines. To do this, Bragg’s law of $\lambda = 2d\sin(\theta)$ was used to solve for $\sin(\theta)$, where 6.271 Å was used for the 2d lattice-spacing of the Si(111) crystal, and for $\lambda$ the 3.982 Å (3114 eV) approximate wavelength value of the He-like Ar lines was applied. The spectrometer’s $\sin(\theta)$ dial was set to 0.6349 Å to observe 3114 eV light with a bandwidth of roughly 120 eV (determined by the size of the CCD chip). At this setting, the spectrometers can measure photon energies from 3054 eV to 3174 eV and cover the He-like $w$ (3140 eV), $x$ (3126 eV), $y$ (3123 eV), and $z$ (3104 eV) lines, and their KLL satellite lines of interest.

Since polarization calculations become more complicated as cascades from higher lying states populate the magnetic sublevels, polarization measurements are typically taken near the excitation threshold to reduce the number of cascades. In our work, the shield voltage was set to 3.99 kV, which is roughly 3.870 keV electron beam energy taking space charge effects into account at an electron beam current of 128.5 mA. This energy is about 730 eV above the excitation energy of the resonance ($w$) line, well above the ionization energy of Li-like Ar ions (918.375 eV), and below the ionization energy of He-like Ar ions (4120.67 eV). This energy is slightly below the $n = 4 \to 1$ direct excitation energy (3875 eV for $1s4p \to 1s^2$) in He-like Ar, excluding cascades from the $n = 4$ energy levels. In addition to collecting near the $n = 2 \to 1$ excitation threshold, measurements were also taken well above the threshold at 8.01 kV shield voltage (approx: 7.928 keV electron beam energy) and with a beam current of 128.1 mA.

Photons were collected with both spectrometers by acquiring signal on the CCD
detectors for 3 minute intervals. Several 3 minute measurements were taken consecutively and later added to improve the signal to noise. The total collection time at 3.99 kV shield voltage was 39 minutes, while collection time at 8.01 kV was 42 minutes.

4.4.2 Setup for DR Measurements

Measurements of KLL dielectronic recombination satellite lines were taken with the same detector setup as described above. The same spectrometer orientations, crystals, voltage cycle, and steady-state mode were used. To find the resonance electron beam energies, the electron beam energy was broadly scanned while taking quick measurements with the HPGe detector. This allowed us to find the maximum intensity of the KLL DR (unresolved in the HPGe spectrum) peak near 2.31 kV. The shield voltage was then finely scanned from 2.25 kV to 2.38 kV in 10 V increments to cover individual resonances. Measurements were taken for 18 minutes at all shield voltage settings, except 2.28 kV, 2.3 kV, and 2.33 kV where 15, 12 and 15 minute measurements were taken respectively. The electron beam current was kept constant at 74 mA for all DR measurements.

4.5 Data Analysis

The goal of our data analysis is to produce intensity values for individual peaks, in both spectrometers. The intensities, combined with the normalization factor then plug into Eqn. 4.47 to determine the experimental linear polarization. The steps required to obtain the intensities are detailed in this section.

Images collected with the CCD detectors were stored as 2048 x 2048 matrices (each matrix element contains a value representing the digitized value of the charge collected in each pixel). The value (intensity) of each element may include contributions from diffracted x-rays, electronic readout noise, cosmic rays, and thermal noise. The capability of CCD detectors to measure the energy and position of incoming x-ray photons was exploited to filter the data following the procedure outlined in [64]. The code used, created at NIST
in IGOR Pro (a scientific data analysis software, numerical computing environment and programming language), produces an “event” intensity histogram that allows the user to specify a range of intensities corresponding to the diffracted x-ray signal. The procedure performs a prediscrimination that sets pixel intensity values below or above the specified range to zero. This first step works well to remove a large portion of the unwanted signal, but it is not effective in removing noise and cosmic rays with energies close to the diffracted x-ray signal. To deal with this issue, an additional step is implemented that looks at event clusters. For this, the code identifies clusters by looking at neighboring pixels and tagging them if they contain a non-zero value. The intensity values in a cluster of pixels are added and placed in the intensity weighted center of the cluster while the remaining pixels are set to zero. The number of pixels in a cluster is saved as the event size. The event size histogram produced allows the user to specify the range of allowed cluster sizes. The code then sets pixel intensities corresponding to event sizes outside of the identified range to zero. This step removes additional cosmic rays, which typically span many pixels.

Fig. 4.9 shows an event size histogram and Fig. 4.10 shows a typical the event intensity histogram. Remembering that the event intensity is proportional to the photon energy, we can think of this as counts vs. photon energy. In this case we are relying on the energy resolving capability (resolution on the order of hundreds of eVs at 3 keV x-ray energy) of the CCD detector, therefore individual transitions are not separated (in fact all peaks within the 120 eV bandwidth of the crystal spectrometer appear as one peak). The largest feature in Fig. 4.10 represents single photon hits in the energy range allowed by the crystal spectrometer (3054 eV - 3174 eV in our case). Sometimes two or more photons can hit a pixel within the data collection time period, and the intensity is exactly double (or triple, etc.) the single photon hit intensity value. The multi-photon hit peaks have been identified in Fig. 4.10 along with a small peak at lower energy, refereed to as an escape peak.

The CCD pixels are made from Si, therefore if an incoming photon has sufficient energy, it can produce a photoelectron from an inner shell of the Si atom. If a K-shell
photoelectron is created the Si atom may respond by producing a K-α photon. The photoelectron will have an energy equal to the incoming x-ray minus the K-α energy \((E_\gamma - E_{k\alpha})\). Typically the K-α photon is reabsorbed, but sometimes it escapes. In this case all of the charge is not accounted for, creating a peak at lower energy (escape peak) equal to \(E_\gamma - E_{k\alpha}\).

Once the image of each frame has been cleaned, they are added to improve the signal to noise. As previously discussed, different orientations of the two spectrometers creates different effective source sizes. In particular the vertically oriented spectrometer sees an extended source size compared to the horizontally oriented spectrometer. As discussed in [131], a finite source size can lead to shape alterations of the diffracted lines. Indeed as shown in Fig. 4.11 (a., top panel), lines diffracted from the vertical spectrometer have a slight curvature along the CCD image. A spectrum produced by summing along the columns shows the broadened lines resulting from the curvature (Fig. 4.11 (a., bottom panel)). To deal with this effect, a script was written in Python language to correct for the curvature. The procedure fits a second order polynomial to two well separated curved features (such as those near pixels 850 and 1250 in Fig. 4.11 (a. top panel)) then performs a linear fit to the coefficients of the polynomials. The results of the straightening procedure are shown in

Figure 4.9: Counts vs. Event (cluster) Size
Comparing Fig. 4.11 (b. bottom panel) to (a. bottom panel) clearly shows the reduction in line broadening resulting from the straightening procedure.

After cleaning, adding, and straightening (vertical only) the images, spectra were created by summing the intensity values along each of the 2048 columns, called channels. Next the intensities, in analogue to digital units (ADU), were converted to photon numbers using Eq. 4.51 provided by Andor Technology Ltd. (the developer and manufacture of the x-ray CCD detectors used in the experiment).

\[
\gamma = \text{Counts (ADU)} \times \text{Sensitivity} \left[ \frac{e^-}{\text{count}} \right] \times W \left[ \frac{eV}{e^-} \right] \\
\text{gain} \times \text{QE} \times E_\gamma
\]

In Eq. 4.51, \( \# \gamma \) is number of photons, \( \text{Counts} \) are the digitized value of the number of electrons recorded, the sensitivity = 1 and gain = 1 are given by Andor Technology Ltd. or set in the software, \( W = 3.66 \text{ eV/e}^- \) is the energy required to produce an electron hole pair in the Si pixels, QE is the quantum efficiency, and \( E_\gamma \) is the photon energy. To obtain energy specific QE values, the QE data provided by Andor Technology Ltd. (Fig. 4.12) was
Figure 4.11: Image from vertically oriented spectrometer.
fit locally with a polynomial around the photon energies of interest. Finally the QE values obtained from the fit were multiplied by 0.92 to account for an 8% drop in QE due to the glass surface which encloses the sensor in the permanent vacuum.

Once the spectra were produced in photon number, individual peaks were fit with single Gaussian functions. Since the width of each channel bin (pixel) is equal to 1, the area value obtained from fitting is equal to the total number of photons under a peak, thus the areas of each peak were used as the intensities in Eqn. 4.47. Areas were produced using the weighted fitting tools in the multi-peak fitting package of IGOR Pro v.6.37. Each peak was included in the fit along with an overall constant background for the horizontal spectra and a cubic background for the vertical spectra. The photon number (N) in each channel was treated as normally distributed statistically and were assigned with weights of $\sqrt{N}$. The overall area uncertainty includes statistical, background, and fitting uncertainties.

Fig. 4.13 shows the horizontal DR spectra at each shield voltage setting with the Li-like satellites identified. By viewing the spectra at each shield voltage setting (Fig. 4.13), the variation in the line strength is seen as a function of the electron beam energy. The electron beam energy at which the maximum intensity of each Li-like line occurs is given in
Figure 4.13: X-ray spectra taken with Horizontal spectrometer.

Table 4.1 along with the description of the transitions for reference. Using this as a guide, the spectra where each line is strong and well separated was summed and peaks were fit with Gaussian functions. The location and widths found from fitting the summed spectra were used as constraints when fitting individual spectra to reduce the uncertainties in the peak locations.

While a number of theoretically unpolarized lines exist in the spectra, the Li-like m line was the strongest, well resolved feature suitable for normalization. The normalization factor (Eqn. 4.45) was determined by fitting the summed 2.25 keV and 2.26 keV horizontal and vertical spectra, shown in Fig.4.14. The ratio of the area of the m line was found to be $2.42 \pm 0.38$, with the uncertainty calculated using:

$$
\alpha_N = N \sqrt{\left(\frac{\alpha_{\text{Area}_{\text{vert}}}}{\text{Area}_{\text{vert}}}\right)^2 + \left(\frac{\alpha_{\text{Area}_{\text{hor}}}}{\text{Area}_{\text{hor}}}\right)^2}
$$

(4.52)

where $\alpha_N$ is the uncertainty in the normalization factor, and $\text{Area}_{\text{vert}}/\text{hor}$ and $\alpha_{\text{Area}_{\text{vert}}/\text{hor}}$ are the area and area uncertainty of the m line measured in the vertical/horizontal summed spectra, respectively.
Figure 4.14: a.) Red shows the sum of the 2.25 keV and 2.26 keV spectra measured with the horizontal spectrometer. b.) Red shows the sum of the 2.25 keV and 2.26 keV spectra measured with the vertical spectrometer. Bottom panels show the individual peaks (constrained to have equal widths, except for the blended t/s line), blue curves show the fit to the data, and top panels show the residuals.
Table 4.1: Li-like satellite transitions from [129], and letters representing the notation of [45]

<table>
<thead>
<tr>
<th>Ion</th>
<th>ID</th>
<th>Transition</th>
<th>Electron Beam Energy of max intensity (keV)</th>
<th>E(Th.) (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>j</td>
<td>$1s2p^2(^1D)^2D_{5/2} \rightarrow 1s^22p_{3/2}^2P_{3/2}^{n}$</td>
<td>2.23</td>
<td>3104.29</td>
</tr>
<tr>
<td>Li</td>
<td>k</td>
<td>$1s2p^2(^1D)^2D_{3/2} \rightarrow 1s^22p_{1/2}^2P_{1/2}^{n}$</td>
<td>2.23</td>
<td>3107.37</td>
</tr>
<tr>
<td>Li</td>
<td>a</td>
<td>$1s2p^2(^3P)^2P_{3/2} \rightarrow 1s^22p_{3/2}^2P_{3/2}^{n}$</td>
<td>2.23</td>
<td>3110.71</td>
</tr>
<tr>
<td>Li</td>
<td>r</td>
<td>$1s2s2p(^3P_0)^2P_{1/2}^{n} \rightarrow 1s^22s^2S_{1/2}$</td>
<td>2.18</td>
<td>3112.47</td>
</tr>
<tr>
<td>Li</td>
<td>q</td>
<td>$1s2s2p(^1P_0)^2P_{3/2}^{n} \rightarrow 1s^22s^2S_{1/2}$</td>
<td>2.19</td>
<td>3114.14</td>
</tr>
<tr>
<td>Li</td>
<td>t</td>
<td>$1s2s2p(^1P_0)^2P_{1/2}^{n} \rightarrow 1s^22s^2S_{1/2}$</td>
<td>2.21</td>
<td>3124.13</td>
</tr>
<tr>
<td>Li</td>
<td>s</td>
<td>$1s2s2p(^1P_0)^2P_{3/2}^{n} \rightarrow 1s^22s^2S_{1/2}$</td>
<td>2.21</td>
<td>3124.80</td>
</tr>
<tr>
<td>Li</td>
<td>m</td>
<td>$1s2p^2(^1S)^2S_{1/2} \rightarrow 1s^22p_{3/2}^2P_{3/2}^{n}$</td>
<td>2.25</td>
<td>3126.35</td>
</tr>
<tr>
<td>Li</td>
<td>n</td>
<td>$1s2p^2(^1S)^2S_{1/2} \rightarrow 1s^22p_{1/2}^2P_{1/2}^{n}$</td>
<td>2.25</td>
<td>3129.52</td>
</tr>
</tbody>
</table>

4.6 Experimental Result

The well known He-like w, x, y and z lines were used to calibrated the spectra (Calibration details are provided in the Appendix A). The spectra taken at 4 kV and 8 kV drift tube voltages are shown in Fig. 4.15, where the vertical spectrum was normalized to the horizontal using the normalization factor described in the previous section. The He-like w, x, y, and z lines are labeled in Fig. 4.15 along with Li-like q and r lines. Lines from the vertical spectrometer are broader than those from the horizontal spectrometer. This results from the larger effective source size as was discussed in the analysis sections.

The sign of the polarization is determined by the numerator ($I_\parallel - I_\perp$) in Eqn. 4.3. Since the horizontal spectrometer preferentially reflects $I_\parallel$ and the vertical preferentially reflects $I_\perp$, Fig. 4.15 shows that the resonance (w) line has a very strong positive polarization at both beam energies. The figure also shows that the x and y lines have a negative polarization, q has a positive polarization, and the z line and r line are almost unpolarized.

Fig. 4.16 shows the KLL DR spectra at each electron beam energy, where again the vertical spectra have been normalized to the horizontal. Spectra were also corrected for differences in collection times. The scan over the Li-like satellites highlights the resonant
nature of the DR process and the energy spread of the electron beam. By visually inspecting the range of electron beam energies each transition appears over in Fig. 4.16, the electron beam energy profile width can be estimated. A more accurate estimate of the width was found by measuring the intensity of the $j$ line at each electron beam energy and then plotting the intensity of the line vs. the electron beam energy as shown in Fig. 4.17. Fitting the data with a Gaussian function weighted with the statistical uncertainty, the electron beam energy FWHM is found to be 40 eV, consistent with previous estimates.

The spectra measured at 2.31 kV drift tube voltage (approximately 2.22 keV beam energy) where the $j$ line is close to its maximum measured value is shown in Fig. 4.18. The $j$, $k$, and $t/s$ blended lines show a strong positive polarization, while the $a$ line shows a negative polarization. As a good verification of our normalization, the fundamentally unpolarized $r$ line shows roughly equal intensity in both spectra.

Using the measured areas and the normalization factor, the polarization of each line was calculated using Eqn. 4.47. To determine the uncertainty we used the calculus approximation for the propagation of errors through multi-variable functions outlined in
Figure 4.16: Scan of electron beam energy over Li-like KLL satellite transitions. a.) Spectra measured with the horizontal spectrometer. b.) Spectra measured with the vertical spectrometer.
Figure 4.17: Electron beam energy profile fit with a Gaussian. Black dashed lines show the 95% confidence bands. Fit equation shown in the text box at the top right.

Figure 4.18: Spectra taken near the maximum intensity of the j line.
Specifically, the uncertainty \((\alpha_P)\) in the measured polarization was defined as:

\[
(\alpha_P)^2 = \left(\frac{\partial P}{\partial I_V}\right)^2 (\alpha_{I_V})^2 + \left(\frac{\partial P}{\partial I_h}\right)^2 (\alpha_{I_h})^2 + \left(\frac{\partial P}{\partial N}\right)^2 (\alpha_N)^2 + \left(\frac{\partial P}{\partial R}\right)^2 (\alpha_R)^2 \tag{4.53}
\]

where:

\[
\left(\frac{\partial P}{\partial I_V}\right) = -\left(\frac{1 + R}{1 - R}\right) \left(\frac{2I_hN}{(I_h + I_vN)^2}\right) \tag{4.54}
\]

\[
\left(\frac{\partial P}{\partial I_h}\right) = \left(\frac{1 + R}{1 - R}\right) \left(\frac{2I_vN}{(I_h + I_vN)^2}\right) \tag{4.55}
\]

\[
\left(\frac{\partial P}{\partial N}\right) = -\left(\frac{1 + R}{1 - R}\right) \left(\frac{2I_vI_h}{(I_h + I_vN)^2}\right) \tag{4.56}
\]

\[
\left(\frac{\partial P}{\partial R}\right) = -\left(\frac{I_h - I_vN}{I_h + I_vN}\right) \left(\frac{2}{(1 - R)^2}\right) \tag{4.57}
\]

In Eqn. 4.53, \(\alpha_{I_V}\), \(\alpha_{I_h}\), \(\alpha_N\), and \(\alpha_R\) are the uncertainties associated with the horizontal and vertical measured intensities \((I_V\) and \(I_h))\), the normalization factor \(N\) and the crystal reflectivity \(R\) respectively. As previously discussed, \(\alpha_{I_V}\) and \(\alpha_{I_h}\) are produced in IGOR Pro from the Gaussian fits to each peak (weighted with \(\sqrt{N}\)). Measured polarization values are given in Table 4.2 along with the uncertainties. The polarization values of the DR transitions were measured from spectra where each line has its maximum intensity (see Table 4.1). The maximum intensity of each line can be graphically seen in Figs. 4.16 and 4.13.

