Simulation of Photoionization in RIMS

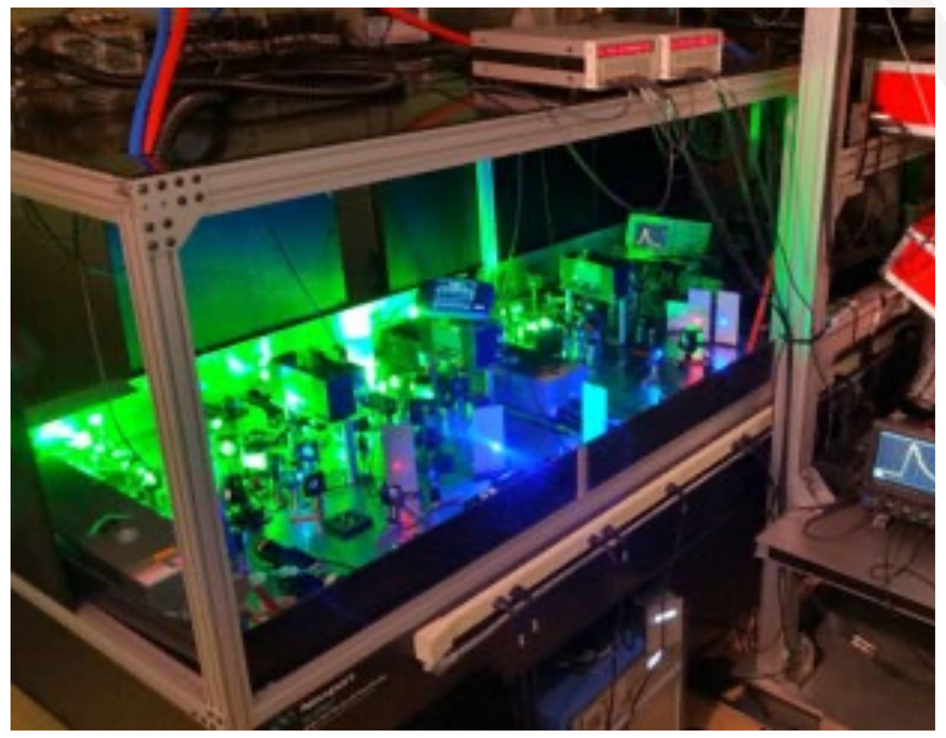
Henry Burns
Georgia Institute of Technology
Steven Biegalski, steven.biegalski@me.gatech.edu
Consortium for Monitoring, Technology, and Verification (MTV)

Introduction and Motivation

- Resonance Ionization Mass Spectrometry (RIMS) uses tuned lasers to selectively ionize the element of interest.
- The ions are accelerated through an electric field. Isotopes can be distinguished from each other by time-of-flight (ToF) measurements.
- Currently, accuracy is hindered by the large cross section of the photoionization zone, which, while necessary to ionize a significant fraction of the sample, produces peak overlap in the time-of-flight detector.

Mission Relevance

- RIMS is a method of mass spectrometry that is particularly well-suited for analyzing isotopic ratios of an element of interest in a sample composed of multiple elements.
- RIMS can measure isotopic ratios even when the element of interest makes up a small proportion of the sample.
- RIMS could therefore be used to analyze uranium isotope ratios from environmental samples for the purpose of nuclear forensics.

