Miniature QMF and LIT using LBMT for HEMS Applications

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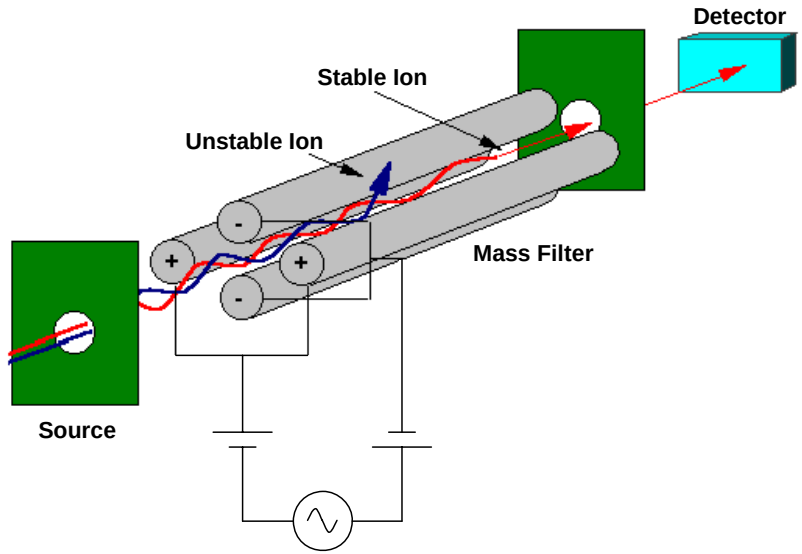
Talk Outline

- Background
  - Silicon MEMS QMS
  - QMS simulation
- Rapid manufacture using layer based manufacturing techniques (LBMT)
  - Digital Light Processing (DLP)
- QMS using DLP
  - Design, fabrication and experimental results
  - HEMS application: 1-6.2 Da
- LIT using DLP
  - Design, fabrication and experimental results
- Conclusions

QMS - principles of operation

$$\frac{d^2u}{d\xi^2} + (a_u - 2q_u \cos(2\xi))u = 0$$



- For given applied voltages only ions of a particular charge to mass ratio have stable trajectories: other ions rejected
- Maximum voltage:

$$V_{max} = f^2 r_0^2 m_{max} / 7x10^6$$

Resolution related to number of RF cycles (n)