### 4.7 Theoretical Results

The Flexible Atomic Code (FAC) [55] was used to produce the atomic data for all calculations. This included the energy levels, radiative and autoionization probabilities, and differential dielectronic capture (and direct excitation) rates.
Table 4.2: Measured and theoretical polarization values. Electron beam energies have been space charged corrected. Li-like satellite energies from [129] in the notation of [45]. He-like energies from [75].

<table>
<thead>
<tr>
<th>Ion</th>
<th>ID</th>
<th>$E_{e\text{-beam}}$ (keV)</th>
<th>$E_{\text{line}}$ (keV)</th>
<th>$P_{\text{exp}}$</th>
<th>$P_{\text{th}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>j</td>
<td>2.23</td>
<td>3104.29</td>
<td>0.46 ± 0.08</td>
<td>0.50</td>
</tr>
<tr>
<td>Li</td>
<td>k</td>
<td>2.23</td>
<td>3107.37</td>
<td>0.55 ± 0.08</td>
<td>0.60</td>
</tr>
<tr>
<td>Li</td>
<td>a</td>
<td>2.23</td>
<td>3110.71</td>
<td>-0.53 ± 0.28</td>
<td>-0.75</td>
</tr>
<tr>
<td>Li</td>
<td>r</td>
<td>2.19</td>
<td>3112.47</td>
<td>-0.06 ± 0.16</td>
<td>0.00</td>
</tr>
<tr>
<td>Li</td>
<td>q</td>
<td>2.19</td>
<td>3114.14</td>
<td>0.47 ± 0.30</td>
<td>0.60</td>
</tr>
<tr>
<td>Li</td>
<td>t/s</td>
<td>2.21</td>
<td>3124.13</td>
<td>0.25 ± 0.12</td>
<td>0.24</td>
</tr>
<tr>
<td>Li</td>
<td>m</td>
<td>2.25</td>
<td>3126.35</td>
<td>0.00 ± 0.17</td>
<td>0.00</td>
</tr>
<tr>
<td>He</td>
<td>w</td>
<td>3.87</td>
<td>3139.58</td>
<td>0.54 ± 0.07</td>
<td>0.58</td>
</tr>
<tr>
<td>He</td>
<td>x</td>
<td>3.87</td>
<td>3126.29</td>
<td>-0.42 ± 0.10</td>
<td>-0.49</td>
</tr>
<tr>
<td>He</td>
<td>y</td>
<td>3.87</td>
<td>3123.53</td>
<td>-0.32 ± 0.10</td>
<td>-0.31</td>
</tr>
<tr>
<td>He</td>
<td>z</td>
<td>3.87</td>
<td>3104.15</td>
<td>-0.14± 0.09</td>
<td>-0.17</td>
</tr>
<tr>
<td>He</td>
<td>w</td>
<td>7.93</td>
<td>3139.58</td>
<td>0.44 ± 0.08</td>
<td>0.46</td>
</tr>
<tr>
<td>He</td>
<td>x</td>
<td>7.93</td>
<td>3126.29</td>
<td>-0.46 ± 0.17</td>
<td>-0.26</td>
</tr>
<tr>
<td>He</td>
<td>y</td>
<td>7.93</td>
<td>3123.53</td>
<td>-0.03 ± 0.15</td>
<td>-0.04</td>
</tr>
<tr>
<td>He</td>
<td>z</td>
<td>7.93</td>
<td>3104.15</td>
<td>-0.05 ± 0.10</td>
<td>-0.07</td>
</tr>
</tbody>
</table>

**DR analysis:** Only dielectronic capture from the ground state of He- and Li-like Ar was considered to populate the doubly excited states of Li- and Be-like ions, respectively. This assumption is generally valid for low density EBIT plasmas where most of the population is in the ground states of the respective ion stages. Since the DR measurements were taken at electron beam energies close to the resonance energy of each line, cascades were not expected to contribute to the populations and were therefore not included in our analysis. The electron beam energy profile, atomic data (for $Q_d$ and $E_{AI}$), and polarization values calculated using the differential cross-sections from FAC were used directly with Eqns. 4.7 and 4.8 to produce the polarized intensity components and to create synthetic DR spectra.

**He-like analysis:** For the He-like transitions, a collisional-radiative (CR) atomic kinetics model of magnetic sublevel populations was used to calculate the polarization. The non-Maxwellian CR model NOMAD uses atomic data form external sources (FAC in this case) and solves the system of steady-state rate equations for the magnetic sublevel populations. The CR model included configurations with single electron excitation up to n
= 5, and autoionizing states with single K-shell electron excitation to \( n = 3 \) for H-like to Be-like ions. The CR model includes atomic processes such as radiative decay, excitation (de-excitation), ionization (3-body recombination), autoionization, and dielectronic capture for magnetic sublevels. Since the model includes all feeding channels for the upper level, the magnetic sublevel populations (cross-sections) produced can be directly used in the equations for the alignment parameter (Eqn. 4.31) and no correction factors (such as the de-orientation parameter, Eqn. 4.14) are required [57].

Linear polarization results from our theoretical calculations are shown in Table 4.2. The theoretical and experimental DR spectra taken at an electron beam energy of 2.22 keV (near the peak of the \( j \) line), and 2.25 keV (near the peak of the Be-like features) are shown in Figs. 4.19 - 4.21. To produce the spectra, the theoretical intensities (Eqn. 4.7 and 4.8) were weighted with the crystal reflectivities (see Eqn. 4.33) for comparison with experiment. The theoretical spectra were normalized to the experimental spectra using the unpolarized \( m \) line at 2.25 keV beam energy. The figures show that there is an overall agreement between experiment and theory. The \( j \), \( k \), and \( t/s \) lines show a positive polarization in both the experimental and synthetic with comparable relative intensities between the horizontal and vertical spectra. Similarly the \( a \) line shows negative polarization in both spectra, and the \( m \), \( n \) and \( r \) lines appear unpolarized in both the theoretical and experimental spectra.

### 4.8 Depolarization Effects

In comparing our experimental and theoretical polarization values in Table 4.2, we see that the strongest \( w \), \( j \) and \( k \) lines seem systematically lower than the theoretical values. The equations used in our analysis assumed that the electron beam travels in a single (\( z \)) direction along the axis of the EBIT. While a good approximation, this is not physically true as electrons follow a spiral path as they interact with the magnetic field. Typically EBITs are designed to minimize the magnetic field in the electron gun region, which means that as electrons travel from the electron gun (zero magnetic field) to the trap (2.7 T field), they...
Figure 4.19: Experimental and synthetic spectra at 2.22 keV beam energy showing the Li-like satellite lines.

Figure 4.20: Experimental and synthetic spectra at 2.25 keV beam energy showing the Li-like satellite lines.
Figure 4.21: Experimental and synthetic spectra at 2.25 keV beam energy showing the lower energy Be-like satellite lines.

travel along a converging helical path as depicted in Fig. 4.22. As a result, the quantization axis may be rotated away from the z-axis (called the pitch angle), and the observation angle may be off from the assumed 90° (shown in Fig. 4.23). These effects may lead to an amount of depolarization of the spectral lines.

Early polarization measurements performed at the NIST EBIT facility [119] estimated these effects by first calculating the maximum transverse kinetic energy using the equation for the cyclotron frequency:

\[ \omega = \frac{eB_0}{m_e} \]  \hspace{1cm} (4.58)

where \( \omega \) is the cyclotron frequency, \( B_0 \) is the magnetic field at the trap, and \( e \) and \( m_e \) are the electron charge and mass respectively. From the cyclotron frequency, the transverse kinetic energy can be calculated using the relation:

\[ v = r\omega \rightarrow E_\perp = \frac{1}{2}m_ev^2 \]  \hspace{1cm} (4.59)
Figure 4.22: Path of an electron as it travel through the EBIT.
Figure 4.23: Cartoon showing how the quantization axis and observation angle change as the electron travels.

where \( r \) is the electron beam radius in the trap region, \( E_\perp \) is the transverse kinetic energy, and \( v \) is the transverse velocity. Plugging in 35 µm for the beam radius and 2.7 T for \( B_0 \) (conditions in the trap), the transverse KE is found to be 785 eV. The pitch angle is found using:

\[
\sin^2(\gamma) = \left( \frac{v_\perp}{v_{\text{total}}} \right)^2 = \frac{E_\perp}{E_{\text{beam}}} \tag{4.60}
\]

where \( v_\perp \) is the transverse electron velocity, and \( v_{\text{total}} \) is the total velocity as shown in Fig. 4.24. \( E_{\text{beam}} \) is the total electron beam energy determined by the potential set on the middle drift tube. Using 785 eV previously calculated for \( E_\perp \), and a total electron beam energy of 3.87 keV, we obtain a pitch angle of 27°.

Following the procedure of [119], we next correct for the angle of observation by
calculating the cosine of the average deviation from 90° as:

\[
\langle \cos(\beta) \rangle = \frac{2}{\pi} \int_0^{\pi/2} \sin(\gamma) \cos(\theta) d\theta = \frac{2\sin(\gamma)}{\pi}
\] (4.61)

In the limit of small angles, the polarization is corrected by applying the factor $1 - \langle \cos(\beta) \rangle^2$ to the theoretical values to compare with the experimental observations. For a pitch angle of 27°, this gives a factor of 0.92. To correct for the quantization axis being off from the true z-axis, we use Eqn. 4.62 to produce a second correction factor.

\[
\langle \cos(\phi) \rangle = 1 - \tan^2(\gamma)
\] (4.62)

Using the values for the current experiment again gives a second correction factor of 0.75. The combined factor from 1.) the off (z-axis) quantization axis and 2.) the off from 90° observation angle correction is 0.68, meaning our measured polarization is 68% of the true, perfectly aligned and laminar result. For example, a theoretical polarization value of 0.74 would be measured as 0.5. It needs to be noted that these estimates are upper limits and the true depolarization effect is somewhat lower, depending on the conditions of the electron beam.

In the years following the [119] study, there have been a few investigations of depolarization effects ([16, 54]). In particular Beiersdorfer & Slater ([16]) inferred $E_\perp$ from
polarization measurements of He-like Mg lines. Using one crystal spectrometer (in first and second order diffraction at a Bragg angle of 45°), they measured the w, x, y and z lines 50 eV above the excitation threshold and compared measurements to theory. They used Eqn. 4.63 (where the (-) sign is used for E1 transitions, and (+) is used for M1 transitions [54]) and 4.60 to calculate the transverse energy (Eqn. 4.64).

\[
P = P_0 \frac{2 - 3 \sin(\gamma)^2}{2 \mp \sin(\gamma)^2 P_0}
\]

(4.63)

\[
E_\perp = E_{\text{beam}} \frac{2(P_0 - P)}{P_0(3 \mp P)}
\]

(4.64)

In the equations above, \(P_0\) is the polarization for the true (pitch angle 0° and observation angle 90°) case and \(P\) is the measured polarization. Eqn. 4.64 allows one to used calculated \(P_0\) (assumed to be accurate) and measured P values to determine \(E_\perp\). In doing this Beiersdorfer & Slater [16] found an average \(E_\perp\) value of 190 ± 30 eV. They found that their results are consistent with the Herrmann theory of optical electron beam propagation [60] which gives an \(E_\perp\) value of 194 eV. They note though that since parameters such as the electron beam radius, temperature, and magnetic field near the electron gun are not exactly known, \(E_\perp\) predicted by Herrmann may vary between 50 and 250 eV.

The Herrmann theory outlined in [60] states that the product of the beam area and the transverse temperature is a constant. This can be used to equate the area and transverse energy at the cathode (c) to the area and transverse energy in the trap (t):

\[
E_\perp(\pi r_c^2) = \frac{1}{2} m v_\perp^2 (\pi r_t^2)
\]

(4.65)

where \(r_c\) and \(r_t\) are the beam radius at the cathode and trap respectively. By estimating the transverse velocity \((v_\perp)\) at the cathode to be \(\sqrt{\frac{2kT}{m}}\), the transverse energy at the trap can be expressed as:

\[
E_\perp = kT \left( \frac{r_c^2}{r_t^2} \right)
\]

(4.66)
The cathode temperature is then estimated by equating the electrical power to the radiative power:
\[
\sigma AT^4 = IV
\] 
(4.67)
where A is the area of the cathode \((2\pi r^2)\), T is the temperature of the cathode, \(\sigma\) is the Stefan-Boltzmann constant, I is the current applied to the filament, and V is the voltage applied. Using a filament voltage of 6.3 V, a current of 0.487 A, and a cathode radius of 1.5 mm, we get \(T = 1400\) K. Then using \(T=1400\) K, \(r_c = 1.5\) mm (maximum beam radius at the cathode equal to the radius of the cathode), \(r_t = 35\) \(\mu\)m, we get \(E_\perp = 221\) eV and a pitch angle of 13.84°. We also note that the parameters including the beam radius at the cathode and trap, magnetic field at the egun, and cathode temperature are not exactly know. The values used are the maximum estimated values, however using lower limits such as \(T=1200\) K and \(r_c = 1\) mm, and \(r_t = 40\) \(\mu\)m gives \(E_\perp = 65\) eV.

Given the range of possible \(E_\perp\) values, we tested the results calculated from Eqn. 4.66, by estimating the transverse energy using Eqn. 4.64. Since the resonance (w) line had the highest counts (and lowest uncertainty) in the 3870 keV spectrum, we inserted the measured and theoretical polarization values into Eqn. 4.64 and calculated \(E_\perp = 219\) eV \(\pm 31\) and \(\gamma = 18.76 \pm 2^\circ\), where the uncertainty comes from the quadrature sum of the errors associated with the electron beam energy and measured polarization. This is in excellent agreement with the value from Herrmann theory, giving us confidence in the 222 eV estimate of the transverse energy at 3870 eV beam energy.

To approximate the true polarization and determine the systematic uncertainty, we rearrange Eqn. 4.63 to express \(P_0\) in terms of the measured polarization, the electron beam energy, and the transverse energy:
\[
P_0 = \frac{2P}{2 - \sin(\gamma)^2(3 \pm P)} = \frac{2P}{2 - \frac{E_\perp}{E_{beam}}(3 \pm P)}
\] 
(4.68)
where (-) is used for electric dipole transitions and (+) for magnetic dipole transitions [54]. Plugging in 222 eV for \(E_\perp\), and \(E_{beam}\) and P values from Table 4.2, we get the estimated
Table 4.3: Comparison of experimental and theoretical polarization values. $P_0$ represents the measured polarization values corrected for the spiral motion of the electrons. The offset values are the difference between the measured and corrected values, showing that the corrected values fall within the experimental uncertainties.

<table>
<thead>
<tr>
<th>Ion</th>
<th>ID</th>
<th>$E_{e\text{-beam}}$ (keV)</th>
<th>$P_{th}$</th>
<th>$P_{exp}$</th>
<th>$P_0$</th>
<th>Offset</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>j</td>
<td>2.23</td>
<td>0.50</td>
<td>0.46 ± 0.08</td>
<td>0.52</td>
<td>0.07</td>
</tr>
<tr>
<td>Li</td>
<td>k</td>
<td>2.23</td>
<td>0.60</td>
<td>0.55 ± 0.08</td>
<td>0.62</td>
<td>0.08</td>
</tr>
<tr>
<td>Li</td>
<td>a</td>
<td>2.23</td>
<td>-0.75</td>
<td>-0.53 ± 0.28</td>
<td>-0.64</td>
<td>-0.11</td>
</tr>
<tr>
<td>Li</td>
<td>r</td>
<td>2.19</td>
<td>0.00</td>
<td>-0.06 ± 0.16</td>
<td>-0.08</td>
<td>-0.01</td>
</tr>
<tr>
<td>Li</td>
<td>q</td>
<td>2.19</td>
<td>0.60</td>
<td>0.47 ± 0.30</td>
<td>0.53</td>
<td>0.07</td>
</tr>
<tr>
<td>Li</td>
<td>t/s</td>
<td>2.21</td>
<td>0.24</td>
<td>0.25 ± 0.12</td>
<td>0.29</td>
<td>0.04</td>
</tr>
<tr>
<td>Li</td>
<td>m</td>
<td>2.25</td>
<td>0.00</td>
<td>0.00 ± 0.17</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>He</td>
<td>w</td>
<td>3.87</td>
<td>0.58</td>
<td>0.54 ± 0.07</td>
<td>0.58</td>
<td>0.04</td>
</tr>
<tr>
<td>He</td>
<td>x</td>
<td>3.87</td>
<td>-0.49</td>
<td>-0.42 ± 0.10</td>
<td>-0.47</td>
<td>-0.05</td>
</tr>
<tr>
<td>He</td>
<td>y</td>
<td>3.87</td>
<td>-0.31</td>
<td>-0.32 ± 0.10</td>
<td>-0.35</td>
<td>-0.03</td>
</tr>
<tr>
<td>He</td>
<td>z</td>
<td>3.87</td>
<td>-0.17</td>
<td>-0.14 ± 0.09</td>
<td>-0.16</td>
<td>-0.01</td>
</tr>
<tr>
<td>He</td>
<td>w</td>
<td>7.93</td>
<td>0.46</td>
<td>0.44 ± 0.08</td>
<td>0.46</td>
<td>0.02</td>
</tr>
<tr>
<td>He</td>
<td>x</td>
<td>7.93</td>
<td>-0.26</td>
<td>-0.46 ± 0.17</td>
<td>-0.49</td>
<td>-0.02</td>
</tr>
<tr>
<td>He</td>
<td>y</td>
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<td>-0.04</td>
<td>-0.03 ± 0.15</td>
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</tr>
<tr>
<td>He</td>
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<td>-0.07</td>
<td>-0.05 ± 0.10</td>
<td>-0.06</td>
<td>0.00</td>
</tr>
</tbody>
</table>

$P_0$ values shown in Table 4.3. The offset values given in 4.3 are calculated as the difference between $P_0$ and $P$ and represents the maximum systematic uncertainty of our measured $P$ values.

