Metrology and Transport of Multiply Charged Ions

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METROLOGY AND TRANSPORT OF MULTIPLY CHARGED IONS

A Dissertation
Presented to
the Graduate School of
Clemson University

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

by
Dhruva Kulkarni
May 2017

Accepted by:
Dr. Chad Sosolik, Committee Chair
Dr. W. Rod Harrell
Dr. Endre Takacs
Dr. Steve Stuart
Abstract

The transport and interaction of singly- and multiply-charged ions with matter has been studied. The experiments were performed in an ultra-high vacuum environment. The low- and hyperthermal-energy ion beamline was used as a source of singly charged ions, while the CUEBIT facility was used as a source of multiply charged ions.

The kinetic energy of the ion beam obtained from the CUEBIT is offset from the nominal value expected from the applied electrostatic potentials. These offsets were studied by measuring the kinetic energy of the beam using a retarding field analyzer (RFA). The offset was attributed to the space charge of the electron beam that is used to create the multiply charged ions. The charge density of the electron beam was varied by changing operational parameters of the electron beam, namely the electron beam current and the energy of the electron beam. Ion beams of Ar\(^{4+}\) and Ar\(^{8+}\) were extracted from the source and the offsets observed in the kinetic energy were related to the variation in the space charge potential of the electron beam. Measurements of these offsets, ranging from 100 eV/Q to 300 eV/Q, are significant and important for experiments that aim to utilize the potential energy of slow multiply charged ions.

The transport of ions using capillaries has been studied to investigate the viability of ion-guiding as a means for a novel ion delivery mechanism. Results on transport through large bore capillaries (macrocapillaries) that probe both the geometric and ion-guided mechanisms are presented. The angle- and position-dependent transport properties
were found to depend on the material of the capillary (specifically, whether metal or insulator) and the geometry of the capillary. Rb$^+$ ions at a kinetic energy of 1 keV were transmitted through metal and glass capillaries that were a few centimeters in length and a few millimeters in diameter. Oscillations were observed in the capillaries made of glass which were absent in the metal capillaries. Calculations based on the geometry of the experimental setup and kinematics of the ions showed that these oscillations could be attributed to the charge patches formed on the capillary walls.

Electronic excitations in solids due to energetic ions at low kinetic energy were measured by using Schottky diodes. Hot electron currents measured at the backside of an Ag/n-Si Schottky diode due to ion bombardment on the frontside were found to depend on the kinetic energy (500 eV to 1500 eV) and angle of incidence ($\pm 30^\circ$) of the ion (Rb$^+$) beam. A sharp upturn in the energy dependent yield is consistent with a kinetic emission model for electronic excitations utilizing the device Schottky barrier as determined from current-voltage characteristics. Backside currents measured for ion incident angle are strongly peaked about normal incidence. Accounting for the increased transport distance for excited charges at non-normal incidence, the mean free path for electrons in silver was found to be $5.2 \pm 1.4$ nm, which is consistent with values reported in the literature.
Dedication

I dedicate this thesis to my parents, my wife, my family and to the memories of my dear departed grandparents Pappa and Mandajji.
Acknowledgments

Considering that, on average, this section of any thesis is probably the most read one, and perhaps the only one read in most cases, I was seriously tempted to reproduce here the abstract disguised as acknowledgments; however, in the end, I decided that expressing my gratitude towards all those involved directly or indirectly in this work trumped such an underhanded promotion of this thesis.

I am grateful for the opportunity to hereby thank the people that have contributed to the successful completion of this work. Let me begin by saying that if you, as the reader perusing this page, do not find your name listed as you may have expected, then I apologize for my oversight and hope that you will be gracious enough in your forgiveness to consider the omission as careless rather than intended. Also, the order/length of any of the mentions in this section should not be interpreted as a quantitative measure of their contribution, for such a ranking is not my intention.

At the outset, I would like to thank my committee - Drs. Sosolik, Harrell, Takacs and Stuart - for proof-reading and accepting this thesis. I have had the opportunity to collaborate with Dr. Harrell and his group from the ECE department due to our common interest in device physics. I thank them for their help in characterizing the Schottky diode samples and also for educating me on the various innuendoes of several electrical characterization techniques. I thank Dr. Takacs for his flexibility with the scheduling of the defense as well as many insightful discussions regarding EBIT-related and medical physics-related work.
Dr. Stuart’s observations about the conical capillary were astute, and I am sure that I will remember 22.4 liters/mole for the rest of my life.

This thesis would be incomplete if I did not thank my adviser Prof. Chad Sosolik for all his help over the last few years. To list the specific skills that I have developed due to my association with him will take too much space; so I will suffice it to say that, looking back, I walked into the lab several years ago greener than a blade of grass, and now, after graduating with a doctorate, I owe to him, directly or indirectly, everything that I have learned in this field. I have always appreciated his high standards of scientific rigor, his excellent work ethic, his practical attitude, his patience as well as his persistence, and also his noteworthy people skills. The enthusiasm and energy he has for science emerges in many forms - through research, education, outreach and also just general conversation - and has been inspiring for me as a graduate student. I have enjoyed all my interactions with Chad, whether as his graduate student or teaching assistant or outreach helper, and consider myself very lucky to have had him as my adviser. Also, I would like to thank his wife Janet, for being so friendly and welcoming, for her helpful tips on website development and resume formatting, and also for that delicious Christmas dinner.

I would like to thank the Department of Physics and Astronomy for their continued support over the years. A big thank you to the Physics machine shop is definitely warranted here: without their willingness to work with graduate students in a tireless and inviting manner and their expertise in design and machining, these experiments would have taken much longer to complete. Dr. Jim Harriss has been invaluable for the successful completion of these experiments as well, due to his expertise in thin film growth and general vacuum know-how as well as also being the person in charge of running the CUEBIT facility and providing me a beam of ions to tune into the target chamber. It was nice to work with Dr. Marler briefly towards the end of my graduate student career. I wish her the best of luck in the charge-exchange and other experiments that she is planning on conducting in the near
future. I would also like to thank the faculty for their excellent instruction and approachable presence. In particular, I loved Dr. Dieter Hartmann’s courses in Classical Mechanics with differential geometry, Statistical Mechanics, and GR, and I hope he continues to teach those courses in the future.

I gratefully acknowledge the financial support from DARPA and NSF along with the College of Science and Engineering. I would also like to acknowledge the Graduate Student Government sponsored Professional Enrichment Grants (PEGs), which enabled me to attend quite a few conferences. Along with the PEGs and travel support from Chad, I believe the exposure I have gained by attending these conferences has been extremely helpful for my professional development and also in terms of professional networking. It was at one of these conferences that I overheard an unsolicited remark about my rather heavy smoking habits that led to me escaping the conference at every possible break, and turns out that remark was exactly the catalyst I needed to quit the habit. I quit the day I returned from the conference, and it has been a relief for me that it is now close to three years as of today since I smoked my last cigarette.

I reserve a special thanks for all my fellow graduate student group members - all of you have contributed in no small measure to my development as an experimental physicist. I would like to thank Jason Puls for his general lab awareness and experimental acumen, though he graduated within a year or so of my joining the group. Radhey Shyam, Endu Srinadhu and the two Daniels - Field and Cutshall - each had unique views and skillsets that made collaborating with each one an interesting and educational experience. Of course, Daniel F. and I have become close personal friends as well, due to our collaboration on the DARPA project and also our mutual interest in billiards. I would like to wish all of you the very best in your future endeavors, and hopefully we can all keep in touch.

I remember the day I walked into the administrative office and haltingly asked if there was any way I could 'transfer' to the physics program. I spoke to Dr. Meyer about
whether such a switch had been attempted before at Clemson - he answered that it been attempted before, but not successfully. Like I needed any more motivation! A few quizzical looks and clarifications later, I was on my way to applying for an admit into the Physics Ph.D. program at Clemson. None of this would have been possible if the admissions committee - Drs. Daw, Meyer and Sosolik - had not taken the chance to admit me to the program based partly upon merely my claimed interest in physics. I will always be grateful to them for admitting me to the program under such unique circumstances.

On the personal front, no amount of thanks is enough for the unconditional support and love of my parents. I understand that this period has been particularly stressful for them given my switch to physics from computer science. I have not been able to visit home in six years - and that cannot have been easy on them at all. I admire the fortitude they have shown in putting on a brave face over their uncertainty and not letting their unease filter through to me. I thank them for their understanding and their support of my decision to pursue a graduate education in physics, not to mention a couple of timely financial bailouts! A similar thank you to my parents-in-law as well - their patience has been sorely tested during the course of this degree. I am glad that they are attending the convocation ceremony and look forward to seeing them in a couple of weeks. Dhawal’s annual visits are the highlight of our year, and due to the nearly constant Whatsapp stream, I hardly feel as if I have left home. Prateek’s visit here was also a memorable one for us and I look forward to many more in the future - they will have to upgrade the IT infrastructure back home to support his latest Macbook! My only regret will be that my mother did not get a chance to visit Clemson, I think she would have enjoyed this place the most.

I have formed many new friendships during my time here at Clemson, and renewed many old ones. To the 'tapri' gang - those impromptu getaway weekends were always the pressure release I needed. You guys remain at the top of my list to ask for help burying the body. While our lives have moved forward with varying degrees of joys and sorrow, I know
once we meet again at some hastily arranged rendezvous, we will pick up the threads like we just met yesterday - and for such friendships I am truly thankful. To Daniel, Mike and Trisha, Jim and Robert, Shyam and Shwetha - these years would not have been half the fun without all of you. In between Daniel, Mike’s parents and Trisha, Priyanka and I always had a great Thanksgiving dinner every year! No mention of Thanksgiving can be complete without remembering the Epic Thanksgiving Day Massacre - I will never forget it. A shout out to all my pool league friends as well - I will surely miss their company over a rack of eight ball. You all made me feel at home, and I am afraid I will miss this place more than I imagine.

And last, but not the least, I am thankful for the unwavering love of my wife. Somehow, through the various timezones and continents and with the help of a well-placed phone call by Chad, we finally made it to the same place at the same time, and for that Clemson will always be special for the both of us. Also, to our very own Hercule Poirot and Arthur Hastings - they made everything doubly fun! And especially Hercule, for all the nights that he kept me company as I wrote this thesis. Now for our next great adventure together!
# Table of Contents

Title Page .............................................. i
Abstract .................................................. ii
Dedication ................................................ iv
Acknowledgments ........................................ v
List of Tables .......................................... xii
List of Figures ......................................... xiii

1 Introduction .......................................... 1
   1.1 Ion-solid interactions ........................... 1
   1.2 CUEBIT facility .................................. 7
   1.3 Outline .......................................... 10

2 Space charge effects .............................. 13
   2.1 Introduction .................................. 13
   2.2 Experiment .................................... 16
   2.3 Results and Discussion ....................... 20
   2.4 Summary ....................................... 26

3 Ion transport through macrocapillaries ........ 28
   3.1 Experiment .................................... 30
   3.2 Results and Discussion ....................... 37
   3.3 Summary and Outlook ......................... 58

4 Metrology of ion-solid interactions .......... 66
   4.1 Hot electron current - Schottky diodes .... 67
   4.2 Metal-oxide-semiconductor(MOS) device irradiations .... 90

5 Future Work .......................................... 91
   5.1 Charge Exchange ............................... 91
<table>
<thead>
<tr>
<th>Appendices</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Ion transport through macrocapillaries - Oscillations due to charge patch formation</td>
<td>101</td>
</tr>
<tr>
<td>B Probing kinetically excited hot electrons using Schottky diodes</td>
<td>108</td>
</tr>
<tr>
<td>C Tracking subsurface ion radiation damage with metal-oxide-semiconductor device encapsulation</td>
<td>114</td>
</tr>
<tr>
<td>D Encapsulating Ion-Solid Interactions in Metal-Oxide-Semiconductor(MOS) Devices</td>
<td>124</td>
</tr>
<tr>
<td>E Area of conical capillary</td>
<td>132</td>
</tr>
<tr>
<td>F Computer Programs</td>
<td>136</td>
</tr>
<tr>
<td>A Interfacing with GPIB</td>
<td>137</td>
</tr>
<tr>
<td>B Interfacing Electrometers</td>
<td>139</td>
</tr>
<tr>
<td>C Auger Measurements</td>
<td>160</td>
</tr>
<tr>
<td>D EBIT Beam tuning and profiling</td>
<td>168</td>
</tr>
<tr>
<td>E Obtaining RFA spectrum</td>
<td>189</td>
</tr>
<tr>
<td>F Picoreader</td>
<td>204</td>
</tr>
<tr>
<td>G Lab Automation Framework</td>
<td>212</td>
</tr>
<tr>
<td>H HCI nanocapillary beam shaping</td>
<td>250</td>
</tr>
<tr>
<td>I modified Safari</td>
<td>275</td>
</tr>
<tr>
<td>J List of programs</td>
<td>279</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Bibliography</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>281</td>
</tr>
</tbody>
</table>
List of Tables

3.1 Table showing the material, length ($l$), inlet diameter ($d_{in}$), outlet diameter ($d_{out}$) and critical angle ($\theta_c$) for the various macrocapillaries used in this experiment ........................................ 35

4.1 Ion beam settings used for the Schottky diode irradiations ............... 73

F.1 Table showing details regarding the computers used to store programs and record data. .......................................................... 137
List of Figures

1.1 Figure showing the different processes that take place according to the kinetic energy of the incident ion beam .................................................. 3

1.2 Potential energy of different ions (Ar, Xe, and U) as a function of the charge state ................................................................. 5

1.3 Variation in energy deposition using different types of ions at varying kinetic energies ................................................................. 6

1.4 A schematic of the ion source (EBIS-SC) and the extraction beamline (Sections I and II) present in the CUEBIT facility ............................................. 8

2.1 A schematic of the experimental setup for the EBIS, beamline and RFA ................................................................. 15

2.2 Model of the RFA along with an example spectrum ................................................................. 18

2.3 Offsets in kinetic energy as a function of electron beam current ................................................................. 22

2.4 Offsets in kinetic energy as a function of the kinetic energy of the electron beam ................................................................. 23

2.5 Measured ΔE values versus the ratio of the electron beam parameters ................................................................. 25

3.1 A schematic of the beamline used for the ion transport studies ................................................................. 32

3.2 Figure showing the dimensions of the capillary used in this study ................................................................. 34

3.3 Position-dependent raw data for the metal capillary (Sample # 1, l=2.10 cm, \(d_{in}=d_{out}=0.23\) cm) ................................................................. 39

3.4 Angle-dependent raw data for the metal capillary (Sample # 1, l=2.10 cm, \(d_{in}=d_{out}=0.23\) cm) ................................................................. 41

3.5 Effective area of the opening of the capillary as a function of the angle of tilt ................................................................. 43
3.6 Maximum, mean and minimum of transmitted current as a function of varying tilt angle for the metal capillary (Sample # 1, $l=2.10 \text{ cm}$, $d_{in}=d_{out}=0.23 \text{ cm}$) 45

3.7 Position-dependent raw data for an insulating capillary (Sample # 2, $l=3.55 \text{ cm}$, $d_{in}=d_{out}=0.54 \text{ cm}$) 47

3.8 Angle-dependent raw data for an insulating capillary (Sample # 2, $l=3.55 \text{ cm}$, $d_{in}=d_{out}=0.54 \text{ cm}$) 48

3.9 Maximum, mean and minimum of transmitted current as a function of varying tilt angle for an insulating capillary (Sample # 2, $l=3.55 \text{ cm}$, $d_{in}=d_{out}=0.54 \text{ cm}$) 50

3.10 Position-dependent raw data for the conical capillary (Sample # 4, $l=1.96 \text{ cm}$, $d_{in}=0.54 \text{ cm}$, $d_{out}=0.23 \text{ cm}$) 55

3.11 Angle-dependent raw data for the conical capillary (Sample # 4, $l=1.96 \text{ cm}$, $d_{in}=0.54 \text{ cm}$, $d_{out}=0.23 \text{ cm}$) 56

3.12 Maximum, mean and minimum of transmitted current as a function of varying tilt angle for the conical insulating capillary (Sample # 4, $l=1.96 \text{ cm}$, $d_{in}=0.54 \text{ cm}$, $d_{out}=0.23 \text{ cm}$) 57

3.13 Proposed design using circular electrodes embedded within an optical fiber for flexible ion transport 60

3.14 Proposed design using hyperbolic electrodes embedded within an optical fiber for flexible ion transport 61

3.15 Equipotentials calculated for a static voltage applied to the circular electrodes embedded within an optical fiber 62

3.16 Equipotentials calculated for a static voltage applied to the hyperbolic electrodes embedded within an optical fiber 63

3.17 Example of the trajectory of an $\text{Ar}^+$ ion in the proposed design using circular electrodes 64

3.18 Example of the trajectory of an $\text{Ar}^+$ ion in the proposed design using hyperbolic electrodes 65

4.1 Various channels of energy dissipation for exothermic reactions at a surface 68

4.2 Schematic and I-V curve of the Schottky diodes used for this experiment 71
<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.3</td>
<td>A schematic representation of the experimental setup used to conduct the</td>
<td>75</td>
</tr>
<tr>
<td></td>
<td>Schottky diode irradiations</td>
<td></td>
</tr>
<tr>
<td>4.4</td>
<td>A photograph of the experimental setup used to conduct the Schottky diode</td>
<td>76</td>
</tr>
<tr>
<td></td>
<td>irradiations</td>
<td></td>
</tr>
<tr>
<td>4.5</td>
<td>Hot electron current measured through a fabricated device in response to a</td>
<td>80</td>
</tr>
<tr>
<td></td>
<td>pulsed Rb(^+) beam at a kinetic energy of 1000 eV</td>
<td></td>
</tr>
<tr>
<td>4.6</td>
<td>Yield of hot electrons plotted as a function of the kinetic energy of the</td>
<td>82</td>
</tr>
<tr>
<td></td>
<td>incident ions</td>
<td></td>
</tr>
<tr>
<td>4.7</td>
<td>Variation in hot electron current as a function of the angle of incidence of</td>
<td>85</td>
</tr>
<tr>
<td></td>
<td>a 5 keV Ar(^+) beam</td>
<td></td>
</tr>
<tr>
<td>4.8</td>
<td>An illustration of the relationship between the detected hot electron current</td>
<td>86</td>
</tr>
<tr>
<td></td>
<td>and path length</td>
<td></td>
</tr>
<tr>
<td>5.1</td>
<td>Figure illustrating the basic measurement of charge exchange</td>
<td>93</td>
</tr>
<tr>
<td>5.2</td>
<td>Figure showing important experimental parameters in studies of charge</td>
<td>94</td>
</tr>
<tr>
<td></td>
<td>exchange</td>
<td></td>
</tr>
<tr>
<td>5.3</td>
<td>Absolute cross-sections for charge exchange involving Ar and Ne ions and</td>
<td>97</td>
</tr>
<tr>
<td></td>
<td>various targets</td>
<td></td>
</tr>
<tr>
<td>5.4</td>
<td>Figure showing evolution of charge states due to charge exchange</td>
<td>98</td>
</tr>
<tr>
<td>5.5</td>
<td>Single and double electron capture events as a function of target thickness</td>
<td>99</td>
</tr>
<tr>
<td>E.1</td>
<td>Figure showing the effective area of opening of a conical capillary</td>
<td>134</td>
</tr>
<tr>
<td>E.2</td>
<td>The calculated effective area of opening of a conical capillary as a function</td>
<td>135</td>
</tr>
<tr>
<td></td>
<td>of tilt angle</td>
<td></td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

1.1 Ion-solid interactions

Ion-solid interactions have been the focus of many experiments in the last century that have aided in the discovery of fundamental properties and also given rise to technology widely used today[1, 2]. Fundamental insights about the nature of the atom were obtained by studies of particle bombardment on solids in the period between 1910 and 1950[3–9]. In the 1960s, due to technological advancement, well-controlled and clean Ultra-High-Vacuum (UHV) conditions were accessible to experimentalists[10] that spurred on investigations in the field of ion-solid interactions including but not limited to gas-surface interactions[11], ion implantation[12–16], radiation damage[17, 18], and sputter erosion[19].

Material modification utilizing singly charged ions (SCIs) is realized by the transfer of the kinetic energy of the ion to the solid into its nuclear and electronic degrees of freedom. It is technologically convenient to accelerate ions as opposed to neutrals to energies reaching $10^7$ eV, resulting in the wide use of ions. The ion interacts with the solid through an interatomic potential that modulates parameters such as range, energy loss, and distribution within the solid. These parameters govern the implantation, damage and sputtering
processes described above and can be used as 'knobs' to controllably manipulate interactions at the nanoscale. Fundamental ion-solid interactions can be summarily described by sequential binary collision approximations, energy loss processes within the solid including recoiling of ions via collision cascades, and radiation damage and sputtering within the target. The different ion-solid interaction processes depend on the value of the kinetic energy, which has resulted in the classification of different regimes of kinetic energy[20]: thermal (<1 eV), hyperthermal (1 eV-500 eV), low energy (500 eV-10 keV), medium energy (10 keV-500 keV), and high energy (>0.5 MeV). Fig 1.1 shows the various processes that occur in the different energy regimes as indicated.
Figure 1.1: Figure showing the different processes that take place according to the kinetic energy of the incident ion beam. The kinetic energy is classified into five regimes depending upon its value as shown. The figure gives a rough estimate of the ranges of these effects as target-specific effects are excluded and should be treated as a rough guide rather than an exact quantification. Adapted from Ref. [20].
Multiply- and highly-charged ions (M/HCIs) are esoteric entities in the world of ions. Their uniqueness lies in the fact that their charge state (Q) is significantly higher than 1, thus making it possible to use their potential energy instead of only the kinetic energy (as is the case with the more traditional singly charged ions). Figure 1.2 shows the potential energy of different species of ions (Ar, Xe, and U) as a function of the charge state. The potential energy is calculated as the sum of the binding energies of the electrons that are removed from the neutral atom to form the highly charged ion. As can be seen in the figure, the potential energy of Xe$^{44+}$ is $\sim 51$ keV, while that of Ar$^{11+}$ is $\sim 2$ keV. This potential energy couples with the surface by attracting electrons from the surface and thus breaking electronic bonds in the case of insulators. The energy density of deposition can be very high for slow highly charged ions, as the entire potential energy may be deposited into an atomic volume of only a few nm$^3$. Due to the high deposition energy density, utilization of the potential energy of these multiply/highly charged ions leads to new effects at surfaces, which is outside the realm of SCIs[21–27]. A comparison [23] between the different effects of slow heavy SCIs, swift heavy ions (SHIs) and slow highly charged ions (HCIs) is shown in Fig. 1.3, and illustrates the high density of energy deposition into the target. The kinetic energy of SHIs leads to a high penetration distance, or range, of these ions into the solid, while the kinetic energy of the HCIs being very low, the range is typically only a few nm. The potential energy is deposited into this small volume indicated in the figure, leading to the high density of deposition.
Figure 1.2: Potential energy of different ions (Ar, Xe, and U) as a function of the charge state. The potential energy is calculated as the sum of the binding energies of those electrons that have been removed from the neutral gas atom to form the highly charged ion. For example, the potential energies of Ar$^{11+}$ ($\sim 2$ keV) and Xe$^{44+}$ ($\sim 51$ keV), are indicated in the figure. These charge states have been utilized commonly when using Ar and Xe species and serve to provide an estimate of the potential energy in question. Adapted from Ref. [23].
Figure 1.3: Figure showing the different schemes for energy deposition for different types of ions at different kinetic energies. The red shows recoil trajectories of the ions and the blue shows the energy lost to electronic excitations. a) Singly-charged heavy ions with kinetic energy in the range of a few keV to an MeV. b) Swift heavy ions in the energy range of a few MeV to a GeV. c) Slow highly charged ions with potential energy of a few keV and kinetic energy less than 1 keV. Adapted from Ref. [23].
1.2 CUEBIT facility

In the last few decades, there has been considerable interest in the utilization of M/HCIs as sources providing these ions with considerably high charge state and flux have become available. Electron Beam Ion Source/Traps (EBIS/Ts) and Electron-Cyclotron-Resonance (ECR) sources are the two primary sources that are used to provide highly charged ions, while a new multiply charged ion source utilizing lasers is under development at Old Dominion University[28]. An excellent review regarding the details of an EBIT can be found in Refs. [29, 30].

Along with the EBIS/T and ECR sources worldwide[31–38], recently an EBIS/T was commissioned at Clemson University as part of the user facility 'CUEBIT’ designed primarily for materials irradiation experiments using M/HCIs[39]. The ion source was obtained from DREEBIT, GmbH[35, 40–47]. A schematic of the beamline is shown in Fig. 1.4. The ion source is designed based on the EBIS-SC source[35]. The electron beam is formed from a cathode emitter and directed through a three-section drift tube where it can ionize an injected species to form HCIs. Beyond the drift tube lies an extraction region where ions and electrons are separated. From the extraction region, ions leave the source and enter the beamline while the electrons are dumped into a collector. Both the collector and cathode are cooled with a closed cycle deionized water loop which cycles through an external laboratory chiller unit. Surrounding the drift tube region is a 6 T closed-cycle-cooled superconducting magnet which provides compression for the central electron beam.
Figure 1.4: A schematic of the ion source (EBIS-SC) and the extraction beamline (Sections I and II) present in the CUEBIT facility. The Faraday cup and quadrupole are labeled as FC and Q, respectively. Adapted from Ref. [39].
As in all EBIT/EBIS machines, bias voltages applied in the drift tube region along with the electron beam serve to confine ionized species axially and radially. Confinement times can be varied within the EBIS-SC by modulating the voltage of the drift tube section adjacent to the extraction region between 'open' and 'closed' trap configurations. Typical modes involve setting the drift tube at a low voltage such that ions with sufficient kinetic energy can surmount the axial potential continuously (leaky mode) or pulsing the drift tube voltage to lower the axial potential over fixed time intervals (pulsed mode).

Connected to the EBIS-SC ion source are two additional vacuum sections (Sections I and II) which constitute the beamline for the CUEBIT facility as shown in Fig. 1.4. Both sections are oil-free pumped with turbomolecular pumps and are separated from the ion source and each other by pneumatically-controlled gate valves. Within Section I, immediately adjacent to the ion source, are mounted an Einzel lens and deflector assembly. Both are used to focus and deflect ions extracted from the source into a retractable Faraday cup mounted within this section. Also mounted in Section I are a quadrupole beam deflector and a 4-jaw slit system. The quadrupole deflector is currently unused; however, it can be employed as an injection point to transport ions back into the central drift tube or trap region for further ionization.

Extracted HCI beams focused through Section I are brought into Section II through an analyzing dipole magnet. A second deflector assembly lies at the exit of the magnet and is used to bring the beam into alignment for this sections Faraday cup or into user-defined detector assemblies mounted in the target region downstream. The analyzing dipole magnet has a deflection angle of 90°, a bending radius of 350 mm, and produces a maximum field of 0.4 T at a 91.2 A induction current. A water cooling loop, also powered by the laboratory chiller, serves to cool the magnet coils, and a Hall probe is mounted within the magnet yokes and interfaced to the laboratory computer to provide field strength readings. The Section II Faraday cup is mounted at the exiting focus point of the analyzing magnet, and
the collection of current readings under varying field strengths in this cup can be used to generate a spectrum of the ion species extracted from the EBIS-SC source.

The target region of the CUEBIT facility refers to the delivery point for HCI beams extracted and focused from the EBIS-SC ion source. Extending into this region is a custom-designed deceleration lens that is configured to provide 100X reduction in the delivered beam energy. The lens has an inner diameter of 40 mm and is constructed upon a DN100CF flange. Given the flexible operating procedures designated for CUEBIT as a user facility, this base flange is considered the standard mounting point for any desired chamber or experimental end point configuration.

1.3 Outline

It is important to accurately determine the kinetic energy of the highly charged ion beam extracted from the source. However, the EBIT, being a non-traditional ion source, it is not straightforward to calculate the energy of these ions as it is with traditional ion beamlines. The overlap of the electron beam and the ion cloud in the source region leads to lowering of the effective potential leading to an offset in the kinetic energy of the extracted ions. This offset depends upon operational parameters of the electron beam and has been found to be a few hundred eV in magnitude. Details regarding these measurements are presented in Chapter 2.

While these ions have received considerable interest recently as described, the ions are confined in UHV conditions in bulky stainless steel beamlines as shown. The rigidity and inflexibility of this design prohibits convenient integration of these ions into existing frameworks such as those used for surface processing techniques or biological applications of ions. The transport of these ions using flexible capillaries has received considerable attention, since the guiding effect was discovered by the Stolterfoht group[48]. A review
of the existing work can be found in Ref. [49]. Several schemes using nano-sized and macro-sized capillaries have been proposed, while recently investigations of novel transport methods have utilized external electric fields in conjunction with curved and conical capillaries[50–52]. Due to higher cross-section and the possibility of higher transmission efficiency, macrocapillaries are of interest for the design of novel transport systems. Chapter 3 presents investigations on the use of macro-sized cylindrical and conical capillaries made of metal as well as an insulating material. Angle and position dependent measurements are presented that show charge patch formation in only the insulating macrocapillaries.

In chapter 4, two experiments that record the electronic excitations due to ion bombardment are described. Electrically sensitive devices were constructed that enabled tracking of both singly and multiply charged ion induced effects at kinetic energies in the low energy regime. Schottky diodes were fabricated in-house (25 nm Ag/n-Si) as a high-efficiency detector of hot electrons, or 'kinecurrent', analogous to chemicurrent[53]. Angle- and energy-dependent measurements are described using singly charged ions. These measurements should serve as a baseline for future measurements with multiply charged ions, as they represent the part of the effect attributed to kinetic energy. A threshold in the onset of hot electron current was obtained from the energy-dependent measurements that agreed well with a kinetic-electron-emission model, while the angle-dependent measurements yielded a mean free path of hot electrons in the silver film that agrees well with the literature. Shifts in capacitance-voltage (C-V) curves of metal-oxide-semiconductor (MOS) devices due to singly as well as multiply charged ion bombardment are used to track subsurface damage caused by the incident ions. Stopping power dependence of the multiply charged ions on the charge state was inferred from these measurements and yielded a quadratic dependence.

Chapter 5 describes the charge exchange measurements planned in the future. A
method of calculating cross-sections from experimental data obtained from a gas cell mea-
surements is presented. The appendices contain reproductions of related articles and list-
ings of the computer programs used for these measurements.
Chapter 2

Space charge effects

2.1 Introduction

Multicharged ions or MCIs are of interest in multiple contexts due to the high potential energies they possess relative to those typically encountered with singly charged ions[54]. This potential energy component leads to large charge-exchange cross sections for MCIs when they encounter a target atom or molecule. In the case of solid targets, this charge exchange can couple into irreversible changes in the structure, and many have proposed MCIs as a route to single-atom nanostructuring at surfaces[55–57]. However, in order to exploit this potential energy effectively, the interaction time between the MCI and the target must be maximized, which implies a need for ions with low kinetic energies. The unique methods by which MCIs are produced, such as in an electron beam ion trap (EBIT) or source (EBIS), can lead to large (>100 eV) offsets in the extracted energies for such ions[58, 59]. This chapter described the measurements of these offsets for MCIs produced in an EBIS device.

Electron beam ion sources produce MCIs by confining and repetitively ionizing source material using a combination of drift tubes and a coaxial electron beam (see Fig. 2.1).
The drift tubes within an EBIS provide an axial trapping potential, while the electron beam serves to both ionize the beam source material through electron impact ionization and trap the generated ions radially through a `space charge’ effect. The space charge potential produced by the electron beam is dependent on its current and kinetic energy. In general, more negative charge (higher electron beam current) will increase the trapping potential, while a shorter residence time for the negative charge (higher electron beam energy) will lower the trapping potential. These changes in the trap potential due to the space charge will lead to offsets in the kinetic energy of any extracted ions. Therefore, calibrating an EBIS for space charge effects is important if one seeks to produce well-defined MCI beams with low kinetic energy.

EBIS-produced beams of MCIs were characterized utilizing retarding field measurements coupled with a systematic variation in the electron beam parameters. The details of our experimental apparatus, including the EBIS, its attached beamline and deceleration optics, and our retarding field analyzer are presented. The results of the kinetic energy offset measurements for argon MCIs are discussed in relation to the trapping conditions within the EBIS (electron beam current and electron kinetic energy).
Figure 2.1: A schematic of the experimental setup for the EBIS, beamline and RFA (1:electron beam, 2:magnetic field (6 T), 3:trapped ion cloud, 4:extracted ion beam, 5:analyzing magnet, 6: charge-to-mass ratio separated ion beam, 7:deceleration lens, 8:RFA). The potential profile for ions trapped within the EBIS is illustrated above the drift tube sections (DT) along with typical applied electrostatic potentials (U), with subscripts signifying position - L:Leftmost, C:Central and R:Rightmost. The central drift tube section (DT_C) is highlighted as it is the ion trapping region. The ions are trapped axially in section DT_C due to the potential well created as shown, while the space charge of the electron beam produces a trapping potential in the radial direction.
2.2 Experiment

These measurements were conducted on the EBIS-SC at the Clemson University Electron Beam Ion Trap (CUEBIT) facility described in detail in Ref. 39. The EBIS produces MCIs by interacting a neutral gas target with a high current, high energy electron beam. The electrons are compressed in the trap center by a strong magnetic field gradient. By tuning the electron beam characteristics and the trapping time, one can optimize the source to produce a desired MCI charge state distribution. The generated MCIs are trapped axially by the electrostatic potentials ($U_L$, $U_C$, and $U_R$) applied to the three sections of the drift tube ($DT_L$, $DT_C$, and $DT_R$) as illustrated in Fig. 2.1. Radial trapping of MCIs is provided by the strong negative potential of the coaxial electron beam passing through the drift tube. The potential applied to the rightmost drift tube section ($DT_R$) is used to control the manner in which ions are released from the drift tube into the beamline. If $U_R$ is dropped quickly below $U_C$, then the MCIs are released in a pulse. If $U_R$ is maintained slightly higher than $U_C$, then some MCIs escape continuously (“leaky” mode). For these measurements, the EBIS was operated in leaky mode with $U_R$ set to 50 V above $U_C$.

Within the EBIS, the electron beam is continuously dumped to a collector plate, while the MCIs extracted from $DT_R$ are guided down a connected UHV beamline and accelerated to an energy of $(Q \times U_R)$ eV to form an ion beam. To separate out ions with a particular charge state $Q$, this ion beam, consisting of a distribution of masses and charge states, is passed through an analyzing or bending magnet that selectively passes ions based upon their charge-to-mass ratio. The beamline is held at a pressure of $\sim 10^{-9}$ Torr to minimize recombination, while it is floated to a negative potential ($U_{BL}$) to facilitate deceleration. A six-element deceleration lens connected to the end of the beamline both slows down the beam and focuses it within a zone 25 mm to 50 mm beyond the end of the lens. The ions are decelerated to a final kinetic energy of $[Q \times (U_R + U_{BL})]$ eV, where $U_{BL}$ is
negative.
Figure 2.2: a) A model of the RFA using SIMION showing the internal components of the RFA - the faceplate (FP), the main body (MB), the retarding plate (RP) with SS mesh, and the Faraday Cup (FC) detector. b) An example RFA curve for an Ar$_{8}^{+}$ beam (+) and the computed derivative (x) fit to a Gaussian. As seen in the figure, the kinetic energy of the ion beam as measured by the RFA (851.3 eV/Q) is offset from the nominal kinetic energy calculated from the trap potentials (950 eV/Q) by 98.7 eV/Q.
For this study, a retarding field analyzer (RFA), shown schematically in Fig. 2.2, was placed within the range of the focal length of the deceleration lens. The RFA position was held constant for all the measurements reported here. The ion current was optimized for each beam setting by appropriately focusing the ion beam using the energy-conserving elements of the deceleration lens. The purpose of the RFA was to measure the kinetic energy of the extracted MCI beams.

