# Photoionization Simulation for Improved RIMS Accuracy

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## Abstract:

This work focuses on accurate simulation of initial ion positions in a resonance ionization mass spectrometer (RIMS) to isolate sources of peak overlap in the detector and improve its accuracy. RIMS uses tuned lasers to selectively ionize a single element of interest in a sample. Different isotopes of the element of interest are then distinguished using time-of-flight measurement. This process is useful for environmental sampling and nuclear forensics, which require accurate measurement of the ratio of uranium isotopes in a sample containing other elements. 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.

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 simulation delivers a more physically accurate model of the ions' initial positions and improves on the original model, which assumes a circular cross section and uniform photoionization. The model produces an input file that can be used with existing ion flight simulation software. The new model has been benchmarked against experimental data, and preliminary results suggest that some ionization occurs that is unaccounted for by the simplified ionization rate equation currently in use. Further work will focus on identifying the reasons for the discrepancy between model and data. An updated model incorporating ionization rate equations is being tested to resolve the issue. After testing against experimental data and further refinement, the model will be used to predict sources of error and remove noise from the RIMS detector output, thereby increasing detector resolution.