Planar Electrode Quadrupole Ion Traps

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Abstract **We present a linear type ion trap consisting of metal lines that are lithographically patterned onto two ceramic substrates. Trapping fields are realized by applying specific voltage potentials to each line. This arrangement allows miniaturization approaches that are immune to surface roughness issues and increased complexities of precision machining of electrode surfaces. We also present how these traps allow a thorough study of higher order multipoles and their effect on mass analyzer performance.**

Introduction

Ion traps have been used in many mass spectrometry applications. These applications include use in the fields of biology, analytical chemistry, forensics, and space exploration. Additionally, there has been progress towards using ion traps to implement quantum computing[1]. Ion traps have been useful in a broad range of applications due to their inherent sensitivity and specificity. The relative simplicity in miniaturization and higher operating pressures also increase the attractiveness of ion trap mass analyzers[2].

There are many approaches being taken to miniaturize ion trap systems. The quadrupole ion trap lends itself the easiest to miniaturization due to ion stability at relatively high operating pressures[3]. One of the great difficulties in miniaturizing conventional quadrupole ion traps is in the available precision in machining and aligning hyperbolic metal electrodes or circular rods[4]. Some of the approaches to miniaturization have involved the simplification of electrode geometries for easier machining. These approaches include cylindrical and rectilinear ion traps[5]. Other approaches have involved microfabrication techniques with MEMS devices[6], micro-ion trap arrays[7,8], lab-on-a-chip designs[9], and patterned planar electrode ion traps in both the Paul trap[10] and toroidal trap[2] configurations. Our group has led the efforts in development of these planar electrode ion traps.

Planar electrode ion traps present several benefits. First, they only require the fabrication and alignment of two surfaces. This alignment requirement means that careful design need only be done in two dimensions instead of three. Also, the electrodes are patterned onto the surfaces with lithographic processes. This results in a process that is less prone to surface roughness issues seen when miniaturizing machined electrodes. Another benefit is that planar electrode designs allow for trapping field adjustment and optimization after the trap has been fabricated and assembled. The planar electrode design allows for several different types of traps. As mentioned above, we have produced Paul traps and toroidal traps using this approach. In this work, we present a planar electrode linear ion trap.

Our group has been successful in producing quadrupole ion traps of various designs. These designs include a paul trap and toroidal trap

designs. Recent efforts have been directed at development of the coaxial trap, a hybrid design of a paul trap and toroidal trap, and a linear ion trap. Linear ion traps (LIT) have demonstrated superior performance to other quadrupole ion traps in several ways. They have been shown to have improved signal-to-noise ratio, increased trapping efficiency, increased trapping capacity, and increased resistance to deleterious space-charge effects[11,12]. These advantages make them effective as stand-alone mass spectrometers, or as part of a tandem setup with time-of-flight systems. Our planar electrode linear ion trap combines the advantages of linear ion traps with those of planar electrode ion traps.

The planar electrode LIT is implemented with two planar ceramic surfaces. These ceramic surfaces have lithographically patterned metal pairs of lines. The two patterned surfaces are arranged so that they face each other. Specific potentials are applied to each line pair to create a quadrupolar field. In our planar electrode traps, the fields can be tuned after the system's original assembly. A great benefit of this is seen in field optimization and the analysis of higher order multipole effects. It has been demonstrated in previous works that deliberately adding a specific percentage of higher order multipoles into the field can actually improve mass spectrometer performance[13]. Our design of the planar electrode LIT allows easy tuning of deliberate higher order poles and compensation of undesired higher order poles.