The RFA consists of the following electrically isolated components: a faceplate (FP) used for alignment, a hollow cylindrical main body (MB), a retarding plate (RP) and a Faraday cup (FC) detector. The aperture sizes of the FP and RP were 3 mm and 4 mm, respectively. The MB here serves only as a spacer, though it is designed as the body of a gas cell for future experiments to study MCI charge exchange in gases (See Chapter 5). The RP was electrically connected to a high-voltage MHV feed-through, allowing the application of potentials up to 5 kV. To avoid a sag in the potential due to the RP aperture, a grid (SS type 316, mesh 20, wire diameter 0.004”) was spot welded to the RP. The maximum expected value for the potential sag with this mesh was calculated to be 0.2 % (See Eq. 1 in Ref. 60). For all measurements, the nominal kinetic energy of the ion beam was set at 950 eV/Q by appropriately adjusting the trap and beamline voltages. Simulations performed using SIMION[61] showed that the minimum energy required by these ions to pass through the RP was 2 eV/Q lower than the voltage applied to the RP-mesh.

The procedure for measuring the kinetic energy of a given MCI beam involved varying the potential applied to the RP while monitoring the beam current in the FC detector. All extracted MCI beams arrived at the RFA as continuous, i.e. non-pulsed, beams and the current collected in the FC detector was measured by a Keithley 6485 picoammeter interfaced to a digital computer for data acquisition. A significant difference was observed between the kinetic energies of the extracted MCI beams measured with the RFA and the expected kinetic energies based on the drift tube potential settings of the EBIS. To deter-
mine the relationship between this offset in kinetic energy and the negative space charge of the electron beam in the ion source, both the current and the energy of the electron beam were varied while extracting $\text{Ar}^{Q+}$ ($Q=4,8$) ion beams with a nominal energy of 950eV/Q. Specifically, the electron beam current ($I_e$) from the cathode emitter was varied from 60 mA to 220 mA in steps of 40 mA at a cathode potential ($U_{\text{cath}}$) of 600 V, and the electron beam energy ($E_{e0}$) was varied from 3.6 keV to 6.6 keV in steps of 1 keV.

### 2.3 Results and Discussion

For an MCI beam of charge state $Q$ extracted in leaky mode from the EBIS, the expected kinetic energy ($E_0$), excluding effects of the space charge potential, is given by the following:

$$ E_0 / Q = U_R + U_{BL} \tag{2.1} $$

For any ion beam, the space charge effect will reduce the kinetic energy by an amount, $U_{sp}$, as shown here:

$$ E / Q = E_0 / Q - |U_{sp}| \tag{2.2} $$

For the ion beams extracted from the EBIS in this study, the drift tube and beam-line voltages were varied appropriately to generate ions with expected kinetic energies of 950 eV/Q. Subsequent measurements within the RFA of the actual kinetic energy showed shifts from these expected values, which we hereafter refer to as the kinetic energy offset $\Delta E$. Measured kinetic energy offsets for beams of $\text{Ar}^{4+}$ are shown in Fig. 2.3 as a function of the electron beam current $I_e$ within the EBIS for four different values of the electron beam energy $E_{e0}$. From these data one can see there is a linear dependence of $\Delta E$ on the electron
beam current for all electron beam energies. Similar linear dependence was measured for 
Ar$^8^+$ ions as well. At individual values of the electron beam current, it is also clear that the 
offsets vary inversely with the electron beam energy. Similar data for Ar$^8^+$ ions are shown 
in Fig. 2.4, now as a function of the electron beam energy. Here a log-log plot is used to 
highlight the inverse dependence on electron beam energy and the fitted lines shown all 
have a slope of $\sim -0.5$. Similar data analysis of measurements with the Ar$^{4^+}$ ions also 
yielded slopes of $\sim -0.5$. 
Figure 2.3: Offset in the kinetic energy of the MCI beam measured at the RFA from the expected value as a function of the electron beam current ($I_e$) at different values of nominal electron beam energy ($E_{e0}$) for Ar$^{4+}$.
Figure 2.4: A log-log plot of the offset in the kinetic energy of the MCI beam (in eV/Q) measured at the RFA from the expected value as a function of the nominal electron beam energy ($E_{e0}$) (in keV) at different values of electron beam current ($I_e$) for Ar$^{8+}$. 
To understand the dependence of $\Delta E$ on $I_e$ and $E_{e0}$ observed in Figs. 2.3 and 2.4, we note that the space charge potential can be estimated as [62]:

$$U_{sp} \approx \frac{I_e}{4\pi \varepsilon_0 v_e} \left( 2\ln \left[ \frac{r_{\text{drift tube}}}{r_{\text{electron beam}}} \right] + 1 \right)$$ (2.3)

where $v_e = \sqrt{2E_{e0}/m_e}$ is the velocity of the electron beam and $r_{\text{drift tube}}$ and $r_{\text{electron beam}}$ refer to the radii of the EBIS drift tube and the electron beam, respectively. If one assumes the effective electron beam radius in DT$_C$ remains constant for the different beams across all source settings, the primary parameters which determine the magnitude of $U_{sp}$ are the electron beam current and velocity. The linear dependence on $I_e$ is clearly demonstrated in the data of Fig. 2.3, while the inverse dependence on the velocity is present in Fig. 2.4.
Figure 2.5: Measured \( \Delta E \) values versus the ratio of the electron beam parameters with the EBIS-SC source for both \( \text{Ar}^{8+} \) (□) and \( \text{Ar}^{4+} \) (△) ions. A slope of \( 5.1 \times 10^{10} \, \text{Vm/C} \) and an intercept of 16 V is obtained from the shown linear fit and can be used to extract the average electron beam radius (200 \( \mu \text{m} \)) inside the ion trap (see text).
The qualitative agreement illustrated in Figs. 2.3 and 2.4 between our measured kinetic energy offsets and the functional dependencies of the space charge on $I_e$ and $E_{e0}$ (Eq. 2.3) suggest that the radial trapping or space charge potential of the electron beam within the EBIS is the source of these offsets. Knowing that, it becomes important to find a quantitative relationship for a given EBIS source that can be utilized for predicting and accounting for these offsets in any experimental design. In Fig. 2.5 we plot our measured $\Delta E$ values versus the ratio of the electron beam parameters that determine the space charge effect ($I_e$ and $v_e$). As the figure shows, there is a linear relationship between $\Delta E$ and this ratio, as expected. This plot can serve as a guide for any measurements which need to account for this offset in the kinetic energy of the MCIs extracted from our EBIS. In addition, the slope of the fit line can be used to determine the radius of the electron beam within the trap region. In this case we find, using Eq. 2.3, that our effective electron beam radius is 200 $\mu$m. This value is somewhat larger than quoted elsewhere for similar EBIS designs[62]. Nevertheless, for in-trap studies of ion-electron interactions typical of EBIS and EBIT machines, the ability to determine the electron beam radius in this way without internally probing the source itself should prove useful.

2.4 Summary

Measurements of the offset in the kinetic energy of ions extracted from an EBIS source using a downstream RFA have been presented. The dependence of the offsets on the electron beam parameters (current and energy) of the source are in good agreement with an expected variation due to the space charge trapping potential of the electron beam. As the measured beam energies differ by up to a few hundred eV/Q, knowledge of the origin of the offsets and how they can be controlled is important for experiments that seek to use slow MCIs. The linear dependence of the kinetic energy offset on space charge parameters
can also be used to extract the radius of the electron beam itself, which can be an important parameter for modeling measurements that focus on the electron-ion interactions within the trap.
Chapter 3

Ion transport through macrocapillaries

Multiply- and highly-charged ions (M/HCIs) are esoteric entities in the world of ions. Their uniqueness lies in the fact that their charge state (Q) is significantly higher than 1, thus making it possible to use their potential energy instead of only the kinetic energy (as is the case with the more traditional singly charged ions). With the advent of sources such as Electron-Cyclotron-Resonance (ECR) sources and Electron-Beam-Ion-Trap/Sources (EBIT/EBIST) worldwide[31–39], these ions have received increased attention in the last few decades due to their unique interaction with terrestrial materials[21–27]. However, these sources confine the ions in Ultra High Vacuum (UHV) conditions (pressures below $10^{-6}$ Torr) and in beamlines consisting of inflexible and often bulky design, due to which it is currently not possible to easily integrate these ions into existing industrial systems or frameworks.

The difficulty of making these ions easily accessible for industrial application can be classified into two separate problems - the pressure problem and the transport problem. The pressure problem is the problem of mating the UHV conditions these ions are produced in with the non-UHV environments that are typical of real-world applications. The charge-exchange with the gases residing in the relatively higher pressure environment would lead
to loss of the charge state of the beam, limiting the length of transport. The second problem - the transport problem - deals with the rigid and bulky nature of existing beamlines. A flexible design for a beamline that could integrate easily into an existing framework or system without requiring extensive restructuring of the existing facilities is desirable for increasing the usability of these ions.

A novel method of guided ion transport using capillaries that achieve focussing by the self-guiding effect due to charge patch formation or alternative by externally guided electric fields has attracted attention as alternative methods for ion delivery. The "self-guided" effect, which led to the increased attention towards capillaries, was discovered by the Stolterfoht group in 2002 using insulating nanocapillaries[48]. The self-guiding effect involves charge patch formation on the interior walls of the nanocapillaries due to the neutralization of the incoming ions and the emission of secondary electrons. The polarity of the charge patch formed is positive for positive incoming ions. As like charges repel, the charge patch repels the incoming ion beam towards the opposite wall of the capillary further down its length, while the charge patch formed also discharges into the bulk. After a certain time, a steady state condition is reached wherein the ions are guided down the length of the nanocapillary. An extensive review of the work in this field can be found in Ref.[49]. Following the discovery of the guiding effect, subsequent studies of transport can be classified into two categories depending on the diameter \( d \) of the bore of the capillary: nanocapillaries\((d < 10^{-6} \text{ m})\) and macrocapillaries\((d > 10^{-6} \text{ m})\)[63].

Studying the underlying mechanism of transport is necessary to design new beamlines that are efficient in terms of flux and also time required for steady transport conditions. Macro-capillaries have recently been proven to be a promising candidate for ion delivery. Recent studies have investigated the use of external electric fields for guiding to improve transport efficiency, conical capillaries and curved glass capillaries[50–52]. We have studied the angle- and position-dependent characteristics of 1 keV Rb+ ions through
glass and metal capillaries of varying diameter. Oscillations are observed in the transmission through the insulating capillaries but not in the metal capillaries. Simple calculations show that charge patch formation on the interior walls of the insulating capillary can deflect the ions beyond the detector leading to the observed oscillations. Though such deflections due to charge-patch formation on the interior walls of insulating nanocapillaries has been well established in literature, the observations reported here are unique with respect to the materials used and the size of the bore.

3.1 Experiment

The irradiations were performed in the singly-charged beamline described in detail in Ref. [64]. A Colutron ion source[65] equipped with an aluminosilicate emitter[66] was employed as a source of $\text{Rb}^+$ ions. The heater current to the filament, $I_{\text{src}}$ was turned up at a rate of approximately 50 turns per 15 minutes up to 300 turns resulting in a heater current of $\sim 1.5$ A. The Wien filter positioned immediately after the source was used to separate out the $\text{Rb}^+$ ions. The current through the electromagnet producing the magnetic field was $I_{\text{mag}} = 1.0$ A (200 turns) along with an electric field produced by an applied voltage of $V_A = 15$ V, corresponding to $\text{Rb}^+$ ions. A custom vacuum chamber was installed subsequent to the Wien filter as indicated in Fig 3.1 by the red arrow. This chamber housed the capillaries used in this experiment. The distance from the end of the Wien filter to the entrance of the capillary at the center of the custom vacuum chamber was 73.0 mm. The base pressure in the vacuum chamber typically was $1 \times 10^{-8}$ Torr. The Faraday cup located downstream was used as the ion detector. The distance from the center of the custom vacuum chamber to the Faraday cup was 142.8 mm. The Faraday cup was constructed as a cylinder from Oxygen Free High Conductivity (OFHC) copper with outer and inner diameters of 25.4 mm and 22.2 mm and depth of 41.2 mm. The energy of the $\text{Rb}^+$ ions was
fixed at 1 keV by setting $V_{accel}$ to 1000 V. $V_{F1}$ used to focus the beam was set at 820 V and the Pearce electrode was biased at -14 V. The currents recorded in the Faraday cup were few tens of nanoamperes in this section.
Figure 3.1: A schematic of the beamline used for the ion transport studies. The red arrow indicates the position at which the capillaries were inserted into the beam path. Adapted from Ref. [67].
Capillaries of two types of materials were used in this study: metals and insulators. A cylindrical steel tube was used as the metal capillary, while a glass capillary of the geometry shown in Fig. 3.2 was obtained for this study and cleaved in two different places to yield three different insulating capillaries. The dimensions of the capillaries used are recorded in Table 3.1. The diameters and length are represented by \( d \) and \( l \) respectively, while the \( \text{in} \) and \( \text{out} \) subscripts refer to the entrance and exit of the capillary respectively with respect to the incident ion beam. The critical angle \( \theta_c \) is defined as the greatest angle with respect to the incident beam of ions for which an unobstructed flight path exists from the entrance to the capillary through to the detector downstream. It can be thought of as the angle made by a line that touches the farthest and opposite corners in a length-wise cross-section of a capillary and is given by \( \theta_c = \tan^{-1}((d_{\text{in}} + d_{\text{out}}) / 2l) \).
Figure 3.2: Figure showing the dimensions of the capillary used to obtain the three glass capillaries of varying sizes used in this study.
Table 3.1: Table showing the material, length ($l$), inlet diameter ($d_{in}$), outlet diameter ($d_{out}$) and critical angle ($\theta_c$) for the various macrocapillaries used in this experiment. The uncertainties associated with these dimensions are $\pm 0.1$ mm and $\pm 0.12^\circ$.

<table>
<thead>
<tr>
<th>Sample #</th>
<th>Material</th>
<th>$l$ (mm)</th>
<th>$d_{in}$ (mm)</th>
<th>$d_{out}$ (mm)</th>
<th>$\theta_c$ ($^\circ$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Steel</td>
<td>21.0</td>
<td>2.3</td>
<td>2.3</td>
<td>6.25</td>
</tr>
<tr>
<td>2</td>
<td>Glass</td>
<td>35.5</td>
<td>5.4</td>
<td>5.4</td>
<td>8.65</td>
</tr>
<tr>
<td>3</td>
<td>Glass</td>
<td>21.0</td>
<td>5.4</td>
<td>5.4</td>
<td>14.42</td>
</tr>
<tr>
<td>4</td>
<td>Glass</td>
<td>19.6</td>
<td>5.4</td>
<td>2.3</td>
<td>11.11</td>
</tr>
</tbody>
</table>
Before inserting into the vacuum chamber, the capillaries were cleaned by rinsing with deionized water in between ten minute cycles of sonication with soap water, acetone and ethanol in that order. The capillaries were mounted at the end of a linear translator that allowed the capillaries to be translated into the path of the beam and were also rotatable with respect to the incident beam. Adhesive metal tape was used to metallize the entrance of the insulating capillaries to avoid charging effects on the lip of the entrance of the capillary. As the diameter of the beam in this section is considerably wider than the diameter of the capillary, the capillary was surrounded by metallic foil to prevent ions that did not enter the capillary from reaching the detector.

The beam being wider than the capillary, it is necessary to determine the center of the beam for placement of the capillary. The center was determined experimentally as follows. The capillary was completely retracted from the path of the beam and then the capillary was centered with respect to the ion beam by maximizing the current in the Faraday cup by translating the capillary into the path of the ion beam. In addition, the distances on either side of the central maximum point at which the measured transmission through the capillary was zero were also recorded.

The capillary was then placed at one edge and translated to the other edge in steps of 1.6 mm. The transmitted current was then recorded as a function of time at these different distances in the beam path for all capillaries used, while the angle-dependent characteristics were obtained by rotating the capillary with respect to the incident beam keeping the location of the capillary fixed at the central maximum point.

The time step used for recording the current for the position- and angle-dependent characteristics was \(~ 15\) s and \(~ 500\) s respectively. A digital Vernier caliper (±0.1 mm) and a digital sensor connected to a PC (±0.09°) were used to measure distances and angles respectively. A Keithley 617 electrometer was interfaced to a computer via GPIB for automated measurements via a program written in the C programming language. Tribological
effects and AC noise pick-up were issues that were identified as leading to a noisy signal from the electrometer. The electrical connectors for the Faraday cup were polished using sandpaper, and short cables were used for connections as far as possible to minimize capacitive losses. The wall-power outlet used for the electrometer was isolated from all other equipment to reduce power line interference. With these precautions, an error bar of $\pm 5$ pA was established for the measurement of the current.

### 3.2 Results and Discussion

We have measured the position- and angle-dependent characteristics of the transmission of $\text{Rb}^+$ ions through metal and insulating capillaries of the dimensions shown in Table 3.1. These data are now presented for each different capillary.

#### 3.2.1 Sample 1

This capillary was the metal macrocapillary with $d_{\text{in}} = d_{\text{out}} = 2.3$ mm and $l = 21.0$ mm corresponding to a critical angle $\theta_c = 6.25^\circ$. Figure 3.3 shows the position-dependent characteristics and Fig. 3.4 shows the angle dependent characteristics.

The transmitted current through the capillary is plotted as a function of time at different insertion distances in the beam path and angle with respect to the beam in Fig. 3.3 and Fig. 3.4 respectively. The position-dependent characteristics shown in Fig. 3.3 were measured as follows. The capillary was inserted into the beam path and the central maximum location denoted by '$C$', i.e. the position where the transmitted current was maximum, was determined. The edge positions $E_{1,2}$, i.e. the positions where the transmitted current dropped to zero on either side of $C$, were determined. Transmitted current at different positions from $E_1$ to $E_2$ was then measured and is shown in Fig. 3.3. As represented by the arrows in the figure, the transmitted current increased from $E_1$ to $C$ then decreased from
$C$ to $E_2$. The positions of $(E_1, C, E_2)$ were (0.0 mm, 7.2 mm, 14.4 mm) which indicate a beam width of $\sim 14$ mm, which was as expected much wider than the bore of the capillary.
Figure 3.3: Position-dependent raw data for the metal capillary (Sample # 1, \( l=2.10 \) cm, \( d_{in}=d_{out}=0.23 \) cm). The transmitted current is plotted as a function of time at varying positions between the edge positions (\( E \)) and the central position (\( C \)). Adapted from Ref. [68].
The angular-dependent characteristics shown in Fig. 3.4 were measured as follows. The capillary was inserted into the beam path at the central maximum location ‘C’, i.e. at the position where the transmitted current was maximum. The angle at which the beam was normal to the face of the capillary (denoted by $N$), was determined roughly by eye and then by maximizing the transmitted current. The capillary was rotated with respect to the incident beam and the angular positions $\theta_{1,2}$, i.e. the positions where the transmitted current dropped to zero on either side of $N$, were determined. Transmitted current at different angles from $\theta_1$ to $\theta_2$ was then measured and is shown in Fig. 3.4. As represented by the arrows in the figure, the transmitted current increased from $\theta_1$ to $N$ then decreased from $N$ to $\theta_2$. The angles $(\theta_1, \theta_2)$ were $(-6.12^\circ, 7.02^\circ)$ which lead to an experimentally determined critical angle of $\theta_c = 6.57\pm0.09^\circ$ as compared to the theoretically calculated value of $6.25^\circ$. 

40
Figure 3.4: Angle-dependent raw data for the metal capillary (Sample # 1, \( l = 2.10 \) cm, \( d_{\text{in}} = d_{\text{out}} = 0.23 \) cm). The transmitted current is plotted as a function of time at varying angles between the normal (\( N \)) and angles where transmission dropped to zero \( \theta_{1,2} \). Adapted from Ref. [68].
No oscillations were observed in the transmitted current for both the position- and angle-dependent cases, as there is no charge-up of the metal capillary. As presented later in this section, we find that this is no longer true in the case of the insulating capillaries. To analyze the transmitted current, we calculated the maximum, minimum and mean of the transmitted current at each position/angle. For the metal capillary, as the transmitted current did not change for a given position/angle, the mean, maximum and minimum values were very similar for a given position/angle.
Figure 3.5: Figure illustrating the varying area of the effective opening (hatched) as the capillary is tilted by an angle $\theta$ resulting in the observed angle-dependent characteristics for geometric transmission. An exact expression for this dependence is shown in Eq. 3.1 of the text. Adapted from Ref. [68].
For the angular-dependent data, the variation in the transmitted current from $\theta_1$ to $\theta_2$ can be explained by the varying opening presented by the overlap in the entrance and exit faces of the capillary to the ion beam, as shown in Fig. 3.5 for a capillary of diameter 'd' and length 'l'. When the axis of the capillary is aligned with respect to the beam, the entire area of the face of the capillary is available for transmission of the ion beam. As the capillary is rotated about its end, the effective area available for transmission is reduced as the further end of the capillary obstructs some of the opening. The effective area of the opening $A$ as a function of the tilt angle $\theta$ is given by the following equation for a capillary of diameter $d$ and length $l$:

$$A(\theta) = \frac{d^2}{2} \cos(\theta) \left[-\sin^{-1}(\gamma) + \gamma \cos(\sin^{-1}(\gamma)) + \pi/2\right]$$

(3.1)

where $\gamma = (l/d) \tan(\theta)$.

The minimum, mean and maximum of the transmitted current for the metal capillary as a function of tilt angle are shown in Fig. 3.6. The solid line shows the transmitted current calculated according to Eq. 3.1. The minimum, mean and maximum currents are narrower than the calculated values. However, the calculation assumed a zero divergence of the ion beam and a constant current density. In reality, the ion beam has a non-zero divergence and a Gaussian current density. A convolution of $A(\theta)$ with a Gaussian current density as compared to a uniform density coupled with losses due to divergence of the ion beam could lead to a narrower calculated transmitted current. Such a calculation can be possible with detailed profiling of the incident ion beam with a movable detector used to map the current density.
Figure 3.6: Maximum, mean and minimum of transmitted current as a function of varying tilt angle for the metal capillary (Sample # 1, \( l=2.10 \) cm, \( d_{in}=d_{out}=0.23 \) cm). The line shows the expected geometrical transmission from the capillary as a function of tilt angle. Adapted from Ref. [68].
3.2.2 Sample 2

This capillary was the straight glass macrocapillary with \( d_{in}=d_{out}=5.4 \) mm and \( l=35.5 \) mm corresponding to a critical angle \( \theta_c=8.65^\circ \). Similar data was measured similar in all respects for Sample 3 which is not shown here. The position- and angle-dependent characteristics, shown in Fig. 3.7 and Fig. 3.8 respectively, were measured in a manner similar to the metal capillary.

A notable difference in the position- and angle-dependent characteristics of the insulating capillary as compared to the metal capillary is the presence of oscillations. These oscillations are present within \( E_1 \) and \( E_2 \) for the position-dependent and within \( \theta_1 \) and \( \theta_2 \) for the angular dependent measurements as shown. The oscillations occur on the timescale of approximately one second. The ion beam width obtained for the insulating capillary was similar to the width obtained using the metal capillary. In addition, the ratio of the maximum transmitted current in the insulating case and the maximum transmitted current in the metal case was 5.48, which agrees well with the ratio of the areas of the entrance of the insulating and metal capillaries (5.51). These observations support the conclusion that the observed oscillations were due to the different type of material of the capillary used and not due to variation in the ion beam.
Figure 3.7: Position-dependent raw data for an insulating capillary (Sample # 2, \( l = 3.55 \text{ cm}, \ d_{in}=d_{out}=0.54 \text{ cm} \)). The transmitted current is plotted as a function of time at varying positions. Adapted from Ref. [68].
Figure 3.8: Angle-dependent raw data for an insulating capillary (Sample # 2, \(l=3.55\) cm, \(d_{\text{in}}=d_{\text{out}}=0.54\) cm). The transmitted current is plotted as a function of time at varying angles. Adapted from Ref. [68].
The minimum, mean and maximum transmitted current as a function of the tilt angle is shown in Fig. 3.9 along with the calculated transmission according to Eq 3.1. As can be seen from the figure, the angular spread of the measured maximum transmitted current agrees well with the angular spread calculated according to Eq. 3.1. However, the minimum and consequently the mean, have significantly lower angular spread as compared to the calculated angular spread. Examining the angular spreads, we obtain the experimentally determined critical angles for the maximum and minimum cases respectively as \( \theta_{c,\text{max}} = 8.65^\circ \) and \( \theta_{c,\text{min}} = 2.83^\circ \). The experimentally determined critical angle for the case of the maximum transmitted current agrees well with the calculated value of 8.65°.
Figure 3.9: Maximum, mean and minimum of transmitted current as a function of varying tilt angle for an insulating capillary (Sample # 2, \( l=3.55 \) cm, \( d_{in}=d_{out}=0.54 \) cm). The solid line shows the expected geometrical transmission from the capillary as a function of tilt angle, while the dashed lines are drawn to guide the eye. Adapted from Ref. [68].
The results of Fig. 3.9 can be explained by dividing the range of the angular tilt $\theta$ into two regions: $(\theta < \theta_{c,min})$ and $(\theta_{c,min} < \theta < \theta_{c,max})$. The first of these regions is where the angular tilt is lesser than the critical angle experimentally determined for the case of the minimum transmitted current. In this region, the minimum transmitted current always has a value greater than zero, i.e. in this range, there is always some transmission of ions that is taking place. Ion transmission in this region does not vanish due to the effects giving rise to the time dependent oscillations. Such effects, like charging of the walls, are not sufficient to completely block transmission within this range of angular tilt. However, within the second angular range $(\theta_{c,min} < \theta < \theta_{c,max})$, these charging effects are sufficient to temporarily block the transmission of the beam, as seen by the presence of a maximum transmitted current but vanishing minimum current for these angles. Thus, in this angular range, the beam is transmitted and blocked as a function of time. These oscillations in the transmitted beam can be attributed to charge patch formation on the interior walls of the capillary. Electric fields produced from charge patch formation can significantly affect the ion flight path leading to a time-varying transmitted current. Other studies where similar oscillations in the transmitted currents was observed include experiments using glass macrocapillaries, Teflon macrocapillaries and transmission through a pair of parallel glass plates[69–71]. The electric fields formed due to charge patches on the walls are strongest closest to the walls and their strength reduces as one moves closer to the center of the capillary. Ions passing closer to the center of the capillary experience a lesser deflecting force as compared to the ions passing closer to the walls of the capillary. The ions passing closer to the walls of the capillary thus experience the strongest force and experience the greatest deflection. The minimum transmitted current vanishing at certain angles can thus be explained by the deflection of these particles beyond the detection range and thus not being registered as the transmitted current. The maximum transmitted current, which bears similarity in the angular spread to the metallic case, can be attributed to transmission at that point of time.
where the charge patches on the walls have dissipated and ions are transmitted without experiencing any deflecting force, similar to the metal case.

Qualitatively, charge patch formation adequately explains the transmission characteristics measured using metallic and insulating capillaries. While a detailed quantitative analysis is necessary to model the guiding effects due to charge patch formation, we present simple order-of-magnitude calculation to examine the feasibility of charge patch formation as the reason for the observed oscillations. The kinetic energy of the ions was set to 1 keV corresponding to a velocity of $4.75 \times 10^4$ m/s. The flight path to the Faraday cup was 15 cm and the size of the detector was 2.54 cm.

A kinematic calculation based on the geometry of the setup can be used to estimate the electric field required to deflect the ions beyond the detector. The time of flight for Rb$^+$ ions at 1 keV through a capillary of a typical length of 20 mm is $t_{\text{cap}} = \sim 420$ ns. The flight path to the detector from the exit of the capillary is 13 cm, and the time it takes for the ion to reach the detector is $t_d = \sim 2736$ ns. To miss the detector, the radial velocity gained by the impulse during the passage of the ion within the capillary should be enough to cover a radial distance $r_d$ of at least 12.7 mm (radius of the detector) within the time it takes for the ion to reach the detector. The velocity gained in the radial direction must be at least $v_r = r_d/t_d = 4641$ m/s. The acceleration experienced by the ion due to its passage through the capillary must be $a = v_r/t_{\text{cap}} = 1.1 \times 10^{10}$ m/s$^2$. Consequently, the electric field necessary to produce this acceleration can be calculated as the acceleration divided by the charge to mass ratio of the incident ions, yielding 9.77 kV/m, or $\sim 10$ kV/m. The time required to deposit enough charge to form an electric field of this magnitude given the typical flux of the ion beam is on the order of 1 s, which agrees well with the timescale of the oscillations observed in the transmitted current. While transport simulations using classical phase-space dynamics as detailed in Ref. [72] can be used to obtain a detailed quantitative picture, the order-of-magnitude calculation above further supports the conclusion drawn
qualitatively that ion deflection due charge patch formation on the walls of the capillary lead to the observed oscillations in the transmission current.

### 3.2.3 Sample 4

This capillary was the conical glass macrocapillary with $d_{in}=5.4$ mm, $d_{out}=2.3$ mm and $l=19.6$ mm corresponding to a critical angle $\theta_c=11.11^\circ$. Figure 3.10 shows the position-dependent characteristics and Fig. 3.11 shows the angle dependent characteristics. The position-dependent and angle-dependent characteristics, shown in Fig. 3.10 and Fig. 3.11 respectively, were measured in a manner similar to the metal capillary.

The position-dependent characteristics for the conical macrocapillary were similar to the position-dependent characteristics of the straight glass macrocapillaries. The oscillations observed using the conical capillary were of similar amplitude as compared to the oscillations using the straight glass capillaries. However, for the angle-dependent characteristics, the amplitude of oscillations observed for the conical capillary were significantly smaller as compared to the straight capillaries. Due to the smaller amplitudes of oscillations, the minimum, mean and maximum are much closer to each other as shown in Fig. 3.12. The smaller amplitudes of oscillations, or lesser variation in the transmitted currents as a function of time for various angles, points to lesser degree of charge patch formation on the walls of the conical capillary. A qualitative reason for a decreased effect could be the sloping walls of the conical capillary. Due to the conical shape, the force imparted by the electric field is directed such it only partially deflects the ions radially while also slowing the ions axially. Thus, the acceleration experienced in the radial direction, which leads to deflection of the ions beyond the detector, might not be enough to gain a velocity required to miss the detector as in the case of the cylindrical capillaries. To measure whether the conical shape had achieved increased focusing due to the geometry, it would
be necessary to measure the current density of the beam exiting the capillary and compare that density to the current density of the incident ion beam.
Figure 3.10: Position-dependent raw data for the conical capillary (Sample # 4, $l=1.96$ cm, $d_{in}=0.54$ cm, $d_{out}=0.23$ cm). The transmitted current is plotted as a function of time at varying positions. Adapted from Ref. [68].
Figure 3.11: Angle-dependent raw data for the conical capillary (Sample # 4, $l=1.96$ cm, $d_{in}=0.54$ cm, $d_{out}=0.23$ cm). The transmitted current is plotted as a function of time at varying angles. Adapted from Ref. [68].
Figure 3.12: Maximum, mean and minimum of transmitted current as a function of varying tilt angle for the conical insulating capillary (Sample # 4, $l=1.96$ cm, $d_{in}=0.54$ cm, $d_{out}=0.23$ cm). The solid line shows the expected geometrical transmission from the capillary as a function of tilt angle, while the dashed lines are drawn to guide the eye. Adapted from Ref. [68].
3.3 Summary and Outlook

We have studied the transmission of the Rb\(^+\) ions through straight metal capillaries, straight glass capillaries and a conical glass capillary. Transmission of ions was studied as a function of time at different insertion distances in the beam path and also at different angles of tilt with respect to the ion beam. Oscillations were observed in the transmission currents when an insulating capillary was used. No oscillations were observed when the metal capillary was used. Qualitatively, charge patch formation on the interior walls of the capillary leading to ions being deflected out of the flight path was consistent with the measured transmission characteristics. From the geometrical dimensions of the setup and timescale of the oscillations observed, an order-of-magnitude calculation showed that charge patch formation was feasible further supporting the notion that charge patch formation lead to the observed oscillations. Absence of oscillation in the metal capillary also lends further credence to the notion that the oscillations were due to charging of the walls of the insulating capillaries. Such oscillations due to charge patch formation were observed before in nanocapillaries, however, this study is unique in terms of the size of the capillaries used.

The size of the capillaries used here was thought to be amenable for designing new beamlines, however it is seen that the charge patch formation by itself is not enough for guiding. The guiding could be greatly improved by the presence of an electric field that could aid the focusing effect and perhaps a smaller size would be better for guiding. To not lose sight of the required physical flexibility in the delivery method, the electrodes that could apply the electric field could be embedded into the flexible tube used to transport the ions. Two such proposed designs are shown in Fig. 3.13 and Fig. 3.14 with circular and hyperbolic electrodes respectively. The 'r' (radius of the embedded electrode) and 'r\(_0\)' (central hollow bore for passage of ions) in Fig. 3.13 were proposed to be 0.050 mm and
0.075 mm with a wall thickness of .015 mm. The dimensions in Fig. 3.14 were proposed as follows: \( r_0 = 0.050 \) mm, \( r_1 = 0.065 \) mm, \( r_2 = 0.210 \) mm. While these novel fibers are still in the design phase and thus experimental measurement was not possible, an in silico experiment using SIMION [61] was performed using the proposed designs. Figures 3.15 and 3.16 show equipotentials for the circular and hyperbolic designs respectively showing the metastable point at the center. If the frequency of the voltages applied to the four terminals is appropriately chosen, it is possible to transport ions in the central wall without them colliding with the walls of the trap. An example trajectory of an \( \text{Ar}^+ \) ion in the proposed designs is shown in Fig. 3.17 and Fig. 3.18 respectively. The energy of the ion was set to 0.01 eV and the maximum applied voltage was 2 V sinusoidally varying at \( \sim 25 \) MHz. For higher energies, higher frequencies are necessary to transport the ions. Frequencies in the GHz range and higher peak voltages were required for confining ions with ion energies in the hyperthermal range. If most of the energy of the ion is directed axially and if the ion only has a small component in the radial direction, then it may yet be feasible to use this scheme for transporting ions successfully. These designs and initial simulations show that externally aided electric fields applied by using embedded electrodes could be an efficient method for flexibly transporting M/HCIs.
Figure 3.13: Proposed design using circular electrodes embedded within an optical fiber for flexible transport of M/HClIs. Figure not drawn to scale.
$r_0 = 0.050 \text{ mm} ; r_1 = 0.065 \text{ mm} ; r_2 = 0.210 \text{ mm}$

Figure 3.14: Proposed design using hyperbolic electrodes embedded within an optical fiber for flexible transport of M/HCl. Figure not drawn to scale.
Figure 3.15: Equipotentials calculated for a static voltage applied to the electrodes in the proposed design using circular electrodes embedded within an optical fiber for flexible transport of M/HCIs.
Figure 3.16: Equipotentials calculated for a static voltage applied to the electrodes in the proposed design using hyperbolic electrodes embedded within an optical fiber for flexible transport of M/HClS.
Figure 3.17: Example of the trajectory of an Ar$^+$ ion in the proposed design using circular electrodes embedded within an optical fiber for flexible transport of M/HCl's. The energy of the ion was set to 0.01 eV and the frequency required was $\sim 25$ MHz.
Figure 3.18: Example of the trajectory of an Ar\(^{+}\) ion in the proposed design using hyperbolic electrodes embedded within an optical fiber for flexible transport of M/HClS. The energy of the ion was set to 0.01 eV and the frequency required was \(\sim 25\) MHz.
Chapter 4

Metrology of ion-solid interactions

This chapter describes the use of two types of electrically sensitive devices (Schottky diodes and Metal-Oxide-Semiconductor(MOS)) devices in experiments aimed at measuring ion-solid interactions. For singly-charged ions with low kinetic energy (KE < 10 keV), as described in Chapter 1, the kinetic energy of the ions couples with the nuclear and electronic subsystem of the target giving rise to subsurface damage and electronic excitations. The subsurface excitations are hard to experimentally determine using conventional methods (such as irradiating thin foils with ions possessing enough kinetic energy to exit the foil allowing the energy loss to be tracked upon exit), as the ions are implanted into the solid at low kinetic energies. Two methods are described here to track the subsurface excitations caused due to ions - 1. Using Schottky diodes to measure hot electron current caused due to excitation of hot electrons 2. Using MOS devices to track subsurface damage by tracking the shift in the capacitance-voltage (C-V) curves of these devices. In the case of multiply charged ions, the potential energy couples with the surface as well as the kinetic energy, leading to additional damage due to electron capture from the target. MOS devices irradiated with multiply charged ions of the same kinetic energy caused shifts in the C-V curve that depended on the charge state. By relating the shifts in the C-V curve to the stop-
ping 'power' (the drag force \(-dE/dx\) experienced by the ions in the solid), it was shown that the stopping power follows a quadratic dependence on charge state. Irradiations of Schottky diodes with multiply charged ions are currently planned, using the single charged data as a baseline for determining the kinetic energy effects. It will be interesting to learn what the irradiations of Schottky diodes with multiply charged ions will reveal regarding the dependence of hot electron generation on the charge state of the incoming ions.