From Table 4.3 we see that the true polarization values for the the He-like lines measured at 3870 and 7930 eV are close to the theoretical values. Assuming that the theoretical values are correct, this may indicate that $E_\perp = 222$ eV is a good estimate at these electron beam energies. At lower electron beam energies however, we see that the offset value becomes larger. As a test we used the theoretical and experimental polarization values of the resonance line at 3.87 and 7.93 keV, and the strongest DR transition (j) at its peak intensity (2.23 keV) and plugged them into Eqn. 4.64. The results are plotted in Fig. 4.25, where the error bars are calculated as the quadrature sum of the uncertainty in the measured polarization and electron beam energy. The red horizontal line represents the $E_\perp = 222$ eV value calculated from the Herrmann theory. According the the theory
Figure 4.25: Transverse energy calculated from experimental result and from Herrmann theory

as long as the parameters in Eqn. 4.66 are constant, then the transverse energy should remain constant. Our data may show however that as the electron beam energy increases, the transverse energy also increases.

Shah et al. [106] also calculated the transverse energy from experimental and theoretical values over a broad range of electron beam energies (4620 eV to 9500 eV). They calculated the weighted average and found good agreement with the theory. Shah et al. also calculated the pitch angle based on their experimental polarization values. In particular they calculated the weighted average of the pitch angle for two beam energy regions (4500 eV - 5100 eV and 8800 eV - 9600 eV). They found a pitch angle of $16.3^\circ$ for the lower energy range and $17.2^\circ$ for the upper range. Their results generally agree within the error bars with the Herrmann theory, but they see a similar trend as in our case.

As shown in Fig. 4.26, the pitch angle derived from our measured and theoretical values tends to stay constant over the range of electron beam energies. This contrast the Herrmann theory (shown in blue) where a constant transverse energy (222 eV) leads to varying pitch angle with electron beam energy. Our results seem to agree with Shah, where
Figure 4.26: Pitch angle calculated from experimental result and from Herrmann theory at beam energies near 4000 eV - 5000 eV, the theory agrees very well with experimental values. At higher beam energies, the experimental pitch angle tends to be larger than what the Herrmann theory estimates. Our data point at a lower electron beam energy (2230 eV) shows that the discrepancy may grow as the electron beam energy decreases.

This may suggest that the transverse energy may vary with electron beam energy (Herrmann theory keeps it constant), and the pitch angle may vary much less than predicted by Herrmann. In Fig. 4.25, the weighted average of the two data points at 4000 eV and 8000 eV is shown in blue to compare with the energy region used in Shah (2018). The weighted average is slightly above the Herrmann theory estimate and agrees with the trend seen in Shah (2018). If we also include the lowest energy data point, the weighted average shifts below the Herrmann theory estimate (but still within the uncertainty).

While our data are limited, these results suggest that polarization measurements taken over a broad energy range could provide some additional insights into the physics of the transverse motion of the electrons. For now we use the 222 eV transverse energy estimated with the Herrmann theory but note that this may overestimate the systematic uncertainty at lower electron beam energies.
4.9 Summary and Conclusion

Polarization is an important process required to understand spectra from anisotropic laboratory and astrophysical plasma sources. Using the two crystal method, we reported the degree of linear polarization of the diagnostically important $w$, $x$, $y$, and $z$ lines from He-like Ar and their $j$, $k$, $a$, $r$, $q$, and $t/s$ KLL DR satellite transitions from Li-like Ar. The experimental results are summarized in Table 4.2 and 4.3 along with theoretical predictions. The comparison between experimental and theoretical spectra in Figs. 4.19 and 4.20 shows overall good agreement. This is further seen in Table 4.2, where all theoretical predictions fall within the experimental uncertainties. Taking depolarization effects into account shifts the measured polarization to slightly higher values and closer to the theoretical predictions as shown in Table 4.3, however they still fall within the reported uncertainties. The measurements presented are intended to contribute to the small collection of existing EBIT measurements of linear polarization of emission from DR transitions and fill in polarization values of $w$, $x$, $y$, and $z$ lines along the isoelectronic sequence. This collection is a valuable resource to be used to benchmark calculations produced by different theoretical approaches. By improving the accuracy of these calculations, anisotropic astrophysical plasma sources can be better diagnosed, and higher quality data can be produced from anisotropic laboratory plasma sources such as EBITs.
Chapter 5

Analysis of the Contribution of Ar Dielectronic Recombination Lines to the Unknown Faint X-Ray Feature Found in the Stacked Spectrum of Galaxy Clusters

This project began while completing an en-route masters degree, therefore some description was already included in Gall (2017) [47]. This work has since been completed and recently published in the Astrophysical Journal. The corresponding article is included in Appendix B, and many of the figures and text in this chapter are taken from that work [48].

5.1 Introduction

Dark matter, which may consist of about 85% of all the matter in the Universe, is vital to our understanding of cosmology, and its origin is one of the biggest open questions
in astronomy. The term dark is in reference to the fact that it doesn’t seem to interact with electromagnetic radiation. This means that spectroscopy and spectroscopic techniques, traditionally one of the most powerful methods used to study the universe, may not be used to directly observe dark matter.

The existence of dark matter was first postulated by astronomers such as Fritz Zwicky, one of the most cited pioneers of dark matter (see work by Bertone (2018) for a nice summary of the history of dark matter [18]). In his 1933 [132] and 1937 [133] works, Zwicky measured the velocity dispersion of the Coma Cluster, and using the virial theorem estimated the gravitational mass of the cluster. Using the cluster mass, he estimated the average mass per galaxy and compared this with the average absolute luminosity of galaxies. From his analysis, Zwicky discovered that the mass to light ratio was hundreds of times larger than that of local stellar objects, and stated that “[In order to derive the mass of galaxies from their luminosity] we must know how much dark matter is incorporated in nebulae in the form of cool and cold stars, macroscopic and microscopic solid bodies, and gases” [133].

The quality of evidence for dark matter has only increased over the years with advancements in technology and our understanding of physics and astronomy. As a result, there has been great interest in solving the “missing mass” problem, spurring a number of hypothesis of the origins of dark matter. One theory suggest that dark matter may consist of hypothetical particles called sterile neutrinos, that only interact through gravity. The decay of these particles could produce an active neutrino and a photon with energy in the keV range, making them indirectly observable with sensitive x-ray detectors and clever techniques [26].

Searching for the possible x-ray decay signature, Bulbul et al. (2014) [26] combed through the XMM-Newton, Chandra, and Suzaku observations to find bright, various red-shifted galaxy cluster spectra. From the XMM-Newton archive, 73 spectra were selected, blue-shifted to z=0 (using bright Fe lines), and stacked. This procedure enhances any weak features common to all the spectra and smears out local instrumental effects. The back-
ground subtracted stacked spectrum was fit with a nonphysical, line-free, multi-temperature APEC (astrophysical plasma emission code) model that accounts for continuum emission from thermal bremsstrahlung, radiative recombination, and two photon emission. Gaussian features were then added to the model where known strong lines (from AtomDB) exist. After fitting the line-free APEC model with Gaussian lines, analysis of the residuals revealed an unidentified emission feature at \( E \approx 3.55\text{keV} \sim 3.57 \text{keV} \). This feature was also seen when the sample was subdivided. However, when evaluating the nearby, bright Perseus Cluster (single cluster) they found an excess of the line flux that was inconsistent with the other samples. By relaxing the upper limits placed on a nearby weak Ar DR feature, they found that the line could be interpreted as an abnormally bright Ar DR line (near 3.62 keV); however the flux would have to be increased by a factor of 30 above the predicted maximum, requiring something physically difficult to interpret or possible issues with the atomic data.

The exciting results of the Bulbul et al. (2014) study have led to a number of follow up investigations. Some of these studies, such as those from Urban et al. and Iakubovski et al. [122, 67], have confirmed the detection while others have found little to no evidence for the dark matter line (see e.g. [80, 3, 120, 28, 104, 33]). The existence of the dark matter line is still under investigation and may remain so until future x-ray satellite missions are able to measure the spectra from a number of galaxy clusters with good energy resolution and sensitivity. Until then, many groups have been searching for other possible explanations of this line. For example, Gu et al. and Shah et al. made compelling arguments in support of charge exchange between bare sulfur and atomic hydrogen occurring as a result of the interaction between the hot intracluster medium (ICM) and cold dense clouds in galaxy clusters [56, 107].

To help eliminate possible atomic origins and to aid the analysis of future observations near the unidentified line, we utilized the electron beam ion trap (EBIT) at the National Institute of Standards and Technology (NIST) to study the Ar DR transitions discussed in Bulbul et al. (2014). In this work, the details of the experimental setup are
provided along with a discussion of the experimental and theoretical results. Finally we compare our results with spectra produced with APEC, the model used in the Bulbul et al. (2014) work.

5.2 Experiment

As previously discussed, dielectronic recombination is a two step process. In the first step a continuum electron recombines with an ion while a bound atomic electron is simultaneously excited. In the second step, one of the two excited electrons radiatively decays. This may be followed by one or more additional decays until the ion fully stabilizes. Since in the initial step the binding energy plus the kinetic energy of the free electron must be equal to the excitation energy, this process can only occur with the free electrons having a specific kinetic energy. The finely tunable electron beam energy that is characteristic of an EBIT, makes these small scale laboratory devices ideal for studying the resonant DR process.

In our experiment the NIST EBIT was used to produce and trap the highly charged Ar plasma. Neutral Ar was injected into the trap using a differentially pumped, ballistic gas injection system [41]. A gas injection pressure of $2.6 \times 10^{-5}$ Torr, which maximized the x-ray signal, was used. The important Ar satellite line mentioned in Bulbul et al. (2014) is a $1s^22l - 1s2l3l'$ transition with an approximate x-ray emission energy of 3.62 keV. While analyzing the stacked spectra, the two strong satellite lines listed in AtomDB at 3.618 keV and 3.617 keV and relative intensities of 0.39 and 1, respectively, were used in the fitting procedure. These transitions and this energy region were the starting point of our investigation.

Since the first step of DR includes recombination, He-like Ar must be abundant in the EBIT plasma to create the $1s^22l - 1s2l3l'$ transition in Li-like Ar. To this end, the electron beam energy was finely scanned from 2.1 keV to 5.2 keV (well above the Li-like ionization energy of 918.375 eV, from the NIST ASD [75]) in $\approx 15$ eV steps with the electron beam current staying constant at 60 mA.
Measurements were taken simultaneously with a Johann-type crystal spectrometer and a high purity Ge (HPGe) detector, at view ports located radially around the trap region. The plane of dispersion of the crystal was oriented perpendicular to the electron beam to maximize the efficiency and increase the count rate (see Chapter 4). The crystal spectrometer was housed with a Si (111) crystal, with a spectral range of 2.219 keV to 4.592 keV and a 2d spacing of 6.271 Å, and was separated from the EBIT vacuum by a 250 µm thick Beryllium window. Since the bandwidth of the crystal spectrometer is ~ 120 eV, measurements were taken at two crystal spectrometer settings, corresponding to the energy region of the n = 2 → 1 and n = 3 → 1 KLM transitions (described below).

Measurements were taken in a steady-state mode with the electron beam energy and beam current remaining constant throughout the measurements. This mode allows the plasma to reach steady-state and increases the signal to noise. The trap voltage was cycled every 5 seconds to displace any built up contaminants, such as barium from the electron gun cathode. While trapping, a floated voltage of +500 V, 0 V, and +260 V were placed on the lower, middle, and upper drift tubes respectively. During the 10 ms dumping period, the middle drift tube voltage was raised to +400 V, above the upper drift tube voltage (but still below the lower drift tube voltage), to push the ions out of the trap and towards the collector assembly.

Three minute measurements were taken simultaneously with the crystal spectrometer and the HPGE detector at each electron beam energy. An additional four consecutive measurements were taken at the KLL and KLM resonance beam energies with the crystal spectrometer, for a total collection time of 15 minutes at each resonance energy.

5.3 Experimental Analysis and Results

Spectra measured with the HPGe detector were plotted as a function of each electron beam energy as shown in Fig. 5.1. The measured spectra were calibrated using synthetic spectra and atomic data from the Flexible Atomic Code (FAC) [55], therefore the uncer-
tainty in the photon energy is $\pm \sim 2$ eV (see Gall (2017) [47] work for calibration details). Fig. 5.1 is rich in information and showcases the unique capabilities of an EBIT.

The vertical lines in the figure originate from the direct excitation process. The strongest lines around 3.10 keV and 3.70 keV photon energy and above $\sim 3$ keV electron beam energy are due to direct excitation of $n = 2 \rightarrow 1$ and $n = 3 \rightarrow 1$ transitions and have been labeled. The intense spots seen in the figure result from dielectronic recombination. This is evident as they only appear at a few electron beam energies. The shape and size of the spots results from the detector response and the electron beam energy profile. The HPGe detector has a 135 eV full width at half maximum (FWHM) energy resolution at 6.5 keV; therefore narrow individual resonances do not appear on the x-axis. The electron beam energy profile follows a Gaussian shape with a FWHM of about 40 eV (see Chapter 4); therefore many resonances within the same $n$ shell may occur at one electron beam energy setting.

The KLL DR feature is the strongest and shows up around 2.25 keV beam energy. The KLM resonance appears at $\sim$2.73 keV electron beam energy and includes two strong peaks near 3.14 keV and 3.62 keV. Since the doubly excited state of the KLM has an electron in the $n = 2$ and $n = 3$ shells, there are two observable transitions in this energy region. One results from the $n = 2 \rightarrow 1$ transition (with spectator at $n = 3$), and the second originates from the $n = 3 \rightarrow 1$ transition (with spectator at $n = 2$).

As the electron beam energy increases, the free electron is captured to higher and higher $n$ levels. These KL$n$ ($n > 2$) resonances each contain two corresponding peaks as described above, and become closer to each other as the electron beam energy approaches the direct excitation threshold. In Fig. 5.1, the $n = 2 \rightarrow 1$ ($1s^2 \ 1S - 1s2p \ 1P$) direct excitation threshold in He-like Ar has been labeled as I while the $n = 3 \rightarrow 1$ ($1s^2 \ 1S - 1s3p \ 1P$) direct excitation threshold has been labeled as II. Above the threshold, the DR channel is cut off and the direct excitation process dominates.

Once the electron beam energy reaches $\sim$3.25 keV, the KMM DR emerges with two strong peaks. This resonance has two excited electrons in the $n = 3$ shell and decays
dominantly through Auger decay [1]. In this case either of the n = 3 excited electrons may
decay to n = 1 (with a spectator electron at n = 3), or an electron may decay to the n =
2 shell and autoionize the n = 3 electron (other paths are possible, but these are the two
dominant decay paths). For this reason one peak shows up as a satellite to the He-like n =
3 → 1 transition, and a second peak enhances the n = 2 → 1 direct excitation feature from
the parent He-like Ar ion.

The horizontal dashed line labeled III in the figure represent the ionization energy of
He-like Ar (4120 eV from NIST ASD). The ionization energy for H-like Ar is not labeled but
it occurs at 4426 eV (from NIST ASD). At electron beam energies above these ionization
energies, H-like and bare ions are created. As a result, the n = 2 → 1 direct excitation
feature is broader above these ionization energies due to the n = 2 → 1 transition in H-like
Ar around 3323 eV. The n = 3 → 1 feature is also wider above these energies, and a bright
spot is seen near 3935 eV from n = 3 → 1 transitions in H-like Ar.

The diagonal lines seen in Fig. 5.1 result from radiative recombination (RR). The
n = 2 RR occurs when a free electron is captured into the n = 2 shell of the ion and the
energy is released as a photon. Due to the radiative nature, as the electron beam energy
is increased the photon energy is also increased by the same amount. The n = 2 RR also
occurs at the same energy as the KLn (n > 1) DR resonances. These competing processes
produce equal energy photons because the excitation energy equals the binding energy plus
free e− kinetic energy. In the case of DR the energy from the captured electron excites a
bound electron and the photon comes from the de-excitation of the bound electron. In the
RR case the photon comes from the capture process where, rather than using the energy
to simultaneously excite a bound electron, the energy is directly released as a photon. The
n= 1 RR also appears in the figure, above the He-like ionization energy as expected.

Finally, there are a number of features in the measured spectra from trapped barium
ions (emanating from the electron gun cathode) and from heavy Xe ions. The ionization
energy for Na-like Xe is 3334 eV (from NIST ASD), whereas the ionization energy of Ne-like
Xe is 7660 eV (high due to the compact closed shell configuration). The Ne-like 2p5 3d3/2
$2p^6$ and $2p_{1/2}^5 3d_{3/2} - 2p^6$ E1 transitions have energies around 4500 eV and 4900 eV respectively and show up in the measured spectra at higher electron beam energies.