Experiment Setup

The procedure for fabrication of the trapping plates is shown in Figure 1. Construction began with a 0.635mm thick, 99.6% pure alumina substrate (Hybrid-Tek, Clarksburg, NJ). A series of holes were then laser cut through the substrate. Some of these holes were cut for alignment purposes, some were for providing a path for ion ejection, and others were filled with gold to create vias for electrical contacts. The center ejection slit was cut to a width of 500μm. The gold filled vias were holes with a diameter of 125μm. The vias were placed symmetrically on either side of the slit and on either end of the slit. After laser cutting, the ceramic surfaces were polished to a surface roughness of better than 1 μm. Gold metal electrodes were patterned onto the substrate using photolithography in the Brigham Young University Integrated Microfabrication Laboratory. In the lithography process, photoresist was spun on and patterned with chrome masks. The mask design for the trapping side of the plates contained one line to cover the entire ejection slit, four pairs of symmetric 25 μm wide lines about the slit, and one pair of outer lines that were several millimeters wide. After patterning the metal and removing the photoresist, a 100 nm layer of germanium was deposited on the trapping side of the substrates. The germanium layer coated the gold line electrodes to serves as a space charge dissipation layer for the trap. The resistivity of the germanium layer also produces a well-defined transition potential between adjacent lines, reducing edge effects on ions located close to the lines. The final plate surface, both before and after germanium deposition, is seen in Figure 2.
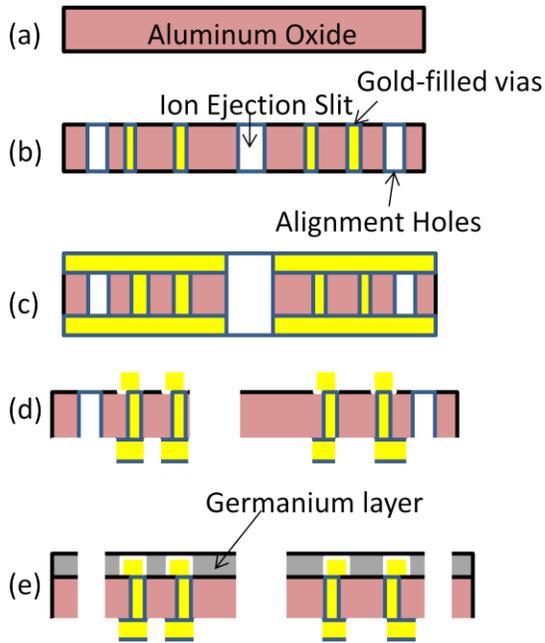
Figure 1 (a) The starting bare alumina substrate, (b) the substrate with gold-filled vias and alignment holes laser drilled, (c) gold deposited onto both sides of the substrate, (d) lithographically patterned gold, and (e) finished plate with germanium layer
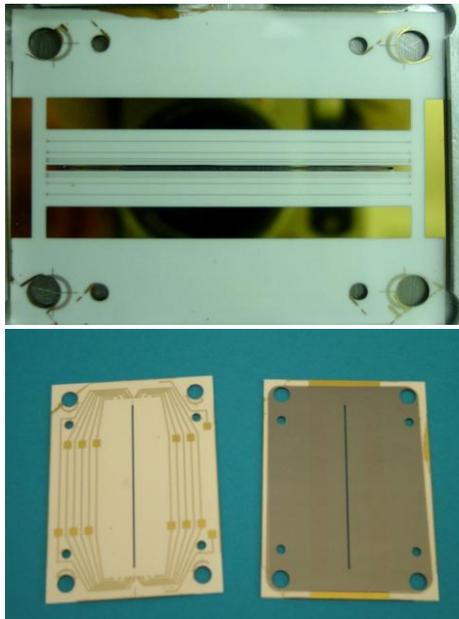
Figure 2 Finished ceramic plate (top) without germanium and (bottom) with germanium and the back side for electrical contact from a PCB.