### 4.1 Hot electron current - Schottky diodes

#### 4.1.1 Introduction

Energy generated by exothermic chemical reactions at surfaces is dissipated into the substrate by a variety of channels, viz. excitation of photons, phonons and electrons, as illustrated in Fig.4.1. The energy loss via the excitation of electron-hole pairs is experimentally the hardest to detect as the lifetime of these excitations is short. Nienhaus et al.[53] measured these excitations using gas molecules of thermal energy incident onto a thin metal film forming a Schottky diode with a semiconductor. By utilizing the barrier of a Schottky diode to provide energy separation, hot electrons ballistically traversing the barrier were detected as chemicurrent in these measurements. These experiments have shown that electron-hole pair excitation is a major non-negligible channel of energy dissipation, whereas earlier it was believed that most of the energy was dissipated into the phononic subsystem of the substrate.
Figure 4.1: Various channels into which energy from exothermic reactions (depicted here as the interaction of the incident reactive gas molecules of thermal energy with the metal surface) is dissipated are shown in the figure. Adapted from Ref. [53].
Our work[73] concentrates on the electron-hole pair excitation caused due to the impact of ions of hyperthermal energy (500 eV - 5000 eV). The earliest report of electron-hole pair detection due to energetic particle bombardment was due to Amirav and Cardillo[74, 75], wherein they measured a transient excitation current originating from a local hot spot upon irradiating Ge(100) and InP(100) surfaces with neutral Xe atoms with energies in the range of 1 eV-10 eV. Other closely related studies were performed by Ray et al.[76] and Wucher et al.[77] using metal-oxide-semiconductor (MOS) and metal-insulator-metal (MIM) devices respectively. The MOS measurements resulted in the discovery of a velocity dependence for the detected hot electrons that was below the expected threshold for transmission over the internal barrier present in the MOS device. The MIM measurements reported the energy-dependence of the hot electron current in the few keV energy range and observed a saturation of the detected hot electron current at ∼5 keV. The study performed here aimed at measurement of the hot electron current, as a function of the energy and angle of incidence of the ion beam, utilizing a device that did not require an insulator and thus eliminated the tunneling necessary for detection in the MOS/MIM devices. As the enhanced sensitivity of Schottky diodes as a detector for hot electrons has been well established in the chemicurrent measurements of Nienhaus and others[53], Schottky diodes were used in this measurement as the detection devices. The measurements are described in detail in the appendices[73].

4.1.2 Experiment

The diodes used for this experiment were fabricated in house at Clemson University. The Schottky diodes were designed as a thin Ag film deposited on silicon substrate with backside Ohmic contacts of Al. Phosphorus doped Si $<111>$ wafers obtained from Monsanto were used as substrates. The resistivity reported for the wafers was $4.0 \pm 0.6 \ \Omega$-cm.
The wafers were etched with diluted HF (2%) to remove the native oxide. The backside Ohmic contacts were formed by depositing 0.5 µm of Al and sintered at 450°C for 45 minutes in a nitrogen environment. The frontside rectifying contact was deposited in the shape of a dot using 99.999% pure Ag in a thermal evaporator, as shown in 4.2a. The thickness of the Ag dot, chosen to be 25 nm, is an important parameter in the design of this experiment for the reasons discussed below in the following paragraphs. I-V characteristics of the Schottky diodes fabricated as stated are shown in 4.2b. The barrier height and ideality factor of the diodes obtained from the I-V characteristics were 0.83 eV and 1.9 respectively.
Figure 4.2: a) A schematic representation of the Schottky diode (25 nm Ag/n-Si) irradiated by a pulsed ion beam with varying kinetic energy and angle of incidence. Current through the device is measured using a Keithley 617 picoammeter. b) Current-voltage characteristics of a typical Schottky diode used in these measurements. Barrier height of 0.83 eV and ideality factor of 1.9 are representative of the parameters for the diodes fabricated for this experiment. Adapted from Ref. [73].
The irradiations were performed in the singly-charged beamline described in detail in Ref. [64]. The experiment was performed as a function of two independent variables with respect to the beam parameters: energy and angle of incidence. The energy-related measurements were performed using Rb$^+$ ions at energies of 500 eV-1500 eV at normal incidence, while the angle-dependent measurements were performed in the target chamber using Ar$^+$ from an Omicron sputter source at a fixed energy of 5 keV. The setup for the energy-dependent measurements utilized a Colutron ion source[65] equipped with an aluminosilicate emitter[66] as a source of Rb$^+$ ions. The heater current to the filament, $I_{src}$ was turned up at a rate of approximately 50 turns per 15 minutes upto 300 turns resulting in a heater current of $\sim 1.81$ A. The bias electrode was set to the usual value of -14 V to produce an ion beam. The Wien filter positioned immediately after the source is usually used to separate out the Rb$^+$ ions. The current through the electromagnet producing the magnetic field was $I_{mag} = 1.0$ A (200 turns) along with an electric field produced by an applied voltage of $V_A = 15$ V, corresponding to Rb$^+$ ions. However, for these measurements, the Wien filter was kept off as this resulted in a stable ion beam. The majority of ions emitted from the source were expected to be Rb$^+$ ions, as seen by the measured current in the Faraday cup, so keeping the Wien filter did not affect the experiment. The electrical deflection voltage was set to 20 V and the horizontal field was set to -1 V. The focusing and the accelerating voltages were set as shown in Table 4.1.
A custom vacuum chamber was installed after the Wien filter that housed the samples for this experiment. The experimental setup used is represented schematically in Fig. 4.3, while Fig. 4.4 is a photograph of the actual setup. The deflectors in the path of the ion beam were used to pulse the ion beam in order to obtain a beam response measurement. The deflectors were toggled in between two values (0 V and 20 V) such that the beam was incident away from/onto the sample. As the beam width in this section is wide (diameter of 14 mm) as seen during the study with the capillaries[68], it was necessary to mask the sample to expose only the metallic portion of the diode to the ion beam. For this purpose, a metal capillary of diameter 2.3 mm housed in a metal shield 125.4 mm wide was mounted on a linear translator and could be moved vertically to align with the sample. The sample itself was mounted on a linear translator that could be moved into the path of the beam behind the capillary as shown. A Faraday cup was mounted in the same plane of the sample and was used to measure ion beam currents and tune the ion beam. The sample was mounted on a platen containing isolated posts at the bottom as shown in Fig.4.4 and placed in an insulating holder. The rectifying contact was connected to one of the posts with a thin silver wire using silver paste from Ted Pella, Inc. The backside was connected to the another post. Isolated copper leads were attached to the housing in a way that they slid on top of the posts providing electrical connections. These copper leads were wired through to electrical feedthroughs using Kapton insulated wires to provide connection points to

<table>
<thead>
<tr>
<th>$V_{\text{accel}}$ (V)</th>
<th>$V_{F1}$ (V)</th>
<th>$I_{FC}$ (nA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>750.2</td>
<td>616.1</td>
<td>19.86</td>
</tr>
<tr>
<td>500.0</td>
<td>416.1</td>
<td>10.46</td>
</tr>
<tr>
<td>1002.0</td>
<td>811.1</td>
<td>28.37</td>
</tr>
<tr>
<td>1250.5</td>
<td>1016.2</td>
<td>35.56</td>
</tr>
<tr>
<td>1500.0</td>
<td>1216.2</td>
<td>38.00</td>
</tr>
</tbody>
</table>

Table 4.1: Table showing the accelerating voltage $V_{\text{accel}}$, focusing voltage $V_{F1}$, and the corresponding current $I_{FC}$ measured in the Faraday cup.
facilitate ex-situ electrical measurements.
Figure 4.3: A schematic representation of the experimental setup used to conduct the ion irradiations. The energy dependence was measured in a custom vacuum chamber inserted into the beamline directly in front of the ion source. The capillary and the sample were translatable in the X and Y directions respectively as indicated. The in-path deflectors were used to pulse the ion beam to measure the response of the sample to the incident beam. Adapted from Ref. [73].
Figure 4.4: A photograph of the experimental setup used to conduct the ion irradiations. The energy dependence was measured in a custom vacuum chamber inserted into the beam-line directly in front of the ion source. The capillary and the sample were translatable in the X and Y directions respectively as indicated. The in-path deflectors were used to pulse the ion beam to measure the response of the sample to the incident beam.
The thickness of the Ag film is an important design parameter in this experiment. If the ions incident onto the metal film penetrated into the semiconductor, these ions would confound the current due to hot carriers. Thus, the contact thickness must be sufficient to stop the ions from penetrating into the semiconductor. Using the Stopping Ranges of Ions in Matter (SRIM) software [78], the range of the ions at the energy range used in this experiment was obtained to be not more than 20 nm, setting a lower limit on the thickness of the film. An upper limit on the thickness of the film also exists as the hot electron current is attenuated exponentially with respect to the path length of the electrons in the metal before reaching the semiconductor. Current is attenuated inside a metal film exponentially with respect to the film thickness \( d \) according to Beer’s Law as shown by the following equation

\[
I \propto I_0 \exp \left( \frac{-d}{\lambda_{mfp}(E) \cos(\theta)} \right)
\]

where the non-scattered current, \( I \), depends on the incident current, \( I_0 \), which is attenuated exponentially according to the mean free path, \( \lambda_{mfp}(E) \), for electrons in the film and the path length, \( d/\cos(\theta) \), of those electrons through the film. The hot electrons are considered to undergo inelastic scattering events both with other cold electrons and the phononic system of the metal film, and both processes have a dependence on the excess energy of the hot electrons, hence the explicit energy dependence shown. The defects in the metal film also play a significant role in determining the mean free path of the electrons. Estimates for the ballistic \( \lambda_{mfp} \) for polycrystalline metal films [79–81]) find them to be tens of nanometers with values that vary depending on the technique used for measurement and on the quality of the film. Here we chose the thickness of our rectifying contact to be \( \sim 25 \) nm, within 5 nm of the lower limit and no more than a factor of two from typical \( \lambda_{mfp} \) values. It is noted here that the samples were photosensitive, so care was taken to block as much light as possible from illuminating the sample. However, some light from the filament which
was in direct line of sight with the samples could not be blocked, resulting in a background
current. The hot electron current was measured as the difference from the background level
in response to the pulsed ion beam incident upon the sample.

It was an interesting problem to determine the correct way to measure the hot elec-
tron current with respect to wiring the sample. We first used two separate electrometers, one
connected to the frontside and the other connected to the backside, to measure the frontside
and backside currents respectively. The frontside current would represent the neutralization
current corresponding to the ion current incident onto the surface of the sample. The back-
side current would represent the hot electron current. The scheme of using two separate
meters was unsuccessful due to the existence of ground loops, which resulted in spurious
currents flowing in between the two meters. Various efforts, including connecting the com-
mon grounds of the two meters, did not result in improvement. Thus, it was determined
that the current measurement should be done using one meter only, which would avoid the
problem of ground loops. The Keithley 617 electrometer was used to measure current using
a triax cable. The signal, shield and ground leads of the triax cable, (colored red, black and
green respectively) were connected across the front and the back in various configurations
to ascertain the consistency of all configurations. Measurements with all these configura-
tions were consistent with respect to the direction of electron flow and sign of the measured
current. The final configuration for measuring the backside current consisted of connecting
the signal (red) lead to the backside contact and connecting the shield and ground (black
and green) to the frontside, while the configuration to measure the frontside was reversed
with respect to the leads i.e. red lead to the frontside and the black and green leads to the
backside.
4.1.3 Results and Discussion

Figure 4.5 shows the measured response of the Schottky diode to the incident 1000 eV Rb\(^+\) ion beam. The label 'ON' signifies the point of time at which the ion beam was incident onto the sample face, while the label 'OFF' signifies when the ion beam was deflected away from the sample face. For example, the ion beam was incident onto the sample face at \(t \approx 10\) s and away from the sample face at \(t \approx 130\) s. The background current, at the time when the beam was OFF, was recorded to be \(-9\) nA. This background signal is attributed to the photosensitive nature of the samples. The beam was incident onto the sample for a period of \(\sim 120\) s. The signal at the time when the beam was ON was recorded to be \(-10.8\) nA. Thus, the ion beam exposure resulted in a negative spike in the current measured at the backside of the sample. A negative spike indicates that electrons were flowing from the semiconductor to the meter, consistent with hot electron generation and transport from the metal film to the semiconductor. This direction of current flow is also consistent with previous measurements[53, 76, 77, 82, 83].
Figure 4.5: Hot electron current measured through a fabricated device in response to a pulsed Rb\(^+\) beam at a kinetic energy of 1000 eV. The label ON signifies that the beam was directed onto the device face (e.g. at \(t \approx 10\) s), while OFF signifies it was deflected away from the device face (e.g. at \(t \approx 130\) s). The background signal when the beam is OFF is approximately \(-9\) nA, while the measured signal is approximately \(-10.8\) nA when the beam is ON. Adapted from Ref. [73].
The current measurements were repeated for incident ion beam energies beginning at 500 eV upto 1500 eV in steps of 250 eV. The hot electrons current measured at the backside was normalized by the incident ion current to obtain a yield. Figure 4.6 shows the yield plotted as a function of the incident kinetic energy of the ions. The error bars were calculated taking into account the 50 pA variation seen in in 1nA current (5%). As seen in the data, no significant hot electron current exists below 1000 eV but a significant onset of hot electron current is observed at 1250 eV. This onset can be interpreted as a threshold lying in between 1000 eV and 1250 eV for the detection of hot electron current using this scheme.
Figure 4.6: Yield of hot electrons plotted as a function of the kinetic energy of the incident ions. The dashed blue line at 1139 eV represents a threshold energy calculated for Rb$^+$ ions on a Ag film using a KEE model (Eq.4.2). Adapted from Ref. [73]. See text for details.
Typically, for exoelectron emission, a threshold is observed within the 'kinetic electron excitation' (KEE) model[76], which can be thought of as an ion-analogue for the photoelectric effect where electron emission from a metal surface into the vacuum arises due to ion bombardment instead of photon bombardment. In the KEE model, the metal surface is idealized as a Fermi gas and a threshold ion velocity ($v_{th}$) for exoelectron emission, analogous to the photon frequency in the photoelectric effect, is calculated taking into account energy transfer to the electronic system of the metal by binary collisions and the depth of the potential barrier trapping the excited electrons. We can apply the KEE model (Eq. 4.2) to the case of hot electron current in the Schottky diode by substituting for the potential barrier the device Schottky barrier height $\phi_b = 0.83$ eV along with Fermi energy $E_f$ and Fermi velocity $v_f$ for our Ag film, $5.49$ eV and $1.39 \times 10^6$ m/s respectively, giving a threshold velocity $v_{th} = 5.06 \times 10^4$ m/s.

$$v_{th} = 0.5 \, v_f \left[ \sqrt{1 + (\phi_b/E_f)} - 1 \right]$$  (4.2)

For the ion species used in our experiment (Rb$^+$), the calculated threshold velocity corresponds to a kinetic energy of 1139 eV, which is represented as the dashed vertical blue line in Fig. 4.6. This threshold value agrees well with the upturn observed in our data near 1000 eV.

For the angular measurements, the energy of the Ar$^+$ ions was kept constant at 5 keV while the angle was varied from -60° to +60°. Figure 4.7 shows the variation in the backside current and also the frontside ion current as a function of the angle of incidence. The backside current obtained in these measurements was also negative as expected, absolute values are plotted for convenience. In Fig. 4.7, the absolute backside current is plotted on the axis to the left, while the frontside current is plotted on the axis to the right. Data in the shaded region in Fig. 4.7 is considered as confounded and discarded, as the ion beam in
this position was hitting some of the exposed leads/wires due to the large angle of rotation. Fluctuation in the frontside current at these positions is also indicative of the ion beam hitting exposed electrical contacts for angles in the shaded region. The frontside current is nearly constant in the non-shaded regions, which is indicative of the fact that at smaller angles the leads were not exposed to the ion beam. The yield at normal incidence is of the same order of magnitude as compared to the energy measurements. This current is strongly peaked about the normal incidence direction and falls off on either side monotonically.

The hot electron current consists of electrons excited by the incoming ion beam which travel ballistically to the metal-semiconductor interface. The spectrum of the energetic excitation as well as the momentum spectrum of these electrons is currently not well known[53]. If we assume an increased intensity of hot electrons in the direction of the ion beam, then as the angle of incidence of the ion beam is increased, the path length to the interface increases as the inverse of the cosine of the angle, as shown in Eq. 4.1. The path length at normal incidence would be the least amongst all angles of incidence and would be equivalent to the thickness $d$ of the metal film. A lower path length implies fewer scattering events with other colder electrons, and thus it is expected that at normal incidence a higher yield will be observed. Figure 4.8 shows the plot of the negative logarithm of the ratio of the hot electron current normalized by the incident ion current and the normalized current at normal incidence versus the inverse of the cosine of the angle of incidence. The slope of the linear fit line is obtained to be $4.8 \pm 1.3$. Using the fact that $d = 25$ nm and Eq. 4.1, we obtain the mean free path of hot electrons in the silver film to be $5.2 \pm 1.4$ nm, which compares well with the values reported in the literature in the range of $4.5 \pm 0.5$ nm obtained by hot electron attenuation measurements using Schottky diodes composed of Ag films of varying thicknesses[84].
Figure 4.7: Variation in hot electron current as a function of the angle of incidence of a 5 keV Ar$^+$ beam. The frontside ion current represented by open circles (○) is approximately constant while the absolute value of the backside hot electron current represented by filled circles (●) is strongly peaked about the normal. The shaded areas correspond to regions where the signal is confounded with ion current and is disregarded. See text for details. Adapted from Ref. [73].
Figure 4.8: Figure illustrating the relation between the detected hot electron current and path length as given by Eq. 4.1. The ordinate is the negative of the logarithm of the ratio of the normalized hot electron current detected at an angle $\theta$ to the normalized hot electron current detected at normal incidence ($\theta = 0^\circ$), while the abscissa is the inverse of the cosine of the angle. The slope ($4.8 \pm 1.3$), obtained from the linear fit, is the ratio of the film thickness to the mean free path of electron inside the film. Adapted from Ref. [73].
4.1.4 Summary and Outlook

We have fabricated Schottky diodes using 25 nm Ag films deposited onto n-type Si substrates and irradiated the top metal contacts with Rb\(^+\) and Ar\(^+\) ion beams of varying kinetic energy and angle of incidence respectively. The kinetic energy was varied between 500 eV and 1500 eV and a threshold for hot electron current detection was observed between 1000 eV and 1250 eV. A kinetic electron emission model applied to the sub-surface Schottky barrier resulted in a calculated threshold value of 1139 eV, in good agreement with our observations. The angular dependent measurements suggest that there is an anisotropic generation and transport of hot electrons through the Ag film as there is a significant drop in the detected current for non-normal incident angles. Using these data and Beer’s Law, an estimate of the mean free path for ballistic electrons in our Ag film is found to be 5.2 ± 1.4 nm. Defects in the metal film as well as non-trivial angular effects similar to those seen in BEEM measurements could contribute to this otherwise low \(\lambda_{\text{mfp}}\) value. We note that as the dependence of the observed hot electron current on the thickness of the metal film can be utilized to obtain the mean free path of hot electrons[85, 86], measurements using diodes fabricated with metal films of varying thickness are currently underway.

Ballistic electron emission microscopy (BEEM), a technique developed by Bell and Kaiser [87–89], can also be used to probe the directional momentum of hot electrons in a Schottky diode and as such is relevant to the angular measurements here. In BEEM, hot electrons from a negatively biased STM tip are injected into a metal surface and are collected, usually at a semiconductor interface, after passing through a Schottky barrier. The hot electron current is observed after a certain threshold bias voltage is reached. The transport of these hot electrons and their scattering within the metal film and at the metal-semiconductor interface is non-trivial. However, if we focus on our angular-dependent measurements, it is worth noting that in BEEM, using concepts of momentum conserva-
tion across the metal-semiconductor interface, there is a critical angle for the direction of the momentum of the hot electrons at the interface [90, 91]. Beyond this angle hot electrons are reflected back into the metal surface instead of passing into the semiconductor, in analogy to total internal reflection of light. These reflected electrons can also undergo multiple reflections in the metal film, depending on its thickness, which can lead to randomization of the original direction and loss of directional information. While further analysis of our method is required before we can compare our measurements directly to such BEEM results, we note that this added angular dependence may serve as an additional factor suppressing the apparent mean free path for electrons in our Ag film. Finally, we note that sputtering of the top layer due to the incoming ion beam can change the effective path length for hot electron transport. Currently measurements are underway to obtain precise sputter yields using the methodology described here [92], however, an estimate of ~70 hours is obtained, using SRIM, as the time required for 25 nm of Ag to be sputtered through by the incoming ions. Our measurements on any particular sample did not exceed a total exposure time of a few hours.

Currently, we have proposed measurements using samples with varying thickness of Ag films - from 25 nm to 100 nm in steps of 25 nm - to verify the MFP using these samples and gain confidence in the claim that the current seen at the backside is due to hot electrons. It would be beneficial to conduct the angular dependence measurements with the same setup and ion beam parameters as the energy dependence, i.e. to conduct the angular dependence measurements in Section 1 of the beamline. This was previously hindered due to lack of space while rotating the sample holder with respect to the beam. This was fixed by using a greater offset in the capillary holder to yield more space allowing rotation of the sample holder without butting into the capillary shield and is currently being installed onto the vacuum chamber. A quick repeat of the measurements with varying angles of incidence and using different species to elucidate any velocity dependence are
interesting measurements that can be obtained relatively quickly given the readiness of the setup. Another measurement of the energy spread of the excited electrons could be obtained by varying the bias of the Schottky diode, effectively varying the height of the barrier the electrons have to overcome - leading to a technique for spectroscopy of the energy levels of the hot electrons. The fact that ionic particles carrying charge were incident onto the sample leads us to question whether the deposited charge is leading to neutralization current within the device that could be interfering with the hot electron current in some unknown manner. Thus, to avoid this problem or to prove it non-significant, it has been proposed to use a gas cell to neutralize the ion beam and repeat the experiment with energetic neutral particles. Measuring neutral particle flux is not as straight forward as measuring charged particle flux. Measurement of the sputter erosion of the thin film by measuring the change in its resistance and correlating that to flux of the charged particle beam seems one way to proceed without a special setup dedicated for neutral flux measurement. Finally, these excited electrons could be sampled by a coincident hyperthermal energy ion beam to study resonant charge transfer with excited electrons and one can use this setup to study Hot Electron Femtochemistry at Surfaces.
4.2 Metal-oxide-semiconductor (MOS) device irradiations

Subsurface interactions of ions with solids at low kinetic energies are not easy to track and quantify. Discrepancies exist at the lower kinetic energy range with the experimental data and noted softwares like SRIM. We have developed a technique to quantify the damage inside an oxide and measure stopping power at low kinetic energies using encapsulated MOS devices. An oxide grown on a semiconductor substrate was irradiated with energetic ions and then capped with a metal layer to form the encapsulated devices. Electrical characterization of these devices via their capacitance-voltage (C-V) curves and shifts therein were used to obtain a quantitative measure of the subsurface damage and stopping power of the incident ions. The effects of incident kinetic and potential energy effects in the low keV regime for Na$^+$ ions and Ar$^{Q+}$($Q = 1, 4, 8, 11$) ions were incident onto the 190 nm SiO$_2$ grown on a Si surface and then capped with an Al layer. The shift in the C-V curves was correlated with internal electron-hole pair generation which in turn depended on the energy lost to the electronic subsystem of the target by the incident ions. The shift in the curves was quadratically dependent on the charge state of the incident ion. Also, a super-linear dependence of the density of the interface states on the kinetic energy of the incident singly charged ions was measured in the experiments with Na$^+$ ions. These measurements are detailed in the publications reproduced in the appendices[25, 93]. Currently, we have obtained data on irradiations of MOS devices with oxide thickness of 50 nm and analysis of the C-V curves is underway in collaboration with Daniel Cutshall and Dr. Harrell in the ECE department.
Chapter 5

Future Work

5.1 Charge Exchange

5.1.1 Introduction

Measurements of cross-sections of charge exchange with neutral gases is an interesting and important topic currently under investigation. There are astrophysical as well as applied motivations underlying these measurements. There are primarily two experimental techniques to study charge exchange - utilizing a gas cell and the other is utilizing a gas jet. The basic measurement utilizing a gas cell is shown in Fig. 5.1. A multiply/highly charged (M/HCl) ion beam is incident onto the opening aperture of the gas cell in some known charge state 'q'. The gas cell consists of a cylindrical body with an inlet for neutral gas and two collinear apertures for the ion beam entrance and exit respectively. The flow rate of neutral gas into the gas cell is usually well monitored utilizing a capacitance manometer to accurately determine the pressure inside the gas cell. The pressure determination, usually calculated taking into account conductance considerations, needs careful attention as the gas inside the cell leaks out of the apertures meant for the entrance and exit of the ion
beam. As the ions, also called projectiles, interact with the neutral gas atoms, also called as 'target atoms' or just 'target', electrons from the target are captured by the ions lowering the charge state of the ions. This process is known as charge exchange and can be quantified by measuring the charge state of the exiting beam. Typically used detectors include retarding field analyzers or hemispherical analyzers which measure ion current as a function of the charge state. The cross-section can be calculated from the dependence of the varying current vs charge state spectrum on the pressure of the gas inside the gas cell. To help facilitate the design of the gas cell, Fig. 5.2 lists important experimental parameters of existing charge exchange studies utilizing Ar ions, as the baseline test of the gas cell under construction will be performed using the sputter Ar source[94–100].
Figure 5.1: Figure illustrating the basic measurement of charge exchange. A multiply/highly charged (M/HCI) ion beam with charge state ‘q’ is incident onto a gas cell containing a neutral gas target. The incident ions undergo charge exchange with the neutral gas atoms by capturing one or more electrons and exit the gas cell in various charge states as shown. A detector, such as a retarding field analyzer or a $127^\circ$ hemispherical analyzer, is used to measure the ion current as a function of the charge state. Repeating these measurements at varying pressures enables us to obtain cross-sections using the ‘growth-rate’ method, as described below.
<table>
<thead>
<tr>
<th>Author</th>
<th>Projectile/Energy</th>
<th>Target Gas</th>
<th>Pressure Gauge</th>
<th>Gas Cell Pressure (Torr)</th>
<th>Gas Cell Length, Entry, exit (mm)</th>
<th>Detector</th>
<th>Absolute Cross-section σ (barn)</th>
<th>Cross-section calculation method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Can (1985)</td>
<td>Ar 2-10, Ne 2-7 0.1 – 3 kV</td>
<td>H₂/H₂</td>
<td>MPS 20 Cap, Man.</td>
<td>4E-4</td>
<td>1E-6</td>
<td>Double-focusing ESA</td>
<td>“1E-15 and lower”</td>
<td>Ratio of yield</td>
</tr>
<tr>
<td>Kosakabe (1986)</td>
<td>Ar 2-7 6.266 keV/u (11.4 keV)</td>
<td>He/H₂</td>
<td></td>
<td>7E-4 to 7E-4</td>
<td>40</td>
<td>PSD after charge separation</td>
<td>1E-15 to 1E-14</td>
<td>Growth rate method</td>
</tr>
<tr>
<td>Elijay (1986)</td>
<td>Ar 1-9 (1.84 keV)</td>
<td>Ne, Ar, Kr</td>
<td>Cap man</td>
<td>5E-4</td>
<td>8</td>
<td>TOF (4% resolution)</td>
<td>“1E-15”</td>
<td>Ratio method</td>
</tr>
<tr>
<td>Vannora (1993)</td>
<td>Ar 6-10 (2.3 keV)</td>
<td>H₂ / H₂</td>
<td>Based on on-line-flow method see text.</td>
<td>1E-5 (main chamber 1E-6 to 1E-5)</td>
<td>122</td>
<td>RFA ESA</td>
<td>1E-15 to 1E-14</td>
<td>Growth rate method</td>
</tr>
<tr>
<td>Kosakabe (2003)</td>
<td>Ar 2-9 (2.0 keV)</td>
<td>CH₄, C₂H₄, C₂H₂, C₂H₂, C₃H₄, C₃H₃, C₃H₂, C₃H₁</td>
<td>Frangiograph Calibrated by cap, man.</td>
<td>7E-4 to 7E-4</td>
<td>40</td>
<td>PSD after charge separation</td>
<td>“1E-12”</td>
<td>Growth rate method</td>
</tr>
<tr>
<td>Zanour (2000)</td>
<td>Theory Ar²⁺</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 5.2: Table showing important experimental parameters in studies of charge exchange using Ar as the projectile species and employing a gas cell.
5.1.2 Calculation of Cross-sections

The cross section, \( \sigma \), depends on the following parameters - the charge state of the incoming beam \( q \), the ionization potential of the gas \( I_p \), and the target thickness \( \rho \). The target thickness is defined as the product of the path length \( L \) and the pressure of the gas \( P \), which is experimentally the knob to turn in these measurements. An example plot for the charge exchange cross sections of Ne and Ar ions with different targets as a function of charge state is shown in Fig. 5.3. A rough estimate of the cross section as a function of the charge state is given by the formula 

\[
\sigma \sim q \times 10^{-15} \text{ cm}^2
\]

(See Ref. [101]).

The cross section is nearly independent of the velocity of the ion at low kinetic energies (velocity less than 1 a.u.)[102]. Velocities to be utilized in the measurements proposed in our lab are approximately 0.01 a.u. to 0.1 a.u. - well below the limit of 1 a.u. The cross section is nearly independent of the projectile species as well[103]. Cross sections are typically reported as they are independent of the geometry/parameter-space of a particular experiment and are a convenient way to describe the underlying physical phenomenon. The cross sections can be calculated from the current measured as a function of the charge state of the beam exiting the gas cell. During the charge exchange process, electrons are captured into high-lying Rydberg states which decay by autoionization leading to some Auger emissions. Thus, a number of paths can lead to the final charge state. Assuming only single or double electron-capture, let \( \sigma_{q,1} \) and \( \sigma_{q,2} \) be the cross-sections of single and double electron capture from charge state \( q \) leading to charge state \( q-1 \) and \( q-2 \) respectively. As seen in Fig. 5.4, an ion with charge state \( q-2 \) can lose an electron by autoionization (Auger) with probability denoted by \( a_{q-21}^q \) and end up in the state \( q-1 \), or can remain in the same state with probability \( 1-a_{q-21}^q \). Similar transitions from different charge states are shown in the figure using which we can derive the functional dependence of the population of a given charge state on the target thickness. Let \( N_q \) denote the number
of ions in state 'q'. The rate of change of $N_q$ with respect to the target thickness depends on the number of ions in that state (i.e. $N_q$) scaled by the cross-sections relating to the various transitions directed into and emanating from the node signifying that state. The transitions coming into that state are forming the charge state, so the transitions directed into a node are assigned a positive sign, while those emanating from are destroying that state and are thus assigned a negative state. Thus, for example, we have $N'_q = -N_q(\sigma_{q,1} + \sigma_{q,2})$ for the charge state 'q', as there are no transitions directed into the node, while there are two transitions emanating from that node. We call the term in the brackets, $(\sigma_{q,1} + \sigma_{q,2})$, as the effective cross-section $\sigma'_{q,t}$, which represents the total cross-section for the ion in charge state 'q'. This effective cross-section is accessible by experiments as the branching probabilities are not known for all transitions. For the state 'q-1', we analogously have

$$N'_{q-1} = +N_q(\sigma_{q,1} + a_{21}^{q-2}) - N_{q-1}(\sigma_{q-1,1} + \sigma_{q-1,2}) = +N_q(\sigma'_{q-1,1}) - N_{q-1}(\sigma'_{q-1,t}).$$

The system of equations for other states is shown in Fig. 5.4. As can be seen from the form of these equations, the solution can be expressed in terms of exponentials. In practice, these are expanded in terms of Taylor polynomials upto second order and are used to obtain the cross-sections. The quadratic equations used to fit the curves obtained experimentally are given below:

$$\frac{N_q(\rho)}{N_q(0)} = 1 - \sigma_{q,t}\rho + \frac{1}{2}(\sigma_{q,t} \rho)^2,$$  \hspace{1cm} (5.1)

$$\frac{N_{q-1}(\rho)}{N_q(0)} = \sigma'_{q-1}\rho - \frac{1}{2}\sigma'_{q-1}(\sigma_{q,t} + \sigma_{q-1,t}) \rho^2,$$  \hspace{1cm} (5.2)

$$\frac{N_{q-2}(\rho)}{N_q(0)} = \sigma'_{q-2}\rho + \frac{1}{2} \left[ \sigma'_{q-1,1} \sigma'_{q-1,1} - \sigma'_{q-2,1} (\sigma_{q,t} + \sigma_{q-2,t}) \right] \rho^2$$  \hspace{1cm} (5.3)

Figure 5.5 shows an example of charge exchange data fit to the quadratic curves obtained above. Ar$^{13+}$ was incident on $H_2$ and only single and double electron capture was considered. The observed ratio of the currents is plotted as a function of varying target thickness.
Figure 5.3: The figure shows measured absolute cross-sections for Ar and Ne ions on various targets. The kinetic energy of the ions was 2q keV, where q signified the charge state of the ions (q=2,3,4,5,6 for Ne ions, and q=2,3,4,5,6,7,8,9 for Ar ions). The different targets are shown in a:CH$_4$, b:C$_2$H$_2$, c:C$_2$H$_4$, d:C$_2$H$_6$, e:a − C$_3$H$_4$ (Allene), f:p − C$_3$H$_4$ (Propyne), g:C$_3$H$_6$, h:(CH$_2$)$_3$. Adapted from Ref. [96].
Figure 5.4: The figure shows the evolution of charge states due to single and double electron capture and also the various paths to obtain a charge state considering Auger emissions. This diagram is useful to derive the differential equations that relate the cross sections to the target thickness $\rho$. Adapted from Ref. [99].
Figure 5.5: The figure shows single and double electron capture as a function of the target thickness (varying pressure in the gas cell) fitted to the quadratic curves shown in Eq. 5.1 - Eq. 5.3. The linear term is dominant in the single electron capture while the quadratic term is dominant in the double electron capture. Adapted from Ref. [99].
Appendices
Appendix A

Ion transport through macrocapillaries - Oscillations due to charge patch formation

The following has been published in *Nuclear Instruments and Methods in Physics Research B*, (NIMB 342, 54 (2016))
Ion transport through macrocapillaries – Oscillations due to charge patch formation

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ABSTRACT

We present results on ion transport through large bore capillaries (macrocapillaries) that probe both the geometric and ion-guided aspects of this ion delivery mechanism. We have demonstrated that guiding in macrocapillaries exhibits position- and angle-dependent transmission properties which are directly related to the capillary material (either metal or insulator) and geometry. Specifically, we have passed 1 keV Rb⁺ ions through glass and metal macrocapillaries, and have observed oscillations for the transmitted ion current passing through the insulating capillaries. Straightforward calculations show that these oscillations can be attributed to beam deflections from charge patches that form on the interior walls of the capillary. The absence of these oscillations in the metal capillary data serve as further confirmation of the role of charge patch formation.