Cuts were taken down the $n=2$ RR feature, and $n = 2 \rightarrow 1$ and $n = 3 \rightarrow 1$ direct excitation features in Fig. 5.1 and projected onto the y (electron beam energy) axis as shown in Fig. 5.2. The width of the direct excitation features (at an off-resonance electron beam energy) was used as the energy bin width and counts within the limits were summed. A similar procedure was used for the RR cut, but for consecutive electron beam energies, the energy range was shifted by the change in electron beam energy. The matlab code used to produce the cuts is provided in Appendix C. The same excitation thresholds and ionization energies (I, II, and III described above) are also included in Fig. 5.2.

In Fig. 5.2, the peaks highlight the resonant nature of the DR process. Above the $n = 2 \rightarrow 1$ threshold the resonances appear as peaks on top of the direct excitation signal. This enhancement of the $K\alpha$ signal is explained by Auger decay as previously discussed. The $n = 2 \rightarrow 1$ cut shows the strongest features, demonstrating that the $K\alpha$ emission dominates. At the KLM peak, both the $n = 2 \rightarrow 1$ and $n = 3 \rightarrow 1$ peaks appear, as explained above. The KLM region also shows that the $K\alpha$ peak is about 3 times stronger than $K\beta$. The $n = 3 \rightarrow 1$ cut dies off rather quickly after the KLN resonance, suggesting that cascade effects are not strong. Emission from higher KLn ($n > N$) resonances becomes blended and unresolved.

The $K\beta$ and $K\gamma$ peaks at KLM and KLN appear at a slightly lower ($\sim 10$ eV lower) electron beam energy than the $K\alpha$ counterpart. This suggest that the states that produce $K\beta$ and $K\gamma$ emission are populated at lower electron beam energies. This was also observed in an earlier work by Ali. et al. [1].

X-rays dispersed by the Johann-type crystal and collected with the CCD were processed (cleaned and summed) using the procedure outline in Section 4.5. The high resolution x-ray measurements are shown in Fig. 5.3. The measurements were taken at the KLM resonance electron beam energy of $\approx 2730$ eV, where the intensity of the $n = 3 \rightarrow 1$ KLM peak is at its maximum value. The lower energy ($\sim 3130$ eV) portion of the spectrum corresponds
Figure 5.1: Spectra measured with HPGe detector at electron beam energies between 2.1 keV and 5 keV
Figure 5.2: Cuts taken down the $n = 2 \rightarrow 1$, $n = 3 \rightarrow 1$, and $n = 2$ RR features in Fig. 5.1. Green lines indicate the I. the $n = 2 \rightarrow 1$ DE threshold, II. the $n = 3 \rightarrow 1$ DE threshold, and III. the ionization energy of He-like Ar.

to $n = 2 \rightarrow 1$ transitions (spectator at $n = 3$), while the higher energy region corresponds to $n = 3 \rightarrow 1$ transitions (spectator at $n = 2$). The lower energy spectra were calibrated using strong $w$, $y$, $z$, and $r$ lines (in Gabriel notation [45]) measured at an off-resonance beam energy of 3348 keV (see Appendix A for an example of the calibration procedure). The 3.6 keV energy region was only measured the KLM resonance beam energy; therefore no strong direct excitation lines could be used for calibration. As a result, the spectrum was calibrated using the synthetic DR spectrum (described below). This is acceptable since we are not reporting line energies and the uncertainty is estimated to be $+/\sim 2$ eV.

5.4 Modeling of the EBIT Plasma

The collisional-radiative model NOMAD [96] was used to calculate the ionization balance, level populations, and line intensities of the highly charged Ar EBIT plasma. NOMAD uses atomic data from external sources to solve the time-dependent system of differential rate equations, and for this work atomic data including the atomic structure,
transition rates, and collisional cross-section data was calculated with the Flexible Atomic Code (FAC) [55]. In the case of our experiment, measurements were taken in a steady-state mode, so NOMAD was used to solve the simplified steady-state rate equations. The NOMAD package allows for an arbitrary electron energy distribution function (EEDF); therefore we were able to include the EBIT’s $\sim$ 40 eV FWHM Gaussian electron beam energy profile in the model.

Charge-exchange occurs in the EBIT plasma between trapped Ar ions and the neutral atoms that are continuously injected. This process can alter the charge state balance by shifting it towards lower charge states. This important process was included in the rate equations as the term: $n_0 v_0 \sigma_{CX}$, where $n_0$ is the density of neutrals in the trap, $v_0$ is the relative velocity between Ar ions and neutrals, and $\sigma_{CX}$ is the charge-exchange cross section [92, 93]. The terms $n_0$ and $v_0$ are generally not known, therefore the product $n_0 v_0$ was used as the only free parameter in the model.

Results from the kinetics simulations are shown in Figs. 5.4 and 5.5. Figure 5.4 shows the simulated spectra at each measured electron beam energy, convolved with a Gaus-
sian of FWHM of 120 eV to match the HPGe detector response. The maximum intensity of the synthetic spectra were normalized to the experimental spectra. The experimental spectra is also shown beside the synthetic for comparison. Looking at the experimental and theoretical results, we see that all of the strong features (DR resonances, DE lines, and RR features) are reproduced at each electron beam energy. This provides a high level of confidence in our model and atomic data. This also shows that the model is able to accurately calculate the charge state balance at each electron beam energy. Comparing the theoretically predicted and experimental spectra also highlights added emission in the experimental spectra from Xe and Ba as previously discussed.

Figure 5.5 shows the simulated spectra at 2730 eV (where the KLM DR intensity is at a maximum) convoluted with a Gaussian of FWHM of 1.4 eV to match the response of the crystal spectrometer. The synthetic spectra is overlaid with the experimental spectra for comparison. Fig. 5.5 shows that the theoretical spectra is able to reproduce the strong features near 3.134 reasonably well. More importantly, our model reproduces the \( n = 3 \rightarrow 1 \) KLM spectra almost perfectly.

As described extensively in Chapter 4, the stationary ions in the EBIT are excited by a unidirectional electron beam. As a result the excited magnetic sublevels can become aligned, meaning they are non-statistically populated. This can lead to anisotropic and polarized emission. Polarization effects were not taken into account in our model; however the relative line intensities of the synthetic spectra match almost exactly with our measured values, especially in the energy region of interest (See Fig. 5.5, bottom panel). This suggest that the lines have a polarization value near zero, or that all the lines have a similar polarization value, which is systematically removed by normalization. In either case, the agreement between measured and theoretical spectra shows that polarization effects were not important for this work.

To identify the measured features, we used the output identifications from the model and FAC. This method of identification has been used in works such as [95, 94, 93, 73, 90, 97, 115] where measurements combined with synthetic spectra were used to identify new
lines. Identifications of strong lines have been added to the Fig. 5.5 for reference. These identifications clearly show the strong KLM DR features from Li-like Ar at $\sim 3.134$ keV and 3.62 keV. The figure also shows a few Be-like Ar features. The Be-like feature near 3.557 keV is almost as strong as the Li-like line near 3.62 keV; however this line was not mentioned in the Bulbul et al. (2014) paper [26].

5.5 Spectra from Collisional-Radiative Models

The goal of our work is to ultimately test the model and atomic data (specifically the Ar satellite transition data near 3.62 keV from AtomDB) used in the Bulbul et al. (2014) study [26]. In the previous section we presented our measured spectra and showed that the CR model NOMAD (using FAC atomic data) reproduced all strong measured features near 3.62 keV in the $n = 3 \rightarrow 1$ KLM spectra, proving that the atomic data used is reliable and accurate. Next we compare our model spectra to spectra produced with APEC.

AtomDB is a database that includes data from the Astrophysical Plasma Emission Database (APED) and outputs from the Astrophysical Plasma Emission Code (APEC)
Figure 5.5: Top panel.) Measured and NOMAD spectrum of $n = 2 \rightarrow 1$ KLM transitions. Bottom panel.) Measured and NOMAD spectrum of $n = 3 \rightarrow 1$ KLM transitions. Both spectra have an electron beam energy of 2730 eV, corresponding to the maximum intensity of the KLM.

model. APED is a database that includes atomic data such as collisional, radiative and dielectronic recombination rates, recombination cross sections, theoretical and measured wavelengths (including satellite line wavelengths), emissivities, and line list collected from literature (including the entire CHIANTI database) for astrophysically abundant elements
APED also includes references to the original source of the data. APEC, created to analyze x-ray data from Chandra and XMM-Newton, calculates the line and continuum emissivities for optically thin, hot plasmas in collisional ionization equilibrium [117].

When analyzing the spectra from galaxy clusters the EEDF is assumed to be Maxwellian. As previously discussed, the EBIT EEDF is a Gaussian with FWHM of 40 eV. Therefore, to compare spectra from APEC and NOMAD we used a Maxwellian EEDF in our NOMAD model. The NOMAD and APEC spectra at an electron temperature ($T_e$) of 1 keV is shown in Fig. 5.6. The NOMAD spectrum was normalized to the APEC spectrum using the strong Li-like satellite of interest near 3.62 keV. The lines have been color coded by charge state, and strong or important features have been identified.

Both spectra contain strong features such as the He-$\alpha$, He-$\beta$, Ly$\alpha$, and Li-like satellite transitions. Looking near the energy region of interest, we see a number of weak features from Li-like Ar missing from the APEC spectrum. The Be-like satellite lines seen in the NOMAD spectrum (also measured in the EBIT) are also noticeably missing from the APEC spectrum.

To focus in on the missing flux, the APEC and NOMAD DR spectra (only DR transitions are included) between 3.55 and 3.67 keV, normalized to the strongest feature, are shown in Fig. 5.7. The spectra were convoluted with a Gaussian of FWHM of 1.4 eV to match the crystal spectrometer response, and strong features have been identified. This figure shows that overall the spectra agree, particularly at the strongest Li-like feature near 3.62 keV that is mentioned in the Bulbul et al. (2014) report. Interestingly though, there are missing lines in the APEC spectrum at 3.56 keV, 3.62 keV, 3.64 keV, and 3.66 keV, all near the observed (potential) dark matter line at 3.55 keV - 3.57 keV.

Much of the missing emission originates from a forest of weak Be-like lines missing from the database AtomDB. There are also few missing or underestimated lines from Li-like transitions. For example, the 3.62 keV and 3.64 keV features are much stronger in our modeled spectra and come from 1s$^2$2s - 1s2s3p transitions. The line missing from APEC at 3.56 keV originates from Be-like transitions (discussed further below), and the 3.66 keV
line comes from missing 1s²3d - 1s3p3d satellite transitions.

### 5.6 Results and Discussion

In the Bulbul *et al.* (2014) analysis, strong Ar emission lines were fit to the stacked galaxy cluster spectrum along with a few weaker features, including the Li-like Ar satellite transitions listed in AtomDB at energies of 3.618 keV and 3.617 keV. These two lines are not fully resolved in our measured spectra, but the blended line is clearly seen around 3.62 keV in Figs. 5.3 and 5.5. This line was also accurately predicted by the CR model NOMAD in Fig. 5.5. Furthermore, this feature was comparable between our NOMAD and APEC spectra in Figs. 5.6 and 5.7. Bulbul *et al.* (2014) calculated the maximum emissivity of the 3.62 keV Ar DR line to be 4% of the He-like Ar triplet at 3.12 keV at $T_e = 0.7$ keV. To check this we calculated the ratio of the emissivity of the 3.62 keV feature to the He-like triplet at $T_e = 1$ keV. In agreement with Bulbul *et al.* (2014), the Ar DR is equal to about 2% of the Ar triplet in both the NOMAD and APEC spectra. This evidence suggest that the data used by Bulbul *et al.* (2014) from AtomDB is correct and not off by the factor of 30 that would be required to explain the dark matter line.

Furthermore, the projected cuts in Fig. 5.2 highlights the relative strength of the $n = 2 \rightarrow 1$ resonance compared to the $n = 3 \rightarrow 1$ KLM resonance. This implies that if something physically unusual is happening in the galaxy clusters that produces a very strong ($n = 3 \rightarrow 1$) KLM resonance, as we have done in the EBIT, then there should be a $n = 2 \rightarrow 1$ KLM counterpart that is almost 3 times stronger. Since this was not the case in the Bulbul *et al.* (2014) work, it is highly unlikely that the Ar DR feature at 3.62 keV is the source of the dark matter line.

While the 3.62 keV resonance is unlikely to be the source of the dark matter line, Figs. 5.6 and 5.7 showed that there is missing emission from APEC/AtomDB from other sources in this energy region. We also showed in our experimental spectra (Fig. 5.5) that the Be-like satellite transitions near 3.56 keV are almost as strong as the 3.62 keV DR
Figure 5.6: Top panel.) Spectra produced with NOMAD at $T_e = 1$ keV. Bottom panel.) Spectra produced with APEC at $T_e = 1$ keV.
feature. This feature was missing from the APEC spectra, and in fact there are no Be-like satellite transitions in AtomDB. To understand the importance of these missing Be-like lines, we used FAC to produce \( 1s^22p^1l^2l''l'' \) and \( 1s^22p^1l^3l''l'' \) data between 3.075 keV and 3.672 keV, and added the data to AtomDB.

APEC was used to produce the Ar spectra over a range of temperatures using the original data in AtomDB, and again with the new Be-like data added. The emissivity in three bands: 1.) 3.1 keV to 3.2 keV (corresponding to the \( \text{Ar}^{16+} \) He-\( \alpha \) complex), 2.) 3.66 keV to 3.72 keV (at \( \text{Ar}^{16+} \) He-\( \beta \)), and 3.) 3.5 keV to 3.66 keV (where the unidentified line, \( \text{Ar}^{16+} \), and \( \text{Ar}^{15+} \) DR lines lie) was added up at each \( T_e \) for both cases. Fig. 5.8 (top panel) shows the emissivity in each energy bin using the original data (solid lines) and with the added data (dashed lines). Fig. 5.8 (bottom panel) shows the ratio of the emissivity in each energy bin with the new data added to the emissivity calculated using the original data.

The figure shows that the added data does not change the total flux in the 3.1 keV - 3.2 keV or 3.66 keV - 3.72 keV energy bands. This is expected as these energy regions are dominated by bright He-\( \alpha \) and He-\( \beta \) lines (see Fig. 5.6), so added weak lines have little effect on the total flux. However, in the 3.5 keV - 3.66 keV energy bin there is some added
Figure 5.8: (top panel) Total emissivity in three energy bands over a range of temperatures. Solid lines show the calculated emissivity using the original data in AtomDB v.3.0.9 while dashed lines show calculated emissivity with added Ar\textsuperscript{15+} data. (bottom panel) Ratio of the total flux with new lines included to the original flux (not including Ar\textsuperscript{15+} lines), shown for each energy band.

flux. At lower temperatures around 1 keV, these new lines increase the flux by a factor of 3. Bulbul et al. (2014) [26] find a range of temperatures for different components used to model their plasma. The lowest of these is $T_e = 2.0$ keV for the “Excluding Nearby Clusters” sample. At this temperature, the new DR data enhances the flux in the 3.5 keV to 3.66 keV band by a factor of 2.

To visualize where the new Be-like lines lie, Fig. 5.9 (top panel) shows the spectrum produced with APEC at $T_e = 1.72$ keV. The features and their constituents are color coded by charge state. The added Be-like lines are also shown in black. Fig. 5.9 (bottom panel) shows the ratio of the spectra calculated with and without the new Be-like satellite data. This shows that the majority of the added emission lies between 3.62 keV - 3.66 keV.

In a recent report, Bulbul et al. (2019) [25], hereafter BUL19, performed experiments similar to ours. Also investigating possible Ar DR atomic origins of the dark matter line, they used the EBIT-I at the Lawrence Livermore National Laboratory to produce and trap the highly charged Ar ions. Rather than taking measurements in a steady-state
mode, they used the Maxwellian simulation mode [101] where the electron beam energy is swept in way that simulates a Maxwell-Boltzmann EEDF. This mode allows for the direct comparison between experiment and simulated spectra using a Maxwellian EEDF (such as APEC); however, the intensities from different ions may not be representative of a true Maxwellian plasma and polarization effects (which depend on electron beam energy) may be difficult to predict [25]. X-ray measurements were taken with an x-ray microcalorimeter spectrometer with a energy resolution of about 5 eV. Fig. 5.10 shows the EBIT spectra (estimated $T_e = 1.74$ keV), and the AtomDB v.3.0.8 spectrum. The bottom left panel shows the spectrum in the energy range of 3.60 keV - 3.70 keV and highlights the discrepancy between the model and experiment near the 3.62 keV Ar DR feature. They report that AtomDB underestimates the flux by a factor of 2.6 in the 3.54 keV to 3.645 keV energy range.

BUL19 also added additional DR data into AtomDB to estimate the effects of missing data. In particular they added data from Tables 5 and 6 from Beiersdorfer et al. (1995)
Figure 5.10: Image from [25] with caption “Zoomed-in energy bands of the AtomDB v3.0.8 and EBIT spectra. The figure compares the EBIT results (solid blue line) with the emission from each ion of argon calculated using AtomDB v3.0.8 with the ion fractions for the EBIT plasma from Table 3.”

Figure 5.11: Table V and caption from [12]

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<th>(\lambda_{\text{theor}}) (Å)</th>
<th>(F_2) (s⁻¹)</th>
<th>Feature</th>
<th>(\lambda_{\text{spec}}) (Å)</th>
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Figure 5.12: Table VI and caption from [12] including 1s3l3l' data spanning 3.645 keV to 3.680 keV and 1s2s2l3l' data between 3.145 keV and 3.588 keV (shown in Figs 5.11 and 5.12). After adding the data to AtomDB, they still saw a factor of ~ 2 in missing flux in the AtomDB spectrum compared with experiment. Their comparison of the EBIT spectrum with AtomDB (with and without the new data) is shown in Fig. 5.13. From the figure it is clear that the added data improved the fit from 3.55 keV - 3.60 keV and 3.65 keV - 3.70 keV; however there no change from 3.60 keV - 3.65 keV. This is expected since the data they added only spans 3.145 keV and 3.588 keV and 3.645 keV to 3.680, not adding anything between 3.588 keV and 3.645 keV.