Sapphire balls were placed in the alignment holes to provide a precise spacing between the two plate surfaces. A capacitive voltage divider circuit was setup onto a printed circuit board (PCB) to place the specific magnitudes of the radio frequency (RF) trapping field onto the desired line. The PCB made contact with the back side of the ceramic plates by way of gold, spring-loaded pogo pins. Figure 3 shows the PCBs and ceramic plates assembled together. The entire PCB and plate assembly was placed inside a copper box for shielding purposes. Custom electronics were built for controlling DC voltages for axial confinement, detector voltage supply, electron gun control, and electron gate control. An Ardara RF supply (Ardara, PA) provided the trapping voltages applied to the PCB. The detector used was a continuous dynode electron multiplier by DeTech (Palmer, MA).
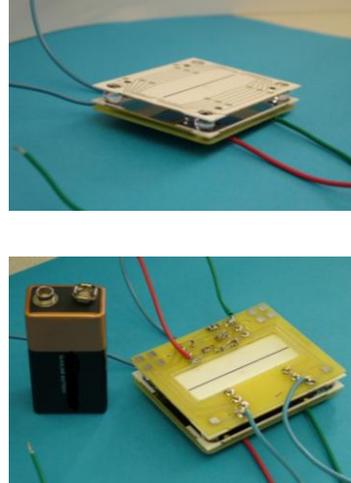

Figure 3 PCB and plate setup

The experiment consisted of four phases: ionization, ion cooling, ion ejection, and then an ion dump to clean out the trap between successive ion scans. During ionization, the electron gate was placed at +100 V to allow electrons into the trap to cause ionization. After ionization, the gate was set to -200 V to

block all electron flow. The RF trapping field was also turned on during ionization. The method of ion ejection for this experiment was sweeping an additional AC signal on the field from a frequency of 1150 kHZ to 100 kHz. This setup is shown in Figure 4. The compounds tested were Isobutylbenzene and Heptane. The resulting mass spectra are shown in Figure 5.
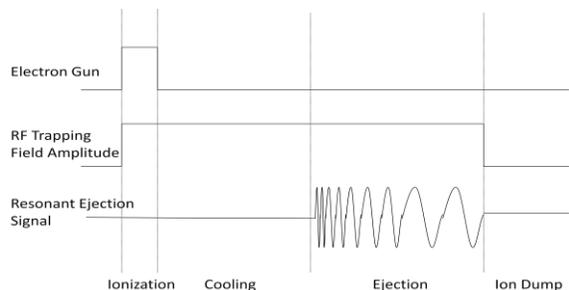
Figure 4 Experimental Setup for Electronics Control
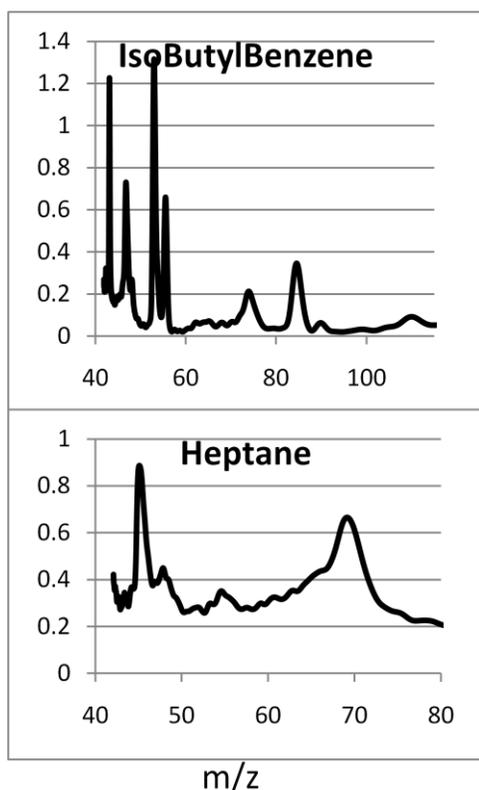
Figure 5 Mass Spectra obtained with planar electrode linear ion trap

Discussion

As discussed earlier, trapping fields can never be purely quadrupolar, and in fact, superior performance has been achieved when a controlled amount of octopolar components are intentionally added to the trapping field. By adjusting the capacitive voltage divider circuit, subtle and precise adjustments can be made to the planar electrode LIT trapping fields. This versatility has allowed an experimental study on the effects of the higher order multipoles on trap performance.