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1. Introduction

Multiply/Highly charged ions (M/HCIs) are unique in the field of ion-related physics as their charge state is significantly higher than the traditional singly-charged ions which dominate the field. This charge state, which is manifest as a non-negligible potential energy of the ions, can be used to modify the surface/subsurface structure of materials in ways that are distinct from other forms of radiation [1–6]. Beams of M/HCIs are obtained from sources such as Electron Beam Ion Source/Traps (EBIS/Ts) and Electron Cyclotron Resonance (ECR) ion sources in laboratories worldwide [7–14] and most recently at our own user facility for surface modification [15] as well as medical physics [16]. Despite this access, a major hurdle in effectively harnessing the potential of these beams for industrial environments is efficient and flexible ion-transport technology.

One approach towards non-conventional ion transport that has garnered significant attention over the last two decades is the use of capillaries as ion guides. In 2002, Stolterfoht et al. observed the so-called “guiding effect” in insulating capillaries [17]. This effect involves charge patch formation on the inside walls of the insulating capillary due to neutralization of and secondary electron emission initiated by the colliding M/HCI beam. Although these charges formed on the wall can dissipate into the capillary bulk or along the surface, they can also interact repulsively with ions of the incoming M/HCI beam to deflect them away from the capillary wall. After sufficient time has elapsed, a steady-state condition can be reached between charge patch formation and charge dissipation such that a charge-state and kinetic energy preserving transmission of the M/HCI beam is established. This is the definition of the guiding effect for ions within a capillary, and an extensive review of the existing research in this field can be found in Ref. [18].

Existing research can be classified into two categories depending on the diameter d of the capillaries used for guiding: nanocapillaries (d < 1μm) and macrocapillaries (d > 1μm) [19]. Recent efforts in macrocapillary transport include the use of external electric fields to guide the ions in conjunction with the guiding effect to improve efficiency of transport [20], use of conical capillaries for guiding antiparticle beams [21] and the use of curved glass capillaries to achieve large bending angles [22]. In this paper, we have studied the transport of singly-charged ions through straight and conical sections of insulating as well as metallic macrocapillaries. Our goal was to measure and understand the position- and angle-dependent characteristics of ion transport through these macrocapillaries.

The organization of this paper is as follows. In Section 2 we describe the experimental setup used in these measurements. In Section 3, we present data measured on a cylindrical metallic, a cylindrical insulating and a conical insulating macrocapillary. Differences and similarities in the data are noted and used to draw conclusions regarding charging effects, which are summarized in Section 4.
2. Experiment

We have measured the position- and angle-dependent transmission properties of singly-charged ions for macrocapillaries with diameters and lengths of a few millimeters and a few centimeters respectively. The experiment was conducted at Clemson University using the singly charged ion beamline described in detail in Ref. [23]. An aluminosilicate emitter (HeatWave Labs, Inc.) was installed as the ion source in the beamline to obtain Rb⁺ ions. The kinetic energy of the Rb⁺ ions was fixed at 1 keV for all measurements. The energy spread of the beam is less than 1% [24].

Macrocapillaries of two types were used in this study: metals (stainless steel) and insulators (glass). The dimensions of the capillaries are shown in Table 1. The inlet refers to the side of the capillary through which the ions were incident, while the outlet is the exit side of the capillary. The critical angle \( \theta_c \) is defined as the maximum angle of the capillary with respect to the incident beam of ions for which geometric transmission is possible. This angle is equivalent to the angle made by a line that touches the farthest and opposite corners in a length-wise cross-section of a capillary and is given by \( \theta_c = \frac{1}{2} \arctan \left( \frac{d_{in} + d_{out}}{2l} \right) \). We note that for our study, all capillaries were cylindrical \( d_{in} = d_{out} \) except one conical capillary denoted by Sample # 4 which had a taper of 4.52° ± 0.12°.

Before inserting the capillaries into our vacuum system, they were cleaned using standard UHV procedures, i.e. ten minute cycles of sonication with soap-water, acetone, and ethanol interspersed with rinsing in distilled water. Each macrocapillary was then mounted in a custom vacuum chamber inserted immediately after our Colutron G2 ion source [25]. The typical pressure in the chamber for these measurements was \( \sim 1 \times 10^{-8} \) Torr. The macrocapillaries were secured along the beamline axis on a rotary feedthrough mounted on a linear translator. The translator allowed us to move the capillary perpendicular to the path of the beam to measure position dependent characteristics, while the rotary feedthrough allowed us to change the incident angle of the incoming ions relative to the capillary inlet. Each capillary was mounted with an adhesive metal tape on the exposed edge of the inlet to avoid entrance charging effects. The space around the capillary was shielded using a metal foil held in place by metal adhesive tape. The shield was necessary to ensure that only those ions that passed through the inside of the capillary and not around it were detected in these measurements.

A Faraday cup located \( \sim 15 \) cm downstream from the capillary mounting was used to measure the current of ions transmitted through the capillaries. For each measurement, the Rb⁺ ion beam was tuned into the Faraday cup with the capillary retracted from the beam path. The capillary was then inserted into the path of the beam and the cup current was monitored to determine the insertion distance at which transmission of ions through the capillary was maximized. In addition, the insertion distances (on either side of this maximum point) at which the measured transmission through the capillary was zero were also recorded. Following these baseline measurements, the transmitted current was monitored as a function of time at multiple distances between the zero measurement end-points to obtain position-dependent characteristics (see, e.g. Fig. 1a). Angle-dependent characteristics for each capillary were obtained at the insertion distance of maximum transmission by varying the angle in steps of \( 0.2°-0.3° \) and monitoring the transmitted current as a function of time (see, e.g. Fig. 1b). For these position- and angle-dependent measurements, the transmitted current through the metal and insulating capillaries was recorded in time steps of \( 15 \) s and \( 500 \) s respectively. Insertion distances were measured using a Vernier caliper (±0.1 mm), while a digital sensor connected to a PC was used to measure angles (±0.09°). The Faraday cup was connected to a Keithley 617 electrometer interfaced to a computer via GPIB for automated measurements. To improve the current measurement precision, the connection points for the Faraday cup were sanded down and connected using extremely short cables to reduce capacitive losses and the electrometer power connection was isolated from other laboratory connections to minimize AC pick-up. These steps resulted in a precision of ±5 pA for our measurements of transmitted current.

3. Results and discussion

Position- and angle-dependent data were obtained for the four macrocapillaries listed in Table 1 using the methods described in the previous section. Fig. 1 shows transmitted currents as a function of time measured for the metal capillary (Sample # 1). Each line in the figure refers to a measurement conducted when the capillary was inserted to a specific distance (Fig. 1a) or rotated to a specific angle (Fig. 1b) in the presence of the incident ion beam. In Fig. 1a, the positions \( E_1, E_2, \) and \( C \) refer to the insertion distances where the transmitted ion current through the capillary are zero \( (E_1 \text{ and } E_2) \) or maximum \( (C) \). The up and down arrows in the figure indicate that as the capillary was moved away from the \( E_1/\text{ or } C \) position the transmitted current increased or decreased respectively. For this metal macrocapillary these positions were \( (E_1, E_2, C) = (0.0 \text{ mm, 14.4 mm, 7.2 mm}) \). These data indicate that the width of the incident ion beam was \( 14 \) mm, which is much wider than the diameter of all of the capillaries used in this study. For the angular data shown in Fig. 1b, \( \theta_{1,2} \) refer to the angles at which transmission dropped to zero while \( N \) refers to maximum transmission observed at normal incidence. As with the insertion data, the arrows on this figure refer to the increase or decrease of the transmitted current for rotations of the angle away from or toward the positions \( \theta_1 \text{ and } \theta_2 \). For this metal macrocapillary the zero transmission angles were \( (\theta_1, \theta_2) = (-6.12°, 7.02°) \), which lead to a measured critical angle \( \theta_c = 6.57 ± 0.09 \) as compared to the theoretical value of 6.25°.

For the angular data of Fig. 1b, the maximum, minimum and mean transmitted current values measured at each angle were calculated and are plotted in Fig. 2. For this metal macrocapillary, these values are nearly equivalent and the plotted data lie on top of each other in the figure. For the glass capillaries (discussed below) this will no longer be the case. To understand the angular dependence shown in these data, we note that the tilt of the capillary modifies the effective opening area presented to the incident beam, as illustrated in Fig. 3 for a capillary of diameter \( d \) and length \( l \). The functional form of this angular-dependent area, \( A(\theta) \), is given by

\[
A(\theta) = \frac{d^2}{2} \cos(\theta) \left[ -\sin^{-1}(\gamma) + \gamma \cos(\sin^{-1}(\gamma)) + \pi/2 \right]
\]

where \( \gamma = (l/d) \tan(\theta) \).

The solid line in Fig. 2, which corresponds to this equation for our metal macrocapillary, shows that the measured angular-dependence of the transmitted current has a narrower angular

<table>
<thead>
<tr>
<th>Sample #</th>
<th>Material</th>
<th>( l ) (mm)</th>
<th>( d_{in} ) (mm)</th>
<th>( d_{out} ) (mm)</th>
<th>( \theta_c ) (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Steel</td>
<td>21.0</td>
<td>2.3</td>
<td>2.3</td>
<td>6.25</td>
</tr>
<tr>
<td>2</td>
<td>Glass</td>
<td>35.5</td>
<td>5.4</td>
<td>5.4</td>
<td>8.65</td>
</tr>
<tr>
<td>3</td>
<td>Glass</td>
<td>21.0</td>
<td>5.4</td>
<td>5.4</td>
<td>14.42</td>
</tr>
<tr>
<td>4</td>
<td>Glass</td>
<td>19.6</td>
<td>5.4</td>
<td>2.3</td>
<td>11.11</td>
</tr>
</tbody>
</table>
range than this calculated geometrical limit. We note that our assumption of a constant current density and zero divergence for our incident ion beam could give rise to this discrepancy between the measured and calculated transmission values. For example, a Gaussian current density convolved with the functional form for $A(h)$ along with losses due to divergence would decrease the angular range of the calculated transmission. These corrections, which require more detailed incident ion beam measurements, will be pursued in future measurements.

Representative data for a straight glass macrocapillary (Sample # 2) is shown in Figs. 4 and 5. A comparison of the time-dependent results for the both the position (Fig. 4a) and tilt angle (Fig. 4b) with those discussed above for the metal macrocapillary (Fig. 1) reveals the primary difference between these capillary types, which is the oscillations in the transmitted current for the glass macrocapillary. Specifically, within the measurement ranges of $E_{1,2}$ and $\theta_{1,2}$ there are significant, time-dependent excursions in the transmitted current on a timescale of approximately one second. We note that the incident beam conditions for these capillary types (metal vs. insulating) was similar, which can be verified by examining the beam width and maximum transmitted current across the various measurements. For example, for these Sample # 2 data we obtained an ion beam width of $d_{in} = 0.23$ cm, which is similar to the beam width determined for the metal macrocapillary (Sample # 1). In addition, the ratio of the maximum transmitted current in the metal and insulating capillaries ($\approx 5.48$) is close to the ratio of the inlet area of the two capillaries ($\approx 5.51$). Similar results were found for the other macrocapillaries listed in Table 1. Therefore, we conclude that the transmitted current excursions observed for the insulating macrocapillaries are material-dependent.

Fig. 5 shows the maximum, minimum and mean transmitted ion beam currents along with the calculated geometric transmission from Eq. (1) as a function of the corresponding tilt angles for the glass macrocapillary data shown in Fig. 4b. The angular spread for the maximum transmission is consistent with that predicted for geometric transmission. However, the angular spread for minimum, maximum and mean transmitted ion beam currents differs significantly. This can be seen by examining the critical angles for the maximum and minimum cases: $(\theta_{c,\text{min}}, \theta_{c,\text{max}}) = (8.65^\circ, 2.83^\circ)$.

In order to understand the results of Fig. 5, we first constrain our discussion to two angular ranges: $(\theta < \theta_{c,\text{min}})$ and $(\theta_{c,\text{min}} < \theta < \theta_{c,\text{max}})$. Within the first of these ranges, we see that
the minimum transmitted current is always non-zero. Therefore, we can interpret this as a region where ions are always transmitted regardless of time-dependent effects, e.g. charging of the walls. In the second angular range, we see that the minimum transmitted current is always zero, which implies that a time-dependent blocking of ion transmission is occurring. This variation or equivalently oscillation in the beam transmission may be linked to charge patch formation on the inside walls of the macrocapillary. It is well known that electric fields produced by charge patches can significantly affect the flight path of the ions. Similar oscillations in transmitted currents have been observed for glass macrocapillaries [26], Teflon macrocapillaries [27] and also for transmission through parallel glass plates [28]. In this context, our data indicate a preferential deflection of ions that pass closer to the walls as compared to the center of the capillary. That is, ions passing closest to the center of the capillary are not subjected to a deflection from electric fields originating from the capillary walls sufficient to make them escape detection. Conversely, those ions that are not near the center are more deflected such that they fall outside the range of detection and the minimum current falls to zero [29]. For the maximum transmitted current data shown in Fig. 5, we can interpret it as indicative of the time during which the walls of the macrocapillary have discharged and the deflection forces are no longer present. The similarities between these data and the metallic macrocapillary result (Fig. 2) then become obvious, as both are governed primarily by the geometric constraints of Eq. (1).

Although our data qualitatively point to beam deflection due to charge patch formation as the underlying origin of the observed oscillations of transmitted currents in insulating macrocapillaries, it is instructive to examine the order of magnitude of the fields required to give rise to it within our parameter space. Specifically, the kinetic energy of our incident ions is fixed at 1 keV, the path length to the Faraday cup detector is 15 cm, and the size of the detector is 2.54 cm. The distance and size of the detector together with the velocity of the ions set a constraint on the minimum electric field required to deflect the ions outside the detector's acceptance angle. For ions passing along the capillary axis, this electric field is calculated to be \( \approx 10 \text{ kV/m} \). The time taken to form such an electric field, assuming no discharge, is on the order of 1 s for the incident flux of our beam, which agrees well with the time period of our observed oscillations. Transport simulations utilizing classical phase-space dynamics for beam deflection along with temporal and spatial charge patch evolution are necessary for a detailed quantitative picture [30] of guiding; however, our calculation is sufficient to show that charge patch formation can give rise to our observed results.

Fig. 6 shows the transmitted currents as a function of time for the conical insulating macrocapillary (Sample #4) where, as before, Fig. 6a and b show the position- and angle-dependent data, respectively. The oscillations in the transmitted ion current as a function of position are qualitatively similar to those seen in the straight insulating capillaries (Samples #2 and #3). The oscillations in the transmitted current as a function of angle, however, are significantly smaller in amplitude as compared to both the position-dependent transmission of the conical capillary itself and to the straight insulating capillaries in general. As a consequence, the maximum, mean and minimum of the transmitted current for the conical insulating macrocapillary appear much closer to each other, as shown in Fig. 7. We note that we have used the average radius for the calculated transmitted current as opposed to using...
a more general form of Eq. (1). The smaller amplitude of oscillation, or decreased variation in the maximum and minimum transmitted currents, indicates that charging effects were less pronounced for this macrocapillary.

4. Summary

We have measured the position- and angle-dependent transmission characteristics of 1 keV Rb\(^+\) ions through metallic and insulating macrocapillaries. Transmission through the metal capillary was constant over time and no oscillations were observed in the recorded signal. The position-dependent data were used to calculate the beam width and also served to verify the stability of the beam over the duration of the experiment. The measured critical angles for transmission agreed well with those calculated from the geometry of the metal capillary, which implies that transmission through the capillary was consistent with straight-through line-of-sight transmission. For the insulating capillaries, the transmitted current was not constant and significant oscillations were observed that were absent in the case of the metal capillary. For a range of angles consistent with ion transmission parallel to the capillary axis, non-zero transmission was always observed; however, outside of this range (but within the geometrical critical angle) the transmission fell to zero intermittently. These observations indicate that electric fields due to charge patch formation preferentially deflect ions that are near the walls of the insulating macrocapillary. The absence of oscillations for the metal macrocapillary is consistent with this conclusion. In addition, a straightforward calculation involving the physical parameters of the setup shows that electric fields necessary to deflect the ions beyond the acceptance angle of the detector can form within the timescale of the observed oscillations.

Acknowledgments

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References


[19] See Section 2.2 in Reference Aumayr-capillary-review.


[25] See Figure 1 in reference Beamline.


Appendix B

Probing kinetically excited hot electrons using Schottky diodes

The following has been accepted for publication in Journal of Vacuum Science and Technology "B", (JVST B 35, 03D103 (2017) ).
Probing kinetically excited hot electrons using Schottky diodes

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Hot electron generation was measured under the impact of energetic Ar and Rb ions on Ag thin film Schottky diodes. The energy- and angular-dependence of the current measured at the backside of the device due to ion bombardment at the frontside is reported. A sharp upturn in the energy dependent yield is consistent with a kinetic emission model for electronic excitations utilizing the device Schottky barrier as determined from current–voltage characteristics. Backside currents measured for ion incident angles of $\pm 30^\circ$ are strongly peaked about $0^\circ$ (normal incidence) and resemble results seen in other contexts, e.g., ballistic electron emission microscopy. Accounting for the increased transport distance for excited charges at non-normal incidence, the angular results are consistent with the accepted mean free path for electrons in Ag films. © 2017 American Vacuum Society.

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I. INTRODUCTION

In exothermic gas interactions at metal surfaces the dissipation of energy into the nuclear and electronic degrees of freedom of the metal typically occurs through the excitation of photons, phonons, or electrons. Of these energy loss channels, the most difficult to detect experimentally has been the excitation of electron-hole pairs. Using Schottky diode gas sensing devices, Nienhaus and others have performed measurements which give clear evidence for the electron–hole pair excitation channel under thermal energy gas exposure.\(^1,2\) While their results indicate that electron–hole pair excitations are a common avenue for energy loss during a gas–surface interaction at thermal energies, there have been few studies that measure the role of this channel for higher energy projectiles.

One of the first experimental demonstrations of electron–hole pair detection in energetic beam scattering was the work of Amirav and Cardillo who were able to measure excitations at Ge(100) and InP(100) surfaces under Xe exposure.\(^3,4\) Using neutral Xe, with incident energies of 1–10 eV, a transient excitation current was seen upon impact that appeared to coincide with the creation of a local thermal “hot spot” at the surface. Other works have focused on metals and device-based measurements, such as the metal-oxide-semiconductor (MOS) results of Ref. 5 and the metal-insulator-metal (MIM) results of Ref. 6. The MOS measurements showed a velocity-dependence that was below the so-called classical threshold for excitation of hot carriers over the internal barrier height of the device while the MIM data showed an energy-dependence which appeared to saturate at low incident energies (5–6 keV). In both cases, the detected hot carrier currents were required to overcome the tunnel barriers imposed by the buried insulating layers of the devices. In the work presented here, we revisit the problem of hot carrier generation using devices with no insulting barrier (Schottky diodes), measuring device currents generated as a function of the incident ion energy and angle.

In Sec. II, we present the details of our experiment including our Schottky device design. In Sec. III, we discuss the results of our measurements for Ar and Rb ions taken as a function of the ion energy and angle, respectively. A summary is presented in Sec. IV.

II. EXPERIMENT

The Schottky diodes used in these measurements were fabricated in-house at Clemson University. Silicon wafers (phosphorus doped Si (111)) with resistivities of 4.0 ± 0.6 $\Omega$cm (Monsanto, Inc.) served as substrates for the diodes. To form backside contacts, the wafers were etched with diluted hydrofluoric acid (2%) to remove native oxide and then 0.5 $\mu$m of Al was deposited and sintered at 450 °C for 45 min in a nitrogen environment. Front-side rectifying contacts were deposited by thermal evaporation in the shape of a 6 mm dot of 99.999% Ag, as shown in Fig. 1(a). The thickness of the Ag dot was chosen to be 25 nm as discussed below. Figure 1(b) shows current–voltage (I-V) characteristics typical of
one of our fabricated diodes. Ideality factors of \(1.9\) and barrier heights of \(0.83\) eV were obtained for the diodes, which is similar to the characteristics of Schottky diodes used in previous studies.\(^2\) For in situ measurements, electrical contacts to the front-side were made using conductive silver paste (Ted Pella, Inc.).\(^7\)

The ion beam irradiations of fabricated devices were performed using the singly charged ion beamline at Clemson University.\(^8\) Beams were incident on the front-side Ag contact of each device, and the resulting current through the device was measured using a Keithley 617 picoammeter connected as shown in Fig. 1(a). This current was measured as a function of two beam parameters: kinetic energy and angle of incidence. The kinetic energy was varied from 500 to 1500 eV at normal incidence. The angle of incidence was varied from \(-60^\circ\) to \(+60^\circ\) at a fixed kinetic energy of 5 keV.

The kinetic energy dependent measurements were performed using Rb\(^+\) ions in a five-port custom vacuum chamber mounted directly in front of an aluminosilicate emitter ion source obtained from Heatwave Tech.\(^9\) The energy spread of the beam was less than 1%. The setup is shown schematically in Fig. 2 where the ion beam was directed along the Z-axis while the device could be translated along the X-axis. The beam passed through a metal capillary (diameter 2.3 mm) mounted on a wide metal plate (width 25.4 mm) before reaching the diode surface. The capillary served as a mask to ensure that the ion beam interacted only with the top rectifying contact. The capillary was mounted on a translator parallel to the Y-axis, placing it \(~5\) mm from the device surface. Beam transmission through the metal capillary was measured previously and is detailed elsewhere.\(^10\) A Faraday cup in plane with the sample (not shown in the schematic) was used for beam tuning and for measuring ion beam currents pre- and postexposure. As the devices used in this experiment were photosensitive, care was taken to cover all vacuum port windows and limit signals arising from external light sources. However, a direct line-of-sight with the filament producing the ion beam led to a background signal. To measure the response of the sample separated from the background, the ion beams were pulsed in front of the devices using in-path defectors resulting in a time-dependent current response such as that shown in Fig. 3. The difference between the signal with the ion beam incident on the device and the background level was determined to be the current response to the ion beam.

Angular-dependent measurements were performed on a device mounted in the beamline scattering chamber using Ar\(^+\) ions from a sputter ion source (Scienta Omicron...
ISE-10). Here, a six-axis manipulator was used to position the device in the beam path, and the angle of incidence was varied by rotating the sample with respect to the incident beam axis.

One important parameter for these measurements was the thickness of the rectifying contact. First, a lower limit was placed on the metal contact thickness such that it would be greater than the penetration depth of the incident ions and avoid confounding our interpretation of hot electron current measurements. The software SRIM (Ref. 12) was used to obtain penetration depths for our range of incident kinetic energies and a lower limit of 20 nm was obtained for the Ag film. An upper limit on the film thickness was set by considering the attenuation of any hot electron current by scattering events. It has been shown previously that the current attenuation inside a metal film depends exponentially on the film thickness (d) according to Beer’s law

\[ I = I_0 \exp \left( -\frac{d}{\lambda_{mfp}(E) \cos(\theta)} \right) \]  

where the nonscattered current, I, depends on the incident current, I_0, which is attenuated exponentially according to the mean free path, \( \lambda_{mfp}(E) \), for electrons in the film and the path length, d/cos(\( \theta \)), of those electrons through the film. The hot electrons are considered to undergo inelastic scattering events both with other cold electrons and the phononic system of the metal film, and both processes have a dependence on the excess energy of the hot electrons, hence the explicit energy dependence shown. The mean free path can also depend on the concentration of defects in the metal film. Estimates for the ballistic \( \lambda_{mfp} \) for polycrystalline metal films [see, e.g., Refs. 2, 13, and 14] find them to be tens of nanometers with values that vary depending on the technique used for measurement and on the quality of the film. Here, we chose the thickness of our rectifying contact to be \( \sim 25 \) nm, within 5 nm of the lower limit and no more than a factor of two from typical \( \lambda_{mfp} \) values.

### III. RESULTS AND DISCUSSION

A typical measurement of the current response of our fabricated Schottky diodes to a pulsed beam of Rb\(^+\) ions is shown in Fig. 3 for a kinetic energy of 1000 eV. In Fig. 3, the label ON signifies that the beam was directed onto the device face (e.g., at \( t \approx 10 \) s), while OFF signifies it was deflected away from the device face (e.g., at \( t \approx 130 \) s). The background signal when the beam is OFF is approximately \(-9 \) nA, while the measured signal is approximately \(-10.8 \) nA when the beam in ON.

The hot electrons are considered to undergo inelastic scattering in the metal film, and both processes have a dependence on the excess energy of the hot electrons, hence the explicit energy dependence shown. The mean free path can also depend on the concentration of defects in the metal film. Estimates for the ballistic \( \lambda_{mfp} \) for polycrystalline metal films [see, e.g., Refs. 2, 13, and 14] find them to be tens of nanometers with values that vary depending on the technique used for measurement and on the quality of the film. Here,
barrier trapping the excited electrons. We can apply the KEE model [Eq. (2)] to the case of hot electron current in the Schottky diode by substituting for the potential barrier the device Schottky barrier height \( \phi_B = 0.83 \text{ eV} \) along with Fermi energy \( E_F \) and Fermi velocity \( v_f \) for our Ag film, 5.49 eV and 1.39 \( \times 10^6 \text{ m/s} \), respectively, giving a threshold velocity \( v_{th} = 5.06 \times 10^4 \text{ m/s} \)

\[
v_{th} = 0.5 v_f \left[ \sqrt{1 + (\phi_B/E_F)} - 1 \right].
\]

For the ion species used in our experiment (Rb\(^+\)), the calculated threshold velocity corresponds to a kinetic energy of 1139 eV, which is represented as the dashed vertical blue line in Fig. 4. This threshold value agrees well with the upturn observed in our data near 1000 eV.

The incident angular dependence of the hot electron generation, measured for Ar\(^+\) ions at a fixed kinetic energy of 5 keV, is shown in Fig. 5. We were constrained to an energy of 5 keV by the experimental setup for these measurements. For angles within the range \(-45^\circ \leq \theta \leq 30^\circ\), we consider that the ion beam was directed fully onto the sample face, which is consistent with the constant front-side current observed in this range. As above, the hot electron current measured at the backside was negative in polarity and consistent with the data shown in Figs. 3 and 4. The absolute value of the hot electron current is plotted in Fig. 5 as a function of the angle of incidence. The yield at normal incidence is of the same order of magnitude as compared to the energy measurements. This current is strongly peaked about the normal incidence direction and falls off on either side monotonically. We note that as the device was rotated with respect to the incoming ion beam for angles beyond the range \(-45^\circ \leq \theta \leq 30^\circ\), ions made contact with exposed wires. Therefore, data within these angular ranges (indicated by the shaded areas) are ignored in our analysis.

To understand the angular data, we note that as the angle of incidence is increased, the path length for the generated hot electrons to reach the Schottky barrier increases as \( \cos^{-1}(\theta) \), as shown in Eq. (1). In Fig. 6, we plot the negative of the logarithm of the ratio of the normalized hot electron current measured at each angle \( \theta \) to the normalized hot electron current measured at normal incidence versus the inverse of the cosine of the angle of incidence. If we interpret these data according to Eq. (1), the slope of the resulting line is the ratio of the film thickness to the mean free path of the hot electrons in the Ag film. The linear fit shown gives a slope of 4.8 \( \pm 1.3 \) which, given that \( d = 25 \text{ nm} \), corresponds to a mean free path of 5.2 \( \pm 1.4 \text{ nm} \). This mean free path value compares well with a value of 4.5 \( \pm 0.5 \text{ nm} \) previously reported from a hot electron current attenuation measurement conducted using Schottky diodes of varying Ag film thicknesses (p. 45 in Ref. 2). However, these values are lower than the values reported in the literature for MFP using other techniques, which could be attributed to the presence of a higher number of defects in the metal film.
Ballistic electron emission microscopy (BEEM), a technique developed by Bell and Kaiser,\textsuperscript{16–18} can also be used to probe the directional momentum of hot electrons in a Schottky diode and as such is relevant to the angular measurements here. In BEEM, hot electrons from a negatively biased STM tip are injected into a metal surface and are collected, usually at a semiconductor interface, after passing through a Schottky barrier. The hot electron current is observed after a certain threshold bias voltage is reached. The transport of these hot electrons and their scattering within the metal film and at the metal–semiconductor interface is nontrivial. However, if we focus on our angular-dependent measurements, it is worth noting that in BEEM, using concepts of momentum conservation across the metal–semiconductor interface, there is a critical angle for the direction of the momentum of the hot electrons at the interface.\textsuperscript{19,20} Beyond this angle, hot electrons are reflected back into the metal surface instead of passing into the semiconductor, in analogy to total internal reflection of light. These reflected electrons can also undergo multiple reflections in the metal film, depending on its thickness, which can lead to randomization of the original direction and loss of directional information. While further analysis of our method is required before we can compare our measurements directly to such BEEM results, we note that this added angular dependence may serve as an additional factor suppressing the apparent mean free path for electrons in our Ag film.

IV. SUMMARY

We have fabricated Schottky diodes using 25 nm Ag films deposited onto n-type Si substrates and irradiated the top metal contacts with Rb\textsuperscript{+} and Ar\textsuperscript{+} ion beams of varying kinetic energy and angle of incidence, respectively. The kinetic energy was varied between 500 and 1500 eV, and a threshold for hot electron current detection was observed between 1000 and 1250 eV. A kinetic electron emission model applied to the subsurface Schottky barrier resulted in a calculated threshold value of 1139 eV, in good agreement with our observations. The angular dependent measurements suggest that there is an anisotropic generation and transport of hot electrons through the Ag film as there is a significant drop in the detected current for non-normal incident angles. Using these data and Beer’s law, an estimate of the mean free path for ballistic electrons in our Ag film is found to be $5.2 \pm 1.4$ nm. Defects in the metal film as well as nontrivial angular effects similar to those seen in BEEM measurements could contribute to this otherwise low $\lambda_{\text{mfp}}$ value. We note that as the dependence of the observed hot electron current on the thickness of the metal film can be utilized to obtain the mean free path of hot electrons,\textsuperscript{21,22} measurements using diodes fabricated with metal films of varying thickness are currently underway.

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7Ted Pella, Inc., \textit{http://www.tedpella.com/}.
11Scienta Omicron GmBh, \textit{http://www.scientaomicron.com/}.
Appendix C

Tracking subsurface ion radiation damage with metal-oxide-semiconductor device encapsulation

The following has been published in Journal of Materials Research, (JMR 30, 1413 (2015))
Tracking subsurface ion radiation damage with metal–oxide–semiconductor device encapsulation

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We describe measurements aimed at tracking the subsurface energy deposition of ionic radiation by encapsulating an irradiated oxide target within multiple, spatially separated metal–oxide–semiconductor (MOS) capacitors. In particular, we look at incident kinetic energy and potential energy effects in the low keV regime for alkali ions (Na\textsuperscript{+}) and multicharged ions (MCIs) of Ar\textsuperscript{Q+} (Q = 1, 4, 8, and 11) incident on the as-grown layers of SiO\textsubscript{2} on Si. With the irradiated oxide encapsulated under Al top contacts, we record an electronic signature of the incident ionic radiation through capacitance–voltage (C–V) measurements. Both kinetic and potential energy depositions give rise to shifted C–V signatures that can be directly related to internal electron–hole pair excitations. The MCI data reveal an apparent power law dependence on charge state, which is at odds with some prior thin foil studies obtained at higher incident energies.

I. INTRODUCTION

Test and commercial-level fusion reactor designs contain materials to fuel the fusion reaction (e.g., deuterium and tritium) as well as materials to confine the reaction, which can include both the magnetic confinement components and the plasma-facing walls (first wall and divertor).\textsuperscript{1} For these walls or plasma-facing materials (PFMs), considerable effort has gone into their evaluation given that they must endure impacts from a wide range of radiation sources: neutrons, alpha particles, electrons, ions, and electromagnetic radiation (IR, UV, visible, and x-ray).\textsuperscript{2} For ions, this evaluation has focused primarily on their role in the sputtering of material away from the wall, which can inject impurities into the fusion plasma or trap fuel components within redeposited wall layers. Sputtering of PFMs, however, is an inherently above-surface aspect of the ion–target interaction, and it ignores routes for the below-surface energy deposition by the ions.

Although subsurface energy deposition does not directly influence the fusion reaction, the overall energy budget of the PFM and its ability to withstand thermal cycling must account for this route of energy transfer.

For singly charged ions, subsurface energy deposition has been extensively studied and can be reliably calculated using stopping power (\(S(E)\)) formulations which, depending on the ion velocity, manifest as either nuclear stopping (\(S_n(E)\)) or electronic stopping (\(S_e(E)\)). The readily available code SRIM (Stopping and Range of Ions in Matter) incorporates this route effectively and can be configured for most ion–target combinations.\textsuperscript{3} In a man-made fusion reaction, however, other ion charge states will appear, much as they do in the natural fusion reactions of the stellar environment.\textsuperscript{4–6} A significant amount of the energy transported by these ions can shift, as a function of charge state \(Q\), from the ion’s kinetic energy to its potential energy. The dissipation of an ion’s potential energy upon impact with a PFM is not a simple process, as it can begin well outside the target material through electron transfer and secondary deexcitations (electron and photon) and can continue as the ion penetrates the target and slows in the subsurface region.
Significant postmortem analysis has focused on the above-surface components of this energy dissipation, looking at surface feature formation and sputtering.  

Similarly, the above-surface charge exchange component has been successfully treated through the so-called over-the-barrier model.  

Below the surface, however, little data or theoretical treatments exist, and those that do point to a $Q$-dependent role for the ion stopping which has not been explored in depth.  

In the work presented here, we seek to demonstrate that semiconductor device platforms can be utilized to track subsurface energy deposition by ions, in particular for multiply charged ions (MCIs). Semiconductor devices have a long history in radiation effects testing, which was indirectly initiated by U.S. and Soviet high-altitude nuclear detonation tests in the early 1960s. These nuclear tests led to the failure of a communications satellite, Telstar I, whose onboard transistor operation had been altered by the increased levels of radiation. Ground-based efforts at understanding this failure led to a successful repair scheme that involved modifying the bias protocol for the satellite’s onboard transistors. While the satellite ultimately failed due to further radiation exposure, the experience contributed to a shift from the traditional approach of making radiation-effect studies on bulk properties of semiconductor materials and devices toward directed efforts at understanding the effects of radiation on the operational characteristics of these devices.  