$$m/\Delta m \approx n^2/20 = f^2 L^2 m / 40 e V_z$$

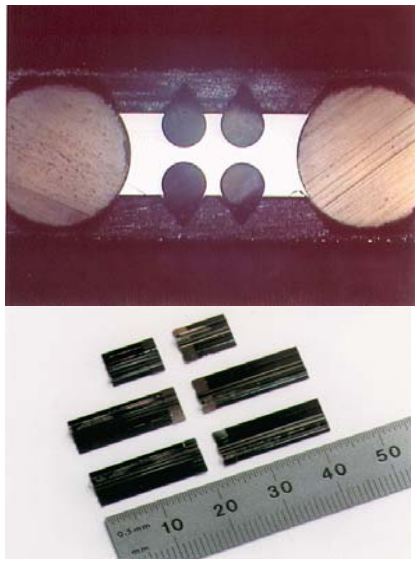
where L = QMF length, V_z= ion energy

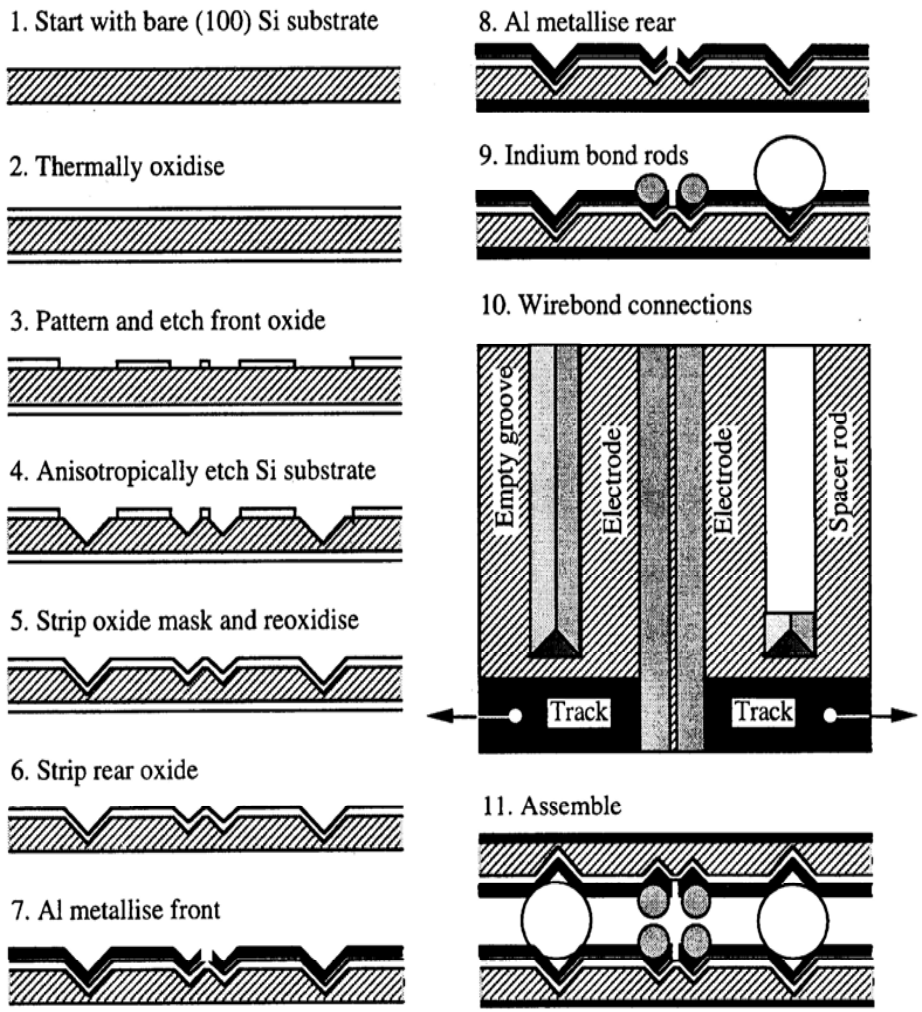
V_{max} falls with r_0^2 : low voltage
L reduction is offset by increasing f : resolution maintained

MEMS QMF (Microquad): circular electrodes

Right: Process schematic

Below: End on cross section of the MEMS QMS (r0=222μm) and disassembled QMFs





S.Taylor, R.F.Tindall and R.R.A Syms, 'Silicon based quadrupole mass spectrometry using micro-electromechanical systems' JVST, B19(2), 557 (2001)

Silicon MEMS QMS

	Conventional QMS	MEMS QMS
Electrode radius (mm)	3.175	0.25
Frequency (MHz)	2.75	6
Length	120	30
V_{max} (V)	1100	32
Δm (at 2eV)	0.05	1

Advantages:

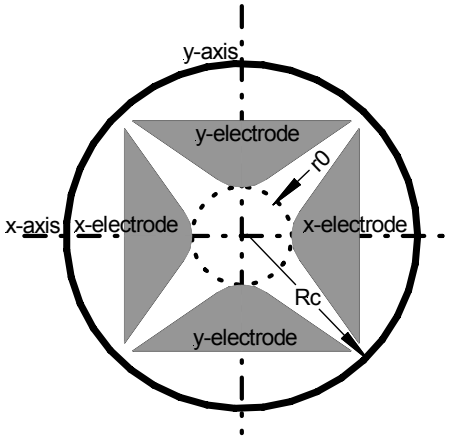
Low voltage, low cost, small size: ability to operate at higher pressures, less vacuum demand (smaller/cheaper pumps)

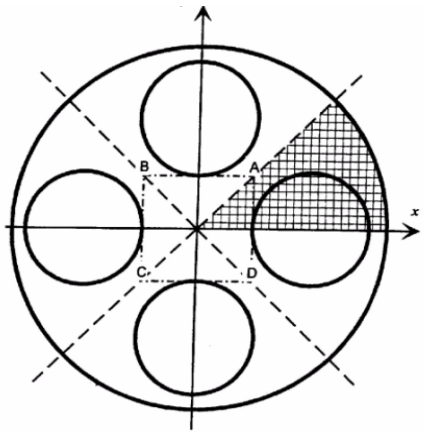
Current instrument status:

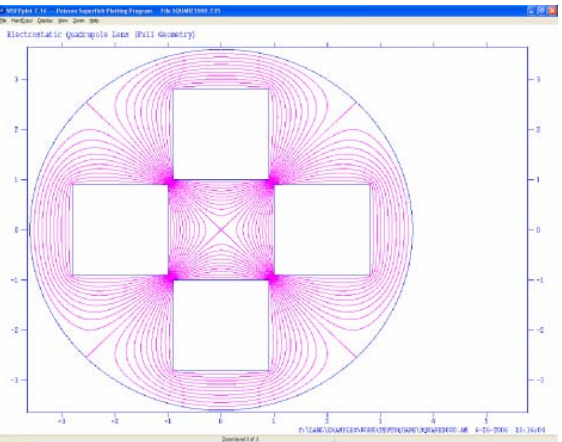
- **r0 = 0.22 mm**
- **Sensitivity: down to ppm, mass range to 400 amu**
- **Resolution = 200 (Syms et al, Microsaic)**
- **Pressure range: up to 10^{-3} mbar**

Miniature QMF and LIT using LBMT...