In our work, we showed that at $T_e = 1.72$ keV, the data added to AtomDB from FAC increases the emissivity by a factor of 2 between 3.5 keV and 3.66 keV. Fig. 5.9 shows

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<th>$F_s$ ($s^{-1}$)</th>
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TABLE VI. Atomic data for 1s2s2l3l' dielectronic satellite lines excited in the capture of a free electron by lithiumlike ions in the 1s2s2 ground state. Numbers in square brackets are powers of ten. Only lines with line strength $F_s \geq 5.0 \times 10^{11}$ s$^{-1}$ are listed.
that the majority of our added data falls between 3.63 keV and 3.67 keV, exactly where BUL19 did not add any new data. This suggests that the factor of 2 discrepancy that they report originates from satellite transitions from Be-like Ar.

### 5.7 Summary and Conclusion

Motivated by the unidentified, potential dark matter line found in the stacked spectrum of galaxy clusters [26], we aimed to help rule out possible atomic origins. During the analysis of the stacked spectrum, it was suggested that an abnormally bright Ar DR line from 1s\(^2\)2l - 1s2l\(^3\)l\(^\prime\) transitions in Li-like Ar could be the source of the unidentified line; however, something physically unusual would have to occur, or the atomic data used in the analysis could be flawed.

Using the NIST EBIT and a high-resolution Johann-type crystal spectrometer we produced the highly charged Ar ions and measured the DR lines of interest. In comparing measurements with a spectra simulated with the non-Maxwellian CR model NOMAD, we
found excellent agreement. This proved that the atomic data used in the model accurately reproduces measured DR features in the energy region near the dark matter line.

Next we compared a $T_e = 1$ keV spectrum produced with the NOMAD and APEC. The spectra generally agreed, but a number of weak features surrounding the 3.62 keV DR were missing in the APEC spectrum. The ratio of the 3.62 keV line to the He-like triple in both NOMAD and APEC spectra were in agreement with the calculation from Bulbul et al. 2014, indicating that the 3.62 keV DR feature was not the source of the dark matter line.

To check if the missing lines near 3.62 keV could be the source, we added missing Be-like data to AtomDB. This produced a factor of 2 increase in the total flux in the energy range between 3.5 and 3.66 keV that was not accounted for in the Bulbul et al. (2014) work. While not enough to explain the dark matter feature, this is still significant. Furthermore, we showed that the majority of the missing flux falls between 3.63 and 3.67 keV and likely explains the discrepancy seen between LLNL EBIT measurements and AtomDB [25].

The strong Be-like line seen in our EBIT spectrum is strongest around $T_e = 750 - 1000$ eV as shown in Fig. 5.14. While Be- and Li- like charge-states may not contribute sig-
nificantly to individual galaxy cluster emission (which are typically at higher temperatures where these ions are less abundant), they may be important in lower temperature astrophysical objects, in stacked spectra where weak features can be greatly enhanced, and in non-Maxwellian plasma sources where resonant processes can dominate. This was clearly demonstrated by comparing spectra produced in a controlled laboratory environment to modeled spectra. However, in messy astrophysical plasmas, which may contain multiple elements, charge states, and electron energies, the effects of weak features can be subtle and could lead to physical misinterpretations, making the inclusion and accuracy of this data important.
Chapter 6

Summary and Outlook

Highly charged ions (HCIs) are found throughout the Universe and in many laboratory plasmas on Earth. Therefore, the data produced from HCI studies can be useful to research scientist in astrophysics, fusion device, and EUV lithography communities, just to name a few. In this work we have shown how the electron beam ion trap (EBIT) can be used to produce a clean environment of basically one element and a few (somewhat selectable) charge states. The tunable almost mono-energetic electron beam also allows a degree of excitation selectivity, making these perfect devices for producing and probing HCIs.

In Chapter 4, we describe linear polarization measurements of He- and Li-like Ar transitions ($w, x, y, z, r, q, t/s, j, k$, in the notation of [45]), taken at the NIST EBIT facility. Measurements were taken with two polarization sensitive crystal spectrometers. The two orientations (horizontal and vertical) of the spectrometers produce preferential reflection of different polarization components and allowed us to use the same crystal (Si(111)) in both spectrometers. This greatly simplified our system of equations and allowed us to determine the polarization of each line independently. Using an unpolarized line, we were able to normalize the vertical spectrometer to the horizontal and remove differences due to efficiency and geometry. We found that the horizontal spectrometer is about 1.4 times more efficient than the vertical, in agreement with reports by Henderson et al. and Takacs et al. [58, 119].
The polarization measurements of the DR satellite lines were taken at the resonance energy while the He-like direct excitation transitions were measured at 4 keV and 8 keV, well above the excitation threshold of all of the lines. Our measurements showed that the \( w \), \( j \), \( k \), and \( q \) lines have a strong positive polarization, the \( a \), and \( x \) lines have a strong negative polarization, and the \( z \), \( m \), and \( r \) lines have a small or zero polarization. The polarization of the \( y \) line decreased sharply between 4 keV (\( P = -0.32 \)) to 8 keV (\( P = -0.03 \)) electron beam energy, while the \( w \), \( x \), and \( z \) lines showed little change. Correcting measured values for depolarization effects from the spiral motion of the electrons shifts the measurements to higher values (but still within the uncertainty).

The linear polarization of each transition was calculated using the density matrix formalism for comparison with experiment. The polarization of the DR satellite transitions were calculated using atomic data from the Flexible Atomic Code (FAC). Since measurements were taken at the resonance energies, cascade effects were ignored. The theoretical polarization values of the direct excitation transitions were found using a collisional-radiative kinetics model of magnetic-sublevel populations, and included excitation up to \( n = 5 \). Theoretical values for the \( w \), \( x \), and \( z \) lines are in excellent agreement with experiment at both 4 keV and 8 keV. The theoretical values for the DR transitions fall within the uncertainties, also showing agreement with experiment. These measurements add to the small collection of EBIT polarization measurements that can be used to benchmark different theories. These theories are important not only for interpretation of EBIT (and other laboratory) spectra, but also for the accurate interpretation of spectra from anisotropic astrophysical sources.

In Chapter 5, we discussed measurements taken at the NIST EBIT facility that were motivated by the famous unknown, possible dark matter feature found in the stacked spectrum of galaxy clusters [26]. Our work aimed to rule out possible atomic origins of this line, specifically contributions from the dielectronic recombination process in He-like Ar. Measurements were taken with a crystal spectrometer and high purity Ge (HPGe) detector. HPGe measurements allowed us to locate the electron beam energies of important resonances and observe the relative strength of the \( n = 2\text{-}1 \) to \( n= 3\text{-}1 \) branches of the KLM
DR of interest.

High resolution measurements, aided by a collision-radiative model, allowed us to identify important DR transitions near the unidentified line. The agreement between our measured and synthetic spectra produced with NOMAD, verified the accuracy of atomic data used. Comparisons between the NOMAD and APEC spectra confirmed the accuracy of the Li-like atomic data used in the galaxy cluster analysis. However, the comparison also revealed a number of Be-like DR features missing from AtomDB, the database used in the galaxy cluster analysis. By adding the missing data into AtomDB, we showed that there is a factor of 2 in missing flux at $T_e = 1.72$ keV that was not accounted for in the cluster analysis. While this is not enough to explain the unidentified line, it could be important for studies involving lower temperature or anisotropic astrophysical objects.

In Chapter 3, the NIST and updated SAO EBIT facilities were described. EBIT facilities continue to drive the field of precision highly charged ion spectroscopic research. Once the SAO EBIT becomes fully operational again, there are plans to install an x-ray microcalorimeter that has previously been successfully used on the NIST EBIT [114]. Similarly, a new x-ray microcalorimeter has been installed at the NIST EBIT facility.

Looking into the future, my assessment is that microcalorimeters will play important role in laboratory and observational x-ray astrophysics. It is a nondispersive spectrometer that measures photon energy by detecting a small change in temperature of an absorbing material, such as superconducting tin. Typically the temperature change is detected by measuring the voltage across a thermistor that has a constant current applied (see [112]). The system is cooled into the mK range using adiabatic demagnetization where a paramagnetic salt pill is initially externally cooled using liquid He (or a cryogen free cryocooler). The paramagnetic material is then magnetized isothermally by applying a magnetic field. This reduces the entropy of the system. Finally the salt pill is adiabatically demagnetized resulting in a temperature drop (see Fig. 6.1).

Microcalorimeters can have energy resolutions of a few eV (FWHM) at 6 keV x-ray energy [112], almost as good as a crystal spectrometer, and have a broad bandwidth, sim-
Figure 6.1: Entropy vs. Temperature during ideal magnetic cooling process from [8].

Similar to the HPGe detector, providing the best qualities of both types of detectors in one. Furthermore, future x-ray satellite missions, such as XARM will include a microcalorimeter and will require atomic data at the level of or better than observations. This is expected to drive a demand for high quality laboratory measurements. As a result, the SAO and NIST microcalorimeters are expected to become the new workhorse of the EBIT facilities, providing high resolution x-ray atomic data, including cross-sections, line positions, and polarization measurements, much more efficiently for astrophysics and plasma physics communities.
Appendices
Appendix A  Calibration of Crystal Spectrometers

In Chapter 4, measurements taken with two Johann-type crystal spectrometers were used to determined the linear polarization of a number of direct excitation and dielectronic recombination lines. Here the details of the calibration are provided. The He-like and DR lines were measured at the same crystal spectrometer setting, therefore the same calibration is used for both data sets. The well known He-like w, x, y and z lines were used for calibration.

To increase the signal of the He-like lines, the spectra collected with an electron beam energy of 3.870 and 7.928 keV were added. The summed spectra were fit using a multi-peak fitting package. Each peak was fit with a single Gaussian and all of the peaks were constrained to have equal widths (shown in the bottom panels of Figs. 2 and 3). The red curve in the center panel of Figs. 2 and 3 shows the summed spectrum taken with the horizontal and vertical spectrometer respectively. The fit is shown as a blue curve over the experimental data with the green line showing the background fit. A constant background was used in the horizontal spectrum while a cubic function was used to fit the background of the vertical x-ray spectrum. The top panel in each figure shows the residuals between the fit and the experimental data. The He-like w, x, y and z lines have been labeled along with the Li-like r and q lines (in the notation of [45]).

The NIST Atomic Spectra Database (ADS) [75] was used to find the line energies of the w, x, y, and z lines. The line energies were plotted vs. the experimental peak positions in channel number and fit with a 3rd order polynomial, as shown in Figs. 4 and 5.

This polynomial was used to convert the experimental uncertainty (in channel number) to uncertainty in energy (eV) (see Fig. 6).

The line energy vs. channel number data points were then fit again with a 3rd order polynomial, but this time weighted with the total uncertainty, where the total uncertainty
Figure 2: Summed x-ray spectra measured with horizontally oriented crystal spectrometer at 7.928 and 3.870 keV electron beam energy

Figure 3: Summed x-ray spectra measured with vertically oriented crystal spectrometer at 7.928 and 3.870 keV electron beam energy

is given as:

\[ \alpha_{total} = \sqrt{\alpha_{exp}^2 + \alpha_{LE}^2} \]  

(1)
Figure 4: Line energy vs. channel number from fits to the horizontal spectrum.

where $\alpha_{total}$ is the total uncertainty, $\alpha_{exp}$ is the uncertainty from fitting the experimental spectra, and $\alpha_{LE}$ is the uncertainty of the line energies from the NIST ASD [75].

The final calibration plots are shown in Figs. 7 and 8, were the data points are shown as crosses with the error bars representing the total uncertainty. The polynomial fit is show...
Figure 6: Line energy vs. channel number from fits to the vertical spectrum.

in red, while the 95% confidence bands are shown in blue. To find the uncertainty in the calibration, the 98% (upper and lower) confidence bands were fit with a 6\textsuperscript{th} order polynomial. From the figures it is obvious that the vertical data have much larger errors due to the lower efficiency.

![Figure 6: Line energy vs. channel number from fits to the vertical spectrum.]

Figure 7: Line energy vs. channel number from fits to the horizontal spectrum. Red line shows 3\textsuperscript{rd} order polynomial fit to the data points, weighted with the total uncertainty. Blue lines show 95% confidence intervals.

![Figure 7: Line energy vs. channel number from fits to the horizontal spectrum.]

From the calibration, the measured spectra were converted from channel number to eV and their uncertainties were calculated from the fits to the confidence bands. The results are shown in Fig. 9, where the Li-like line energies were taken from Yerokhin
Figure 8: Line energy vs. channel number from fits to the vertical spectrum. Red line shows 3rd order polynomial fit to the data points, weighted with the total uncertainty. Blue lines show 95% confidence intervals.

& Surzhykov (2018) [129]. From the table we see that the uncertainties in the spectra measured with the horizontal spectrometer are less than 0.30 eV, while the spectra from the vertical spectrometer are less than 0.81 eV.

<table>
<thead>
<tr>
<th>Line</th>
<th>Exp. peak position (channel number)</th>
<th>Line Energy from literature (eV)</th>
<th>Exp Energy (eV)</th>
<th>Exp. Uncertainty (eV)</th>
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<tr>
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</tr>
<tr>
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<td>3126.33</td>
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<tr>
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<tr>
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<tr>
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<td>3112.47</td>
<td>3112.45</td>
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</table>

Figure 9: Measured lines converted from channel number to eV using calibration curves.

To test the calibration, the calibrated DR spectra measured near the maximum intensity of the j and m line are shown in Figs. 10 and 11 respectively, with Li-like line.
energies taken from Yerokhin & Surzhykov (2018) [129]. The measured features agree well with the values from the literature, giving us confidence in the calibration.

Figure 10: Calibrated measured spectra taken at 2.22 keV beam energy with literature line energies overlaid for reference.

Figure 11: Calibrated measured spectra taken at 2.25 keV beam energy with literature line energies overlaid for reference.
EBIT Observation of Ar Dielectronic Recombination Lines near the Unknown Faint X-Ray Feature Found in the Stacked Spectrum of Galaxy Clusters

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Abstract

Motivated by possible atomic origins of the unidentified emission line detected at 3.55–3.57 keV in a stacked spectrum of galaxy clusters, an electron beam ion trap (EBIT) was used to investigate the resonant dielectronic recombination (DR) process in highly charged argon ions as a possible contributor to the emission feature. The He-like Ar DR-induced transition 1s2 2s2p^3P→1s2p^3P was suggested to produce a 3.62 keV photon near the unidentified line at 3.57 keV and was the starting point of our investigation. The collisional-radiative model NOMAD was used to create synthetic spectra for comparison with both our EBIT measurements and with spectra produced with the AtomDB database. Simultaneous propagation into an energetically higher bound state of the electron resulted in the unknown X-ray emission feature. The unknown feature has been reported in a number of galaxy clusters.

Key words: atomic processes – line: identification – methods: laboratory: atomic – techniques: spectroscopic – X-rays: galaxies: clusters

1. Introduction

Studies of galaxy clusters driven by the search for a dark matter candidate, the sterile neutrino, whose decay may produce an X-ray photon, have found a promising unidentified X-ray emission feature. The unknown feature has been reported at 3.55–3.57 keV (Bulbul et al. 2014) in the stacked X-ray Multi-Mirror (XMM-Newton) spectrum of high-count galaxy clusters and at 3.52 keV ± 0.02 keV (Boyarsky et al. 2014) in the XMM-Newton spectrum of the Perseus galaxy cluster and the Andromeda galaxy. Bulbul et al. (2014) noted that the observed feature could be due to a number of atomic transitions including lines from Ar and K, while Gu et al. and Shah et al. made arguments in support of charge exchange between bare sulfur and atomic hydrogen occurring as a result of the interaction between the hot intracluster medium (ICM) and cold dense clouds in galaxy clusters (Gu et al. 2015; Shah et al. 2016).

The possibility that the feature could be a signature of dark matter has spurred many follow-up studies: some confirmed the detection (Iakubovskyi et al. 2015; Urban et al. 2015) while others, including the high-resolution broadband Hitomi results from the Perseus cluster (Aharonian et al. 2017), found little evidence for the unidentified line (Malyshev et al. 2014; Anderson et al. 2015; Carlson et al. 2015; Tamura et al. 2015; Sekiya et al. 2016). The existence of the unidentified line is still under investigation and may remain in question until future high-energy resolution X-ray satellite missions are able to measure the spectra with good energy resolution and sensitivity in a number of galaxy clusters.

To help eliminate possible atomic origins and to aid the analysis of future observations near the unidentified line, we utilized the electron beam ion trap (EBIT) at the National Institute of Standards and Technology (NIST) to study the 1s2p^3P→1s2p^3P resonant dielectronic recombination (DR) transitions in Li-like Ar (Ar^12+), which produce X-ray photons close to the energy of the unknown line. In this work, we show measured and calculated Ar X-ray spectra that include many DR satellites from lower charge-state ions that were not listed in AtomDB (Foster et al. 2012), the atomic database that was used in the Bulbul et al. (2014) analysis and often used in astrophysical X-ray spectral modeling. We further demonstrate that inclusion of these lines leads to a significant increase in emission in this energy region and produces agreement with measurements.