For satellite systems, the move in technology from bipolar transistors to metal–oxide–semiconductor field effect transistors (MOSFETs) also shifted the emphasis on radiation effects studies. Metal–oxide–semiconductor (MOS) devices in particular were found to be a powerful tool to study the effects of radiation. For example, changes observed in the MOS capacitor threshold and flatband voltages led to the conclusion that the major effects of radiation on these devices were the buildup of positive charge in the oxide which was able to drift under an applied electric field. By examining silicon-based MOS structures under many types of radiation ($\gamma$ rays, low-energy electrons, high-energy electrons, ultraviolet rays, and x-rays), it was concluded that any ionizing radiation with an energy greater than the band gap of $\text{SiO}_2$ ($\sim 8$ eV) leads to the buildup of positive space charge within the oxide and the creation of interface states at the oxide/semiconductor interface.  

While MCIs can be more accurately described as “ionized radiation”, they too can generate electron–hole pairs and lead to charge buildup within a MOS structure. In the following sections, we describe an experimental setup aimed at tracking the dependence of ion-induced radiation effects on the ion energy and charge state for embedded insulators within MOS devices. We use both singly charged and multiply charged ions for this study, with the MCIs coming from a new electron beam ion trap (EBIT) ion source at Clemson University. As shown in these data, there occurs within an irradiated MOS structure a spatially dependent shift in the capacitance–voltage ($C–V$) signature that is correlated with the current density profile of the incident ion beam. These results are consistent with internal radiation damage inflicted by the ions, and by tracking this damage for different energies and charge states, we find that the MOS can record the subsurface component of the kinetic and potential energy dissipation for incident ionic radiation.  

II. EXPERIMENT  

We have probed radiation damage in oxides due to low-energy ion impacts by measuring capacitance–voltage ($C–V$) characteristics of MOS devices. Specifically, we have irradiated as-grown oxide-on-semiconductor samples ($\text{SiO}_2/\text{Si}$) and then encapsulated them postirradiation with metal dots to fabricate MOS devices (Al/$\text{SiO}_2/\text{Si}$). Irradiations of the oxides focused on separate investigations of ion kinetic energy effects for focused beams of singly charged ions in the few keV range and the ion potential energy effects for MCIs with a fixed kinetic energy. Below, we describe our multistep sample fabrication–irradiation–encapsulation procedure and present the details of the irradiation and characterization techniques used.  

A. Fabrication  

Raw materials (3-inch p-type Si $<100>$ wafers) were purchased from Silica-Source, Inc. with resistivities of 1–10 $\Omega$ cm. Prior to the $\text{SiO}_2$ oxide growth, these wafers were cleaned to remove any organic surface contaminants. The cleaning procedure was a standard RCA clean (1:1:5 solution of $\text{NH}_4\text{OH} + \text{H}_2\text{O}_2 + \text{H}_2\text{O}$) for five minutes under ultrasonic agitation. The cleaned surface was then etched with dilute 1% HF for two minutes to remove any native oxide followed by a triple rinse in deionized water for a total of six minutes. A thick oxide layer was grown on these cleaned wafers in an oxidation furnace at 1000 °C under steam flow. For the singly and multiply charged ion irradiations, the oxide thicknesses were 1900 Å ($1887$ Å $\pm 43$ Å) and 1750 Å ($1746$ Å $\pm 41$ Å), respectively. Following the oxide layer growth, a metal film was deposited on the backside of the wafer as an Ohmic contact. The Ohmic contact deposition involved etching the wafer backside with 1% HF solution to remove any native oxide and then growing a 0.5 μm Al contact using a thermal evaporator. The contact was sintered at 450 °C in a nitrogen environment. The completed wafers were diced into 12 mm square samples to conform to the sample mounting requirements of our ion beamline setups.
B. Singly charged ion irradiation

Singly charged Na\(^+\) ions were used to irradiate the 1900 Å SiO\(_2\) samples at kinetic energies of 1–5 keV to investigate MOS device sensitivity to kinetic energy induced damage. The ion source and beamline used to carry out these irradiations are described in detail elsewhere.\(^\text{24}\) Briefly, the Na\(^+\) ions were obtained from an aluminosilicate emitter (Heatwave Labs, Inc.) by thermionic emission which was mounted in a custom-built ion source. The SiO\(_2\) samples were mounted in the beamline just beyond the ion source section on a translator that was custom-designed for these irradiations. The sample mount included a plate with two holes of 0.25\(^\circ\) diameter which could be moved into the path of the beam. The first hole on the plate served as a mask for the irradiation, with the sample mounted directly behind it. The second hole served as an initial focus point for the beam, where the ion source’s einzel lens and Wien filter were used to focus the ion beam into a Faraday cup mounted behind the plate. During initial setup, a beam viewer was temporarily placed in the Faraday cup position to determine the spatial profile of the ion beam. A circular current density profile which approximately matched the diameter of the focusing aperture within the sample plate was obtained in this way. The total beam current was \(~5\) nA and the on-sample doses for the irradiations were in the range of \(6 \times 10^{12}\) to \(8 \times 10^{12}\) ions/cm\(^2\). The pressure in the source and beamline during these irradiations was \(5 \times 10^{-7}\) Torr. Following each irradiation, the SiO\(_2\) target was removed from the beamline so that MOS top contacts of Al could be deposited in a thermal evaporator. We note that the deposition, which occurred at a pressure of \(5 \times 10^{-6}\) Torr, led to a sample frontside temperature no higher than 80 °C, as based on prior characterization measurements. For these depositions, a custom-built mask was used which placed four Al top contacts in the central, irradiated region and four Al top contacts in the corner, unirradiated regions of the target, as shown in Fig. 1(a). The diameter of the metal dots is 1 mm, and the dots in the central, irradiated region are placed symmetrically at a distance of 1 mm from the center.

![Figure 1](image_url)

**FIG. 1.** (a) A diced, oxidized Si sample mounted on an Omicron-style sample holder showing four central (irradiated) and four corner (unirradiated) MOS devices. (b) HF and LF capacitance–voltage (C–V) curves for an unirradiated device. (c) HF and LF C–V curves for a device encapsulating an oxide layer irradiated by 3 keV Na\(^+\) ions.
C. MCI irradiation

Irradiations of the 1750 Å SiO2 samples by MCIs were carried out in the CUEBIT facility at Clemson University, which is described in detail in Ref. 25. For these irradiations, the SiO2 targets were exposed to the focused beams of Ar\(^{Q+}\) with charge states of \(Q = 1, 4, 8,\) and 11. The potential energy of these ions, which is the sum of the ionization energies of the electrons that have been removed from the neutral Ar atom, varies from 15 eV (\(Q = 1\)) to 2004 eV (\(Q = 11\)). During the irradiation process, the targets were load-locked into the target region of the CUEBIT beamline (base pressure \(1 \times 10^{-8}\) Torr). Argon ions of the desired charge state were selected by an analyzing dipole magnet and then transported down the beamline to the target area for the irradiation. As the cross-section for charge transfer for MCIs is three to four orders of magnitude higher than that for singly charged ions, the pressure in the beamline was maintained in the low \(10^{-9}\) Torr range to avoid neutralization during transport. Space charge spreading of the beam was also avoided by floating the beamline to a transport voltage (-3 kV) and then decelerating the ions at the entry point to the target chamber using a custom-designed deceleration lens (Dreebit, GmbH). The kinetic energy for all of the incident charge states was fixed at 1 keV. Beam currents at the target position were measured using a Faraday cup mounted in the sample plane and were found to vary for different charge states from tens of pA for \(Q = 11\) to ~100 pA for \(Q = 4\) and \(Q = 8\). As in the singly charged ion irradiations, beam profiles, like the one shown in Fig. 2, were obtained using a beam viewer (HRBIS-4000 from Beam Imaging Solutions) as well as a Faraday cup.

To isolate the radiation damage dependence on charge state or potential energy, the dose dependence for each charge state was recorded across multiple exposures with doses ranging from \(5 \times 10^{11}\) to \(5 \times 10^{12}\) ions/cm\(^2\) for \(Q = 4, 8,\) and 11 ions. One control point for singly charged Ar (\(Q = 1\)) ions was also recorded. The listed dose range was chosen based on those used in the singly charged Na\(^+\) work, both for comparison and to avoid saturating the MOS device flatband response. Following each irradiation, top metal contacts were deposited on the sample by moving the sample from the target region and into a thermal evaporator. A 5 \(\times\) 5 grid of Al dots, each with a diameter of 1 mm and a center-to-center distance of 2.5 mm, was deposited on the sample to complete the fabrication of the MOS devices.

D. Device characterization

Both the singly charged ion and MCI irradiation–encapsulation steps produced samples that contained multiple MOS devices. These spatially separated Al-capped regions represented pristine and irradiated regions of the targets which were characterized using C–V measurements. High-frequency (HF) and low-frequency (LF) C–V measurements were carried out on all samples, and Figs. 1(b) and 1(c) show typical C–V curves for pristine and irradiated devices, respectively. Details about the C–V data are discussed in detail in the following sections, and here, we mention only the details specific to the C–V measurement technique. A micromanipulator probe station connected to a HP4280A for HF measurements and a HP4140B for LF measurements was used to obtain the C–V characteristics of each individual MOS device. Each sample was loaded on the chuck of the micromanipulator, where the backside Ohmic contact was connected through suction provided by a small vacuum pump. The top Al contact was connected using a probe tip mounted on the manipulator. A characteristic C–V curve was recorded for each device on a sample, and shifts in the curve shape were found to correspond to the level of irradiation damage at that position on the sample. To quantify these curve shifts, the flatband voltage (\(V_{FB}\)) was determined for each sample, where \(V_{FB}\) was calculated based on the average doping concentration of the underlying Si substrate \((5 \times 10^{16}\) cm\(^{-3}\)) as described in Ref. 26. The difference in flatband voltages \((\Delta V_{FB})\) taken relative to a pristine (unirradiated) device/sample region was tracked for different samples across dose and charge states explored in these measurements.

III. DISCUSSION

Here, we discuss separately the two measurements performed for irradiations of thick SiO2 by singly or multiply charged ions, looking at the kinetic energy dependence and the potential energy dependence of the results, respectively.
A. Singly charged ion irradiation

For the irradiations performed with singly charged ions, the 1900 Å oxide samples were exposed to well-defined beams of Na$^+$ ions as described above. Each SiO$_2$/Si sample was then capped with Al metal dots to form finished MOS devices that were $C$–$V$ characterized. For these measurements, variations in the $C$–$V$ curves are taken as the recorded shift in the flatband voltage, $ΔV_{FB}$, which is determined relative to a reference or unirradiated result.

The flatband value, $V_{FB}$, was chosen as a standard comparison point for these measurements as it is a universally accepted reference point on the $C$–$V$ curve of MOS devices. Physically, $V_{FB}$ corresponds to the point where, for an ideal system, the gate voltage equals the work function difference between the Al gate and the Si substrate. In this case, an ideal pristine device of Al and Si would have a $V_{FB}$ value of $–0.8$ V; however, in our pristine devices a value of $–3.8$ V was obtained for $V_{FB}$ across all samples. This shifted value can be attributed to charge trapping which occurs during the device fabrication. Quantitatively, a flatband shift of $–3.8$ V for the unirradiated devices relative to the ideal value ($–0.8$ V) corresponds to a trapped charge concentration of approximately $3.43 \times 10^{11}$ cm$^{-2}$ at the oxide–semiconductor interface, which is considered an acceptable value for the thick oxides utilized here.

For the irradiated samples, the masked areas at the sample corners produced MOS devices which gave $V_{FB}$ values of $–3.8$ V, indicating that they were pristine or unirradiated in those positions. In contrast, the central sample areas gave MOS devices whose $V_{FB}$ values were consistently shifted to more negative values, indicating shifts induced by the ion irradiation at those positions. Figure 3 shows the $V_{FB}$ values as well as the shifts or $ΔV_{FB}$ values obtained for the irradiated MOS device positions on the samples as a function of the incident kinetic energy of the Na$^+$ ions. The observed trend is approximately linear in energy for the dose and energy ranges in this study.

Before considering the role of kinetic energy dissipation for the observed $ΔV_{FB}$ trend in these Na$^+$ results, it must be noted that alkali ions, in general, are considered to be an “ionized impurity” within SiO$_2$. Therefore, the presence of these ions in the subsurface region can lead to a measurable shift in $V_{FB}$ relative to a pristine device unexposed to Na$^+$ ions. To account for this possibility, we calculated the $V_{FB}$ shift that would be introduced by the Na$^+$ ions, assuming that they were distributed in the SiO$_2$ layer at implantation depths given by SRIM. For the kinetic energy range used here (2–5 keV), the ions are implanted at a mean depth ranging from 6 to 12 nm, respectively, which is confined to the top 5% of the oxide layer. Therefore, the ions account for no more than 25% of the measured shift in $V_{FB}$ and these results are included in Fig. 3.

After accounting for the possibility of an ionic impurity component in the $V_{FB}$ shift, it is clear that the remaining shift and observed linear trend with respect to kinetic energy are directly attributable to the loss of kinetic energy by the stopped Na$^+$ ions within the SiO$_2$ layer. Microscopically, this can be considered as reflecting the energy lost per unit length by the ions as they travel through the layer, which is defined as the stopping power ($S(E) = –dE/dx$). While stopping power is traditionally divided into two components: nuclear stopping and electronic stopping, it is not immediately clear that our measurements can distinguish between them. However, if we focus on the known fact that a MOS-encapsulated oxide is sensitive to electron–hole pair excitations above a certain threshold then we can assume that electronic stopping of the ions is the most probable route to those excitations. For SiO$_2$, the threshold energy required to create an electron–hole pair is 18 eV$^{34}$ and the transport of electron–hole pairs induced by radiation energy losses is well described by the columnar recombination model. This model is represented as

$$\frac{\partial n_+}{\partial t} = D_\pm \nabla^2 n_\pm - \mu_\pm E \frac{\partial n_\pm}{\partial x} - \alpha n_\pm n_\mp,$$

where $n_\pm$ represents the hole (+) or electron density (−) and the terms on the right-hand side are, from left to right, the diffusion term, the drift term, and the recombination term. $D$ represents the diffusion constant, $\mu$ is...
the mobility of carriers (\( \mu_+ = 40 \text{ cm}^2/\text{V s} \) and \( \mu_- = 10^{-11} \text{ cm}^2/\text{V s} \)) in SiO\(_2\), \( E \) is the applied/internal field, and \( \alpha \) is the recombination coefficient. For our measurements, we first note that the mobility of electrons is much higher than that of holes. Therefore, we can assume a process where recombination can take place initially with surviving electrons being swept away into the semiconductor substrate. Considering that we are not applying a gate voltage, we can neglect the electric field term in the model and arrive at a uniform distribution of holes in the oxide.

Looking at our data, we can then interpret our measured \( \Delta V_{FB} \) as a representation of a hole distribution within the oxide and we can calculate an “experimental” density of holes (\( N_{H-\text{EXPERIMENTAL}} \)). Here, we simply adapt the standard formalism for the flatband shift in a MOS device and assume that the entire hole concentration is represented by a charge sheet centered at half the depth of the oxide, which gives

\[
N_{H-\text{EXPERIMENTAL}} = \frac{2 \times \Delta V_{FB} \times C_{ox}}{e},
\]

where \( C_{ox} \) is the maximum capacitance of the oxide per unit area and \( e \) is the electron charge.

Using SRIM, we can compare with \( N_{H-\text{EXPERIMENTAL}} \) by calculating the energy lost to electronic stopping in the oxide and converting that value to an expected density of holes. To do so, we obtain a theoretical hole density (\( N_{H-\text{SRIM}} \)) due to the energetic ions as

\[
N_{H-\text{SRIM}} = \frac{D \times \frac{dE}{dx}}{18} \int_{0}^{x_{ox}} G(\mu, \sigma) \times x dx
\]

where \( D \) is the dose (ions/cm\(^2\)), and \( \frac{dE}{dx} \) is the electronic loss (units of eV/Å) obtained from SRIM calculations. A Gaussian distribution of holes obtained from SRIM (\( G(\mu, \sigma) \)) is also included and is weighted by the depth \( x \) to account for linear energy loss of the ions across the oxide thickness, \( x_{ox} \).

By comparing the experimental and theoretical yields for holes, we define the fractional yield of holes that have survived the initial recombination step as

\[
f(E) = \frac{N_{H-\text{EXPERIMENTAL}}}{N_{H-\text{SRIM}}}
\]

Figure 4 shows this fractional yield as the slope of a linear fit to the plot of \( N_{H-\text{EXPERIMENTAL}} \) versus \( N_{H-\text{SRIM}} \). The value obtained is 0.0124, which is comparable to the fractional yield for holes within SiO\(_2\) obtained using different forms of radiation excitation.\(^{36}\)

We note that annealing of our irradiated samples at 200 °C in the presence of a bias removed the observed shifts in \( V_{FB} \), leading to a full recovery of pristine \( V_{FB} \) voltage values. This is clear evidence that the subsurface energy loss of the ions causes reversible damage in the SiO\(_2\) layer in the form of trapped charge. This has been observed in other radiation studies of MOS devices\(^{32}\) and can be explained by the thermally initiated release and subsequent neutralization of the trapped charge in the oxide.

### B. MCI irradiation

As with the singly charged ion irradiations, our MCI data consisted of \( C-V \) results obtained after individual SiO\(_2\)/Si samples were irradiated, encapsulated, and probed through multiple Al/SiO\(_2\)/Si devices that had been deposited on each sample. Specifically, we have irradiated 1750 Å thick SiO\(_2\) layers with Ar\(^{+}\) ions (\( Q = 1, 4, 8, \) and \( 11 \)) at a fixed kinetic energy of 1 keV.

To accommodate the target chamber requirements of CUBEIT, no mask was used during these MCI irradiations. Instead, the entire sample was exposed to the beam and then capped with a larger grid of metal dots as shown in Fig. 5. The \( C-V \) results, expressed as \( \Delta V_{FB} \), are also shown in Fig. 5, plotted as a function of position for a single sample. It is clear from this figure that the \( \Delta V_{FB} \) values are spatially varying and that this variation is consistent with the typical spatially resolved intensity of the MCI beam such as the example in Fig. 2. To compare these observed shifts in \( V_{FB} \) on any given sample to the respective fluence used to dose that sample, an across-sample average was calculated. Additionally, in calculating the fluence for each sample, a correction for Faraday cup area, which was used to measure the dose, was applied. In general, a two-dimensional Gaussian
function can be used to fit the beam profiles, and by extension, the observed spatially varying $\Delta V_{FB}$ results. The average shift in $\Delta V_{FB}$ across the sample was calculated as

$$
\Delta V_{FB,\text{avg}} = \frac{\int_A V(\text{Gaussian fit})dA}{\int_A dA},
$$

(5)

where $V(\text{Gaussian-fit})$ represents the two-dimensional Gaussian function fit to the measured $\Delta V_{FB}$ data and $A$ represents the area of the sample. The calculated average $\Delta V_{FB,\text{avg}}$ corresponds to the shift that would have resulted for devices on the sample if the incident MCI beam had been spatially uniform with a flat, non-Gaussian profile. Geometrically, the definition above corresponds to the volume under the interpolated surface of the $\Delta V_{FB}$ profile over the area of the sample, and $\Delta V_{FB,\text{avg}}$ represents the height of a rectangular prism with cross-sectional area of the sample that would contain the same volume.

Figure 6 shows the dependence of $\Delta V_{FB,\text{avg}}$ on fluence for different charge states. The linear dependence observed for each charge state indicates that the fluences used here are within a linear regime for radiation dosing of these devices. That is, each MCI has an independent and additive effect on the flatband shift, and the slope of these lines can be used to quantify this effect per ion. The clear differences in slopes also indicate a nonlinear charge state dependence which can be seen in Fig. 7 where the $\Delta V_{FB,\text{avg}}$ shift per ion is plotted as a function of MCI charge state. If the shift caused by $Ar^{1+}$ ions is taken as a kinetic energy control and the remaining charge states are plotted relative to this point, we obtain a power law ($V_{FB} \sim Q^{2.2}$) for the flatband shifts due to MCI irradiation. This near quadratic dependence of $\Delta V_{FB,\text{avg}}$ on the charge state could be an indicator that the stopping power of MCIs depends on $Q$ via an intrinsic power law.

A comparison of our result with other efforts to investigate the charge state dependence for stopping power shows that this is an open question. In particular, Herrmann et al. found no $Q$-dependence as described in Ref. 34, while Schenkel et al. have found evidence of $Q$-dependent stopping as described in Refs. 22 and 23.
Most of these experiments involved the passage of MCIs through a thin foil and the subsequent measurement of their kinetic energy and charge. As such, the requirement of foil penetration and emergence places a fundamental limit on the kinetic energy required to pass through the foil and can be considered a nonviable method for low-kinetic energies. The nearest experiment to our subsurface result is that described in Ref. 33 where a low-kinetic and potential energy deposition by ions and Sb1+ ions implanted in SiO2 was measured by SIMS (Secondary Ion Mass Spectroscopy) and used as a measure of enhanced stopping power within the oxide. We also note that a quadratic dependency of electronic stopping power on effective charge state has been previously used in the literature. Finally, using extensions of the theory behind the SRIM code, Biersack has predicted a Qdependence of stopping power.21

IV. SUMMARY AND CONCLUSIONS

The as-grown samples of SiO2 were irradiated with singly and multiply charged ions to investigate the use of C–V measurements in tracking kinetic and potential energy deposition within the subsurface region of a target material. By encapsulating irradiated oxide samples with Al contacts, spatially resolved signatures of the ionic radiation below the surface were revealed in shifted C–V characteristics. These shifts scaled linearly with the ion dose and kinetic energy. The potential energy, however, gave rise to C–V shifts that, when calibrated for dose, appear to follow a power law in a charge state with an exponent of ~2.2. This result is at odds with prior data obtained with similar ions that had penetrated thin foils. Overall, our results indicate that MOS encapsulation and C–V measurements can serve as a method to track low-kinetic and potential energy deposition by ions into the subsurface regions of a solid.

REFERENCES

Appendix D

Encapsulating Ion-Solid Interactions in Metal-Oxide-Semiconductor (MOS) Devices

The following has been published in *IEEE Transactions on Nuclear Science*, (IEEE Trans. Nucl. Sci. 62, 3346 (2015))
Encapsulating Ion-Solid Interactions in Metal-Oxide-Semiconductor (MOS) Devices

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Abstract—We report on a measurement of low energy ion irradiation effects on as-grown films of SiO₂ on a Si substrate. Beams of normally incident Na⁺ ions with kinetic energies of 2 keV to 5 keV were focused onto ~ 1900 Å SiO₂ films. Aluminum top metal contacts were subsequently deposited onto these targets such that irradiated regions and unexposed (pristine) regions of the target could be compared using capacitance–voltage (C–V) measurements of individual metal-oxide-semiconductor (MOS) devices. The C–V data reveal an energy-dependent shift in the flatband voltage (VFB) that can be returned to its near-pristine value by a low temperature anneal. An increase in the density of interface states (Dit) inferred from the C–V curves is found to have a superlinear dependence on the incident kinetic energy. These data are consistent with previously observed UV radiation effects on MOS oxides, where transferred energy leads to electron-hole pair production and the diffusion and trapping of holes throughout the oxide. Our measured trapped hole densities are compared with calculated densities, which are based on the incident ion dose and the predicted ion implantation range, to arrive at a fractional yield for hole survival and measurement within an encapsulated MOS device.

Index Terms—Electron-hole pairs, hole-trapping, interface traps, ion beams, ion implantation, ion radiation effects, linear energy transfer, metal-oxide-semiconductor (MOS) devices, radiation damage.

I. INTRODUCTION

EXPERIMENTAL measurements of the effects of low energy ion irradiation on insulating solids can be challenging to interpret, as the primary probe, atomic force microscopy, is a top layer specific technique [1], [2]. In this paper, we demonstrate that irradiation effects from ions can be probed after an insulator is encapsulated into a finished metal-oxide-semiconductor (MOS) device. Specifically, by measuring capacitance–voltage (C–V) of the MOS structure we can resolve the residue of energy-dependent electron-hole pair excitations induced by the passage of ions into the subsurface of the previously exposed insulator.

In our previous work on encapsulation of irradiation effects, we were able to show that crater formation on a thin film dielectric (Al₂O₃) can be probed in a metal-insulator-metal (MIM) device [3]. Each device was probed using differential conductance measurements through films that had been exposed to highly charged ions, and the conductance change per ion impact was interpreted as a single ion effect dependent on charge state. In this work we focus on singly-charged ions which are embedded near the surface of an oxide film. The unique sensitivity of an MOS device to interstitial ions and trapped charge effects through C–V measurements [4] is then exploited to explore how the kinetic energy of the stopped ions was dissipated.

Studies of the dependence of MOS device performance on radiation damage have a long history in the context of applied device physics [5]–[10] given their relevance to fabrication-induced effects, such as those arising from the passage of dopant ions through the oxide and bound for the underlying semiconductor substrate [11]–[16]. To understand these effects as well as those arising in deployed MOS devices, i.e., devices in harsh radiation-intensive environments, numerous investigations have employed intentional sources of radiation damage, such as gamma rays [5], [6], high energy ions [6], [7], [9], [10], and UV sources [17]. It is from these experiments that a detailed picture was developed for oxide radiation damage in MOS structures, incorporating data on depth, time, and voltage-dependent observations. In the context of applied devices, however, the transition of MOS and MOSFET structures to ever thinner oxides has diminished the role that radiation damage plays in device physics [5]–[10] given their relevance to fabrication-induced effects through C–V measurements [4] is then exploited to explore how the kinetic energy of the stopped ions was dissipated.

The organization of this paper is as follows. In Section II we describe our MOS device fabrication and characterization both pre- and post-irradiation with low energy Na⁺ ions. Results for irradiated devices are discussed in Section III and compared with a phenomenological model based on ion stopping values extracted from SRIM [18]. Conclusions from these data are summarized in Section IV.

II. EXPERIMENT

Our MOS devices were fabricated in-house at Clemson University. The starting materials were 3-in p-type Si(100) wafers.
purchased from Silica-Source, Inc. The wafers, which had resistivities of $1 \to 10 \, \Omega \cdot \text{cm}$, were precleaned to remove organic surface contaminants prior to oxide growth. The cleaning procedure was a standard RCA clean ($1:1:5$ solution of NH$_3$OH + H$_2$O$_2$ + H$_2$O) for five minutes under ultrasonic agitation. The cleaned surface was then etched with dilute $1\%$ hydrofluoric acid for two minutes to remove any native oxide followed by a triple rinse in deionized water for a total of six minutes.

Oxide was grown on the samples by placing them in an oxidation furnace for 25 min at $1000^\circ\text{C}$ under a steam flow. Measurements of the resulting film thickness with a Nanometrics NanoSpec AFT (Automatic Film Thickness) gave a nominal value of $1900 \, \text{Å} (1887 \, \text{Å} \pm 43 \, \text{Å})$. Preparation of the wafer backside involved etching with concentrated hydrofluoric acid to remove the grown oxide, triple-rinsing with deionized water and subsequent deposition of $0.5 \, \mu\text{m}$ of Al from a thermal evaporator. The as-deposited Al contacts were sintered at $450^\circ\text{C}$ for 30 min in a nitrogen environment. Finally, the wafers were diced into $12 \, \text{mm} \times 12 \, \text{mm}$ squares to accommodate the sample mount for our ion irradiation setup.

Sample irradiations were carried out using Na$^+$ ions obtained from an aluminosilicate emitter (Heatwave Tech) mounted in a custom-built ion source. The oxidized and diced Si wafer targets were mounted directly in front of this source in the first section of our ion beamline, which is described in detail elsewhere [19]. The plate holding each target was masked so that only a central circular region (~ $6 \, \text{mm}$ diameter) would be exposed to the incident ions. Prior to each irradiation, an initial beam tuning was obtained by focusing the beam through an aperture that was equivalent in size to the central mask and into a Faraday cup mounted directly behind the sample position. Ion doses in the $1 \times 10^{12} \, \text{ions} \cdot \text{cm}^2$ range with incident energies between 2 and 5 keV were used. Beam profiles were obtained using a beam viewer located directly behind the Faraday cup. The base pressure within the beamline during irradiations was $6.67 \times 10^{-5} \, \text{Pa}$.

After each irradiation, the target was removed from the beamline so that MOS top contacts of Al could be deposited. For these depositions, a custom-built mask was used which placed four Al top contacts in the central, irradiated region and four Al top contacts in the corner, unirradiated regions of the target. This gave eight MOS devices per target (four irradiation-encapsulated and four pristine). We note that the deposition, which occurred at a pressure of $1.33 \times 10^{-4} \, \text{Pa}$, led to a sample frontside temperature no higher than $80^\circ\text{C}$, as based on prior characterization measurements. Fig. 1 shows the devices obtained after deposition with reference to the area exposed to the beam.

Both pristine and irradiated devices were characterized using C–V measurements. A micromanipulator probe station connected to a HP4280A for high frequency (HF) measurements and a HP4140B for low frequency (LF) measurements was used to obtain the C–V characteristics of each individual MOS device. The HF measurements were carried out at 1 MHz while the LF measurements were carried out in a quasi-static manner resulting in a frequency less than 10 Hz. The variation in typical LF and HF signatures of one of our irradiated MOS capacitors as compared to a pristine MOS capacitor is shown in Fig. 2. The pristine device C–V signature is shown by lighter curves while the dark curves are the signature of the irradiated device. As a function of the applied gate voltage, both the LF and HF C–V curves show accumulation behavior at the most negative applied voltages and hence give similar capacitance values due to the intrinsic capacitance of the $1900 \, \text{Å}$ oxide layer. For the LF C–V this result is mirrored at the most positive applied gate voltage where the MOS device goes into inversion whereas the HF C–V is lower due to the capacitance of the depletion layer. Between these two extremes, both LF and HF C–V curves for the pristine device show a distinct drop at a point in voltage that is near to the so-called flatband voltage ($V_{\text{FB}}$) where, for an ideal system, the applied gate voltage equals the difference in work function between the Al gate and the Si substrate ($\approx 0.8 \, \text{eV}$). This flatband voltage is identified in our experiment as the voltage at which the capacitance is 0.91 times the maximum capacitance of the oxide [20]. More generally, however, $V_{\text{FB}}$ can be considered as sensitive to the detailed conditions of the oxide and its interfaces and, in particular, to implanted charged species and any additional charges, such as excited holes, left by irradiation. For example, the $3 \, \text{keV}$ Na$^+$ irradiated device in Fig. 2 shows a significant shift in the $V_{\text{FB}}$ position. Another feature of the data is the increased skew of the irradiated C–V curve as compared to the pristine curve, as shown by the dash-dot line in Fig. 2, which is related to an increase in the interface trap density, $D_{\text{it}}$. Therefore, it is through the shifted flatband voltage, $(\Delta V_{\text{FB}})$, and the increase in interface trap density, $D_{\text{it}}$, that we track the energetics of kinetic energy dissipation for our Na$^+$ ions within the MOS oxide layer.

III. RESULTS AND DISCUSSION

For this study, we irradiated our as-prepared SiO$_2$ ($\approx 1900 \, \text{Å}$) targets with beams of Na$^+$ ions that had energies between 2 and 5 keV. All target doses were in the range of $6 \times 8 \times 10^{12} \, \text{ions} \cdot \text{cm}^{-2}$. Following each irradiation, Al top
contacts were deposited as noted in Section II and the finished MOS devices were characterized by C–V measurements. Representative C–V data for four devices in the irradiated energy range are shown in Fig. 3. It is clear from these spectra that there is a significant shift in the position of the flatband toward more negative gate voltage values as the incident beam energy is increased. Additionally, we note that the shift is not a parallel shift but includes stretching out the C–V curve. Our results showing \( \Delta V_{FB} \) for irradiated target regions are summarized in Fig. 5. The devices constructed on the masked or unirradiated regions of the targets, not shown in the figure, have a nearly constant value of \(-3.8 \text{ V}\) across all samples. This reproducible value served as a consistency check on our fabrication technique, and we attribute the shift away from the ideal value of \(-0.8 \text{ V}\) to the trapping of positive charge during the fabrication process [20].

Fig. 4 schematically depicts the processes occurring as a consequence of the irradiation that lead to a shift in the flatband voltage and also to creation of radiation-induced interface traps. The large unfilled circles represent the implanted Na\(^{+}\) ions. The mean depth of implantation, or range “R,” of these incident ions is expected, via simulations, to be less than 12 nm. As these ions remain in the charged state in the oxide, it is reasonable to expect a flatband shift due to the ions themselves. However, the shift expected due to the ions themselves is only approximately a third to a fourth of the measured flatband shift. The additional shift is attributed to the creation of holes due to electron-hole pair excitation along the short track of these ions. Electrons are depicted by filled circles while holes are depicted by small unfilled circles. Most of these electron-hole pairs recombine, however, a fraction (\(~1\%\)) escape recombination.

The electrons that escape recombination are swept away due to their high mobility and do not contribute further to the radiation-response of the MOS structure; however, the surviving holes, having a mobility many orders of magnitude lower than the electrons, are trapped in the oxide. These trapped holes undergo a stochastic hopping transport through the oxide, activated by internal electric fields of the ions themselves and possibly internal contact potentials, and migrate towards the semiconductor interface where they are trapped in deep trapping sites, and can remain trapped for a period ranging from hours to years. This additional positive charge trapped in the oxide leads to the observed additional shift in the C–V curve of the MOS capacitor. This shift has been observed to persist for a period of at least one year for our devices.

Imperfections, due to imbalance in the proportion of silicon and oxygen, are always present in the interface between the oxide and semiconductor leading to dangling silicon bonds or equivalently the so-called interface traps. The energy levels of these traps lie within the bandgap and their occupancy depends on the Fermi level, and consequently, on the applied gate voltage. In addition to the flatband shift, post-irradiation response of the MOS devices also shows an increased skew, or distortion, in the C–V curves as compared to the pristine curves. Thus we infer that radiation-induced interface traps were created as a result of ion irradiation.
The shift and skew in the $C-V$ curves of the MOS devices thus represents the energy lost by the impacting ions to electronic excitations within the oxide. The ions themselves are implanted in the first $\sim 10$ nm; however, carrier transport in the oxide results in interface-trapped states at the Si–SiO$_2$ interface $\sim 200$ nm away from the implanted ions. As the flatband shift depends on the first moment of the charge trapped in the oxide, the MOS structure is inherently sensitive to radiation damage, which consequently results in a measurable signal in terms of the flatband shift and creation of interface states. Thus, MOS devices can be a useful tool for measuring energy loss of low energy ions in dielectric films, which is otherwise experimentally refractory. In the remainder of this section, we explore quantitatively the energy dependence of the voltage shift and also the increase in populated interface trap density.