QMS simulation:
Aim: 3D model of QMF with EI source, including pressure dependence and space charge effects







- 10^5 ion trajectories calculated for each point on mass scale, using 4th order Runge Kutta numerical integration of Mathieu equation.
- Total input ions typically: 10^8
- Ions randomised in space and time relative to the RF field.

- Motion for non-hyperbolic and displaced electrode case[1] defined by:
  - $qE_x = m(\partial^2x/\partial t^2)$ and $qE_y = m(\partial^2y/\partial t^2)$

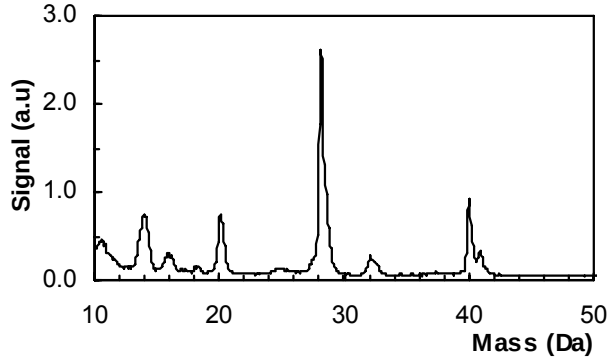
- BEB theory allows electron current and pressure dependence in ion source
- BEM method faster than POISSON Superfish (FD) and allows 3D effects to be incorporated.

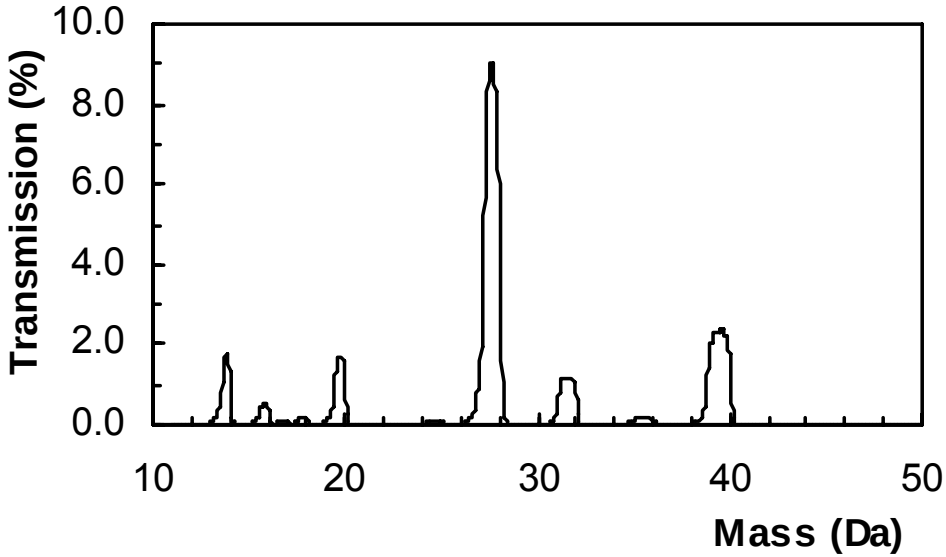
[1] *S. Taylor and J.R.Gibson JMS **43,** 5, p609 (2008)*

MEMS QMF circular electrodes: theoretical simulation

Simulation of MicroQuad spectra and performance by injecting >10^7 ions into the mass filter and calculating the trajectories

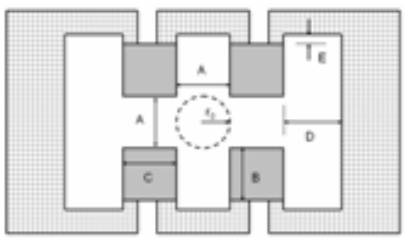
(upper figure shows experimental results)

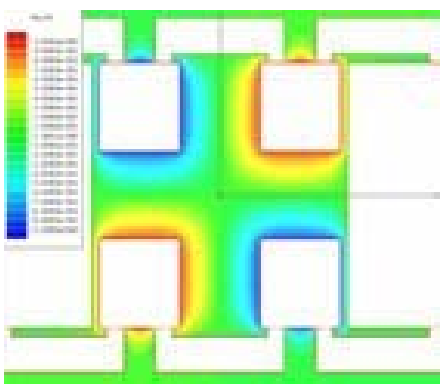




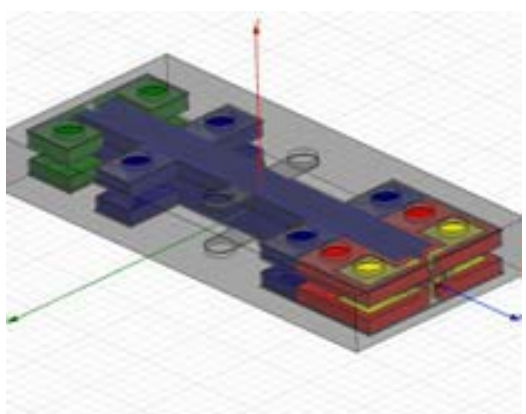
S.Taylor, B, Srigengan and J. R. Gibson, Sensor Review, 23 (2) (2003)