The total trapping field potential in a 2-D ion trap is described by

$$\Phi(x,y) = \phi_0(t)\sum_{N=0}^{\infty} A_N \Phi_N \qquad (1)$$

where, A_N is the multipole expansion coefficient, and Φ_N is the potential associated with a specific pole. Or in other words, the electric field is a summation of all the multipole components. In the planar electrode LIT, the trapping field potential is a linear superposition of the contributions from each pair of line electrodes. Fields were calculated using SIMION and Matlab. In SIMION, the electrode arrangement was setup so that only one pair of electrode lines was turned on to a maximum normalized voltage, and all other electrodes were grounded at 0 V. A neutral particle was then flown from one plate surface to the other, across the middle of the trapping region, to measure the field potential created by each line pair. Figure 6 shows the fields from each line pair under these conditions.

The quadrupole trapping field is created by picking the right coefficient by which to multiply each of the curves in Figure 6, and then adding up the results. These coefficients lead to the specific voltages to apply to each line pair on the plate surface. This summation not only

helps calculate the total trapping potential, but also the components of each higher order multipole. This is calculated by

Quadrupole of whole trap: $A_2 = A_{21}\Phi_{01} + A_{22}\Phi_{02} + A_{23}\Phi_{03} + ... + A_{2m}\Phi$

Octopole of whole trap: $A_4 = A_{41}\Phi_{01} + A_{42}\Phi_{02} + A_{43}\Phi_{03} + ... + A_{4m}\Phi$

Dodecapole of whole trap: $A_6 = A_{61}\Phi_{01} + A_{62}\Phi_{02} + A_{63}\Phi_{03} + ... + A_{6m}\Phi$

$\underbrace{\qquad}_{\substack{\text{Line 1} \\ \text{contribution}}} \underbrace{\qquad}_{\text{Line 2 contrib.}} \underbrace{\qquad}_{\text{Line 3 contrib.}}$

where for A_{nm}, n is the multipole number (quadrupole, octopole, etc.), m is the line pair numbered from the center slit, and where Φ_m is the RF amplitudes applied to line m. The optimal field used in these experiments is shown in Figure 7.
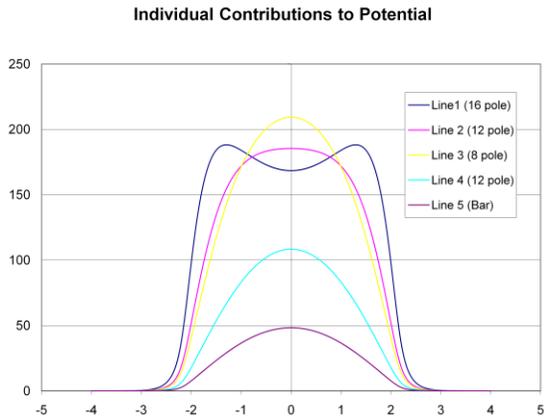
Figure 6 Individual contributions from each line pair to overall field potential spanning the distance between plates in mm
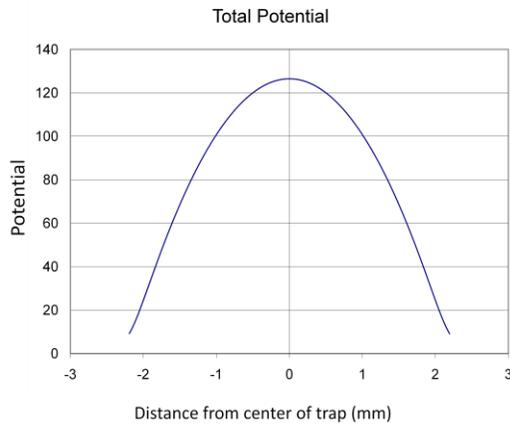
Figure 7 Total field potential used in these experiments

Conclusion

We have demonstrated the implementation of a linear type ion trap using patterned planar electrodes. We have achieved favorable mass resolution on the mass range of 35-120 mass units. We have explored the use of different magnitudes of various higher order multipole effects on the fields, and are continuing work on trap optimization.

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