2. Dielectronic Recombination

DR is a two-step resonant process, in which a free electron is captured into a bound state of an ion while an atomic electron is simultaneously propagated into an energetically higher bound state. The doubly excited ion then stabilizes through spontaneous decay, emitting a photon. The DR process is described by Equation (1).

\[ e^- + X^\text{+} \rightarrow (X^\text{+(1)}) + e^- \rightarrow X^\text{+(1)} + h\nu, \]  

(1)

where \( e^- \) represents the free electron, \( X^\text{+} \) is an ion (X) with positive charge \( q^+ \), \( (X^\text{+(1)} + e^-) \) is the doubly excited ion with charge \( (q-1)^+ \), \( X^\text{+(1)} \) is the stabilized ion, and \( h\nu \) denotes an emitted photon.

DR resonances are labeled using three-letter notation, with the first, second, and third letters representing the principal quantum number of the initial unexcited bound electron, the excited electron, and the capture shell of the recombined ion.
electron, respectively. As a relevant example, during the KLM DR process, a free electron may be captured into the \( n = 3 \) (M) shell while a bound electron is excited from \( n = 1 \) (K) to \( n = 2 \) (L).

DR can play an important role in determining the charge-state balance of plasmas. This has motivated a number of EBIT and electron beam ion source (EBIS) measurements. For \( \text{Ar}^{+2} \) in particular, measurements of cross sections for DR on He-like Ar were performed by Ali et al. (1990, 1991). These measurements were later expanded upon by Smith et al. (2000) where good agreement was found between measurement and theory. Later EBIT measurements by Biedermann et al. (2002) explored He-like Ar satellite lines for plasma temperature diagnostics.

3. Experiment

X-ray spectra of highly charged Ar ions were measured at the NIST EBIT facility. Its quasi-monoenergetic electron beam, with an energy spread and radius of approximately 50 eV and 35 \( \mu \)m, respectively, allows for ion charge state and excitation selectivity (Gillaspy 1996). The electron beam is compressed to about a 10\(^{11}\) cm\(^{-3}\) density by a 2.7 T magnetic field produced by a pair of superconducting Helmholtz coils. The drift tube assembly, consisting of three sequentially aligned cylindrical tubes, traps ions axially while the space charge potential of the electron beam confines them radially. The voltages on the three drift tubes are floated on top of that of a shield electrode surrounding the drift tubes. The energy of the electrons in the interaction region is determined by the voltage of the middle drift tube, finely adjustable up to 30 kV, and the space charge of the electron beam (Porto et al. 2000). Neutral atoms can be continuously injected into the interaction region using a ballistic gas injection system (Fahy et al. 2007) attached to one of the side ports oriented perpendicular to the electron beam. Additional ports located radially around the trap region are used for spectroscopic observations of the EBIT plasma.

Presently, X-ray and EUV spectral regions can be accessed. Further details of the design and operation of the NIST EBIT can be found in Gillaspy (1997).

For our investigation, neutral argon atoms were injected into the EBIT, and the electron beam current was set to 60 mA. The electron beam energy was initially set to 2.1 keV, well above the ionization threshold of \( \text{Ar}^{1 \div +} \) (918.375 eV from the NIST database (Kramida et al. 2018)). The trap voltage cycle included a charge breeding time of 5 s followed by a 10 ms dumping interval to displace any build-up of contaminants such as barium ions sputtered out of the dispenser cathode of the electron gun. The measurements were performed in a steady-state mode where the electron beam energy was set to remain constant during measurements. In this mode, the EBIT plasma attains steady-state at each individual electron beam energy setting, and the charge-state balance at each energy can be properly accounted for by a non-Maxwellian collisional-radiative (CR) model.

During our study, the electron beam energy was scanned from 2.1 to 5.2 keV in 15 eV steps to identify DR resonances. X-rays were collected for 3 minutes at each electron beam energy using a broadband solid-state high purity germanium (HPGe) detector with 135 eV full width at half maximum (FWHM) energy resolution at 6.5 keV. Simultaneous measurements were taken with a high-resolution (less than 2 eV FWHM at 3 keV) Johann-type crystal spectrometer (Henins 1987) using a Si (111) crystal and an X-ray CCD detector.

4. Analysis and Results

4.1. Experimental Broadband Results

Spectra obtained from the 3-minute measurements taken with the HPGe detector are plotted at each electron beam energy as shown in Figure 1 (left panel). The plot highlights some of the atomic processes occurring inside the EBIT including radiative recombination (RR), resonant DR, and...
direct excitation (DE). These processes present themselves in Figure 1 as diagonal lines, intense spots, and vertical lines, respectively. Important Ar features have been labeled in Figure 1 as diagonal lines, intense spots, and vertical lines, \((\text{direct excitation})\). Cuts projected onto the vertical axis from Figure 1 were projected onto the vertical axis for a more comprehensive view as shown in Figure 2. For reference, the \(n = 2 \rightarrow 1 \text{ DE thresholds and the He-like ionization energy have been labeled as I, II, and III, respectively, in Figure 1 (left panel) and Figure 2.}\)

The \(1s^2n^1l\) DR transitions in Li-like Ar are seen in the \(n = 2 \rightarrow 1 \text{ cut of Figure 2, as sharp peaks below the } n = 2 \rightarrow 1 \text{ DE energy threshold. Above this threshold, the He-like direct excitation is enhanced by KMM and KMN resonances. This results from L-shell Auger decay (Ali et al. 1991; Smith et al. 1996). The } n = 2 \text{ RR cut exposes the higher } n \text{ counterpart of the } 1s^22l-1s2ln^1f \text{ DRs.}\)

4.2. High-resolution Results

Argon spectra measured with the high-resolution crystal spectrometer at the electron beam energy corresponding to a maximum intensity of the \(n = 3 \rightarrow 1 \text{ transition of the KLM resonance is shown as the solid black curve in Figure 3. Measurements at the KLM resonance energy were collected with a total dwell time of 15 minutes.}\)

The detailed structure of the \(n = 2 \rightarrow 1 \text{ DR transitions with a spectator electron at } n = 3 \text{ in Li-like Ar is seen between 3.100 and 3.150 keV, while the } n = 3 \rightarrow 1 \text{ transitions, with a spectator at } n = 2, \text{ are seen between 3.600 and 3.650 keV.}\) The spectrum also shows corresponding lines from lower charge states, in particular around 3.560 keV, very close in energy to the reported unidentified line as discussed in the following sections. Features have been labeled with the strongest lines for more detailed identifications.

4.3. Collisional-radiative Modeling of the EBIT Plasma

The collisional-radiative package NOMAD (Ralchenko & Maron 2001), which allows for an arbitrary electron energy distribution function, was used to calculate the ionization balance, level populations, and line intensities of the EBIT plasma. The NOMAD code uses atomic data from external sources to solve the steady-state rate equations. To this end, the flexible atomic code (FAC; Gu 2008) was used to calculate atomic structure, transition rates, and collisional cross-section data. Charge-exchange occurring between trapped Ar ions and neutral atoms, which can shift the charge-state balance toward lower charge states, was included in the rate equations as the term: \(n_0\sigma_{\text{CX}}\), where \(n_0\) is the density of neutrals in the trap, \(v_r\) is the relative velocity between Ar ions and neutrals, and \(\sigma_{\text{CX}}\) is the charge-exchange cross section (Ralchenko et al. 2008, 2011). Since \(n_0\) and \(v_r\) are not well known, the product \(n_0\sigma_{\text{CX}}\) was used as the only free parameter in the model. The simulated spectra were compared with measurements to understand the charge-state balance and correctly identify measured lines. This method has been used in previous works to accurately identify emission features from highly charged ions in X-ray and EUV spectral regions (see, e.g., Ralchenko et al. 2006, 2007, 2011; Kilbane et al. 2014; Poply et al. 2014; Reader et al. 2014; Sitiwal et al. 2017). Many of the earlier works also provide a thorough explanation of the calculations, which are omitted here.

**Figure 1** (right panel) shows the modeled EBIT plasma convolved with a Gaussian of FWHM of 120 eV. Measured features including the intense DR resonances, direct-excitation lines, and RR diagonals are clearly reproduced, verifying our model at each electron beam energy. The theoretical spectrum, calculated at an electron beam energy of 2.730 keV and convolved with a Gaussian of FWHM of 1.4 eV, is shown with our EBIT spectra in Figure 3. Measured KLM DR features seen in our EBIT spectra are well reproduced, providing additional confidence in our model.

It is important to note that the emission produced by the unidirectional electron beam in the EBIT can be polarized and...
anisotropic. Furthermore, the crystal spectrometer is sensitive to the polarization (see, e.g., Henderson et al. 1990; Beiersdorfer et al. 1996; Takács et al. 1996). The agreement seen between our modeled and experimental spectra, particularly at the $1s^22p - 1s^2p^3$ and $1s^22s2p - 1s^2s^2p^3$ DR peaks of interest, suggest that polarization effects from these sources were not significant and were not considered for the DR analysis in this work. Additional efforts are currently underway to investigate polarization of DR transitions in Li-like Ar.

4.4. Spectra from Collisional-radiative Maxwellian Models

The ions present in the EBIT trap are produced and excited by a quasi-monoenergetic electron beam, producing a non-Maxwellian plasma; however, the hot ICM of galaxy clusters, responsible for producing the majority of the emission, is assumed to follow a Maxwellian distribution. To predict the importance of experimentally observed features under these conditions, we applied our CR model, which accurately reproduces measured spectra, to a Maxwellian-distributed electron energy distribution with electron temperature $T_e$.

The calculated Ar spectra at $T_e = 1$ keV detailed in Figure 4 (top panel) includes strong He-like direct-excitation features, Li-like DR transitions, and weaker Be-like DR transitions. The two strong Li-like DR transitions of interest mentioned in Bulbul et al. (2014) are observed near 3.62 keV along with a number of weaker Li-like DR transitions. Close in energy to the unidentified line, near 3.57 keV, we see lower charge-state Be-like Ar DR transitions and additional Li-like DR transitions.

AtomDB is an atomic database that includes the Astrophysical Plasma Emission Database (APED) containing fundamental atomic data such as wavelengths, radiative transition rates, and electron collisional excitation rate coefficients. AtomDB also includes the spectral models output from the Astrophysical Plasma Emission Code (APEC; Smith et al. 2001). APEC uses the data from APED to calculate line...
emissivities for optically thin plasmas in collisional ionization equilibrium. In Figure 4 (bottom panel) we utilized APEC to calculate the same Ar spectrum at \( T_e = 1 \text{ keV} \) for comparison with NOMAD. Lines with an emissivity below \( 10^{-20} \text{ (ph cm}^{-3} \text{ s}^{-1}) \) are typically not included as individual emission features in the AtomDB data but are instead included in a pseudo-continuum consisting of weak lines. For our calculation, the emissivity cutoff was lowered to \( 10^{-22} \text{ ph cm}^{-3} \text{ s}^{-1} \), and as a result, the calculated spectra from AtomDB is seen to have more weak lines when compared to our calculated spectra in Figure 4 (top panel). However, the strongest lines show the same overall structure.

Focusing only on DR transitions, we overlaid our NOMAD DR spectra, convolved with a 1.4 eV FWHM Gaussian to match the resolution of the crystal spectrometer, with that produced by APEC in the energy region of interest. The spectra were normalized to the strongest DR feature near 3.616 keV. The DR intensities in Figure 5 are generally in good agreement with a few features missing in the APEC spectra near 3.56, 3.62, 3.64, and 3.66 keV. While much of the missing emission is due to a forest of weak Be-like lines missing from the database AtomDB, we also found a few missing or underestimated intensities from Li-like transitions also contributing. In particular, the 1s'2s - 1s2s3p transitions at 3.62 keV and 3.64 keV are much stronger in our model and are partially responsible for the missing emission. The missing emission near 3.56 keV is solely due to Be-like transitions (discussed further in Section 5), and the 3.66 keV line originates from missing 1s'3d - 1s3p3d DR transitions.

5. Discussion

The astrophysical atomic database AtomDB was used in the analysis of the stacked spectra of galaxy clusters (Bulbul et al. 2014). Strong Ar emission lines were fit along with a few weaker features, including the He-like Ar DR satellites listed in AtomDB at energies of 3.616 keV and 3.617 keV and relative intensities of 0.39 and 1, respectively. Though these two lines...
are not fully resolved, even in our measured high-resolution spectra, we do see the blended line in Figure 3. The projected cuts taken through the EBIT data plot shown in Figure 2 highlight strong DR resonances and show the relative strength of the $n = 2 \to 1$ to the $n = 3 \to 1$ satellite transitions of interest at the KLM DR peak.

In their report, Bulbul et al. (2014) calculated the maximum emissivity of the 3.62 keV Ar DR line to be 4% of the He-like Ar triplet at 3.12 keV, at $T_e = 0.7$ keV. They also note that if the unidentified galaxy cluster line results from the 3.62 keV DR resonance, then the flux would need to be increased by a factor of 30 from the current AtomDB estimate. As a check, we looked at the 3.62 keV DR resonance feature in the NOMAD and APEC spectra and compared its emissivity to the He-like triplet. In agreement with Bulbul et al. (2014), at $T_e = 1$ keV, the 3.62 keV DR is roughly 2% of the Ar triplet in both spectra. Given that the relative intensity ratio of the strong He-like lines to the 3.62 keV DR line is also comparable between our EBIT measurements and calculated spectra, we conclude that the He-like DR features are not off as much as the factor of 30 needed for known atomic physics to resolve the problem.

During our investigation, we measured an interesting feature very close in energy to the unidentified line near 3.56 keV. This line, seen in the measured EBIT spectrum and replicated in our NOMAD calculated spectrum (Figure 3), has an intensity comparable to the Ar DR satellite feature near 3.62 keV. Using the NOMAD model, we were able to identify this as $1s^22s2p-1s2p2p3p$ electric dipole DR transitions from $Ar^{15+}$ with an approximate energy of 3.557 keV. AtomDB does not include DR satellite lines for $Ar^{15+}$ recombining to $Ar^{14+}$; therefore, the 3.557 keV feature was not included in Bulbul et al. (2014), and it is not in the AtomDB spectra in Figure 4 (bottom panel) and Figure 5. It can clearly be seen in our $T_e = 1$ keV NOMAD spectrum (Figure 4 (top panel) and Figure 5).

Using FAC, we produced data for 1s22f'2f'' and 1s22f'3f'' DR satellite lines between 3.075 and 3.672 keV. This data was added to AtomDB and the ratio of the flux with and without the new lines was evaluated in three energy bands and over a range of electron temperatures. The three energy bands include: 3.1–3.2 keV (corresponding to the $Ar^{16+}$ HeII complex), 3.66–3.72 keV (at $Ar^{16+}$ HeI), and 3.5–3.66 keV (where the unidentified line, $Ar^{15+}$, and $Ar^{15+}$ DR lines lie). As shown in Figure 6, the added data has minimal effects on the HeII and HeI complexes, as these lines were already very bright. However, the new DR data leads to significant enhancement of the DR feature around 3.6 keV, especially at lower temperatures.

In Figure 7 (top panel), the Ar emissivity was calculated at $T_e = 1.72$ keV using the original AtomDB data and again with the newly included DR data. The emission is broken up for each Ar charge state, demonstrating the lack of $Ar^{15+}$ features in the original spectrum. The new $Ar^{15+}$ DR features are seen predominately around 3.64 keV. Their effect is further highlighted in Figure 7 (bottom panel) where the ratio of the total emissivity with and without the features is calculated for each energy bin. This produces a maximum factor of 44 increase in emissivity around 3.65 keV.

Bulbul et al. (2014) find a range of temperatures for different components used to model their plasma. The lowest of these is $T_e = 2.0$ keV for the “Excluding Nearby Clusters” sample. At this temperature, the new DR data enhances the flux in the 3.5–3.66 keV band by a factor of 2. While significant, this is much smaller than the factor of 30 that Bulbul et al. (2014) state is required for this line to explain the 3.55 keV feature.

In a recently released preprint, Bulbul et al. (2019, hereafter BUL19) report EBIT experiments in a similar vein to these, aiming to measure the effect of the Ar DR emission. Their results are similar to ours in that they also find that their measured Ar DR is more intense than allowed for in AtomDB and therefore in Bulbul et al. (2014), but not by the factor of 30 required for Ar DR to explain the unidentified feature. In particular at $T_e = 1.74$ keV, BUL19 report a factor of 2.6 in missing flux in the 3.54–3.645 keV range (from BUL19, Table 4) when comparing EBIT measurements to spectra produced with AtomDB v3.0.8. They added DR data from Beiersdorfer et al. (1995) Tables V and VI including 1s3f' data spanning 3.645–3.680 keV and 1s22f' data between 3.145 and 3.588 keV. With the added lines, a better fit at

![Figure 5. Comparison of the DR spectra produced with APEC and spectra produced with NOMAD near the unidentified line at 3.57 keV.](image)
3.55–3.59 keV was obtained, but no improvement between 3.6 and 3.65 keV was observed. BUL19 mention that the additional lines cannot explain the extra flux they measured in the Ar16+ + Heβ DR lines. Since the Ar15+ DR lines added in their work only spanned 3.145–3.588 keV, conclusions cannot be made regarding their effect on the total flux in this region.

As previously discussed in this work, we added Be-like DR data to AtomDB covering a wider energy range (3.075–3.672 keV). At $T_e = 1.72$ keV (close to the BUL19 temperature), the addition of these lines produced a factor of 2 increase in the total flux between 3.5 and 3.66 keV. As demonstrated in Figure 7, we saw the largest increase in flux between 3.63 and 3.67 keV, suggesting these lines account for a large portion of missing flux reported by BUL19 in Table 4. The largest discrepancy they report between experiment and AtomDB is a factor of 10.7 difference in flux in the energy region between 3.630 and 3.645 keV. Inclusion of the Be-like data in this work increases the flux in this energy region by a factor of 14.5 at $T_e = 1.72$ keV. Finally, as discussed in Section 4.4, we also found 1s2s−1s2s3p transitions at 3.62 keV and 3.64 keV that were either missing or greatly underestimated in AtomDB. Amending these issues will add more to the missing flux in this region.