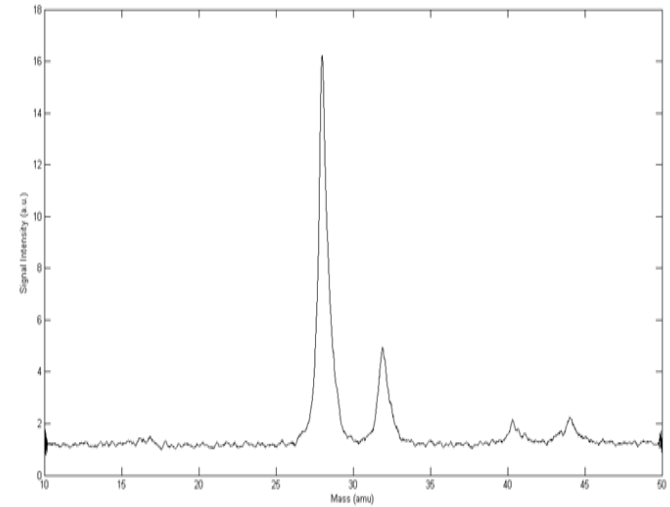
MEMS QMF: rectilinear electrodes (Zone 3)



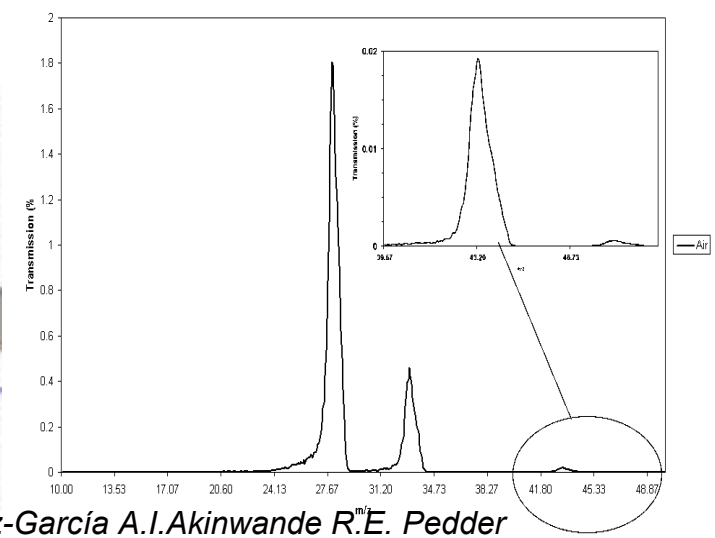


Upper right:
Experimental air spectra from square electrode MEMS QMF (MIT),
Below right: simulation using QMS-2H (UoL)





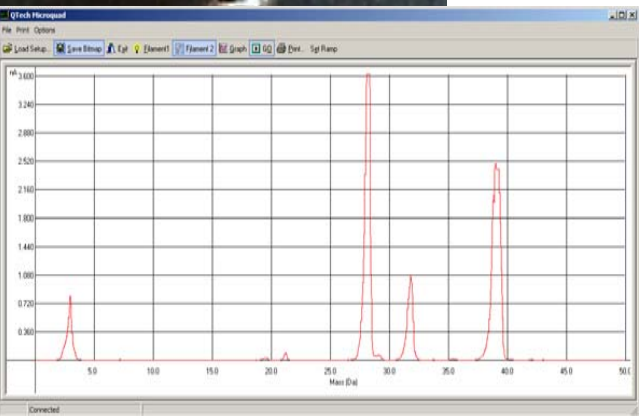
Zone 3 operation for Ei = 18eV and f = 2MHz.