For the irradiated devices, the measured $\Delta V_{FB}$ values shown in Fig. 5 lie between approximately $-4$ V and $-14$ V and increase monotonically across the incident Na$^+$ kinetic energy range. In general, $\Delta V_{FB}$ in MOS devices can be attributed to the presence of charges in the oxide and is given by [21]

$$\Delta V_{FB} = \frac{1}{C_{ox}} \int_0^{x_{ox}} \rho(x) dx$$  \hspace{1cm} (1)

where $\rho(x)$ is the charge distribution within the oxide, $C_{ox}$ is the maximum capacitance of the oxide per unit area, $x$ is distance within the oxide measured from the metal-oxide interface and $x_{ox}$ is the thickness of the oxide. From (1) it is clear that observed shifts in $V_{FB}$ are proportional to the amount of charge present in the oxide. For the parameters of these measurements (Na$^+$ kinetic energy and oxide thickness) it is reasonable to assume that the incident ions penetrate into and are implanted within the oxide. Additionally, Na$^+$ ions are known to remain ionized inside SiO$_2$[13]. Therefore, some fraction of the $V_{FB}$ shifts we observe could be assigned to the presence of implanted ions in the oxide. Since (1) also indicates that $V_{FB}$ shifts will depend on the depth of the charge in the oxide, it is possible that ions of higher kinetic energy, which will travel further into the oxide, could give rise to shifts in $V_{FB}$ that are tied to the implantation depth and its kinetic energy dependence. In order to estimate the contribution of the Na$^+$ ions and their depth within the oxide to our measured $V_{FB}$ values, the Monte Carlo code SRIM [18] was used. SRIM is a collection of well known and widely used computer codes which calculate the stopping range of heavy ions in matter along with related effects such as sputtering, recoils, and damage. Relevant results from SRIM are shown in Table I. The depth profile of the implanted ions obtained from SRIM was Gaussian ($G_{\mu,\sigma}(x)$) in shape, where the mean implantation depth, $\mu$, ranged between 5.9 and 11.8 nm with a standard deviation, $\sigma$, between 2.8 and 5.5 nm. Substituting this distribution for the charge distribution $\rho(x)$ in (1), we find an estimated contribution of the implanted ions to $V_{FB}$ which is plotted in Fig. 5. A linear fit to the measured flatband shift resulted in a slope of $3.0 \pm 0.2$ V/keV, while a slope of $0.8 \pm 0.1$ V/keV was obtained for the calculated shift resulting from only the ions themselves. Relative to the measured $V_{FB}$ values at each kinetic energy, we see from the slopes of the linear fit that the implanted ions contribute no more than $\sim 25\% - 30\%$ of the total $V_{FB}$. Therefore, the observed linear trend in $V_{FB}$ with respect to kinetic energy cannot be fully accounted for by considering only the contribution of the Na$^+$ and their depth within the oxide.

To account for the additional shift in $V_{FB}$ that cannot be attributed to the implanted ions themselves, we consider the interactions of the ions with the oxide. In particular, the nuclear and electronic energy loss channels of these ions, typically treated through the stopping power or stopping force ($-dE/dx$), must be considered. It is known that electronic excitations in the oxide above a certain threshold lead to generation of electron-hole pairs, which can appear, post-excitation, as a form of trapped charge that can shift the MOS $V_{FB}$ signature [22]. For the incident ion kinetic energies used in our experiments, the electronic component of stopping power reported by SRIM, as shown in Table I, is in the range of 26.540–41.967 eV/nm. We can calculate the total energy lost to the electronic subsystem of the oxide target per ion as the product of the electronic component of the stopping power ($s_{\text{electronic}}$) and the depth of the implanted ion. If we represent the depth through the ion implantation profile $G_{\mu,\sigma}(x)$ obtained from SRIM, the total energy lost to the electronic subsystem per unit area ($\Delta E_{\text{electronic}}$) for a given dose $d$ is

$$\Delta E_{\text{electronic}} = d s_{\text{electronic}} \int_0^{x_{oi}} x G_{\mu,\sigma}(x) dx$$  \hspace{1cm} (2)
where the denominator is included as a normalization factor for the Gaussian function. Since it is known that approximately 18 eV is required to generate one electron hole pair in SiO₂[22], we can calculate the number of electron-hole pairs generated per unit area, assuming every electron-hole pair gives rise to a hole in the oxide, as

\[ N_{H-SRIM} = \frac{\Delta E_{\text{electronic}}}{18.0}. \]  

(3)

Although (3) can be used to calculate the density of electron-hole pairs generated in the oxide by the passage of implanted ions, the subsequent recombination and transport of these excitations must be accounted for to determine the final distribution of ion-generated charge. This process is well described by the columnar recombination model developed by Jaffe with subsequent numerical solutions by Oldham [7]–[9]. The model includes terms for diffusion and recombination and is written here as

\[ \frac{\partial n_{p,n}}{\partial t} = D_{p,n} \frac{\partial^2 n_{p,n}}{\partial x^2} + \mu_p n E \frac{\partial n_{p,n}}{\partial x} - \alpha n_{p,n} n_p \]  

(4)

where \( n_{p,n} \) represents the hole (\( p \)) and electron (\( n \)) density, \( D_{p,n} \) is the diffusion constant, \( \mu \) is the mobility of the carriers (electron mobility \( \mu_n = 40 \, \text{cm}^2/\text{V-s} \) and hole mobility \( \mu_p = 10^{-11} \, \text{cm}^2/\text{V-s} \)), \( E \) is electric field resulting from the application of a gate voltage and \( \alpha \) is the recombination coefficient. The diffusion constant \( D \) scales linearly with the mobility \( \mu \) according to Einstein’s relation. Since the mobilities of the generated electrons and holes vary by multiple orders of magnitude, we can assume that the highly mobile electrons are quickly swept away into the bulk, while the holes require longer to migrate through the oxide. For our experimental setup, with an exposed oxide that has no initial top gates, we can ignore the second term on the right hand side in (4), as there is no field \( E \) due to an applied voltage. We note here that though there is no externally applied electric field, there will be an internal field present due to internal contact potentials and the implanted ions themselves. These internal fields serve to activate hole transport even though there is no externally applied field in our experiment [9].

Under these conditions, the solution to this equation is a uniform distribution of holes that are trapped within the oxide. It is these remaining holes, as trapped positive charge, that give rise to the \( V_{FB} \) shifts we observe. Substituting such a uniform distribution into (1), we can determine the \( \Delta V_{FB} \) that would have been measured on the irradiated devices on account of these holes (assuming no recombination, i.e., \( \alpha = 0 \)), as

\[ \Delta V_{FB-CALC} = \frac{\epsilon N_{H-SRIM}}{2C_{ox}}. \]  

(5)

A comparison between the measured shifts, \( \Delta V_{FB-EXPT} \) and the calculated shifts, \( \Delta V_{FB-CALC} \), calculated from kinetic energy induced electronic excitations in the oxide using (5), is shown in Fig. 6. A linear fit to this result gives a slope of 1.2±0.2 which corresponds to a yield of \( \sim 1\% \), or equivalently the result that about 1 out of every 100 holes that are generated give rise to the shift we measure in the MOS flatband voltage, while the remainder are lost to recombination and do not contribute to the measured shift. This is compatible with the trends seen in other types of radiation effects [5]–[7], [9], [10] and in particular with UV source results [17]. Moreover, our result is consistent with values found for the recombination coefficient (\( \alpha \approx 0.98 \)) for SiO₂/Si based devices [9].

The microscopic mechanism of transport of holes within the oxide is described accurately using a continuous-time-random-walk (CTRW) model [23]. The CTRW describes the time dispersion of holes within an oxide with a single value of the disorder parameter, which implies a universal nature of transport of holes within the oxide with respect to temperature, electric field and oxide thickness. The process is activated by an electric field and thermally activated above 140 K [9]. The microscopic transit times for individual carriers vary over many orders of magnitude. For our samples, the CV measurements were performed within six days of irradiation. While information regarding the time evolution of hole distribution within the oxide was lost during this elapsed time between irradiation and first characterization, we have since measured the CV curves again after an elapsed time of one year and report that all samples were consistent with previous measurements.

We have interpreted the shift in the flatband voltage, \( \Delta V_{FB} \), in terms of the electronic excitation caused in the oxide due to energetic ionic radiation. As shown in Fig. 2, \( \Delta V_{FB} \) represents the horizontal shift in the irradiated C–V curve with respect to the pristine C–V curve. A charge distribution in the oxide bulk would result in a parallel shift of the C–V curve but would not induce a skew as observed in the irradiated C–V curves [23]. This parallel shift, in simple terms, is the additional voltage required to overcome the opposing electric field of the oxide-trapped charges. The skew, or equivalently the increased voltage range between accumulation and inversion, of the C–V curve is indicative of an increase in the interface trap density, \( D_{tr} \). The interface traps that lie outside the band gap are equivalent to charge trapped in the oxide, however the occupancy of the interface traps within the band gap changes with band bending at the interface. The interface traps are charged or neutral depending upon whether they are above or below the Fermi level. Since the Fermi level is shifting depending upon the applied gate voltage, the interface charge density varies with gate...
Further measurements are necessary to elucidate the full dependence of $D_{it}$ on the ion impact conditions. We do note, however, that our assumption of a steady state solution for $n_p$ in \( \text{eq} (4) \) has been tested using measurements of irradiated devices that were stored for over a year, and in all cases, the results reported here were reproduced. The reversibility of our ion-induced radiation damage was also verified by annealing the targets at $\sim 250^\circ \text{C}$, a result which is consistent with other radiation effects studies [6], [23].

IV. SUMMARY

We have measured kinetic energy dependent irradiation effects of focused Na$^+$ ion beams on thick SiO$_2$ films ($\sim 1900$ Å) on a Si substrate in the low energy regime (2–5 keV). These effects were encapsulated by depositing top metal contacts on irradiated and unexposed parts of the samples and comparing the C–V data obtained from the resulting individual MOS capacitors. An approximately linear relationship between the kinetic energy of the incident ions and shifts in the flatband voltages of the irradiated devices was observed in these measurements. The measured $V_{FB}$ shifts were significantly ($\sim 3$ times) larger than the values calculated and assigned to the presence of the implanted Na$^+$ ions, and the residual shift was attributed to subsurface excitation caused by the passage of the ions into the oxide. These ion-induced excitations involve the dissipation of the ion kinetic energy to the electronic subsystem of the target and the generation of electron-hole pairs. Using the SRIM code the range of implantation of the ions within the oxide was calculated and used along with the electronic component of the stopping power to determine an expected density of generated holes. Within the columnar recombination model, it was shown that the subsequent transport and trapping of these holes will lead to a steady-state, uniform hole distribution in the oxide. A comparison of this expected trap density with that required to give the measured $V_{FB}$ shifts shows a linear relationship that we use to infer a fractional yield of $\sim 1\%$ for hole survival. Interface trap states at the oxide-semiconductor interface are observed even though the ions are implanted only within the top 10% of the depth of the oxide. The density of the observed interface traps is calculated to be in the $\sim 10^{11}$ cm$^{-2}$ V$^{-1}$ range and a superlinear dependence on kinetic energy is observed. The results for hole survival and density of interface traps as well as the long term stability and annealing behavior of the irradiated oxides is consistent with results found under other forms of radiation [5]–[7], [9], [10], [17], [23]–[25], and overall, these measurements show that MOS devices can be used to track subsurface energy dissipation for impacting ions.

ACKNOWLEDGMENT

The authors would like to thank S. Chambers for his assistance in the characterization of MOS devices.

REFERENCES


Appendix E

Area of conical capillary

It is noted here that the formula provided in Eq. 3.1 applies as presented only to cylindrical capillaries. A similar calculation is shown here for conical capillaries. With the length, inlet diameter (radius) and outlet diameter (radius) of the capillary denoted by \( l, d_1(r_1), \) and \( d_2(r_2) \) respectively \((d_1 > d_2)\), the dependence of the effective area of the opening of the capillary depends on the angle of tilt \( \theta \) can be divided into three cases.

Case 1: \((\theta) < \arctan((r_1 - r_2)/l)\)

The first case is when the tilt angle is such that there is no obstruction of the opening at the exit of the capillary due to the tilt angle. This case occurs when \( \tan(\theta) < (r_1 - r_2)/l \).

The area of the opening is the same as the area of the opening at the exit of the capillary modulated by the cosine of the angle i.e. for angles such that \((\theta) < \arctan((r_1 - r_2)/l)\), \(A(\theta) = \pi r_2^2\).

Case 2: \((\theta) > \arctan((r_1 + r_2)/l)\)

The second case is the case when the tilt angle is such that the opening of the capillary is completely shielded and thus the area of the opening is zero i.e for angles such that \((\theta) > \arctan((r_1 + r_2)/l)\), \(A(\theta)=0\).

Case 3: \(\arctan((r_1 - r_2)/l) < (\theta) \leq \arctan((r_1 + r_2)/l)\)
This case involves the angles not covered in the first two cases and represents the case where there is an overlap in the effective area of the openings at the entrance and the exit of the capillary. The area of overlap is the intersection of the two ellipses as shown in Fig. E.1 for two angles $\theta_1$ and $\theta_2$ such that these angles satisfy the condition $\arctan((r_1 - r_2)/l) < (\theta_1 < (\theta_2 < \arctan((r_1 + r_2)/l)$. This area can be calculated numerically as the area of intersection between the two curves that lies within the opening of the ellipse representing the opening of the entrance of the capillary, or we can also use the formulae for the area of a sector of an ellipse bounded by a line[104].

For illustrating the shape of the curve, calculations for a few points are shown in Fig. E.2 for the dimensions of the capillary used in this experiment.
Figure E.1: Figure showing the effective area of opening of a conical capillary at a) $\theta_1$ and b) $\theta_2$ such that $\arctan((r_1 - r_2)/l) < (\theta_1) < (\theta_2) < \arctan((r_1 + r_2)/l)$.
Figure E.2: Figure showing the numerically calculated approximate area of opening of the capillary at a few tilt angles.
Appendix F

Computer Programs

The programs written during the course of this work are listed here for reference. Listing all the codes in their entirety would be prohibitive and unnecessary, so only those programs deemed important are included in this document, while the computer and directory where the electronic and binary versions of all programs are provided. The programs can be categorized as programs for interfacing data acquisition equipment, a lab automation framework, modifications to a molecular dynamics code, a numerical partial differential equation solver, and other miscellaneous topics. The following table F.1 lists the computers where these programs are stored along with their Internet Protocol (IP) addresses, physical locations, usernames, and passwords. Though the IP addresses are dynamically assigned, they are not expected to change as long as the machine is not down before the address lease expires (typically 24 hours).

Interfacing equipment so data can be recorded with low latency is the preferred method of data collection. The methods used generally in laboratories involve some type of third party software that interfaces to the device (e.g. LabView). While this is convenient and works in most cases, it is better in terms of latency to interact with the devices themselves through the drivers provided for the operating system. Low latency requirements
<table>
<thead>
<tr>
<th>Computer</th>
<th>IP Address</th>
<th>Location</th>
<th>Username</th>
<th>Password</th>
</tr>
</thead>
<tbody>
<tr>
<td>cerebellum</td>
<td>130.127.188.194</td>
<td>EBIT lab</td>
<td>root</td>
<td>N@Noscience</td>
</tr>
<tr>
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<td>130.127.188.87</td>
<td>Lab 13</td>
<td>root</td>
<td>cattac</td>
</tr>
<tr>
<td>kaa</td>
<td>130.127.189.181</td>
<td>Office 13</td>
<td>sinuser</td>
<td>cattac</td>
</tr>
</tbody>
</table>

Table F.1: Table showing details regarding the computers used to store programs and record data.

are often present in industrial contexts (low latency platforms are preferred for example in high frequency trading) and such experience in writing low latency measurement programs is relevant in many such cases. The two methods of interfacing that were preferred here, as they were the most common for all the devices used, were utilizing the GPIB (General Purpose Interface Bus) and RS232 (serial port) protocols. While the serial port configuration already exists on a modern operating system (e.g. Linux, Windows), GPIB drivers need to be installed separately. Note that it is recommended, though might not be necessary, to compile the source against the headers of the particular kernel version in use if it is required to reinstall these drivers. After the installation is successful, the file `/etc/gpib.conf` should be modified to reflect the setup being used. The current version of the file is shown below. It includes the settings for the devices (electrometers, source meters etc.) used to record data in the lab.

**Appendix A   Interfacing with GPIB**

- `/etc/gpib.conf` : Located on 'raksha'

```python
device {
    minor = 0
    name = "keithley617"
}```
pad = 27
sad = 0
}

device {
    minor = 0
    name = "keithley485"
    pad = 12
    sad = 0
}

device {
    minor = 0
    name = "keithley2000"
    pad = 15
    sad = 0
}

device {
    minor = 0
    name = "keithley6485"
    pad = 14
    sad = 0
}

138
device {
    minor = 0
    name = "HP3478a"
    pad = 10
    sad = 0
}
device {
    minor = 0
    name = "agilent34401a"
    pad = 24
    sad = 0
}
device {
    minor = 0
    name = "keithleysmu_2400"
    pad = 26
    sad = 0
}

Appendix B  Interfacing Electrometers

The C code written to interface to the GPIB drivers to communicate with the devices are listed below. The following code utilizes two electrometers simultaneously - the Keithley 485 and the Keithley 2400 SMU

- '/electrometers/measure_485_2400.c' : Located on 'raksha'
#include <stdio.h>
#include <stdlib.h>
#include <fcntl.h>
#include <errno.h>
#include <unistd.h>
#include <termios.h>
#include <string.h>
#include <time.h>
#include <ib.h>    /* GPIB header file */

struct timespec timespec_diff(struct timespec start, struct timespec end)
{
    struct timespec temp;
    if ((end.tv_nsec - start.tv_nsec) < 0) {
        temp.tv_sec = end.tv_sec - start.tv_sec - 1;
        temp.tv_nsec = 1000000000 + end.tv_nsec - start.tv_nsec;
    } else {
        temp.tv_sec = end.tv_sec - start.tv_sec;
        temp.tv_nsec = end.tv_nsec - start.tv_nsec;
    }
    return temp;
}
```c
int main(int argc, char* argv[]) {
    struct termios options;
    int fd1, fd2;
    int ret1, ret2;
    float samprate, sleepms;
    char buff1[256] = {0};
    char buff2[256] = {0};
    char formatted[2560] = {0};
    int i = 0;
    FILE *fp;
    struct timespec st, ct, diff;
    float tdiff;
    float val1, val2;
    if (argc != 3) {
        printf("Usage: ./measure filename samprate \n");
        printf("This will write time(s) Current Keithley_SMU_2400 (uA) \n Current Keithley485 (uA) to specified file \n");
        printf("Configure SMU by front panel turn output on, and make sure READ? output has only one element (:FORM:ELEM:CURR) \n");
    }
}
```
exit(1);
}

fp=fopen(argv[1],"w");
samplerate=atof(argv[2]);
sleepms=1000.0/samplerate;

/*
 fd1=open("/dev/ttyUSB0",O_RDWR);
 if(fd1==-1)
 perror("port not open - ");

tcgetattr(fd1,&options);
cfsetispeed(&options,B9600);
cfsetspeed(&options,B9600);
tcssetattr(fd1,TCSANOW,&options);
*/

fd1=ibfind("keithleysmu_2400");
fd2=ibfind("keithley485");

clock_gettime(CLOCK_MONOTONIC,&st);
sprintf(formatted,"#Time(s)\tCurrent_SMU_2400(uA)\n
tCurrent_485(uA)\n");
fprintf(fp,"%s",formatted);
printf("%s\n",formatted);
while (1) //CTRL+C to break out of this program
{
    sprintf(buf1,"READ?");
    ibwrt(fd1,buf1,strlen(buf1));
    ret1=ibcnt;
    sprintf(buf1,"\n");
    ibwrt(fd2,buf1,strlen(buf1));
    ret2=ibcnt;
    // printf(" Wrote %d bytes\n", ret1);
    memset(buf1,256,0);
    memset(buf2,256,0);
    usleep(sleepms*1000);
    ibrd(fd1,(char *)(buf1),256);
    ret1=ibcnt;
    ibrd(fd2,(char *)(buf2),256);
    ret2=ibcnt;
    clock_gettime(CLOCK_MONOTONIC,&ct);
    diff=timespec_diff(st,ct);
    tdiff=diff.tv_sec + diff.tv_nsec*1e-9;
    // printf("Read %d bytes\n", ret1);
    // printf("%s\n", buf1);
    // for (i=0;i<strlen(buf1);i++)
    // {
    //     if (buf1[i]==',')
    // }
//
//  {
//  buff1[i - 1] = 0;
//  break;
//  }
//}

val1 = atof(buff1);
val1 *= 1E6;

for (i = 0; i < strlen(buff2); i++)
{
    buff2[i] = buff2[i + 4];
}

val2 = atof(buff2);
val2 *= 1E6;

// sprintf(formatted,"%f",((float)diff.tv_sec + (float)(diff.tv_nsec/1000000000.0)));
// strcat(formatted," ");
// strcat(formatted,buff1,buff2,"\n");

printf("%f\t%f\t%f\n", tdiff, val1, val2);
sprintf(formatted, "%f\t%f\t%f\n", tdiff, val1, val2);
fprintf(fp, "%s", formatted);
flush(fp);
}
fclose(fp);
ibloc(fd1);
ibloc(fd2);
}

The following code utilizes two electrometers simultaneously - the Keithley 485 and the Keithley 617

- `/electrometers/measure_617_485.c` : Located on 'raksha'

```c
#include <stdio.h>
#include <stdlib.h>
#include <fcntl.h>
#include <errno.h>
#include <unistd.h>
#include <termios.h>
#include <string.h>
#include <time.h>
#include <ib.h>            /* GPIB header file */

struct timespec timespec_diff(struct timespec start, struct
timespec end)
{
    struct timespec temp;
    if (((end.tv_nsec - start.tv_nsec) < 0) {
        temp.tv_sec = end.tv_sec - start.tv_sec - 1;
```
temp.tv_nsec = 1000000000+end.tv_nsec-start.tv_nsec;

} else {
    temp.tv_sec = end.tv_sec-start.tv_sec;
    temp.tv_nsec = end.tv_nsec-start.tv_nsec;
}
return temp;

int main(int argc, char*argv[])
{
    struct termios options;
    int fd1,fd2;
    int ret1,ret2;
    float sleepms;
    int samplerate;
    char buff1[256]={0};
    char buff2[256]={0};
    char formatted[2560]={0};
    int i=0;
    FILE *fp;
    struct timespec st,ct,diff;
    float tdiff;
    float val1,val2;
    if(argc!=3)
```c
{
    printf("Usage: ./measure filename samplerate\n");
    printf("This will write time(s) Current Keithley485(nA) to specified file\n");
    exit(1);
}

fp=fopen(argv[1], "w");
samplerate=atoi(argv[2]);
if (samplerate != 0)
sleepms=1000.0/samplerate;
else
    sleepms=0;

/*
fd1=open("/dev/ttyUSB0", O_RDWR);
if (fd1 == -1)
    perror("port not open - ");

tcgetattr(fd1, &options);
cfsetispeed(&options, B9600);
cfsetospeed(&options, B9600);
tcsetattr(fd1, TCSANOW, &options);
*/
```
/*
fd1 = ibfind("keithley617");
fd2 = ibfind("keithley485");

clock_gettime(CLOCK_MONOTONIC, &st);
sprintf(formatted, "#Time(s)\tCurrent_617_Current_485
(nA)\n");
fprintf(fp, "%s", formatted);
printf("%s\n", formatted);
while (1) // CTRL+C to break out of this program
{
    //
    sprintf(buf1, "*CLS;READ?;CLS;\n");
    //
    ibwrt(fd1, buff1, strlen(buff1));
    //
    ret1 = ibcnt;
    sprintf(buff1, "\n");
    ibwrt(fd1, buff1, strlen(buff1));
    ibwrt(fd2, buff1, strlen(buff1));
    ret2 = ibcnt;
    //
    printf("Wrote %d bytes\n", ret1);
    memset(buff1, 256, 0);
    memset(buff2, 256, 0);
    usleep(sleeplex*1000);
    ibrd(fd1,(char *)(buff1),256);
    //
    ret1 = ibcnt;
    ibrd(fd2,(char *)(buff2),256);
*/
ret2=ibcnt;
clock_gettime(CLOCK_MONOTONIC,&ct);
diff=timespec_diff(st,ct);
tdiff=diff.tv_sec + diff.tv_nsec*1e-9;

// printf("Read %d bytes\n", ret1);
// printf("%s\n", buff1);
// for(i=0;i<strlen(buff1);i++)
// {  
//     if(buff1[i]==',')
//     {  
//         buff1[i-1]=0;
//         break;
//     }
// }
// val1=atof(buff1);

for(i=0;i<strlen(buff1);i++)
{
    buff1[i]=buff1[i+4];
}

for(i=0;i<strlen(buff2);i++)
{

buff2[i] = buff2[i + 4];
}
val1 = atof(buff1);
val2 = atof(buff2);

// sprintf(formatted,"%f",((float)(diff.tv_sec)
  +(float)(diff.tv_nsec/1000000000.0)));

// strcat(formatted," ");

// strcat(formatted, buff1, buff2,"\n");

printf("%f \t%f \t%f \n", tdiff, val1*1.0E+3, val2*
  *1.0E+9);

sprintf(formatted,"%f \t%f \t%f \n", tdiff, val1*
  *1.0E+3, val2*1.0E+9);

fprintf(fp,"%s",formatted);

fflush(fp);
}
fclose(fp);
ibloc(fd1);
ibloc(fd2);
}

The C code written to interface to the RS232 drivers to communicate with the device
Keithley 2000 are listed below.

- 'electrometers/keithley2000.c' : Located on 'cerebellum'

#include <stdio.h>
#include <stdlib.h>
#include <fcntl.h>
#include <errno.h>
#include <unistd.h>
#include <termios.h>
#include <string.h>
#include <time.h>

struct timespec timespec_diff(struct timespec start, struct timespec end)
{
    struct timespec temp;
    if ((end.tv_nsec-start.tv_nsec)<0) {
        temp.tv_sec = end.tv_sec-start.tv_sec-1;
        temp.tv_nsec = 1000000000+end.tv_nsec-start.tv_nsec;
    } else {
        temp.tv_sec = end.tv_sec-start.tv_sec;
        temp.tv_nsec = end.tv_nsec-start.tv_nsec;
    }
    return temp;
}

int main(int argc, char*argv[])
{

struct termios options;
int fd;
int ret;
float samplerate, sleepms;
char buff[256] = {0};
char formatted[2560] = {0};
int i = 0;
FILE *fp;
struct timespec st, ct, diff;
if (argc != 3)
{
    printf("Usage: ./keithley filename samplerate \n");
    printf("This will write t(secs) Volts(V) (space delimited) to specified file \n");
    exit(1);
}

fp=fopen(argv[1], "w");
samplerate = atoi(argv[2]);
sleepms = 1000.0 / samplerate;
fd=open("/dev/ttyS1", O_RDWR);
if (fd == -1)
    perror("port not open");
tcgetattr(fd,&options);
cfsetispeed(&options,B9600);
cfsetospeed(&options,B9600);
tcgetattr(fd,TCSANOW,&options);

clock_gettime(CLOCK_MONOTONIC,&st);

while(1) //CTRL+C to break out of this program
{
    sprintf(buff,"READ?\n");
    ret=write(fd,buff,strlen(buff));
    printf("Wrote %d bytes\n",ret);
    memset(buff,256,0);
    usleep(sleepms*1000);
    ret=read(fd,(char *)(buff),256);
    clock_gettime(CLOCK_MONOTONIC,&ct);
    diff=timespec_diff(st,ct);
    printf("Read %d bytes\n",ret);
    buff[ret]=0;
    printf("%s\n",buff);
    sprintf(formatted,"%f",((float)(diff.tv_sec)
        +(float)(diff.tv_nsec/1000000000.0)));
    strcat(formatted,"\n");
}
The following code was used to interface the Keithley 2000 for thermocouple measurements.

- ’electrometers/keithley2000_thermocoupletypeC’ : Located on ’cerebellum’

```c
#include <stdio.h>
#include <stdlib.h>
#include <fcntl.h>
#include <errno.h>
#include <unistd.h>
#include <termios.h>
#include <string.h>
#include <time.h>

float mvols[2400]={0};

int lookup(float val)
{
    int i;
```
for (i=0; i<2315; i++)
{
    if (val>=mvols[i] && val<mvols[i+1])
    {
        // printf("i=%d val=%f mvols[%d]=%f
                   mvols[%d]=%f\n", i, val, i, mvols[i], i+1, mvols[i+1]);
        return i;
    }
}
return 6666;

struct timespec timespec_diff(struct timespec start, struct timespec end)
{
    struct timespec temp;
    if ((end.tv_nsec-start.tv_nsec)<0) {
        temp.tv_sec = end.tv_sec-start.tv_sec-1;
        temp.tv_nsec = 1000000000+end.tv_nsec-start.tv_nsec;
    }
} else {
    temp.tv_sec = end.tv_sec - start.tv_sec;
    temp.tv_nsec = end.tv_nsec - start.tv_nsec;
}

return temp;

int main(int argc, char* argv[])
{
    struct termios options;
    int fd;
    int ret;
    float samplerate, sleepms;
    char buff[256] = {0};
    char buffC[256] = {0};
    char formatted[2560] = {0};
    int i = 0;
    FILE *fp, *tabf;
    struct timespec st, ct, diff;
    float offset, val;
    int temperature = 0;
    int index;
    char *token;
\begin{verbatim}
if ( argc != 4 )
{
    printf( "Usage: ./keithley_sample rate offset

    Sam plerate offset \n" );
    printf( "This will write t ( secs ) Volts ( V )

    Temper ature ( Celcius ) ( space delimited ) to

    specified file . Offset is offset in mV for

    reference junction temper ature .\n" );
    printf( "Expects reading from Keithley to be

    in Volts\n" );
    exit ( 1 );
}

fp = fopen ( argv [ 1 ] , "w" );
tabs = fopen ( "typeC_conversion_chart.txt" , "r" );
fgets ( buff , 1000 , tabs ); // ignore first line.
temperature = 0;
while ( temperature < 2316 )
{
    fgets ( buff , 1000 , tabs );
token = strtok ( buff , "\t\n" );
token = strtok ( NULL , "\t\n" );
mvolts[ temperature ] = atof ( token );
temperature ++;
} // read table
\end{verbatim}
fclose(tabf);

samplerate=atoi(argv[2]);
offset=atof(argv[3]);
sleepms=1000.0/samplerate;
fd=open("/dev/ttyS1",O_RDWR);
if (fd==−1)
    perror("port not open");

tcgetattr(fd,&options);
cfsetspeed(&options,B9600);
cfsetospeed(&options,B9600);
tcsetattr(fd,TCSANOW,&options);

clock_gettime(CLOCK_MONOTONIC,&st);

while(1) //CTRL+C to break out of this program
{
    printf(buff,"READ?\n");
    ret=write(fd,buff,strlen(buff));
    printf("Wrote %d bytes\n",ret);
    memset(buff,256,0);
    usleep(sleepms*1000);
}
ret=\texttt{read}(fd,(\texttt{char} *)\texttt{buff},256);
\texttt{clock\_get\_time}(\texttt{CLOCK\_MONOTONIC},&ct);
diff=\texttt{timespec\_diff}(st,ct);
\texttt{printf}("Read\_%d\_bytes\n",ret);
\texttt{buff[ret}-1]=0;
\texttt{printf}("\%s\n",\texttt{buff});

val=\texttt{atof}(\texttt{buff});
\texttt{val}*=1000.0;
\texttt{val}+=\texttt{offset};

\texttt{temperature=lookup(val);}
\texttt{printf}("\%d\n",\texttt{temperature});
\texttt{sprintf(buffC,\"\%d\n\",\texttt{temperature});

\texttt{sprintf(formatted,\"\%f\",(\texttt{float})(\texttt{diff.t}\_\texttt{v}\_\texttt{sec})
+(\texttt{float})(\texttt{diff.t}\_\texttt{v}\_\texttt{n}\_\texttt{sec}/1000000000.0)));}
\texttt{strcat(formatted,"\_\_");}
\texttt{strcat(formatted,\texttt{buff});}
\texttt{strcat(formatted,"\_\_";}
\texttt{strcat(formatted,\texttt{buffC});}
\texttt{fprintf(fp,\"\%s\",\texttt{formatted});}
\texttt{fflush(fp);}
Appendix C  Auger Measurements

For Auger measurements, the SRS locking was interfaced via GPIB and RS232. The code listed here is used to obtain Auger measurements. The file 'compile.sh' lists compilations instructions. The file 'params.sh' lists all parameters used by the script to run the Auger measurements. The file 'auger.sh' runs the Auger measurements and sources 'params.sh'. The file 'srs830.c' contains the code to interface to the SRS lock-in amplifier. The flow is as follows: modify params.sh, run auger.sh, hit Ctrl+C to terminate measurements, run auger_plot.sh to save measurements. The file 'rtplot.sh' can be used to view the plot realtime as it is collected, however, the data needs to saved separately by running the auger_plot.sh file. These files are located under the the '/root/interfacing/srs/' directory.

- 'auger/params.sh' : Located on 'raksha'

