

A Coded Aperture Mattauch-Herzog Mass Spectrograph

Zachary E Russell, Shane T DiDona, Jason J Amsden, Charles B Parker, Michael E Gehm, Jeffrey T Glass

Duke University, Durham, NC

In order to combat losses in signal intensity often present in mass spectrometry miniaturization efforts [1], we have applied the principles of spatially coded apertures [2] to magnetic sector mass spectrometry showing increases in signal to background ratios of greater than 10X with no loss in mass resolution [3][4]. We are investigating the compatibility of this technique with other common mass spectrometer and mass spectrograph configurations, as well as perturbations from these classic geometries that may be more compatible with spatial aperture coding. In this work we will present a compatibility assessment with the popular Mattauch-Herzog mass spectrograph geometry, and a computational methodology used to evaluate new geometries to optimize performance.

Experimental results demonstrating compatibility were obtained using the commercially available miniature Mattauch-Herzog type mass spectrograph from OI-Analytical/Xylem [5]. COMSOL Multiphysics [6] finite element solvers were used to simulate electric and magnetic fields, and a custom particle tracing routine written in C# that allowed for calculations of more than 15 million particle trajectory time steps per second. A parametric optimization routine [7] was used to perform geometric optimization and simulation results indicated adjustments to the electric sector that would allow intensity gains of greater than 10X for the Mattauch-Herzog geometry, with no accompanying loss in mass resolution. This work was sponsored in part by The Department of Homeland Security Science and Technology Directorate.

[1] Badman, E. R.; Cooks, R. G., Special feature: Perspective - Miniature mass analyzers. *J Mass Spectrom* 2000, 35 (6), 659-671. **[2]** Brady, D. J., *Optical Imaging and Spectroscopy*. Wiley: 2009. **[3]** Russell, Z. E.; Chen, E. X.; Amsden, J. J.; Wolter, S. D.; Danell, R. M.; Parker, C. B.; Stoner, B. R.; Gehm, M. E.; Brady, D. J.; Glass, J. T., Two-Dimensional Aperture Coding for Magnetic Sector Mass Spectrometry. *J Am Soc Mass Spectr* 2015, 26 (2), 248-256. **[4]** Chen, E. X.; Russell, Z. E.; Amsden, J. J.; Wolter, S. D.; Danell, R. M.; Parker, C. B.; Stoner, B. R.; Gehm, M. E.; Glass, J. T.; Brady, D. J., Order of Magnitude Signal Gain in Magnetic Sector Mass Spectrometry Via Aperture Coding. *J Am Soc Mass Spectr* 2015, 1-8. **[5]** OI Analytical, A Xylem brand, IonCam Product **[6]** COMSOL COMSOL Multiphysics, 4.3b; 1988-2013. **[7]** Brent, R. P. *Algorithms for Minimization without Derivatives*. Dover, 2002 (Original edition 1973).