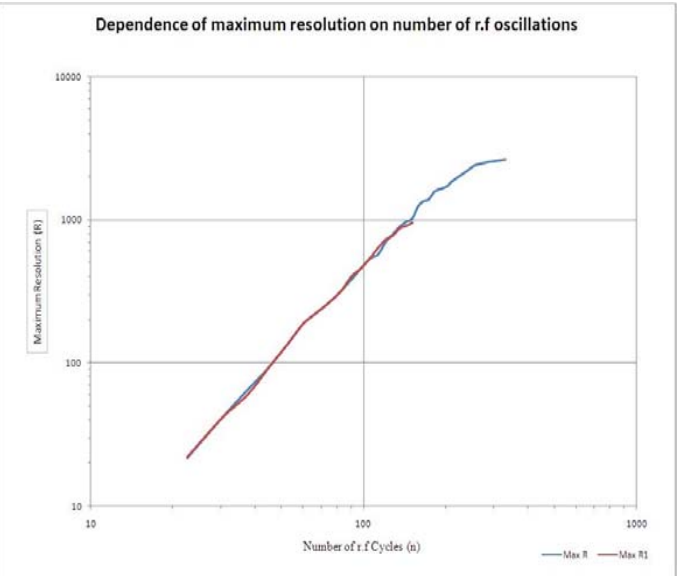


Left and centre: results from K. Cheung et al, HEMS Workshop, 2007

T.J. Hogan S.Taylor K.Cheung, L.Velásquez-García A.I.Akinwande R.E. Pedder submitted to IEEE Trans on Instrumentation and Measurement, 2009

Hyperbolic vs Circular





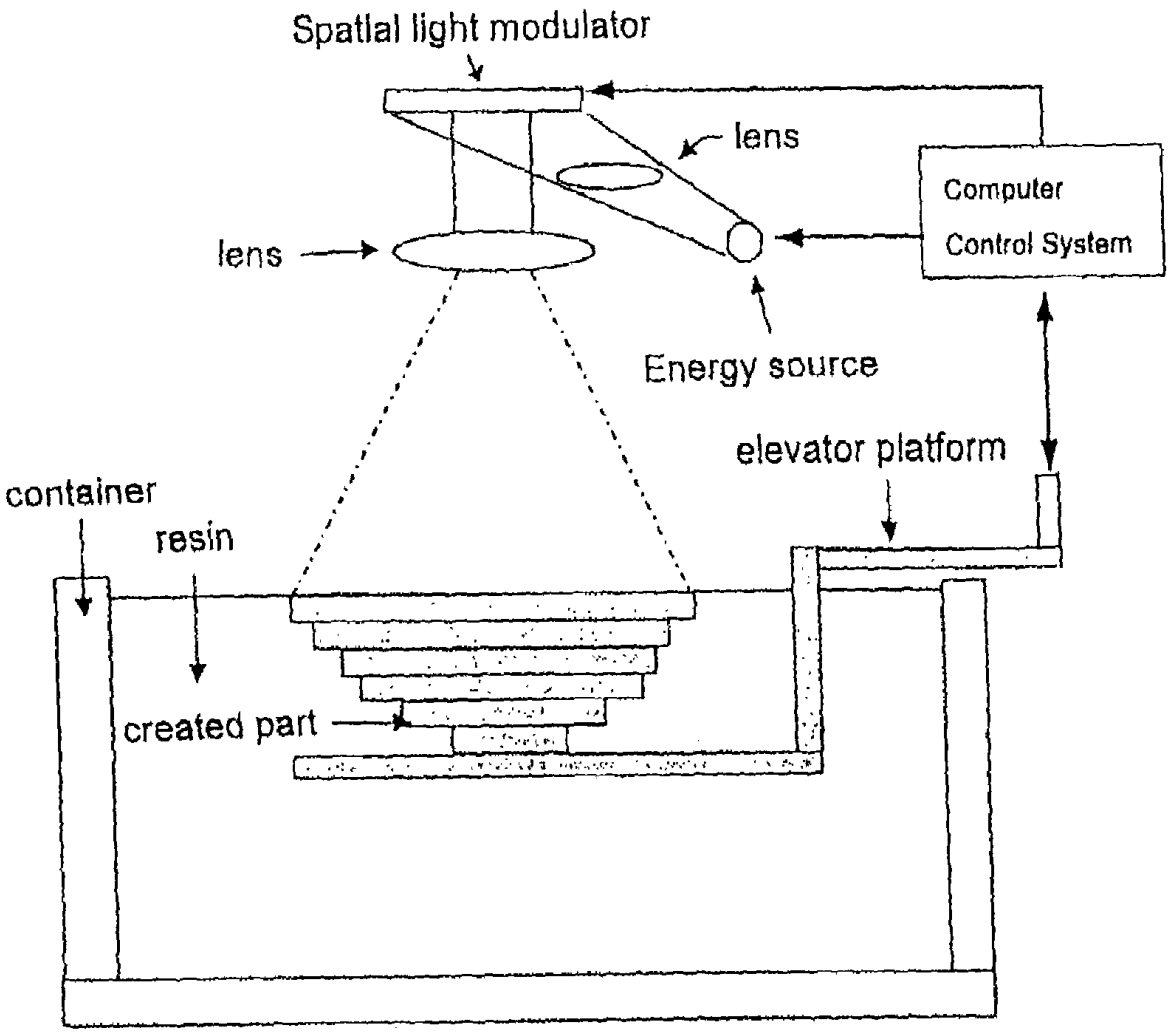
- Ideal quadrupole field from hyperbolic electrodes
- Resolution x3
- Transmission x2
- Better peak shape (especially in Zone 3)
- How to make low cost hyperbolic electrodes at the microscale ?

