Design and Simulation of a Micromachined Cylindrical Ion Trap (CIT) Array

Dolores Cruz[1, 3], Matthew G. Blain[1], Daniel E. Austin[1], Leah S. Riter[2], Guangxiang Wu[2], R. Graham Cooks[2], and Jane P. Chang[3], *[1]MicroAnalytical Systems Department, Sandia National Laboratories, Albuquerque, NM, [2]Chemistry Department, Purdue University, West Lafayette, IN, [3]Dept. of Chemical Engineering, UCLA, Los Angeles, CA*

Breakthrough improvements in microsensors for high-consequence applications, including chemical/biological warfare agents, medical diagnostics, and explosives and contraband detection, will be realized only with the development of ultrasensitive and ultraselective microfabricated detectors which are able to *unambiguously* identify the compound of interest. A micron-scaled mass spectrometer on a chip could set the performance standard for such micro-detectors. For example, the combination of a micro-gas chromatographic (μGC) separation column with a micro-mass spectrometer (μMS) detector could provide an extremely sophisticated capability for specific and unambiguous molecular identification. A μMS could also serve as a standalone microanalytical system. While the effort to develop a complete μMS system must include sample introduction, ion source, mass analyzer, ion detector, vacuum, and power subsystems, we will describe in this paper the design considerations and simulation of a micron-scaled (cylinder radius r_0=1□m) cylindrical ion trap (CIT) mass analyzer and our efforts to microfabricate a cm^2-sized array of $\geq 10^6$ micron-scaled cylindrical ion traps (CITs) on a silicon substrate. The analyzer design includes an integrated ion detector. The theoretical mass range of the design would allow for detecting high mass species. The objective is to develop and test an inexpensive, compact chip-based mass-spectrometer system for use in portable chemical sensors such as Sandia's MicroChemLab™.

We will also describe our initial efforts, which are currently in progress, to fabricate the CIT array using silicon micromachining techniques and tungsten metallization processes. A first-generation ion trap array using aluminum has been microfabricated, however cylinder profile control issues have led to microfabrication of the next-generation prototype using molded tungsten and chemical mechanical polishing. The individual trap array element consists of two endcap electrodes, one ring electrode, and a detector/collector plate, fabricated in seven metal layers. The layers are defined by molding tungsten around features (0.5□m minimum dimension) etched into SiO_2 using standard lithography and plasma etching techniques. Each layer of tungsten is then polished back in damascene fashion. The SiO_2 is removed using a standard MEMS release processes to realize a free-hung ion trap element. Common anchor points of adjacent elements allow for the entire array of traps to be operated in parallel.

Calculations of the electric fields produced by the CIT and simulation of ion trajectories using ITSIM and SIMION software have been performed in order to understand and optimize ion trap design. Important considerations include implications of imperfections that may be encountered on this scale of fabrication, such as misalignment of end-cap holes, non-cylindrical ring electrode walls and surface roughness. The simulations have been used to elucidate excitation conditions and trap operational sequences and to study the unique properties of small ion traps, including space charge, potential well depth (thus trapping efficiency), capacitive heating, and geometry, e.g. endcap to ring electrode gap and r_0 to z_0 (cylinder radius to half-length) ratio.

[1]Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.