```plaintext
sample="SRNL_Cr_sample1"
run="run1"
resultdir="./"
#scanrate on auger ( eV/s ), lower limit (eV) , higher limit (eV)
scanrate="1.0"
startenergy="200.0"
endenergy="1000.0"
```
# rate at which to read data from SRS830. (samples/sec).

# works well at 10, works upto 20, but do not stress machine out with any other program when running above 10. Do not exceed 20.

samplerate="10.0"

num_pts='echo "($endenergy-$startenergy)*$samplerate/$scanrate" | bc`

filename=$sample"_"$run"_"$scanrate"_"$startenergy"_"$endenergy"

title=$sample

f=save.gp

• `auger/auger.sh`: Located on `raksha`

source ./params.sh

./snapdata temp $num_pts $scanrate $startenergy $samplerate $samplerate

• `auger/auger_plot.sh`: Located on `raksha`

source ./params.sh

line="#" 'date +%D-%R'

sed "1~$line" -i temp

 cp temp $filename

 cp temp $resultdir"/$filename

 echo "set terminal png" > $f

161
echo "set size square" >> $f
echo "set border lw 5" >> $f
echo "set xlabel 'Energy (eV)'" >> $f

echo "set output 'temp_X.png'" >> $f
echo "plot 'temp' u 1:2 t '$title w l'" >> $f
echo "set output" >> $f

echo "set output 'temp_Y.png'" >> $f
echo "plot 'temp' u 1:3 t '$title w l'" >> $f
echo "set output" >> $f

echo "set output 'temp_R.png'" >> $f
echo "plot 'temp' u 1:(sqrt($2**2+$3**2)) t '$title w l'" >> $f
echo "set output" >> $f

echo "set terminal x11" >> $f

gnuplot save.gp
cp temp_X.png $filename"_X.png"
cp temp_X.png $resultdir"/$filename"_X.png"
cp temp_Y.png $filename"_Y.png"

cp temp_Y.png $resultdir"/$filename"_Y.png"

cp temp_R.png $filename"_R.png"

cp temp_R.png $resultdir"/$filename"_R.png"

echo "Raw data in $filename"

echo "plot in $filename"_X.png,"$filename"_Y.png,"$filename"_R.png"

    $filename"_R.png"

• 'auger/srs830.c': Located on 'raksha'

#include <stdio.h>
#include <stdlib.h>
#include <fcntl.h>
#include <errno.h>
#include <unistd.h>
#include <termios.h>
#include <string.h>
#include <time.h>

struct timespec timespec_diff(struct timespec start, struct timespec end)
{

struct timespec temp;

if ( (end.tv_nsec - start.tv_nsec) < 0 ) {
    temp.tv_sec = end.tv_sec - start.tv_sec - 1;
    temp.tv_nsec = 1000000000 + end.tv_nsec - start.tv_nsec;
} else {
    temp.tv_sec = end.tv_sec - start.tv_sec;
    temp.tv_nsec = end.tv_nsec - start.tv_nsec;
}

return temp;
}

int main(int argc, char*argv[])
{

    struct termios options;
    int fd;
    int ret;
    int num_pts;
    float scanrate, startenergy, samplerate, sleepms;
    char buff[256] = {0};
    char formatted[2560] = {0};
    char *x,*y;
    int i=0;
    FILE *fp;
    time_t starttime, currt ime;
struct timespec st, ct, diff;
float msecs;
if (argc != 6)
{
    printf("Usage: ./snapdata filename num_pts scanrate startenergy samplerate \n");
    printf("This will write E(eV) X Y (space delimited) to specified file \n");
    exit(1);
}

fp=fopen(argv[1],"w");
num_pts=atoi(argv[2]);
scanrate=atof(argv[3]);
startenergy=atof(argv[4]);
samplerate=atof(argv[5]);
sleepms=1000.0/samplerate;
printf("Num_pts=%d \n", num_pts);
f=opend("/dev/ttyUSB0",O_RDWR);
if (fd==-1)
    perror("port not open - ");

tcgetattr(fd,&options);
cfsetispeed(&options,B9600);
cfsetospeed(&options,B9600);

165
tcsetattr(fd, TCSANOW, &options);

clock_gettime(CLOCK_MONOTONIC, &st);

while(1)  // Ctrl+C to break
{
    sprintf(buf, "SNAP\n1,2\n");
    ret = write(fd, buf, strlen(buf));
    printf("Wrote %d bytes\n", ret);
    memset(buf, 256, 0);
    usleep(sleepms * 1000);
    ret = read(fd, (char *)(buf), 256);
    clock_gettime(CLOCK_MONOTONIC, &ct);
    diff = timespec_diff(st, ct);
    printf("Read %d bytes\n", ret);
    buf[ret] = 0;
    printf("%s", buf);
    x = strtok(buf, ",\n");
    y = strtok(NULL, ",\n");
    printf("x=%s", x);
    printf("y=%s", y);
    if (x == NULL || y == NULL)
    {
        166
    }
printf("bad data!\n");
strcat(formatted,"\#Got bad data here!\n");

else
{
    // sprintf(formatted,"%f",((float)(diff.tv_sec)+(float)(diff.tv_nsec/1000000000.0))*scanrate + startenergy);
sprintf(formatted,"%f",((float)(diff.tv_sec)+(float)(diff.tv_nsec/1000000000.0)));
strcat(formatted,"\n");
strcat(formatted,x);
strcat(formatted,"\n");
strcat(formatted,y);
strcat(formatted,"\n");
}
fprintf(fp,"%s",formatted);
fflush(fp);
}
fclose(fp);
close(fd);
Appendix D  EBIT Beam tuning and profiling

The following programs were used to tune the beam and obtain a beam profile. The beam profile program can accept input from a TV remote (IR) if an IR receiver is connected to the computer (typically via USB). There are various versions of the programs to tune the beam and obtain the profile. These are all located in the '/crap' directory on cerbellum and a list can be obtained by running a 'ls -l tuning*' command. The latest versions are listed here. The file 'tuning_v3.c' contains code to tune the beam onto a faceplate and a Faraday cup. The file 'tuning_profile.ver4.c' contains code to obtain a spatial distribution of the current density of the beam.

- 'ebit-beam-tuning-profiling/tuning_v3.c' : Located on 'cerebellum'

```c
#include <stdio.h>
#include <stdlib.h>
#include <fcntl.h>
#include <errno.h>
#include <unistd.h>
#include <termios.h>
#include <string.h>
#include <time.h>

struct timespec timespec_diff(struct timespec start, struct timespec end)
{
    struct timespec temp;
}```
if ((end.tv_nsec - start.tv_nsec) < 0) {
    temp.tv_sec = end.tv_sec - start.tv_sec - 1;
    temp.tv_nsec = 1000000000 + end.tv_nsec - start.tv_nsec;
} else {
    temp.tv_sec = end.tv_sec - start.tv_sec;
    temp.tv_nsec = end.tv_nsec - start.tv_nsec;
}
return temp;
}

int main(int argc, char* argv[]) {
    struct termios options;
    int fd1, fd2;
    int ret1, ret2;
    float samplerate, sleepms;
    char buff1[256] = {0};
    char buff2[256] = {0};
    char formatted[2560] = {0};
    char formatted2[2560] = {0};
    int i = 0;
    FILE *fp;
    struct timespec st, ct, diff;
    float val1, val2;
```c
float tdiff;
if (argc != 3)
{
    printf("Usage: ./tuning_v2 filename samplerate \n");
    printf("Assumptions: Keithley picoammeter connected via RS232 \n");
    printf("Assumptions: Keithley multimeter connected via RS232 and through femptoamp \n");
    printf("This will write Time(s) Current (pA) \nCurrent (mV) to specified file \n");
    exit(1);
}

fp=fopen(argv[1],"w");
samplerate=atoi(argv[2]);
sleepms=1000.0/samplerate;
fd1=open("/dev/ttyS0",O_RDWR);
fd2=open("/dev/ttyS1",O_RDWR);
if (fd1==-1 )
    perror("port not open\n");
if (fd2==-1 )
    perror("port not open\n");
```

tcgetattr(fd1,&options);
cfsetispeed(&options,B9600);
cfsetospeed(&options,B9600);
tcsetattr(fd1,TCSANOW,&options);

tcgetattr(fd2,&options);
cfsetispeed(&options,B9600);
cfsetospeed(&options,B9600);
tcsetattr(fd2,TCSANOW,&options);

clock_gettime(CLOCK_MONOTONIC,&st);

printf("Time(s) Current(pA) Current(mV)\n");
sprintf(formatted,"Time(s) Current(pA) Current(pA)\n");
fprintf(fp,"%s",formatted);

while(1) //CTRL+C to break out of this program
{
    sprintf(buff1,"READ?\n");
    ret1=write(fd1,buff1,strlen(buff1));
    memset(buff1,256,0);

    printf("ret1=%d\n",ret1);
}
printf("READ?\n");
ret2=write(fd2,buff2,strlen(buff2));
memset(buff2,256,0);

printf("READ?\n");
usleep(sleeptime*1000);
ret1=read(fd1,(char *)(buff1),256);
ret2=read(fd2,(char *)(buff2),256);
clock_gettime(CLOCK_MONOTONIC,&ct);
diff=timespec_diff(st,ct);
tdiff=diff.tv_sec + diff.tv_nsec*1e-9;

buff1[ret1]=0;
buff2[ret2]=0;
for(i=0;i<strlen(buff1);i++)
{
    if(buff1[i]==',')
    {
        buff1[i-1]=0;
        break;
    }
}
val1=atof(buff1);
val2=atof(buff2);
```c
// sprintf(formatted,"%f",((float)(diff.tv_sec)
+(float)(diff.tv_nsec/1000000000.0)));
// strcat(formatted," ");
// strcat(formatted,buff1,buff2,"\n");

printf("%f,%f,%f\n",tdiff,val1*1.0E+12,val2
*1.0E+3);
printf(formatted,"%f,%f,%f\n",tdiff,val1
*1.0E+12,val2*1.0E+3);
fflush(fp);
}
fclose(fp);
close(fd1);
close(fd2);
}

• ’ebit-beam-tuning-profiling/tuning_profile_ver4.c’: Located on ’cerebellum’

#include <stdio.h>
#include <stdlib.h>
#include <fcntl.h>
#include <errno.h>
#include <unistd.h>
#include <termios.h>
#include <string.h>
```
#include <time.h>
#include <curses.h>
#include <unistd.h>
#include <signal.h>

struct termios oldtermios;
#define TOTAL_READINGS (1.0)

/
This is tuning_profile_ver3 with following additions:
1. Set terminal to raw – added code for that
2. Key 7 accepts (intention is to use remote which
   already has numerical
   keys programmed
3. Added beeps for:
   a. ready to take reading
   b. multiple beeps for end of stripe.
   (modprobe pcspkr if not working in console)
   (the play .wav is slow, uncomment for fun if
   you wish)
4. Accept main filename (previously RFA.profile) at
   command line
5. Not writing sub-files anymore – waste of space
*/
```c
int ttyraw(int fd)
{
    /* Set terminal mode as follows:
       Noncanonical mode – turn off ICANON.
       Turn off signal-generation (ISIG)
           including BREAK character (BRKINT).
       Turn off any possible preprocessing of input (IEXTEN).
       Turn ECHO mode off.
       Disable CR-to-NL mapping on input.
       Disable input parity detection (INPCK).
       Disable stripping of eighth bit on input (ISTRIP)
           .
       Disable flow control (IXON).
       Use eight bit characters (CS8).
       Disable parity checking (PARENB).
       Disable any implementation-dependent output
           processing (OPOST).
       One byte at a time input (MIN=1, TIME=0).
    */
    struct termios newtermios;
    if (tcgetattr(fd, &oldtermios) < 0)
        return(-1);
    newtermios = oldtermios;
```
newtermios.c_iflag &= ~(ECHO | ICANON | IEXTEN | ISIG);

/* OK, why IEXTEN? If IEXTEN is on, the DISCARD character is recognized and is not passed to the process. This character causes output to be suspended until another DISCARD is received. The DSUSP character for job control, the LNEXT character that removes any special meaning of the following character, the REPRINT character, and some others are also in this category.
*/

newtermios.c_iflag &= ~(BRKINT | ICRNL | INPCK | ISTRIP | IXON);

/* If an input character arrives with the wrong parity, then INPCK is checked. If this flag is set, then IGNPAR is checked to see if input bytes with parity errors should be ignored. */
If it shouldn’t be ignored, then PARMRK determines what character sequence the process will actually see.

When we turn off IXON, the start and stop characters can be read.

/*

newtermios.c_cflag &= ~(CSIZE | PARENB);
/* CSIZE is a mask that determines the number of bits per byte.
   PARENB enables parity checking on input and parity generation on output.
*/

newtermios.c_cflag |= CS8;
/* Set 8 bits per character. */

newtermios.c_oflag &= ~(OPOST);
/* This includes things like expanding tabs to spaces. */

newtermios.c_cc[VMIN] = 1;
newtermios.c_cc[VTIME] = 0;
/ * You tell me why TCSAFLUSH. */

if ( tcsetattr(fd, TCSAFLUSH, &newtermios) < 0)
    return(-1);

return(0);

int ttyreset(int fd)
{
    if (tcsetattr(fd, TCSAFLUSH, &oldtermios) < 0)
        return(-1);

    return(0);
}

void sigcatch(int sig)
{
    ttyreset(0);
    exit(0);
}

void init_raw_mode()
{


/* Catch the most popular signals. */

if ( signal(SIGINT, sigcatch) < 0 )
{
    perror("signal");
    exit(1);
}

if ( signal(SIGQUIT, sigcatch) < 0 )
{
    perror("signal");
    exit(1);
}

if ( signal(SIGTERM, sigcatch) < 0 )
{
    perror("signal");
    exit(1);
}

/* Set raw mode on stdin. */

if ( ttyraw(0) < 0 )
{
    fprintf(stderr, "Can't go to raw mode.\n");
    exit(1);
}
float get_reading(char *filename, int fd1, float sleepms, int total_readings, int write_flag)
{
    // takes 'total_readings' number of readings by talking to port 'fd1' with interval of 'sleepms', writes each of them to file 'filename' if 'write_flag' is enabled
    // returns average of all readings taken

    int i, ret1, count;
    char buff1[256];
    float val1, val2;
    FILE *fp;

    if (write_flag)
        fp=fopen(filename, "w");
    val2 = 0.0;
    for (count = 0; count < total_readings; count++)
    {
        val1 = 0.0;
        printf(buff1,"READ?\n");
ret1 = write(fd1, buff1, strlen(buff1));
memset(buff1, 256, 0);
usleep(sleepms*1000);
ret1 = read(fd1, (char *)buff1, 256);
buff1[ret1] = 0;
for (i = 0; i < strlen(buff1); i++)
{
    if (buff1[i] == ',', ')
    {
        buff1[i - 1] = 0;
        break;
    }
}
val1 = atof(buff1);
val1 *= 1.0E+12;
printf("%f\r\n", val1);
if (write_flag)
    fprintf(fp, "%f\n", val1);
    val2 += val1;
}
if (write_flag)
    fclose(fp);
val2 /= total_readings;
printf("Average Reading=%f\r\n", val2);
return val2;

}

int main(int argc, char*argv[])
{
    struct termios options;
    int fd1;
    float samplerate, sleepms;
    int count1=0;
    FILE *fm;
    float x1_start, x1_end, x1_step, x2_start, x2_end,
         x2_step, x1_num_readings, x
         2_num_readings;
    float x1_curr, x2_curr;
    char filename[256];
    char formatted[256];
    char master[256];
    float val[256];
    char ch;
    int i;
    int x1_count=0, x2_count=0;
    float avg_val;

    if(argc!=10)

\!
\n\n\n\n∗∗∗∗∗∗∗∗∗∗∗∗∗∗∗
\n\nUsage:

./tuning_profile_v4

axis

x1_start

x1_step

x1_num

readings

axis

x2_start

x2_step

x2_num

readings

filename

\n
ne.g.

./tuning_profile_v4

Y

0.0

0.2

10

Z

5.6

0.2

10

RFA

.profile
\n
The

above

command
would
result
in

readings

(Y,Z)=

n(0.0,

5.6)
\nt(0.0,5.8)\t...
\nt(0.0,7.4)\n\tn(0.2,5.6)\t\nt(0.2,5.8)\t\t...
\nt(0.2,7.4)\n\n...
\n\n\nn(1.8

,5.6)\t\nt(1.8,5.8)\t\t...
\nt(1.8,7.4)\n\n"

\n
ne.g.

./tuning_profile_v4

Z

0.0

-0.2

10

X

5.6

0.2

10

RF

A.

profile
\n
The

above

command
would
result
in

readings

(Z,X)=

n(0.0,

5.6)
\nt(0.0,5.8)\t...
\nt(0.0,7.4)\n\tn(-0.2,5.6)\t\nt(-0.2,5.8)\t\t...
\nt(-0.2,7.4)\n\n...
\n\n\nn(-1.8,5.6)\t\tn(-1.8,5.8)\t\t...
\nt(-1.8,7.4)\n\n"

\n
The

path

is

from

(x1, x2_start)

to

x1, (x2+(x2step-1)*x2_
num_readings) for different x1s. 

e.g. do a vertical stripe with Y, go back to t

op Y, move Z inwards by dz and repeat vertical stripe, till reaached bounds as use t above 

Most recent changes

ntty set to raw mode, so no need to press enter.

remember to enter filename at command line. we will no longer make subfiles

*

exit (1);

x1_start=atof(argv[2]);
x1_step=atof(argv[3]);
x1_num_readings=atoi(argv[4]);
x1_end=x1_start+(float)((x1_step)*(x1_num_readings-1));

x2_start=atof(argv[6]);
x2_step=atof(argv[7]);
x2_num_readings=atof(argv[8]);
\[ x_{2\_end} = x_{2\_start} + (\texttt{float})((x_{2\_step} \times (x_{2\_num\_readings} - 1))) ; \]

\[ x_{1\_curr} = x_{1\_start} ; \]
\[ x_{2\_curr} = x_{2\_start} ; \]

\texttt{printf(}"\text{The desired grid bounds are }%s:%%f \text{ to } %f \text{ in }%steps of }%f, \text{ and }%s:%%f \text{ to } %f \text{ in }%steps of }%f", \text{argv[1]}, x_{1\_start}, x_{1\_end}, x_{1\_step}, \text{argv[5]}, x_{2\_start}, x_{2\_end}, x_{2\_step}) ; \]

samplerate = 1.0;
sleepms = 1000.0 / samplerate;
fd1 = \texttt{open("/dev/ttyS0", O_RDWR)} ;
\texttt{if} (fd1 == -1)
    perror("port not open") ;

tcgetattr(fd1, &options) ;
cfsetspeed(&options, B9600) ;
cfsetospeed(&options, B9600) ;
tcsetattr(fd1, TCSANOW, &options) ;
printf(master, argv[9]);
fm=fopen(master,"a");
fprintf(fm,"#%s(inches)\t%"s(inches)\tFC3(pA)\n",argv[1],argv[5]);

init_raw_mode();

for(x1_count=0;x1_count<x1_num_readings;x1_count++,x1_curr+=x1_step)
{
    for(x2_count=0,x2_curr=x2_start;x2_count<x2_num_readings;x2_count++,
x2_curr+=x2_step)
    {
        printf("\nMove_RFA_to_\%s=\%.4f_and\_\%
        \%s=\%.4f_and_hit_"7\n\to_confirm.\r\n",argv[1],x1_curr,argv[5],x2_curr);
        do{
            i = read(0,&ch,1);
            if(ch=='3')
            {
                fclose(fm);
                close(fd1);
                ttyreset(0);
                exit(1);
            }
        }
    }
}

186
while(ch!='7');

sprintf(filename,"RFA%s%.4f%s%.4f.profile",argv[1],x1_curr,argv[2],x2_curr);

avg_val=get_reading(filename,fd1,
sleepms,TOTAL_READINGS,0);

sprintf(formatted,"%.4f\t%.4f\t%.4f\n",x1_curr,x2_curr,avg_val);

fprintf(fm,formatted);
fflush(fm);
printf("Wrote%d bytes to master file\n",strlen(formatted));

if(x2_count!=x2_num_readings-1)
{
    system("echo\n\n\n"); // for console
    system("play lines1.wav"); // for XII
// dont play sound for last reading, as we will p

lay end of stripe sound

}
Appendix E  Obtaining RFA spectrum

The following code was used to obtain the RFA spectrum. The RFA spectrum program can accept input from a TV remote (IR) if an IR receiver is connected to the computer (typically via USB). The file is located in the '/crap' directory on 'cerebellum'.

- 'ebit-beam-tuning-profiling/RFA_spectrum.c' : Located on 'cerebellum'

```c
#include <stdio.h>
#include <stdlib.h>
#include <fcntl.h>
#include <errno.h>
#include <unistd.h>
#include <termios.h>
#include <string.h>
#include <time.h>
#include <curses.h>
#include <unistd.h>
#include <signal.h>

struct termios oldtermios;
#define TOTAL_READINGS (1.0)
```
```c
struct timespec timespec_diff(struct timespec start, struct
timespec end)
{
    struct timespec temp;
    if ((end.tv_nsec-start.tv_nsec)<0) {
        temp.tv_sec = end.tv_sec-start.tv_sec-1;
        temp.tv_nsec = 1000000000+end.tv_nsec-start.tv_nsec;
    } else {
        temp.tv_sec = end.tv_sec-start.tv_sec;
        temp.tv_nsec = end.tv_nsec-start.tv_nsec;
    }
    return temp;
}

int ttyraw(int fd)
{
    /* Set terminal mode as follows:
       Noncanonical mode – turn off ICANON.
       Turn off signal-generation (ISIG)
            including BREAK character (BRKINT).
       Turn off any possible preprocessing of input (IEXTEN).
       Turn ECHO mode off.
       Disable CR-to-NL mapping on input.
    */
}
```
Disable input parity detection (INPCK).
Disable stripping of eighth bit on input (ISTRIP).
Disable flow control (IXON).
Use eight bit characters (CS8).
Disable parity checking (PARENB).
Disable any implementation-dependent output processing (OPOST).
One byte at a time input (MIN=1, TIME=0).

*/
struct termios newtermios;
if (tcgetattr(fd, &oldtermios) < 0)
    return(-1);
newtermios = oldtermios;

newtermios.c_lflag &= ~(ECHO | ICANON | IEXTEN | ISIG);

/* OK, why IEXTEN? If IEXTEN is on, the DISCARD character is recognized and is not passed to the process.
   This character causes output to be suspended until another DISCARD is received. The DSUSP character for job control,
the LNEXT character that removes any special meaning of
the following character, the REPRINT character, and some
others are also in this category.

/*

newtermios.c_iflag &= ~(BRKINT | ICRNL | INPCK |
ISTRIP | IXON);

/* If an input character arrives with the wrong parity, then INPCK
is checked. If this flag is set, then IGNPAR is checked
to see if input bytes with parity errors should be ignored.
If it shouldn’t be ignored, then PARMRK determines what
character sequence the process will actually see.

When we turn off IXON, the start and stop characters can be read.

*/

newtermios.c_cflag &= ~(CSIZE | PARENB);
/* CSIZE is a mask that determines the number of bits per byte.

PARENB enables parity checking on input and parity generation on output.
*/

newtermios.c_cflag |= CS8;
/* Set 8 bits per character. */

newtermios.c_oflag &= ~(OPOST);
/* This includes things like expanding tabs to spaces. */

newtermios.c_cc[VMIN] = 1;
newtermios.c_cc[VTIME] = 0;

/* You tell me why TCSAFLUSH. */
if(tcsattr(fd, TCSAFLUSH, &newtermios) < 0)
    return(-1);
return(0);

}

int ttyreset(int fd)
if (tcsetattr(fd, TCSAFLUSH, &oldtermios) < 0)
    return(-1);

return(0);

void sigcatch(int sig)
{
    ttyreset(0);
    exit(0);
}

void init_raw_mode()
{

    /* Catch the most popular signals. */
    if (signal(SIGINT, sigcatch) < 0)
    {
        perror("signal");
        exit(1);
    }

    if (signal(SIGQUIT, sigcatch) < 0)
    {
        perror("signal");
}
exit(1);
}
if( signal(SIGTERM, sigcatch) < 0 )
{
    perror("signal");
    exit(1);
}

/* Set raw mode on stdin. */
if( ttyraw(0) < 0 )
{
    fprintf(stderr,"Can't go to raw mode.\n");
    exit(1);
}

int main(int argc, char*argv[])
{
    struct termios options;
    int fd1,fd2,fd3;
    int ret1,ret2,ret3;
    int total_readings;
    float samplerate,sleepms;
int start_v, stop_v, step_v, voltage;
char buff1[256]={0};
char buff2[256]={0};
char buff3[256]={0};
char formatted[2560]={0};
char formatted2[2560]={0};
int i=0;
FILE *fp;
struct timespec st, ct, diff;
float val1, val2, val3;
float avg_val1, avg_val2, avg_val3;
float tdiff;
int count;
char ch;

if (argc!=6)
{
    printf("Usage: ./tuning_v2 filename
    readingspersample\start_v\stop_v\step_v\(votages\ are \ integers\)\n\n")
    printf("Assumptions: Keithley multimeter 2010 connected via RS232 and through femptoamp
    Keithley 617 connected via GPIB–USB
    Keithley 485 connected via*
    SEPARATE* GPIB–USB will write other\n")

196
code to use just one
Remember to
initialize the GPIB controller to correct
address using ++addr xx, and to
initialize the Keithley to read Amps in
the appropriate range

printf(“This will write Time(s) Current 617 (pA) Current 485 (pA) Current 2010 (mV) to
specified file
”);
exit(1);
}

fp=fopen(argv[1],”w”);
total_readings=atoi(argv[2]);
sleepms=1000.0/1.0;

start_v=atoi(argv[3]);
stop_v=atoi(argv[4]);
step_v=atoi(argv[5]);

fd1=open(”/dev/ttyUSB0”,O_RDWR);
fd2=open(”/dev/ttyS1”,O_RDWR);
fd3=open(”/dev/ttyUSB1”,O_RDWR);

if (fd1==−1 )
```c
perro("port not open - ");

if (fd2 == -1)
  perro("port not open - ");

tcgetattr(fd1,&options);
cfsetspeed(&options,B9600);
cfsetospeed(&options,B9600);
tcsetattr(fd1,TCSANOW,&options);

tcgetattr(fd2,&options);
cfsetspeed(&options,B9600);
cfsetospeed(&options,B9600);
tcsetattr(fd2,TCSANOW,&options);

tcgetattr(fd3,&options);
cfsetspeed(&options,B9600);
cfsetospeed(&options,B9600);
tcsetattr(fd3,TCSANOW,&options);

clock_gettime(CLOCK_MONOTONIC,&st);
```
printf("\#Voltage Current_617 (pA) Current_485 (pA) Current_2010 (mV)\n");
sprintf(formatted,"\#Voltage Current_617 (pA) Current_485 (pA) Current_2010 (mV)\n");
fprintf(fp,"%s",formatted);
memset(buf1,256,0);
sprintf(buf1,"++addr\n27\n");
ret1=write(fd1,buf1,strlen(buf1));
sprintf(buf1,"++auto\n0\n");
ret1=write(fd1,buf1,strlen(buf1));
memset(buf1,256,0);
sprintf(buf1,"++addr\n12\n");
ret3=write(fd3,buf1,strlen(buf1));
sprintf(buf1,"++auto\n0\n");
ret3=write(fd3,buf1,strlen(buf1));

init_raw_mode();
for(voltage=start_v;voltage<=stop_v;voltage+=step_v){
    printf("\r\nAdjust Voltage to %dV and hit \n'7' to confirm or \n'3' to exit.\r\n",voltage);
    do{
        
    }while
199
i = read(0,&ch,1);

if(ch=='3')
{
    fclose(fp);
    close(fd1);
    close(fd2);
    close(fd3);
}
} while(ch!='7');

avg_val1=0.0; avg_val2=0.0; avg_val3=0.0;

for(count=0;count<total_readings;count++)
{
    val1 =0.0; val2 =0.0; val3 =0.0;

    memset(buff1,256,0);
    memset(buff2,256,0);
    memset(buff3,256,0);
    sprintf(buff1,"++ read\n");
    ret1=write(fd1,buff1,strlen(buff1));
    ret3=write(fd3,buff1,strlen(buff1));
    ret2=write(fd2,buff2,strlen(buff2));
memset(buff2, 256, 0);

usleep(sleepms*1000);

ret1 = read(fd1, (char *)buff1, 256);
if (ret1 != 17)
    ret1 = read(fd1, (char *)buff1, 256);

ret3 = read(fd3, (char *)buff3, 256);
if (ret3 != 15)
    ret3 = read(fd3, (char *)buff3, 256);

ret2 = read(fd2, (char *)buff2, 256);

clock_gettime(CLOCK_MONOTONIC, &ct);
diff = timespec_diff(st, ct);
tdiff = diff.tv_sec + diff.tv_nsec*1e-9;

if (ret1 != 17 && ret2 != 16)
    continue;
buff1 [ ret1 ] = 0;
buff2 [ ret2 ] = 0;
buff3 [ ret3 ] = 0;
for (i = 0; i < strlen (buff1); i++)
{
    printf ("%d = %c\n", i, buff1 [ i ]);
    buff1 [ i ] = buff1 [ i + 4 ];
}

for (i = 0; i < strlen (buff3); i++)
{
    printf ("%d = %c\n", i, buff3 [ i ]);
    buff3 [ i ] = buff3 [ i + 4 ];
}

val1 = atof (buff1);
val2 = atof (buff2);
val3 = atof (buff3);

avg_val1 += val1;
avg_val2 += val2;
avg_val3 += val3;

printf("\r\n%f %f %f %f \r\n", tdiff, val1 * 1.0E+12, val3 * 1.0E+12, val2 * 1.0E+3);
}

avg_val1 /= total_readings;
avg_val2 /= total_readings;
avg_val3 /= total_readings;

printf("\r\n****************************************\r\n", voltage, avg_val1 * 1.0E+12, avg_val3 * 1.0E+12, avg_val2 * 1.0E+3);

sprintf(formatted, "%d%f%f%f\n", voltage, avg_val1 * 1.0E+12, avg_val3 * 1.0E+12, avg_val2 * 1.0E+3);
fprintf(fp, "%s", formatted);
fflush(fp);
}

if(ttyreset(0) < 0)
{

203
Appendix F  Picoreader

The following code is used to read the data saved by the picoreader logging tool. Note the #pragma pack(1) compiler directive. Modern compilers enforce a 4-byte or 8-byte alignment restrictions, however we need to force the program to respect a 1-byte alignment when reading data saved by the picoreader. The data is saved in Little Endian format. The file is located in the '/crap' directory on 'cerebellum'.

- 'picoreader.c' : Located on 'cerebellum'

```
#pragma pack (1)

#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <math.h>
```
#define MAX_CHANNELS 16

typedef unsigned short int uint16;
typedef unsigned int uint32;
typedef unsigned char uint8;

typedef struct
{
    uint16 header_size;
    char signature[40];
    uint32 version;
    uint32 no_of_parameters;
    uint16 parameters[250];
    uint32 sample_no;
    uint32 no_of_samples;
    uint32 max_samples;
    uint32 interval;
    uint16 interval_units;
    uint32 trigger_sample;
    uint16 triggered;
    uint32 first_sample;
    uint32 sample_bytes;
    uint32 settings_bytes;
    uint32 start_date;
}
void getdata(FILE *infp ,FILE *outfp , FILE *masterfp) {
{
    plw_header hdr;
    int i,j;
    uint32 t;
    float ch[MAX_CHANNELS];
    char output_str[4096];
    char temp[4096];
float *integrated_intensity;

static int first_file_flag = 1;
uint32 start_time_of_first_file;

fread(&hdr, sizeof(hdr), 1, infp);
printf("header_size=%u, sample_bytes=%u, no_of_samples=%u, interval=%u, interval_units=%u, settings_bytes=%u, no_of_parameters=%d\n", hdr.header_size, hdr.sample_bytes, hdr.no_of_samples, hdr.interval, hdr.interval_units, hdr.settings_bytes, hdr.no_of_parameters);
printf("current_time=%u, startTimeMsAccuracy=%u, start_date=%u, start_time=%u, noOfDays=%u\n", hdr.current_time, hdr.startTimeMsAccuracy, hdr.start_date, hdr.start_time, hdr.noOfDays);
printf("%d\n", sizeof(float));

integrated_intensity = (float *)malloc(hdr.no_of_parameters * sizeof(float));

if (first_file_flag == 1)
{

start_time_of_first_file = hdr.start_time;
first_file_flag = 0;
}

for (i=0; i<hdr.no_of_samples; i++)
{
    fread(&t, sizeof(t), 1, infp);
    sprintf(output_str, "%u\t", t);

    fread(ch, sizeof(float), hdr.no_of_parameters, infp);
    for (j=0; j<hdr.no_of_parameters; j++)
    {
        if (j != hdr.no_of_parameters - 1)
        {
            sprintf(temp, "%f\t", ch[j]);
            strcat(output_str, temp);
        }
        else
        {
            sprintf(temp, "%f\n", ch[j]);
            strcat(output_str, temp);
        }
        if (ch[j] != 2.5)
integrated_intensity[j] += (float)ch[j];

}

fprintf(outfp, output_str);

// ignoring the .pls file that is appended to
// the .plw file.

}

// outputting integrated intensity to master file
sprintf(output_str, "%u\t", hdr.start_time -
    start_time_of_first_file);

for (j = 0; j < hdr.no_of_parameters; j++)
{
    if (j != hdr.no_of_parameters - 1)
    {
        sprintf(temp, "%f\t",
                integrated_intensity[j]);
        strcat(output_str, temp);
    }
    else
    {

209
printf(temp,"%fn",
integrated_intensity[j]);
strcat(output_str,temp);
}
}

fprintf(masterfp,output_str);

}

int main(int argc, char **argv)
{

FILE *infp,*outfp,*masterfp;
int i,start,end;
char filename[512];

printf("%d,%d,%d\n",sizeof(uint16),sizeof(uint32),sizeof(uint8));

if(argc!=4)
{
    printf("Usage: executable_name file_prefix start_index end_index\n");
}

210
exit(1);

}

start=atoi(argv[2]);
end=atoi(argv[3]);

sprintf(filename,"integrated\%s\%s\%s.txt",argv[1],argv[2],argv[1],argv[3]);
masterfp=fopen(filename,"w");
fprintf(masterfp,"\#Data from files \%s\%s.PLW to \%s\%s.PLW\n\# First columns is Time in seconds from \%s\%s; subsequent columns are integrated intensities over respective channels for that one burst\n",argv[1],argv[2],argv[1],argv[3]);

for (i=start;i<=end;i++)
{
    sprintf(filename,"\%s\%d.PLW",argv[1],i);
infp=fopen(filename,"r");

    sprintf(filename,"\%s\%d.txt",argv[1],i);
outfp=fopen(filename,"w");
fprintf(outfp,"\#Data from file \%s\%d.PLW\n",argv[1],i);

}
getdata(infp, outfp, masterfp);

fclose(outfp);
fclose(infp);
}

fclose(masterfp);

Appendix G  Lab Automation Framework

The following programs were used to create a lab automation framework. This involved a central server communicating in the background to various processes while taking in user input at the command line interface (CLI). The processes the CLI communicated with in the background were responsible for controlling the various instruments that were required to be controlled remotely. The devices controlled by the CLI were two turbopumps and two electrometers. Some devices also had analog output that necessitated the use of a microcontroller. For this purpose, a Rabbit microcontroller was utilized. The framework made provisions to read Auger output as well as control gate valves using the Rabbit. A remote could also operated using the Rabbit for measurements requiring physical action at a distance. The Rabbit was interfaced to the computer running the central CLI server via ethernet. A local area network was setup for just the two computers manually using the 10.***.** address range. If necessary, the route and ARP tables on the computer need
to be populated to facilitate TCP/IP communication. A telnet server was coded on top of the Rabbit TCP/IP stack to accept commands from the CLI. The following files - cli.c, tpumpD.c, tpumpB.c, electrometer0.c, electrometer1.c, and globals.h - are located on ‘cerebellum’ in /crap, while the file telnet.c contains the code for the Rabbit microcontroller on ’kaa’.

- ‘automation/globals.h’ : Located on ‘cerebellum’

```c
// define globals here.
#define MAXBUF 256
#define MAXARGS 64
#define MAXARGLEN 64
char *nargv[MAXARGS];
int nargc = 0;

#define ON 1
#define OFF 0

#define CLOSED 0
#define OPEN 1

#define MPUMPB 1
#define MPUMPD 2
#define GVALVEB 3
#define GVALVED 4
#define TPUMPB 5
```
#define TPUMP 6
#define ELECTROMETER0 7
#define ELECTROMETER1 8
#define MAX_DEVICES 10

struct dev
{
    int dev_id;
    int status;
};

struct global_state_structure
{
    struct dev devices[MAX_DEVICES];
    // populate in init: currently assuming everything is OFF when starting u
    p.

    int lock_mode;
}
global_state;

#define CLIPORT 19999 // this is the port on which cli will listen on... future g
ui purposes.
// this order of remote ports is followed in the port−fd map.

#define ETHPORT0_INDEX 0
#define ETHPORT1_INDEX 1
#define ETHPORT2_INDEX 2
#define ETHPORT3_INDEX 3
#define ETHPORT4_INDEX 4
#define ETHPORT5_INDEX 5
#define ETHPORT6_INDEX 6
#define ETHPORT7_INDEX 7
#define RABBITPORT_INDEX 8

#define MAXPORTS 9 // increase if you want to connect to more remote ports.