Layer Based Manufacturing Techniques

- http://www.envisiontec.com/uploads/pics/PIII.Maschine2_12.png

- LBMT's are a class of rapid manufacturing technologies, which allow direct manufacture at the microscale without the need for expensive toolingusing
- Digital Light Processing (DLP), which is a low-cost 3D Layer Based Manufacturing Technique (LBMT).
- Instead of removing material via a reductive process, there is a repetitive addition of material in a layer wise manner.
- An advantage of DLP is that smooth, lightweight, electrode structures of any geometry may be quickly realized at low cost. The density of PMMA is ≈ 1.2 g/cm^3 whereas the density of stainless steel is ≈ 7.8 g/cm^3.

Digital (or direct) light processing



DLP is based on the TI digital micromirror device (DMD), a MEMS microchip with microscopic mirrors aligned on a matrix.

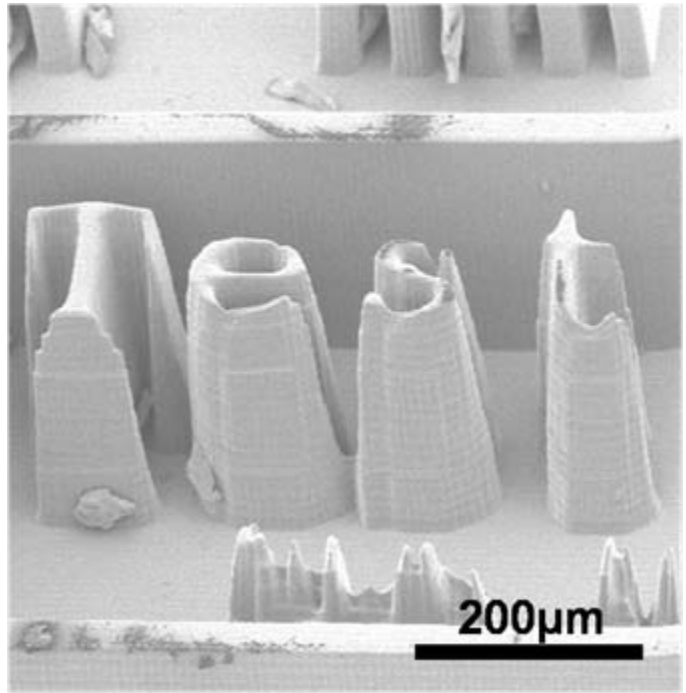
DMD enables precise control of lasers to achieve high resolution video projection or to process materials like PMMA.

DLP has dynamic masking capability to selectively expose photosensitive,

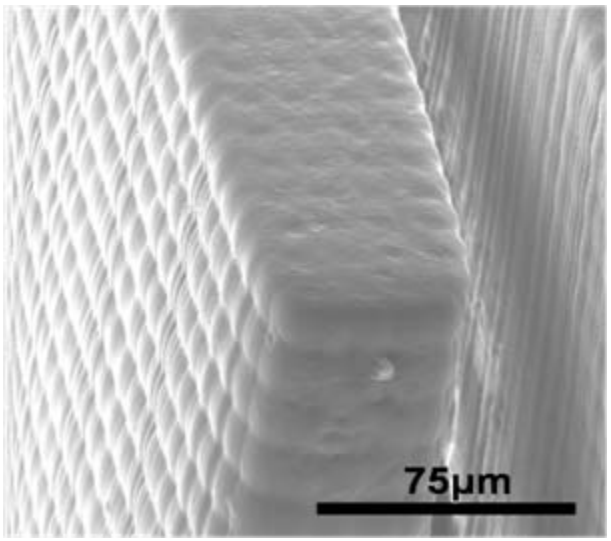
resinous materials causing them to polymerise layer by layer to realise the desired geometry.