### 6. Conclusions

Searching for possible atomic origins of the unidentified line in the stacked spectra of galaxy clusters (Bulbul et al. 2014), we measured X-ray emission from Ar ions at the NIST EBIT facility. The excellent agreement shown between our EBIT and NOMAD modeled non-Maxwellian spectra provides a high level of confidence in the atomic data used in our model. In comparing a $T_e = 1$ keV Maxwellian-distributed spectra...
produced by the NOMAD code to that produced with AtomDB/APEC, we find good agreement in the line intensity ratio of the He-like triplet to the 3.62 keV DR, confirming that the Ar^{15+} DR is not off by the factor of 30 required to explain the unidentified feature. We also found that the AtomDB spectra has significant emission missing in the energy region near the unidentified line due to Ar^{15+} DR features. Including missing Ar^{15+} DR data in AtomDB resulted in a factor of 2 increase in the flux between 3.5 and 3.66 keV at T_e = 1.72 keV. There are also a number of Ar^{16+} DR transitions missing or underestimated in the AtomDB data that show up near 3.64 keV and 3.62 keV in Figure 5. Combined, these features contribute to a significant amount of emission that was not accounted for in AtomDB and therefore not in the Bulbul et al. (2014) work. These missing or inaccurate DR lines also account for the missing emission reported in BUL19 in this energy region.

Finally, while charge-states lower than He-like Ar may not contribute significantly to individual galaxy cluster emission (which are typically at much higher temperatures where these low charge-states are less abundant), they may be important in lower temperature astrophysical objects, in non-Maxwellian plasma sources, and in stacked spectra where weak features can be greatly enhanced. This was clearly demonstrated by comparing spectra from our controlled EBIT plasma to Beiersdorfer et al. 2015, APEC, we find good agreement in the line intensity ratio of the He-like triplet to the 3.62 keV DR, confirming that the Ar^{15+} DR is not off by the factor of 30 required to explain the unidentified feature. We also found that the AtomDB spectra has significant emission missing in the energy region near the unidentified line due to Ar^{15+} DR features. Including missing Ar^{15+} DR data in AtomDB resulted in a factor of 2 increase in the flux between 3.5 and 3.66 keV at T_e = 1.72 keV. There are also a number of Ar^{16+} DR transitions missing or underestimated in the AtomDB data that show up near 3.64 keV and 3.62 keV in Figure 5. Combined, these features contribute to a significant amount of emission that was not accounted for in AtomDB and therefore not in the Bulbul et al. (2014) work. These missing or inaccurate DR lines also account for the missing emission reported in BUL19 in this energy region.

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Measurements of the Linear Polarization of Satellite Transitions from Li-like Ar Ions

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ABSTRACT

Using two polarization sensitive Johann-type crystal spectrometers at the NIST electron beam ion trap facility, we measured the linear polarization of well-known dielectronic recombination satellite transitions from Li-like Ar ions. Measurements were compared with theoretical predictions based on relativistic magnetic sublevel atomic kinetics using the density-matrix theory. The large positive and negative polarization values found for the various strong satellite lines demonstrate that polarization should be considered when these lines are used in plasma diagnostic investigations.

Keywords: atomic processes, methods: laboratory: atomic, techniques: spectroscopic, dielectronic recombination, polarization, highly-charged ions

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1. INTRODUCTION

Physical properties of astrophysical and laboratory plasmas are often determined from spectral observations aided by theoretical models. Deriving accurate information from spectra requires a reliable knowledge of the ionization balance and a detailed understanding of the atomic processes occurring. One such process, dielectronic recombination (DR), can be a dominant collisional process that plays a vital role in determining the equilibrium conditions of hot, electron-ionized plasmas. The radiationless first step of DR occurs when a continuum electron is captured by a recombining ion, while a bound atomic electron is simultaneously excited. As the ion relaxes from the double excited state to the ground state, through a single or multiple radiative decays, the DR process is complete. The required matching of the a.) kinetic energy (KE) of the initial continuum electron plus the binding energy of the captured electron with b.) the excitation energy of the core electron makes DR a resonant process occurring only with electrons of select KE in the plasma. This resonant behavior can greatly alter the ionization balance, making the accuracy of DR data critical when implemented in plasma models.

EBITs, well suited for systematic atomic studies due to the variety of accessible elements and the tuneable quasi mono-energetic electron beam that allows for a degree of charge state and excitation selectivity, are ideal devices for studying DR and producing atomic data such as DR cross sections (Knapp et al. 1993; McLaughlin et al. 1996; Gall et al. 2019). The emission produced in an EBIT originates from ions excited by a unidirectional electron beam, rather than an isotropic electron distribution, therefore the emitted radiation can be anisotropic and linearly polarized (Percival & Seaton 1958). Anisotropic and polarized emission is also observed in astrophysical sources such as jets and solar flares (see e.g. Havag (1979); Akita et al. (1983); Inal & Dubau (1987); Dubau et al. (1996)) where beams of electrons travel along magnetic field lines. The polarized emission in both of these cases originates from non-statistically populated magnetic sublevels, where the sublevels are populated from processes such as electron impact excitation (EIE) or recombination (radiative or dielectronic). Therefore, to understand the emitted line intensity ratios, sublevel specific differential analysis may be required.

The controlled and relatively simple plasma environment created by EBITs (compared with astrophysical environments) is ideal for polarization measurements, needed to benchmark various theoretical approaches used to calculate cross sections (see e.g. Takics et al. (1996); Beiersdorfer et al. (1996); Nakamura et al. (2003)). While the majority of these studies focus on polarized emission following EIE, there have been few measurements of polarized emission from states populated from dielectronic capture. These include measurements from highly charged Xe (Jörg et al. 2015), Kr (Shah et al. 2015), and Fe (Shah et al. 2018; Shlyaptseva et al. 1998).

Adding to the limited collection, we report measurements of the linear polarization from the 1s2p(jD) D1/2 → 1s2p1/2sP0/2 (j in the notation of Gabriel (1972)), 1s2p(jD) D3/2 → 1s2p1/2sP0/2 (k), 1s2p(3P) P0/2 → 1s2p1/2sP0/2 (a), 1s2p(3P) P1/2 → 1s2p1/2s(S)1/2 (τ), 1s2p2(1S)1/2P0/2 → 1s2s2P1/2 S1/2 (q), and the blended 1s2p2(3P) 3P1/2 → 1s2s2S1/2 and 1s2p2(3P) 3P1/2 → 1s2s2S1/2 (k/s) satellite transitions from Li-like Ar.

Finally, the uncertainties stemming from the complicated and challenging calculations required for DR has led to increasingly accurate calculations (e.g. Bryans et al. (2006); Badnell (2006)) and to a number of electron beam ion trap (EBIT) and storage ring experiments (see e.g. Savin (2007); Wargelin et al. (2001); McLaughlin et al. (1996); Beiersdorfer et al. (1992); Ali et al. (1991)) to benchmark the theory (Savin & Laming 2002). The ongoing effort to produce accurate DR data and test of theory will continue as experimental and theoretical methods become increasingly sophisticated and as high-resolution X-ray satellites, such as the X-ray Imaging and Spectroscopy Mission (XRISM), demand more from astrophysical models such as the CHIANTI package (Dere, K. P. et al. 1997) and the astrophysical plasma emission code (APEC) (Smith et al. 2001). Our data add to this effort and are intended to not only improve the quality of atomic DR data that will be produced from anisotropic laboratory plasmas, but also benchmark theories used to interpret spectra from anisotropic astrophysical plasma sources.

In the sections that follow, we outline the details of our measurement followed by our experimental results. This is followed by a comparison with polarization values calculated with the aid of the flexible atomic code (FAC) (Gu 2008).

2. EXPERIMENTAL PROCEDURE

2.1. Polarization of the Emission from the EBIT Plasma

Measurements were taken at the EBIT facility at the National Institute of Standards and Technology (NIST). The NIST EBIT has been described extensively in previous works (see e.g. Gillaspy (1997)), but relevant details are discussed here. In short, the EBIT is a device used to create and trap ions for spectroscopic study. The
main components include the electron gun (egun), drift tube (trap), and collector assemblies. The quasi monoenergetic electron beam is compressed to approximately a 35 µm radius and 10^{13} cm^{-3} density by a 2.7 T superconducting magnet. Electrons emanate from a barium doped, 3 mm diameter, curved cathode in the egun with currents up to 150 mA. The finely tunable high voltages placed on the drift tubes can produce electron beam energies up to 30 keV. (We note that all quoted electron beam energies in our work have been space charge corrected (e.g. Porto et al. (2000)), where space charge effects were estimated by comparing experimental and theoretical resonance beam energies.) Neutral atoms, or low charge state ions, are injected into the drift tube region where they interact with the electron beam and become ionized through electron impact ionization. Ions are electrostatically trapped in the axial direction by the relative voltages placed on the three drift tube electrodes in the central region of the machine. The space charge of the electron beam and the shape of the electrodes provide additional radial trapping of the ions. Measurements are taken through observation ports located around the trap region and perpendicular to the electron beam direction.

The cylindrically symmetric system basically consists of stationary ions interacting with a beam of e^-s traveling vertically through the center of the EBIT. For this geometry, the degree of linear polarization of the emission measured at 90° relative to the electron beam direction is defined as:

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

(1)

Treating light emitted from atomic transitions as transverse waves with the electric field (E), magnetic field (B), and propagation (k) directions perpendicular to each other, polarization is defined by the direction of E. Thus, I_\parallel and I_\perp are two polarization components of the intensity with E parallel and perpendicular to the quantization axis (defined as the electron beam axis), respectively.

In our measurements two polarization sensitive, Johann-type crystal spectrometers with CCD detectors were used to measure the linear polarization using the “two crystal technique” (see e.g. Takács et al. (1996); Beiersdorfer et al. (1996)). One of the crystal spectrometers was oriented with the plane of dispersion of the crystal perpendicular to the electron beam (horizontal orientation), while the second spectrometer was rotated such that the plane of dispersion was parallel with the electron beam (vertical orientation). The measured intensity for the vertical (I_\text{vert}) and horizontal (I_\text{hor}) orientations can be expressed as:

\[ I_\text{vert} = \Omega_v \eta_v \left[ R_\parallel + I_\perp \right] \]  

(2)

\[ I_\text{hor} = \Omega_h \eta_h \left[ I_\parallel + R_\parallel \right] \]  

(3)

where \( \eta_v,h \) is the detection efficiency and \( \Omega_v,h \) is a factor including the geometry with solid angle of acceptance for the vertical and horizontal spectrometers, respectively (Biedermann et al. 2002). Defining \( R_\parallel \) and \( R_\perp \) as the integrated crystal reflectivities for X-rays polarized parallel and perpendicular to the plane of dispersion, then \( R \) is defined as the ratio: \( R = \frac{R_\perp}{R_\parallel} \). Values for \( R \) may be roughly estimated by \( R = \cos^m(2\theta) \), where \( 1 \leq m \leq 2 \) and \( \theta \) is the Bragg angle. The limits of \( m \) correspond to perfect (m=1) and mosaic (m=2) crystals, while real crystals typically have reflectivity values between the two limits. The reflectivity values used for our work were calculated using the X-ray Oriented Program (XOP) software. Reflectivities were calculated for a range of Bragg angles including angles corresponding to 3000, 3100, 3124, 3140, and 3200 eV photon energies. A third order polynomial was fit to these data points to extract the \( R \) value for each measured line.

Eqs. 2 and 3 show that both spectrometers preferentially reflect X-rays polarized perpendicular to the plane of dispersion. In the case of the vertical orientation \( I_\perp \) is perpendicular to the dispersion plane, while in the horizontal orientation \( I_\parallel \) is perpendicular to the plane of dispersion.

Given the vertical slit like shape of the EBIT source, the effective source size will be different for the two spectrometer orientations (Henderson et al. 1990). To account for this, the spectrometers were normalized to one another using an unpolarized line as an intensity reference. If the same crystal is used in both spectrometers (same \( R \) value), the normalization factor (N) reduces to the ratio of the geometrical factors and efficiencies.

\[ \frac{I_\text{hor}}{I_\text{vert}} = \frac{\Omega_v \eta_v}{\Omega_h \eta_h} = N \]  

(4)

This relation can be used to express \( I_\text{vert} \) in terms of \( \Omega_v \eta_v \). Then, combining Eqs. 1, 2, 3, and 4, the measured polarization may be defined in terms of the measured intensities, the normalization factor and the crystal reflectivities:

\[ P = \frac{(1 + R)(I_\text{hor} - N I_\text{vert})}{(1 - R)(I_\text{hor} + N I_\text{vert})} \]  

(5)

2.2. Experimental Setup

Measurements were taken simultaneously with the two crystal spectrometers (capable of resolving features less...
than 2 eV apart at 3 keV X-ray energy) and a high count rate, high purity Ge (HPGe) detector (135 eV energy resolution at 5.9 keV X-ray energy). Both crystal spectrometers housed a Si(111) crystal, with 6.271 Å interplanar spacing (2d value from Henke et al. (1993)). The HPGe signal was used to maximize the X-ray emission by optimizing the EBIT parameters and the Ar gas injection pressure. Measurements were taken in a steady-state mode, where the electron beam energy and current remain constant during measurements. In addition to improving the signal to noise, this mode allows the charge state balance to reach steady-state. The two crystal spectrometers were set to reflect 3114 eV X-ray photons at the center of the spectrum that fit across the CCD detectors. With a bandwidth of roughly 120 eV, the spectrometers measured photon energies ranging from 3054 eV to 3174 eV and covered the KLL (in inverse Auger notation) DR satellite transitions of interest. The He-like resonance $1s^2 1S - 1s2p^1P(\text{w})$, intercombination $1s^2 1S - 1s2p^3P(x, y)$, and forbidden $1s^2 1S - 1s2p^3S(\text{z})$ lines were first measured with an electron beam energy of 3.87 keV and an electron beam current of 128.5 mA for calibration purposes. X-rays were collected in 3 minute intervals for a total of 39 minutes. The KLL resonances were measured while finely scanning the electron beam energy from 2.16 keV to 2.29 keV in 10 eV increments. This electron beam energy range includes the resonance energies of all of the strong Li-like satellite transitions of our interest. The electron beam current was kept constant at 74 mA while measurements were taken for 12-18 minutes at each beam energy setting.

2.3. Experimental Analysis and Results

The data collected by the CCDs included contributions from diffracted x-rays, electronic readout noise, cosmic rays, and thermal noise. Energy and spatial discrimination techniques outlined in Hudson et al. (2007) were used to filter the data and improve the signal to noise. Additional procedures were used to process the data from the vertical spectrometer, since, as discussed in Zschornack et al. (1982), the finite source size (due to the parallel orientation) can lead to shape alterations of the diffracted lines. Features were systematically fit and straightened to reduce the broadening. Additional details of this procedure are given in (Buechele et al. 2019).

Spectral lines were fit with single Gaussian functions using the weighted fitting tools of a multi-peak fitting software package. A constant background was fit to the horizontal spectra while a cubic function was used to fit the background of the vertical spectra. Fits were performed by weighing each data point by the statistical uncertainty, therefore the total uncertainty in line intensities includes statistical, background, and fitting uncertainties. To reduce the uncertainties in the line positions, particularly for very weak features, spectra were summed to increase the signal to noise. Peak locations and widths obtained by fitting the summed spectra were later used as constraints when fitting individual spectra.

While a number of unpolarized lines exist in the spectra, the Li-like $\text{m}$ (Gabriel 1972) line was the strongest, well resolved feature suitable for normalization. The normalization factor (Eqn. 4) was determined by taking the ratio of intensities of the m line in the summed (2.25 keV and 2.26 keV) horizontal and vertical spectra. The normalization factor (4.22 ± 0.38) as described above was used to correct the vertical spectra for differences in efficiencies and geometry.

Results from the electron beam energy scan over the KLL resonances are shown in Fig. 1, where the w, x, y, and z lines (energies from Bruhns et al. (2007); Saloman (2010)) measured at 3.87 keV were used to calibrate the X-ray spectra. The scan highlights the resonant nature of the DR process and the energy spread of the electron beam. The strong Li-like features have been labeled using the notation of Gabriel (1972). Weak features appearing at lower photon energies and at electron beam energies above 2.22 keV are from satellite transitions in Be-like ions.

To estimate the electron beam energy profile and width, the intensity of the j line was measured at each electron beam energy. The line intensity vs. electron beam energy shown in Fig. 4 was fit with a Gaussian function weighted with the statistically uncertainty. The full width at half maximum (FWHM) of the electron beam energy profile was found to be approximately 40 eV in agreement with previous estimates.

The spectra measured at 2.25 keV electron beam energy, where the m line is close to its maximum measured value, are shown in Fig. 2 (top panel). The j and k lines measured with the horizontal spectrometer are much stronger than those measured with vertical, indicating a large, positive polarization. Fig. 2 also shows that the m line, which was used for normalization appears unpolarized as expected. The spectra measured at 2.22 keV electron beam energy, where the j line is close to its maximum measured value, are shown in Fig. 3 (top panel). The spectra shows that the t,s blended line has a positive polarization, while the a line has a negative polarization. As a good verification of our normalization, the r line, which is fundamentally unpolarized, has roughly equal intensity in both spectra.
The polarization values for the j, k, r, q, t/s blend, a and m are given in Table 1 along with the electron beam energy at which they were measured. The values reported were taken at the electron beam energy corresponding to the maximum intensity of each line.