#define ETHPORT0 (20000+ETHPORT0_INDEX) // these are ports to which cli connects.
#define ETHPORT1 (20000+ETHPORT1_INDEX) // these are ports to which cli connects.
#define ETHPORT2 (20000+ETHPORT2_INDEX) // these are ports to which cli connects.
#define ETHPORT3 (20000+ETHPORT3_INDEX) // these are ports to which cli connects.
#define ETHPORT4 (20000+ETHPORT4_INDEX) // these are ports to which cli connects.
```c
#define ETHPORT5 (20000+ETHPORT5_INDEX) // these are ports to which cli connects.
#define ETHPORT6 (20000+ETHPORT6_INDEX) // these are ports to which cli connects.
#define ETHPORT7 (20000+ETHPORT7_INDEX) // these are ports to which cli connects.
#define RABBITPORT 23 // these are ports to which cli connects.

// we will have predefined command_port mapping.
// internally cli should generate a port_fd mapping.
// this is 2_step instead of one hardcoded command_fd mapping for failure cases..
// e.g. proc killed, then proc & conn will be restarted and fd can then change.

// command mapping : assumption: first word is enough to differentiate.
struct cmdstruct
{
    char cmd[64]; // only the first word of cmd.
    //
    int cmd_id;
    int port;
};
```
int dev_id; // populated if the command relates to a specific device, else 0.

void (∗fnptr)();

};
void fnmpumpB();
void fnmpumpD();
void fnpumpB();
void fnpumpD();
void fnvalveB();
void fnvalveD();
void fnzc0();
void fnzc1();
void fnlock();
void fnunlock();
void fnauger();
void fnshowstatus();

struct cmdstruct cmd_list[] =
{
    {"mpumpB", RABBITPORT, MPUMP_B, fnmpumpB},
    {"mpumpD", RABBITPORT, MPUMP_D, fnmpumpD},
};
{"gvalveB" ,RABBITPORT , GVALVEB , fngvalveB }
{"gvalveD" ,RABBITPORT , GVALVED , fngvalveD }
{"tpumpB" ,ETHPORT2 , TPUMPB , fnpumpB }
{"tpumpD" ,ETHPORT3 , TPUMPD , fnpumpD }
{"zc0" ,ETHPORT0 , ELECTROMETER0 , fnzc0 }
{"zc1" ,ETHPORT1 , ELECTROMETER1 , fnzc1 }
{"lock" ,RABBITPORT , 0 , fnlock }
{"unlock" ,RABBITPORT , 0 , fnunlock }
{"auger_scan" ,RABBITPORT , 0 , fnauger }
{"showstatus" ,0 , 0 , fnshowstatus } ,
};

int port_fd_map[MAXPORTS];

// populate at startup during connects.
//only stores fd's for remote ports, indexed by *****
PORT_INDEX. we assume we do not need to store fds corresponding to those connections connecting to cli.

int cli_listener_fd;
int gui_fd;
int cli_conn_count=0; //use this to count connections, also first connection to cli will be gui.

fd_set masterfds;
fd_set readfds;

int fdmax=0;
char bufrecv[MAXBUF];
char bufsend[MAXBUF];
char buftemp[MAXBUF];

FILE *logfd;

int rcvd;
int sent;
int cmd_id;
• 'automation/cli.c': Located on 'cerebellum'

// this is the cli file
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <sys/socket.h>  /* socket definitions */
#include <sys/types.h>    /* socket types */
#include <arpa/inet.h>    /* inet (3) functions */
#include <unistd.h>       /* misc. UNIX functions */

#include <fcntl.h>
#include <errno.h>
#include "globals.h"  // use this to define global variables.

extern int errno;

int myConnect(char *remote_addr, short int remote_port) {

int sock;
struct sockaddr_in serv_addr;

// create socket

if ( (sock=socket(AF_INET, SOCK_STREAM, 0)) == -1 )
{
    perror("Cant create socket!");
    exit(1);
}

// fill serv_addr

memset(&serv_addr,0,sizeof(serv_addr));
serv_addr.sin_family = AF_INET;
serv_addr.sin_port = htons(remote_port);
if ( inet_aton(remote_addr, &serv_addr.sin_addr) == 0 )
{
    perror("inet_aton fail");
    exit(1);
}

// all set, connect.
if ( connect(sock, (struct sockaddr *) &serv_addr,
    sizeof(serv_addr) ) == -1 )
{
    perror("connect fail");
    exit(1);
}

return sock;

int myListen(short int port)
{
    int sock;

    int yes=1; // socket option resuable address set
    struct sockaddr_in serv_addr;
    if ( (sock=socket(AF_INET, SOCK_STREAM, 0)) == -1 )
    {
        perror("Can't create socket!");
        exit(1);
    }
    if ( setsockopt(sock, SOL_SOCKET, SO_REUSEADDR, &yes,
        sizeof(int)) == -1)
    {
        perror("setsockopt");
}
exit(1);
}

memset(&serv_addr, 0, sizeof(serv_addr));
serv_addr.sin_family = AF_INET;
serv_addr.sin_port = htons(port);
serv_addr.sin_addr.s_addr = htonl(INADDR_ANY);
if (bind(sock, (struct sockaddr *)&serv_addr, sizeof(serv_addr)) == -1)
{
    perror("bind");
    exit(1);
}
if (listen(sock, 10) == -1)
{
    perror("listen");
    exit(1);
}
return sock;

int ReceiverTimeout ( int s, char *buf, int len, int timeout )
{

    fd_set fds;

    223
int n;
struct timeval tv;
FD_ZERO(&fds);
FD_SET(s, &fds);
    // Set up the struct timeval for the timeout.
tv.tv_sec = timeout;
tv.tv_usec = 0;
n = select(s+1, &fds, NULL, NULL, &tv);
    if ( n == 0 ) return -2;
    if ( n == -1 ) return -1;
    // data must be here, so do a normal recv
    return recv(s, buf, len, 0);
}

int logic_fnmpumpB(){
int logic_fnmpumpD(){
int logic_fntpumpB(){
int logic_fntpumpD(){
int logic_fngvalveB(){
int logic_fngvalveD(){
int logic_fnzc0(){
int logic_fnzc1(){
int logic_fnlock(){
int logic_fnunlock(){
```c
int logic_fnauger () {
}

void togglestate ()
{
    int fd; int port; int dev_id;

    if (nargc != 2)
    {
        printf("Not right number of args!\n");
        fprintf(logfd, "Not right number of args!\n");
        return;
    }

    if (global_state.lock_mode)
    {
        printf("Lock mode is ON. Cannot execute command.\n");
        fprintf(logfd, "Lock mode is ON. Cannot execute command.\n");
        return;
    }

    225
```
port=cmd_list[cmd_id].port;
dev_id=cmd_list[cmd_id].dev_id;

if (port==RABBITPORT)
    fd=port_fd_map[RABBITPORT_INDEX];
else
    fd=port_fd_map[port - 20000];

if (strncmp(nargv[1],"on",2)==0)
{
    if (global_state.devices[dev_id].status==ON)
    {
        printf("Already ON. Cannot execute command.\n");
        fprintf(logfd,"Already ON. Cannot execute command.\n");
    }
    return;
}
else if (strncmp(nargv[1],"off",3)==0)
{
    if (global_state.devices[dev_id].status==OFF)

{  
    printf("Already OFF. Cannot execute command.\n");  
    fprintf(logfd, "Already OFF. Cannot execute command.\n");  

    return;
}
}

switch(dev_id)
{

    //FIXME: add logic checks here:--
    case MPUMPB:  
    case MPUMPD:  
    case GVALVEB:  
    case GVALVED:  
    case TPUMPB:  
    case TPUMPD:  
    default:  
        break;
}

sent=send(fd,bufrecv,strlen(bufrecv),0);
printf("sent \%d bytes\n", sent);

rcvd=RecvTimeout(fd, bufrecv, MAXBUF, 5);
if (rcvd <=0)
{
    printf("Lost connection or process is stuck\nKill that process and restart.");
    //FIXME: Code to kill and restart... if
    rabbit is down you are f*cked.
    return;
}
else
{
    fprintf(logfd, bufrecv);
    printf("\%s", bufrecv);
    if (strcmp(bufrecv, "SUCCESS", strlen("SUCCESS")) ==0)
        global_state.devices[dev_id].status ^=1;
}

void togglezc()
{ 
    int fd; int port; int dev_id;
    char msg[64];

    if (nargc != 1)
    {
        printf("Not right number of args!\n");
        fprintf(logfd, "Not right number of args!\n");
        return;
    }

    if (global_state.lock_mode)
    {
        printf("Lock mode is ON. Cannot execute command.\n");
        fprintf(logfd, "Lock mode is ON. Cannot execute command.\n");
        return;
    }

    port=cmd_list[cmd_id].port;
    dev_id=cmd_list[cmd_id].dev_id;
    if (port==RABBITPORT)
        fd=port_fd_map[RABBITPORT_INDEX];
else
    fd = port_fd_map[ port - 20000 ];

if ( global_state . devices [ dev_id ] . status == OFF )
    sprintf ( bufrecv , "zcon\n" );
else
    sprintf ( bufrecv , "zcoff\n" );

sent = send ( fd , bufrecv , strlen ( bufrecv ) , 0 );
printf ( "sent %d bytes: %s\n" , sent , bufrecv );

rcvd =RecvTimeout ( fd , bufrecv , MAXBUF , 5 );
if ( rcvd <= 0 )
{
    printf ( "Lost connection or process is stuck\nKill that process and restart." );
    //FIXME: Code to kill and restart ... if rabbit is down you are fuccked.
    return ;
}
else
{
    fprintf ( logfd , bufrecv );
```c
printf("%s", bufrecv);
if (strcmp(bufrecv, "SUCCESS", strlen("SUCCESS"))) == 0)
    global_state.devices[dev_id].status ^= 1;
}

void fnmpumpB()
{
togglestate();
}

void fnmpumpD()
{
togglestate();
}

void fnpumpB()
{
togglestate();
}

void fnpumpD()
{
togglestate();
}

void fnzcv()
{
togglezc();
}

void fnzcl()
{
    return; /* togglezc(); FIXME: HACK FOR NOW: REMOVE return and uncomme
```
nt WHEN SECOND ELECTROMETER IS ALSO CONNECTED */

void fnlock () { global_state.lock_mode = ON; }
void fnunlock () { global_state.lock_mode = OFF; }
void fnauger () {}
```c
int i=0;
for (i=0; i<MAXPORTS; i++) {
    if (port_fd_map[i] == fd) {
        if (i == RABBITPORT_INDEX)
            return RABBITPORT;
        else
            return (i+20000);
    }
}
}

int lookup_cmd(char *cmd)
{
    // returns -1 on failure!

    int i=0;

    for (i=0; i<sizeof(cmd_list); i++) {
        
233
```
if(strcmp(cmd, cmd_list[i].cmd, strlen(cmd)) == 0) {
    // we found the command.
    return i;
}

return -1;

void init() {

    int fd, i;

    // do initializations here.
    FD_ZERO(&masterfds);

    // connection for cli: currently using stdin, later
    // switch to gui, [ cli
    //_listener_fd ] defined in globals....

    // myListen here for gui.
    FD_SET(0, &masterfds);

    // connection for rabbit

234
printf("Connecting to Rabbit...
");
fd=myConnect("10.10.6.100",RABBITPORT);
if (fdmax<fd) fdmax=fd;
port_fd_map[RABBITPORT_INDEX]=fd;
FD_SET(fd,&masterfds);
printf("Connected to Rabbit

");

// connection for ETHPORT0
fd=myConnect("127.0.0.1",ETHPORT0);
if (fdmax<fd) fdmax=fd;
port_fd_map[ETHPORT0_INDEX]=fd;
FD_SET(fd,&masterfds);

/*
// connection for ETHPORT1
fd=myConnect("127.0.0.1",ETHPORT1);
if (fdmax<fd) fdmax=fd;
port_fd_map[ETHPORT1_INDEX]=fd;
FD_SET(fd,&masterfds);
*/

// connection for ETHPORT2
/*
fd=myConnect("127.0.0.1",ETHPORT2);
if (fdmax<fd) fdmax=fd;
port_fd_map[ETHPORT2_INDEX]=fd;
FD_SET(fd,&masterfds);
*/
// connection for ETHPORT3
fd=myConnect("127.0.0.1",ETHPORT3);
if (fdmax<fd) fdmax=fd;
port_fd_map[ETHPORT3_INDEX]=fd;
FD_SET(fd,&masterfds);

// connections set up. populate global_state.
// FIXME : currently just setting defaults.... actually should query each device/process and get current state.
// FIXME : implement query command.
    global_state.lock_mode=OFF;
    for (i=0;i<MAX_DEVICES;i++)
    {
        global_state.devices[i].dev_id=i;
        global_state.devices[i].status=OFF;
    }
    global_state.devices[ELECTROMETER0].status=
        global_state.devices[ELECTROMETER1].status=ON; // zc is on by default

    for (i=0;i<MAXARGS;i++)
    //      argv[i]=(char*) realloc(MAXARGLEN, sizeof(char ));

236
memset(bufsend, 0, sizeof(bufsend));
memset(bufrecv, 0, sizeof(bufrecv));

logfd=fopen("log.txt", "a");

printf("Done\nInit!\n");
}

int parsecommand()
{
    //return -1 on error!

    int i;
    char *token;

    nargc = 0;
    argv[0] = strtok(buftemp, "\n");
    if (argv[0] == NULL)
        return -1;
    else
    {
        nargc = 1;
        while ((token = strtok(NULL, "\n")) != NULL)
        {
            
            237
        }
    }
nargv[nargc]=token;
nargc++;
if (nargc>MAXARGS)
    return −1;
}
return 1;

int main()
{
    // ok now cli starts.
    // call init
    int i, j;
    int cmd_fd, cmd_dev_id;
    printf("In main!\n");
    init();
while (1)
{
    // call master select
    cmd_id = -1;
    memset(bufrecv, 0, MAXBUF);
    memset(bufsend, 0, MAXBUF);

    readfds = masterfds;
    select(fdmax + 1, &readfds, NULL, NULL, NULL);
    fflush(stdout);
    fflush(logfd);

    for (i = 0; i < fdmax + 1; i++)
    {

        printf("\n\n\n");
        fprintf(
            logfd, "\n\n\n");
        fflush(
            stdout);
        fflush(logfd);

        if (FD_ISSET(i, &readfds))
        {

{
    // currently don't care where
    // we get the command from,
    // if valid execute!

    if (i == 0)
    {
        fgets(bufrecv, 256, stdin);
        rcvd = strlen(bufrecv);
    }

    else
    {
        rcvd = recv(i, bufrecv, sizeof(bufrecv), 0);
    }

    if (rcvd <= 0)
    {
        printf("Lost connection or process got stuck!\n");
    }

}
..and pray it isn't the rabbit!

```
//add code here to 
restart this 
process.

close(i);
FD_CLR(i,&masterfds);

}
else
{

fprintf(logfd,"
Command: %s \n", 
bufrecv);
memcpy(buftemp,
bufrecv,sizeof(
bufrecv));

if(parsecommand())
==−1)
{
    printf(""
Unable to
parse
command:
```
printf(
    logfd, "Unable to parse command: %s\n", bufrecv);
}
else {
    if ((cmd_id = lookup_cmd (nargv [0])))

        {
        printf
            (  
                " Unable to lookup command: %s\n", bufrecv);


242
fprintf
(
    logfd
    ,
    "Unable to lookup command: %s
    , bufrecv
    ");

    }
else
{
    // we got command cmd_id

    .just call it's associated function.

    printf("Found command cmd
d_id=%d!!\n", cmd_id);

    //

    243
int old()
{
    struct sockaddr_in remoteaddr;

    struct sockadc

```c
int fd0 = myListen(20000);
int fd1 = myConnect("127.0.0.1", 7);
int newfd;
char *msg = "hope this works!";
char bufr[100], bufs[100];
int i, sent, rcvd, fdmax, addrlen;

if (fd1 > fd0)
    fdmax = fd1;
else
    fdmax = fd0;

struct timeval tv;
fd_set readfds;
fd_set master;
tv.tv_sec = 2;
tv.tv_usec = 500000;

FD_ZERO(&master);
FD_SET(0, &master);
FD_SET(fd0, &master);
FD_SET(fd1, &master);
```
```c
printf("fd0=%d, fd1=%d\n", fd0, fd1);

while(1)
{
    memset(bufr, 0, 100);
    memset(bufs, 0, 100);
    readfds=master;
    select(fdmax+1, &readfds, NULL, NULL, NULL);

    for(i=0; i<fdmax+1; i++)
    {
        if(FD_ISSET(i, &readfds))
        {
            printf("%d was set!\n", i);
            if(i==fd1)
            {
                // we got something from the server

                rcvd=recv(i, buf, sizeof(buf), 0);
                printf("rcvd:\%s\n", buf);
            }
        }
        else if(i==fd0)
        {
```
accept(new_connection, &addrrlen = sizeof(remoteaddr));

if((newfd = accept(fd0, (struct sockaddr*)&remoteaddr, &addrrlen)) == -1)
{
 perror("accept");
}
else
{
 FD_SET(newfd, &master); // add to master

 if(newfd > fdmax)
{
 printf("selectserver : new_connection from socket\n", inet_ntoa(remoteaddr.sin_addr), newfd);

 fdmax = newfd;

 printf("server: new connection from socket\n", inet_ntoa(remoteaddr.sin_addr), newfd);

 fflush(stdout);

247
else if (i == 0)
{
    fgets (bufs, 100, stdin);
sent = send(fd1, bufs, strlen(bufs), 0);
    printf("sent %d bytes\n", sent);
    fflush(stdout);
}
else
{
    // this is the connections we accepted... write to fd1 what we got here then get response and send that back.
    rcvd = recv(i, bufr, sizeof(bufr), 0);
    printf("rcvd: %s\n", bufr);
    sent = send(fd1, bufr, strlen(bufr), 0);
    printf("sent %d bytes\n", sent);
memset(bufr, 0, 100);

// now we wait for response
... use _RecvTimeout here

ercvd=RecvTimeout(fd1, bufr, 100, 3);

if (rcvd == -2)
    printf("Timeout from server!\n");
else if (rcvd > 0)
    printf("Received response from server:\n");

sent = send(i, bufr, strlen(bufr), 0);

printf("sent %d bytes back\n", sent);

}
Appendix H  HCI nanocapillary beam shaping

This code was written with the intention of simulating the results reported in Zhang et al.[105] where using nanocapillaries, rhombus shaped and rectangular shaped beam were obtained at the exit when the other shape was incident onto the capillaries. The files are located on 'cerebellum' under '/root/dhruva/hci_nanocapillaries_tailoring'.

- 'nanocapillary-tailoring/tailoring.c' : Located on 'cerebellum'

```c
#include <stdio.h>
#include "globals.h"
```
#include <math.h>

#define PI (3.1415)

// Distance in nm.
// Time in nsec.

/*

FUNCTIONS

1. set up surface function.
   parameters: shape, shape specific params.

2. follow one ion function.
   follow the trajectory of one ion.

3. check whether hit walls
   depending on shape of capillary.

4. do sim: call fn 2 repeatedly for all ions as
dictated by original beam p

rofile.()
I/O

1. input: param file.
2. output: text file with location of all ions that make it through

*/

```c
void follow_ion(vec, vec, vec);
void get_pos(vec *, vec *, vec *, vec *);
void get_acc(vec *, vec *);
void get_vel(vec *, vec *, vec *, vec *);
int wall_hit_check(vec *);
int end_capillary_check(vec *);
void write_to_file(FILE *, vec *, vec *);
void init_surface();
double get_distance_from_point_to_line(vec, vec, vec);
void xform(vec *, vec *);
void print_pos(vec pos) { printf("Pos%.1g,%.1g,%.1g at time=%.7g\n", pos.x[0], pos.x[1], pos.x[2], time);}
void rotate2d(vec * res, double phi);
void get_vector(vec * res, vec pt1, vec pt2);
void get_pos_on_detector(vec * final_pos, vec * pos, vec * vel);
```
```c
void normalize(vec *res);

void initK()
{
    eps_r = 7.0;  // http://iopscience.iop.org
    1478-7814/37/1/304
    K = (eps_r - 1)/(eps_r + 1);
    K = K * q * q / 4;
    K = K * 0.015458653;
    K = K / m;
    K *= 8.98800752 * pow(10, 9);

    // acceleration = K sum(ni_bar/di^2); in nm/nsec, di in nm.
    // K = (0.015458653 * (eps_r - 1) * q^2) / (m in amu) * (eps_r + 1) * 4

    printf("K is \%g\n", K);
}

int main()
{

}
vec a, b, c;

double i, j;

// open files for I/O
ions_reached_fp=fopen("out.txt", "w");
init_surface();
initK();

// calculate ioncoming velocity.
v.x[0]=v.x[1]=0; v.x[2]=1.38913882*sqrt(E/m)*pow((10,4);
printf("velocity_is_\%g\n", v.x[2]);
printf("timestep_is_\%g\n", timestep);

pos.x[0]=pos.x[1]=pos.x[2]=0;
acc.x[0]=acc.x[1]=0; acc.x[2]=0;

printf("Debug: \\
get_distance_from_point_to_line (a, vertex [2], verte
x[3]));

for (i = -30; i <= 30.0; i += 0.1)
{
    for (j = -30.0; j <= 30.0; j += 0.1)
    {
        pos.x[0] = (double)i; pos.x[1] = (double)j;
        v.x[0] = v.x[1] = 0; v.x[2] = 1.38913882 * sqrt(E/m)*pow(10,4);
        acc.x[0] = acc.x[1] = 0; acc.x[2] = 0;
        time = 0;
        total_particles ++;
        follow_ion (pos, v, acc);
    }
}

/*
for (j = 0; j <= 120; j += 1)
{
    for (i = -90; i <= 90; i += 1)
{ 
    pos.x[0] = (double) i; pos.x[1] = (double) j;
    v.x[0] = v.x[1] = 0; v.x[2] = 1.38913882 * sqrt(E/m) * pow(10, 4);
    acc.x[0] = acc.x[1] = 0; acc.x[2] = 0;
    time = 0;
    total_particles ++;
    follow_ion(pos, v, acc);
}

break;
}

/*

/*
    pos.x[0] = 50.0;
    pos.x[1] = 50.0;
    pos.x[2] = 0;
    follow_ion(pos, v, acc);
*/

printf("Total \_particles \_sent:\%lld\n",
        total_particles);

256
printf("Particles through capillary: %lld\n", particles_at_detector);
printf("Particles hit walls: %lld\n", particles_hit_wall);

// close files
fclose(ions_reached_fp);

void follow_ion(vec pos, vec vel, vec acc)
{

/* Using verlet velocity algorithm.
http://research.chem.psu.edu/shsgroup/chem647/newNotes/node6.html
or
http://en.wikipedia.org/wiki/Verlet_integration#
Velocity_Verlet

Algorithm:
Start with r(t) and v(t) and calculate a(t)

Repeat the following steps:
1. calculate r(t+dt) = r(t) + v(t) dt + 0.5 a(t) dt^2
2. calculate $a(t+dt)$

3. calculate $v(t+dt) = v(t) + 0.5[a(t) + a(t+dt)]\, dt$

// this is under the condition that $a(x,t)$ and not $a(x,v,t)$.

*/

vec new_vel, new_pos, new_acc;
vec theta_phi;
int i, j, k;

// init structs
for (i=0; i<3; i++)
{
    new_vel.x[i]=new_pos.x[i]=new_acc.x[i]=0;
}

while (1)
{
    time+=timestep;
    get_pos(&new_pos,&pos,&vel,&acc);
    // print_pos(new_pos);
    if (wall_hit_check(&new_pos))
    {
        
    
}
printf("Particle hit wall at: \lf, \lf, \lf \n", new_pos.x[0], new_pos.x[1], new_pos.x[2]);

particles_hit_wall++;
break;
} 
if (end_capillary_check(&new_pos))
{
    get_pos_on_detector(&new_pos,&pos,&vel);

    xform(&theta_phi,&new_pos);
    write_to_file(ions_reached_fp,&new_pos,&theta_phi);
    print_pos(new_pos);
    particles_at_detector++;
    break;
}

// we are still inside the playfield.
get_acc(&new_acc,&new_pos);
get_vel(&new_vel,&new_acc,&acc,&vel);

pos=new_pos; vel=new_vel; acc=new_acc;
void get_pos( vec * result, vec * pos, vec * vel, vec * acc)
{
    int i;
    for(i=0; i<3; i++)
    {
        // r(t+dt) = r(t) + v(t) dt + 0.5 a(t) dt^2
        result->x[i] = pos->x[i] + vel->x[i] *
                        timestep + 0.5 * acc->x[i]
                        * timestep * timestep;
    }
}

void get_acc( vec * result, vec* pos)
{
    // we are inside the capillary when this fn is called.
    // F = - K ( ni_bar / di^2 ); i =1 to 4 // shape specific.
    int i;
    double d, dsq_inverse;
    switch(shape)
    {

case 1:
case 2:
result -> x[0] = result -> x[1] = result -> x[2] = 0;
for (i = 0; i < 4; i++)
{
    d =
        get_distance_from_point_to_line
        ( *pos, vertex[i], vertex[(i+1)%4] );
    dsq_inverse = (1/(d*d));
    result -> x[0] += -1.0*K*
        dsq_inverse * normals[i].x[0];
    result -> x[1] += -1.0*K*
        dsq_inverse * normals[i].x[1];
    // printf("-------> %g,%g\n", result -> x[0], result -> x[1]);
}
break;
default:
void get_vel ( vec * result, vec * a2, vec * a1, vec * vel )
{
    // v(t+dt) = v(t) + 0.5[ a(t) + a(t+dt) ]dt
    int i;
    for ( i=0; i<3; i++ )
        result->x[i]=vel->x[i] + 0.5*(a1->x[i] + a2
                                     ->x[i])*timestep;
}

void xform ( vec * thph, vec * pos )
{
    // get theta phi of final position.
    // thph->x[0] unused
    // thph->x[1] theta
    // thph->x[2] phi

    double l=detector_z+channel_length;
}
thph->x[1]= atan(pos->x[1]/l);  // tan theta = y/l;
thph->x[2]= atan(pos->x[0]/l);  // tan phi = x/l;

thph->x[1]*=180.0/(PI);
thph->x[2]*=180.0/(PI);

}

void write_to_file(FILE *fp, vec *pos, vec *thph)
{
    fprintf(fp,"%g\%g\%g\n",pos->x[0],pos->x[1],pos->x[2]);
    fprintf(fp,"%g\%g\n",thph->x[1],thph->x[2]);
}

void get_pos_on_detector(vec *final_pos, vec *pos, vec *vel)
{
    // get time to reach detector using z's. use that
time to calc final x,y.
    double t;
    t=(detector_z - pos->x[2])/(vel->x[2]);
    final_pos->x[0] = pos->x[0] + vel->x[0]*t;
    final_pos->x[1] = pos->x[1] + vel->x[1]*t;

263
}

int wall_hit_check(vec *pos)
{
    // return 1 if wallshit, else return 0.
    /* 1. we are always inside the walls when this
        function is called.
        2. calculate distance to each of the walls,
        if less than 1 nm re
        turn true. else return false.
    */

    int i;
    double d;
    for (i=0; i<4; i++)
    {
        d = get_distance_from_point_to_line(*pos,
                                              vertex[i], vertex[(i+1)%4]);
        if (d < 1.0)
            return 1;
    }
}

264
double get_distance_from_point_to_line(vec pt, vec l1, vec l2) {
    // calc distance of point pt from line segment joining l1 and l2.

    // d of (x0, y0) from line joining (x1, y1) and (x2, y2) : |( (x2 - x1)(y1-y0) - (x1-x0)(y2-y1) ) / sqrt( (x2-x1)^2 + (y2-y1)^2 )| |

    double d;
    double x1, x2, y1, y2, x0, y0;
    x1 = l1.x[0]; y1 = l1.x[1];
    x2 = l2.x[0]; y2 = l2.x[1];
    x0 = pt.x[0]; y0 = pt.x[1];

    d = fabs( (x2-x1)*(y1-y0) - (x1-x0)*(y2-y1) ) / sqrt( (x2-x1)^2 + (y2-y1)^2 );
    return d;
}
int end_capillary_check(vec *pos)
{
    // if z is greater than channel length, we are done.
    if (pos->x[2] > channel_length) return 1;
    return 0;
}

void init_surface()
{

    int i, j, k;

    #if 0

        // topmost, leftmost = start of indexing. then following clockwise.
        // e.g.: rhombus:

        A
         |   |
         |   |
         |   |

        D   B
         |   |
         |   |
    #endif

}
\[ C \]

\textit{e.g.: rectangle:}

\[ A \mid \mid \mid \mid B \]

\[ | \quad | \]

\[ | \quad | \]

\[ | \quad | \]

\[ | \quad | \]

\[ D \mid \mid \mid \mid C \]

\( A=0, B=1, C=2, D=3 \quad */

\textbf{switch}(\text{shape})

\{

\textbf{case} 1: // \textit{rectangle}

\textbf{int} i, j;

// \textit{set up vertex array}.

\textbf{for} (i=0; i<4; i++)

\textbf{for} (j=0; j<3; j++)

\hspace{1cm} \text{vertex}[i].x[j]=a.x[j];

\}

\#endif

// \textit{populate normals array} \rightarrow \textit{all normals point inwards into the hole away from walls}.
switch (shape)
{
    case 1: // rectangle
        for (i=0; i<4; i++)
        {
            get_vector(&normals[i],
                        vertex[i], vertex[(i+1)%4]);

            rotate2d(&normals[i], -(PI/2.0));
            normalize(&normals[i]);
            printf("Normal%d = (%g, %g, %g)\n", i, normals[i].x[0], normals[i].x[1], normals[i].x[2]);
        }
        break;

    case 2:
        // rhombus
        for (i=0; i<4; i++)
        {
            get_vector(&normals[i],
                        vertex[i], vertex[(i+1)%4]);
        }
}
rotate2d(&normals[i], -(PI / 2.0));
normalize(&normals[i]);
printf("Normal %d = (%g, %g, %g)\n", i, normals[i].x[0], normals[i].x[1], normals[i].x[2]);
}
break;
default:
break;

void rotate2d(vec * res, double phi)
{
double r2d[2][2];
int i, j;
vec temp=*res;
r2d[0][0]= cos(phi);
r2d[0][1]= -sin(phi);
r2d[1][0]= sin(phi);
r2d[1][1]= cos(phi);

for (i=0; i<2; i++)
{

res->x[i]=0;
for (j=0; j<2; j++)
    res->x[i]+=temp.x[j]*r2d[i][j];
}

res->x[2]=temp.x[2];

}

void normalize(vec *res)
{
    double l=0;
    int i;
    for (i=0; i<3; i++)
        l+=res->x[i]*res->x[i];

    for (i=0; i<3; i++)
        res->x[i]/=sqrt(l);
}

void get_vector(vec *res, vec pt1, vec pt2)
{
    int i;
    for (i=0; i<3; i++)
\[ \text{res} -> x[i] = pt2.x[i] - pt1.x[i]; \]

- `nanocapillary-tailoring/globals.h` : Located on `cerebellum`

```c
/* parameters:
   main box containing capillary x, y.
   shape of capillary:
   1: rectangle
   2: rhombus
   3. ...
*/

// all dimensions in nm.

struct Vector {
    double x[3];
};

typedef struct Vector vec;

double X = 500;
double Y = 500;
```
double eps_r,K;

// topmost, leftmost = start of indexing. then following clockwise.

/* e.g.: rhombus:

   A
   | |
   | |
   D B
   | |
   | |
   C

   e.g.: rectangle:

   A |||| B
   |   |
   |   |
   |   |
   |   |
   D |||| C

A=0, B=1, C=2, D=3
*/

int shape=1;

// rectangle: 200 x 450

/* double ax=-100, ay=225, az=0; */
double bx=100, by=225, bz=0;
double cx=100, cy=-225, cz=0;
double dx=-100, dy=-225, dz=0;
double Ax=-100, Ay=225, Az=20000;
double Bx=100, By=225, Bz=20000;
double Cx=100, Cy=-225, Cz=20000;
double Dx=-100, Dy=-225, Dz=20000;
*/
double channel_length=20000.0;
/
vec a={ {-100,225,0} };
vec b={ {100,225,0} };
vec c={ {100,-225,0} };
vec d={ {-100,-225,0} };
*/
vec vertex[]={
   { -100.0,100.0,0.0 },
   { 100.0,100.0,0.0 },
   { 100.0,-100.0,0.0 },
   { -100.0,-100.0,0.0 };
vec normals [4];
int shape = 2;

// rhombus: 140 x 250
double ax = -70, ay = 0;
double bx = 0, by = 125;
double cx = 70, cy = 0;
double dx = 0, dy = -125;
double channel_length = 10000;

vec normals[4];
*/

// beam parameters

double E = 7000.0; // energy in eV
double m = 20.1797; // mass in amu

double q = 7.0; // charge state

vec v; // velocity in nm/sec
//1 amu = 9.3146x10^6 eV/c^2
//→→ v = sqrt(2E/m) = sqrt(2Ec^2
//9.3146x10^6) =
//sqrt(18E/9.3146m)x10^13 nm/sec
//= sqrt(1.93245E/m) x 10^13 nm/sec
//= sqrt(1.93245E/m) x 10^4 nm/nsec

vec pos; // initial position
vec acc; // initial acceleration

double detector_z=50000.0;

double timestep=1.0E−5; // nanoseconds
FILE * ions_reached_fp;
FILE * ions_walled_fp;
double time=0;

long long int total_particles=0;
long long int particles_hit_wall=0;
long long int particles_at_detector=0;

Appendix I modified Safari

The detector and analysis codes were rewritten in C for the SAFARI program.
These programs, and the associated scripts, are bulky and not reproduced here. Instead,
the readme file that lists instructions on running these programs is listed here. These files are located on 'kaa'.

- 'safari/readme.txt': Located on 'kaa'

***Take care to not disturb directory structure.
***If changing one script, copy that to all directories.
***All input files are assumed to be named *ev.input
  e.g. 20ev.input, 100ev.input etc.

Run scripts in this order:

1. sh convert.sh ——> get input files with correct parameters.

2. sh run.sh ——> runs safari that also generates .trajs files.

3. sh check.sh ——> checks that all ran with same energy... no overlap of queuing and running.

4. qsub cdtect_run.sh ——> get .cdtect files from .trajs files.

5. qsub cdtect_post.sh ——> generates trajcount.txt ... counts trajectories backscattered, stuck, buried, unable to escape for each energy

6. qsub trim.sh ——> removes all stuck and buried
(−100 eV or −200 eV) from .cdtect files and generates .trimmed files.

7. qsub gnuplot.sh ———> plots angle and energy resolved 
spectra from .trimmed files.

8. qsub spot_energy_spectrum.sh
———> reads .trimmed files and generates intensity vs energy 
numbers for particular theta final spots....
generates $energyincoming$_$thetafinal_energy_spectrum.txt 
files
———> also generates individual plots of intensity vs 'k'
for Ein, thetain.

*** Sometimes Palmetto is slow to run after queueing the job :
in this case, due to the wonderful requirement of safari.
   input by Safari,

run "run_with_different_dirs.sh"

then, "collect_with_different_dirs.sh"

then, "remove_different_dirs.sh"
at this point, we are done with step 2, continue from step 3 above.
Appendix J  List of programs

The source code for the programs listed here have been copied onto the ’kaa’ machine and organized conveniently as shown below.

Listings

gpib.conf .......................................................... 137
"electrometers/measure_485_2400.c” .......................... 140
"electrometers/measure_617_485.c” .......................... 145
"electrometers/keithley2000.c” .............................. 150
"electrometers/keithley2000_thermocoupletypeC.c” ........ 154
"auger/params.sh” .............................................. 160
"auger/auger.sh” ................................................ 161
"auger/auger_plot.sh” ........................................ 161
"auger/srs830.c” ................................................. 163
"ebit–beam–tuning–profiling/tuning_v3.c” .................... 168
"ebit–beam–tuning–profiling/tuning_profile_ver4_folded.c” 173
"ebit–beam–tuning–profiling/RFA_spectrum.c” .............. 189
"picoreader.c” .................................................... 204
"automation/globals_folded.h” ................................ 213
"automation/cli_folded_typeset.c” ............................ 220
"nanocapillary–tailoring/tailoring_folded.c” .............. 250
"nanocapillary–tailoring/globals_folded.h” .................. 271
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