DLP micro structures

a)



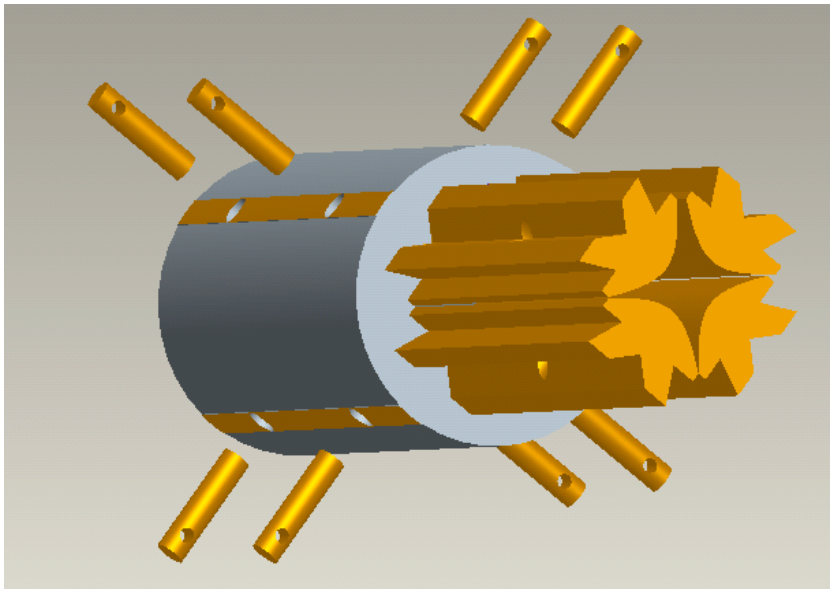
b)



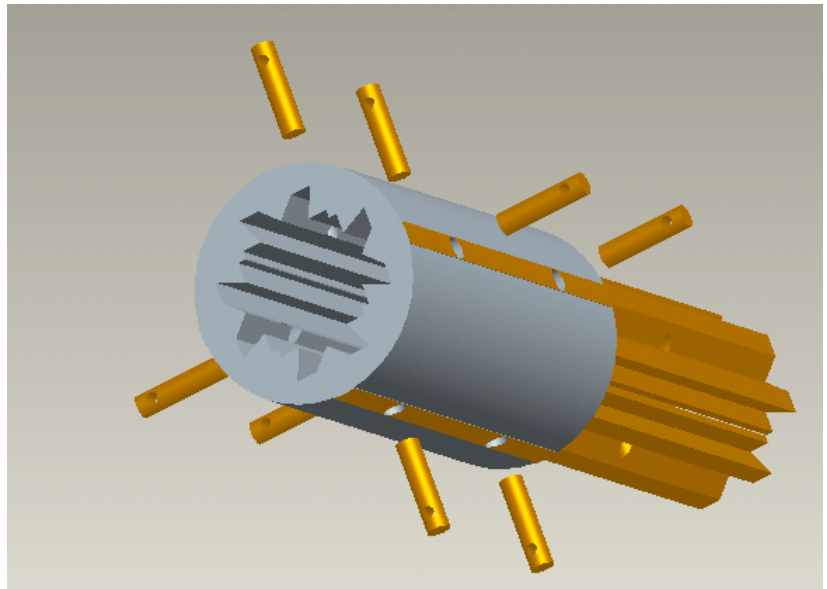
c)

PMMA MEMS structure fabricated using the DLP Envisiontec Perfactory System (**a**, top-left). Enlarged parts of the DLP structure taken by scanning electron microscope (SEM) (**b**, top-right and **c**, bottom-left) showing volumetric pixels (voxels), which represent its building blocks.

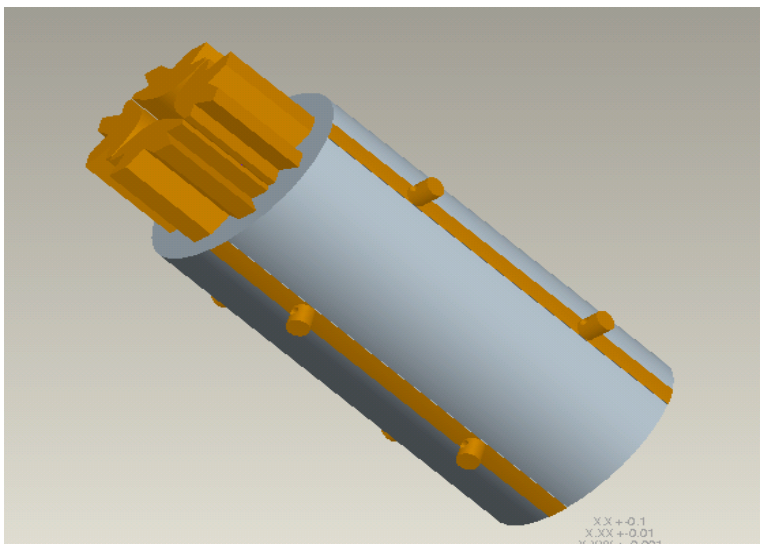
Design process for the DLP QMF



a)



b)