2.4 Theoretical Approach

The theoretical total intensity of lines produced by a beam of electrons observed at 90° relative to the beam direction is given by:

\[ I(90°) = I_1 + I_\perp \]  

(6)

Using the formula describing the angular dependence of dipole radiation given in Percival & Seaton (1958), \( I(90°) \) is related to the 4π-averaged intensity by:

\[ I(90°) = \langle I \rangle = \frac{3}{2} - P \]  

(7)

By combining Eqns. 1, 6, and 7, the polarization components of the intensity can be expressed in terms of the 4π-averaged intensity:

\[ I_1 = \frac{3}{2} \langle I \rangle \left( \frac{1 - P}{3 - P} \right) \]  

(8)

\[ I_\perp = \frac{3}{2} \langle I \rangle \left( \frac{1 + P}{3 - P} \right) \]  

(9)

Following the procedure of Shlyaptseva et al. (1998), \( \langle I \rangle \) can be written in terms of the intensity factor \( Q_i \) (Vainshtein & Safronova (1978)), the electron energy distribution function \( f(E) \), and the autoionization energy \( E_{\text{AI}} \). For this experiment, as previously discussed, the electron energy distribution is characterized by a Gaussian function centered at \( E_0 \) with a FWHM of 40 eV (proportional to \( \Delta E \)).

\[ I_1 = \frac{3}{2} Q_i e^{\exp} \left[ - \left( \frac{E_0 - E_{\text{AI}}}{\Delta E} \right)^2 \right] \left( \frac{1 - P}{3 - P} \right) \]  

(10)

\[ I_\perp = \frac{3}{2} Q_i e^{\exp} \left[ - \left( \frac{E_0 - E_{\text{AI}}}{\Delta E} \right)^2 \right] \left( \frac{1 + P}{3 - P} \right) \]  

(11)

The theoretical polarization (P) values used in the Eqs. 10 and 11, were calculated within the photon density matrix formalism (see e.g. Inal & Dubau (1989); Blum (1996); Shlyaptseva et al. (1998); Balashov et al. (2000); Sharma et al. (2010)). Since transitions from upper levels with total angular momentum \( J=1/2 \) are fundamentally unpolarized (see Inal & Dubau (1987)), the o, p, h, v, c, d, t, r, m, and t lines have \( P=0 \).

Within the electric dipole approximation, the degree of polarization of the remaining DR lines, observed at 90° relative to the electron beam, can be expressed as (Balashov et al. 2000; Sharma et al. 2010):

\[ P = -3 G^2 (\alpha_{a} J_{a} M_{a} J_{f} M_{f} A_{20}) \frac{2 - G^2 (\alpha_{a} J_{a} M_{a} J_{f} M_{f}) A_{20}}{2} \]  

(12)

where \( A_{20} \) and \( G^2 \) are the alignment parameter and the structure function respectively, used for electric dipole transitions. The normalized alignment parameter, \( A_{20} \) describes the non-statistical population distribution among magnetic sublevels of the upper level and is given as:

\[ A_{20} = \frac{\sum_{M_{a}=-J_{a}}^{J_{a}} (-1)^{J_{a}+M_{a}-J_{f}} (J_{a} M_{a} J_{r} M_{r} - M_{r}(20)) \sigma(\alpha_{a} J_{a} M_{a})}{|\langle J_{a} M_{a} | J_{a} M_{a} \rangle|^{2}} \]  

(13)

where J, M, and \( \alpha \) denote the total angular momentum, its corresponding magnetic component, and all other quantum numbers required to describe the state, respectively. For the dielectronic recombination process, the initial state of the ion (prior to \( e^- \) capture), the intermediate doubly excited state, and the final state (after photon emission) are characterized by subscripts i, id, and f, respectively. \( \langle J_{a} M_{a} | J_{a} M_{a} \rangle \) in Eqn. 13 represents the Clebsch-Gordan coefficient, \( \sigma(\alpha_{a} J_{a} M_{a}) \) is the cross section for dielectronic capture of the substate with magnetic quantum number M, \( \sigma(\alpha_{a} J_{a} M_{a}) \) is the total dielectronic capture cross section.

The structure function \( G^2 \), which reflects the angular momentum coupling between the intermediate doubly excited and the final states can be expressed as:

\[ G^2 (\alpha_{a} J_{a} M_{a} J_{f} M_{f}) = (-1)^{(1+J_{a}+J_{f})} \left\{ \begin{array}{ccc} 1 & 1 & 2 \\ J_{a} & J_{a} & I_{f} \end{array} \right\} \sqrt{\frac{12 J_{f}+2}{2}} \]  

(14)

where the quantity in curly brackets denotes the Wigner 6j-symbol.

From Table 1, the k, q, and s lines all have \( J_{a}=3/2 \) and \( I_{f}=1/2 \) values. Solving for the alignment parameter and structure function, the final expression for the degree of polarization for this transition is:

\[ P(90°) = \frac{3}{2} \sigma(1/2) - \sigma(3/2) \]  

(15)

where \( \sigma(M_{a}) \) again represents the cross section for dielectronic capture of the substate with magnetic quantum number \( M_{a} \).

The Flexible Atomic Code (FAC) (Gu 2008) was used to generate the required atomic data for Eqns. 10, 11, and 12. This data included the energy levels, radiative and autoionization probabilities, and dielectronic capture rates. Only dielectronic capture from the ground state of He- and Li-like Ar was considered to populate
Figure 1. Scan of electron beam energies over KLL resonances. a.) Measured spectra from horizontally oriented spectrometer. b.) Measured spectra from vertically oriented spectrometer.
Figure 2. Spectra taken at 2.25 keV beam energy. Top panel: Experimental spectra from horizontally and vertically oriented spectrometers. Bottom panel: Synthetic spectra.

Figure 3. Spectra taken at an electron beam energy near the maximum intensity of the j line. Top panel: Experimental spectra from horizontally and vertically oriented spectrometers. Bottom panel: Synthetic spectra.
Table 1. Measured and theoretical polarization values. Li-like satellite energies from Yerokhin & Surzhykov (2018) in the notation of Gabriel (1972). Line energy of the t/s blended line measured experimentally.

<table>
<thead>
<tr>
<th>Line</th>
<th>Ebeam (keV)</th>
<th>Transition</th>
<th>E_\text{EF}(\text{keV})</th>
<th>E_\text{thex}(\text{keV})</th>
<th>P_{\text{exp}}</th>
<th>P_{\text{th}}</th>
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<td>1s2s'2p'[2P]P_{3/2} \rightarrow 1s^22p_{1/2}P_{1/2}</td>
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<td>-</td>
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<td>p</td>
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<td>2.16</td>
<td>-</td>
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<td>1s2p'[2P]P_{3/2} \rightarrow 1s^22p_{1/2}P_{1/2}</td>
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<td>-</td>
<td>-</td>
<td>0.00</td>
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<tr>
<td>v</td>
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<td>-</td>
<td>0.00</td>
</tr>
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<td>-</td>
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<td>3091.38</td>
<td>1s2p'[2P]P_{3/2}P_{3/2} \rightarrow 1s^22p_{3/2}P_{1/2}</td>
<td>2.21</td>
<td>-</td>
<td>-</td>
<td>0.60</td>
</tr>
<tr>
<td>l</td>
<td>3104.19</td>
<td>1s2p'[2P]P_{3/2}P_{3/2} \rightarrow 1s^22p_{3/2}P_{1/2}</td>
<td>2.23</td>
<td>-</td>
<td>-</td>
<td>-0.75</td>
</tr>
<tr>
<td>j</td>
<td>3104.29</td>
<td>1s2p'[2P]P_{3/2}P_{3/2} \rightarrow 1s^22p_{3/2}P_{1/2}</td>
<td>2.23</td>
<td>2.23</td>
<td>0.46 ± 0.08</td>
<td>0.50</td>
</tr>
<tr>
<td>k</td>
<td>3107.37</td>
<td>1s2p'[2P]P_{3/2}P_{3/2} \rightarrow 1s^22p_{3/2}P_{1/2}</td>
<td>2.23</td>
<td>2.23</td>
<td>0.55 ± 0.08</td>
<td>0.60</td>
</tr>
<tr>
<td>c</td>
<td>3107.526</td>
<td>1s2p'[2P]P_{3/2}P_{3/2} \rightarrow 1s^22p_{3/2}P_{1/2}</td>
<td>2.23</td>
<td>-</td>
<td>-</td>
<td>0.00</td>
</tr>
<tr>
<td>d</td>
<td>3110.70</td>
<td>1s2p'[2P]P_{3/2}P_{3/2} \rightarrow 1s^22p_{3/2}P_{1/2}</td>
<td>2.23</td>
<td>-</td>
<td>-</td>
<td>0.00</td>
</tr>
<tr>
<td>a</td>
<td>3110.71</td>
<td>1s2p'[2P]P_{3/2}P_{3/2} \rightarrow 1s^22p_{3/2}P_{1/2}</td>
<td>2.23</td>
<td>2.23</td>
<td>-0.53 ± 0.28</td>
<td>-0.74</td>
</tr>
<tr>
<td>r</td>
<td>3112.47</td>
<td>1s2s2p'[2P]P_{3/2} \rightarrow 1s^22s'2p_{3/2}</td>
<td>2.20</td>
<td>2.18</td>
<td>0.05 ± 0.14</td>
<td>0.00</td>
</tr>
<tr>
<td>b</td>
<td>3113.88</td>
<td>1s2s2p'[2P]P_{3/2} \rightarrow 1s^22s'2p_{3/2}</td>
<td>2.23</td>
<td>-</td>
<td>-</td>
<td>0.60</td>
</tr>
<tr>
<td>q</td>
<td>3114.14</td>
<td>1s2s2p'[2P]P_{3/2} \rightarrow 1s^22s'2p_{3/2}</td>
<td>2.20</td>
<td>2.19</td>
<td>0.47 ± 0.30</td>
<td>0.60</td>
</tr>
<tr>
<td>t/s blend</td>
<td>3124.30* t</td>
<td>1s2s2p'[2P]P_{3/2} \rightarrow 1s^22s'2p_{3/2}</td>
<td>2.21</td>
<td>2.21</td>
<td>0.25 ± 0.12</td>
<td>0.24</td>
</tr>
<tr>
<td></td>
<td></td>
<td>s 1s2s2p'[2P]P_{3/2} \rightarrow 1s^22s'2p_{3/2}</td>
<td>2.21</td>
<td>2.21</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m</td>
<td>3126.35</td>
<td>1s2s2p'[2P]P_{3/2} \rightarrow 1s^22p_{3/2}P_{1/2}</td>
<td>2.25</td>
<td>2.25</td>
<td>0.00 ± 0.17</td>
<td>0.00</td>
</tr>
<tr>
<td>n</td>
<td>3129.52</td>
<td>1s2s2p'[2P]P_{3/2} \rightarrow 1s^22p_{3/2}P_{1/2}</td>
<td>2.25</td>
<td>-</td>
<td>-</td>
<td>0.00</td>
</tr>
</tbody>
</table>

From the polarization calculations, the intensities in the parallel and perpendicular polarization modes were calculated using Eqs. 10, and 11. In Figs. 2 and 3, the measured and theoretical spectra, taken with an electron beam energy of 2.22 keV and 2.25 keV respectively, are shown for comparison. The calculated crystal reflectivities were applied to the theoretical intensity components to produce the synthetic EBIT spectra according to Eqs. 2 and 3. The theoretical spectra, normalized to the experimental unpolarized m line in the 2.25 keV electron beam energy spectra, shows strong agreement with our experiment. The j, k, and t/s lines show a positive polarization in both the experimental and synthetic spectra with comparable relative intensities between the horizontal and vertical spectra. Similarly the a line shows negative polarization in both spectra, while the m, n and r lines appear unpolarized in both the theoretical and experimental spectra.

In comparing our experimental and theoretical polarization values in Table 1, we see that the strongest j and k lines seem systematically lower than the theoretical values. The equations used in our analysis assumed that the electrons travel in a single (z) direction along the axis of the EBIT. While a good approximation, this
is not physically true as electrons follow a spiral path as they interact with the magnetic field. Typically EBITs are designed to minimize the magnetic field in the electron gun region. This means that as electrons travel from the electron gun (near zero magnetic field) to the trap (2.7 T field), they travel along a converging helical path. As a result, the quantization axis may be rotated from the z-axis (called the pitch angle), and the observation angle may be off from the assumed 90°. These effects may lead to an amount of depolarization of the observed spectral lines.

To estimate the maximum amount of depolarization, we follow the optical approach developed by Herrmann (1958) and verified by Beiersdorfer & Slater (2001). The Herrmann theory shows that the product of the beam area and the transverse temperature is constant. Using this to equate the area and transverse energy ($E_{\perp}$) we may calculate $E_{\perp}$ in the trap as:

$$E_{\perp} = kT \left( \frac{\gamma^2}{c^2} \right)$$

(16)

where $k$ is the Boltzmann constant, $T$ is the temperature of the cathode, and $r_c$ and $r_t$ are the beam radius at the cathode and trap respectively. From the transverse energy, the pitch angle ($\gamma$) is calculated as:

$$\sin(\gamma)^2 = \frac{E_{\perp}}{E_{\text{beam}}}$$

(17)

where $E_{\text{beam}}$ is the electron beam energy determined by the voltage placed on the central drift tube.

Using $T=1400$ K, $r_c = 1.5 \text{ mm}$, and $r_t = 35 \text{ \mu m}$, we find $E_{\perp} = 222$ eV and $\gamma=18.4^\circ$ for an electron beam energy of 2.22 keV. Noting that the parameters including the beam radius at the cathode and trap, magnetic field at the egun, and cathode temperature are not exactly know, the lower limit of $E_{\perp}$ is estimated to be 65 eV with $\gamma = 9.8^\circ$.

From the estimated transverse velocity, the true polarization may be calculated as (Gu et al. 1999):

$$P_0 = \frac{2P}{2 - \frac{2P}{P_{\text{true}}}} \left(3 - P\right)$$

(18)

where $P_0$ is the polarization for the case when $E_{\perp} = 0$, and $P$ is the measured polarization. Using this formula with the maximum $E_{\perp}$ value of 222 eV, the estimated true polarization values are: $P_j = 0.52$, $P_k = 0.62$, $P_n = -0.64$, $P_e = 0.06$, $P_d = 0.53$, and $P_{\text{true}} = 0.29$.

3. CONCLUSIONS

Using the two crystal method, we report the linear polarization of KLL DR transitions from Li-like Ar. The experimental results are summarized in Table 1 along with theoretical predictions. The comparison between experimental and theoretical spectra in Figs. 2 and 3 shows overall good agreement. This is further seen in Table 1, where all theoretical predictions fall within the experimental uncertainties. Taking depolarization effects into account shifts the measured polarization to slightly higher values, however they still fall within the reported uncertainties. The data presented are intended to contribute to the small collection of existing EBIT measurements of linear polarization of emission from DR transitions and may be used to benchmark calculations produced by different theoretical approaches.

4. ACKNOWLEDGMENTS

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Software: FAC (Gu 2008)

REFERENCES


Plenum Press
Appendix C  Codes

Matlab code used to create cuts, taken from [47], is shown below. Cuts were taken in shield voltage (rather than electron beam energy).
%2-1 cut 
clear all 
clc 
intensity = xlsread('Measured_Ge_detector.xlsx','Sheet5','C3:EF477'); 
[m,n] = size(intensity); 
i = 1; 
j=1; 
two = zeros(n,1); 
three = zeros(115,1); 
for i =1:n 
    for j = 116:133 
        two(i)= two(i)+ intensity(j,i); 
        j = j+1; 
    end 
    i = i+1; 
end 
p=20; 
i=1; 
% 3-1 cut 
for p =20:n 
    for j = 144:157 
        three(i)= three(i)+ intensity(j,p); 
        j = j+1; 
    end 
    i = i+1; 
p = p+1; 
end 

% n=2 RR cut 
RR = 0; 
SV = round(xlsread('Measured_Ge_detector.xlsx','Sheet5','C1:EF1')); 
sv = length(SV); 
k = 1; 
diff = zeros(sv,1); 
for k =2:sv 
    diff(k) = SV(k)-SV(k-1); 
end 
i = 1; 
s =1; 
t = l13; 
v = l27; 
RR = zeros(n,1); 
for l = 1:n 
    t = t+ diff(l); 
    v = v + diff(l); 
    for s = t:v 
        RR(l) = RR(l) + intensity(s,l); 
        s = s+1; 
    end 
    l = l+1; 
end

SV2 = xlsread('Measured_Ge_detector.xlsx','Sheet5','C2:EF2');
SV3 = xlsread('Measured_Ge_detector.xlsx', 'Sheet5', 'V2:EF2');
figure
plot(SV2, two, 'b', SV3, three, 'g', SV2, RR, 'r');
xlabel('Shield Voltage (KV)')
ylabel('counts')
legend('n=2 cut', 'n=3 cut', 'RR cut')
figure
subplot(2, 2, 1);
plot(SV2, two, 'b');
xlabel('Shield Voltage (KV)')
ylabel('counts')
title('n=2 cut')
subplot(2, 2, 2);
plot(SV3, three, 'g');
xlabel('Shield Voltage (KV)')
ylabel('counts')
title('n=3 cut')
subplot(2, 2, [3, 4]);
plot(SV2, RR, 'r');
xlabel('Shield Voltage (KV)')
ylabel('counts')
title('n=2 RR cut')
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