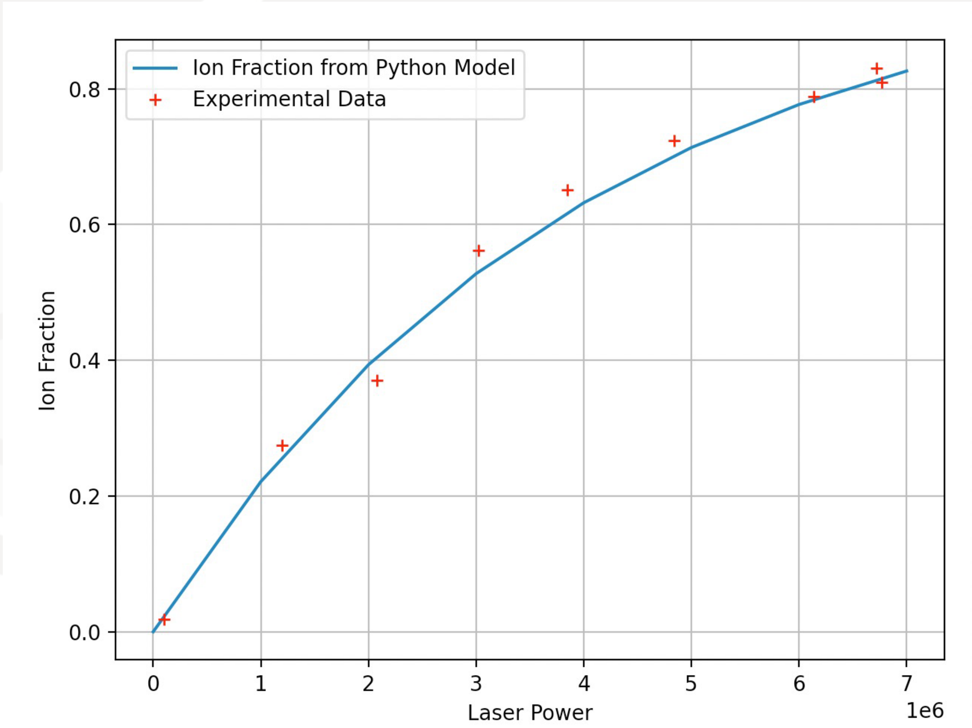


Technical Approach

- Working with researchers at LLNL, a new photoionization model has been developed in Python that simulates an elliptical beam with a Gaussian power distribution passing through a cloud of atoms sputtered from a sample.
- The code allows the user to specify the laser's dimensions and power and calculates ionization probability based on the formula $P = 1 - \exp(-I/I_{sat})$, where I is the laser's intensity and the saturation intensity is determined experimentally.
- The model produces an input file that can be used with existing ion flight simulation software.
- The model is then benchmarked against existing data demonstrating peak overlap.

Results

- Preliminary results suggest that some ionization occurs that is unaccounted for by the simplified ionization rate equation currently in use.
- A corrective factor introduced to the model leads to a charge distribution closely matching experimental data.



Expected Impact

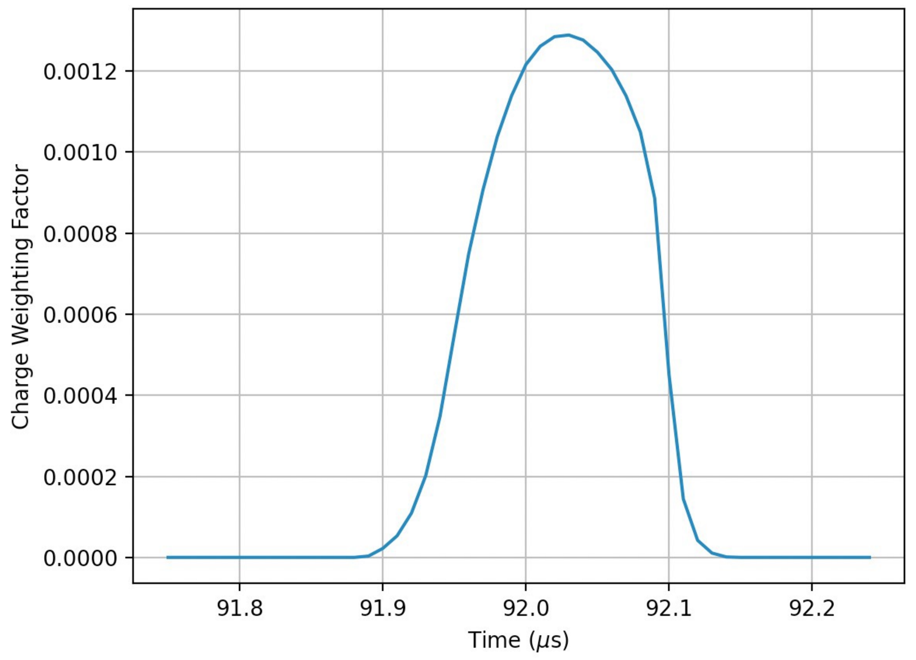
- Accurately modelling sources of noise in RIMS will lead to a more accurate analysis of the data produced by RIMS.
- This should allow use of RIMS on smaller samples and increase precision on larger samples.

MTV Impact

- Parts of this work are the result of collaboration with LLNL and were cleared for release to the general public under IM release number VIDEO-825505
- In summer of 2022, I will be continuing this collaboration as a Seaborg Intern at LLNL.

Conclusion

- The resulting model of photoionization in RIMS is a more physically accurate simulation than the previous model in use.
- Use of more accurate ionization rate equations is expected to remove the need for a corrective factor in the model.



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