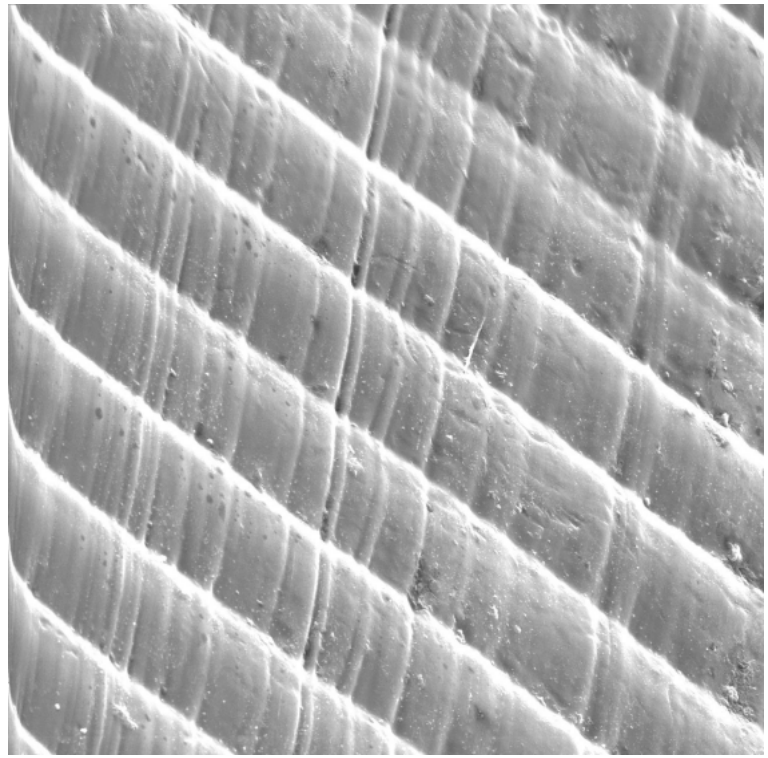


c)

PRO/ENGINEER CAD design drawing for the hyperbolic DLP QMF with r_0 = 2mm showing: QMF electrode design (**a**, top-left), design for the electrode grooves and housing (**b**, top-right) and complete assembly of the QMF with conducting and securing pins (**c**, bottom-left). Shape of the grooves on the housing was carefully chosen to make tight fitting for the rods in order to establish a good alignment and separation. This is especially important for QMFs where small displacement of the electrodes can severely reduce the performance of the instrument.

Fabrication – DLP QMF electrodes

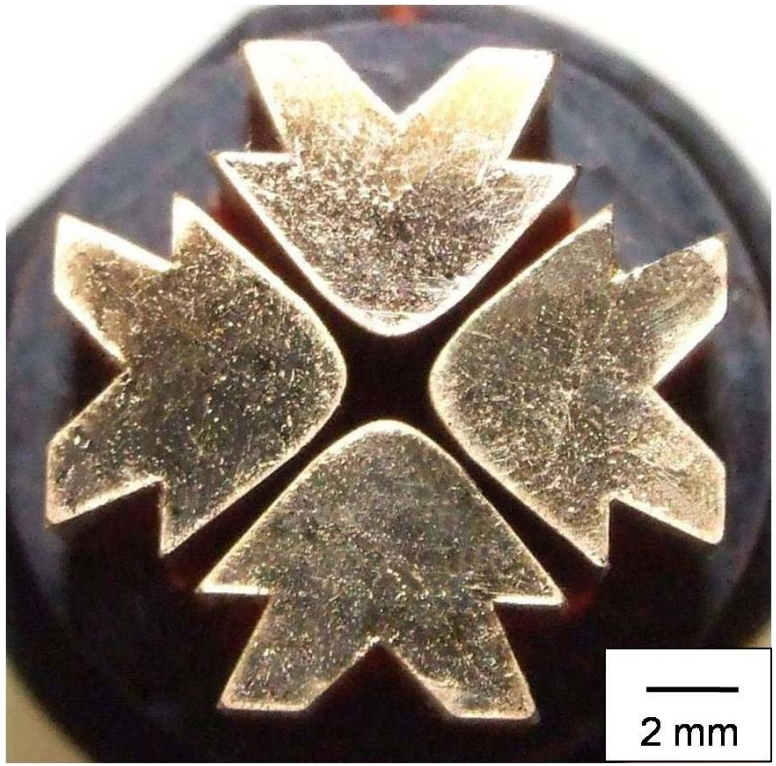
Coated and uncoated QMF rod after the fabrication. The thickness of the gold coating is approximately 1μm. Resistance of the conducting electrode from one end to another is approximately 40Ω. By improving the gold coating, the resistance can be further reduced, which will give more accurate driving voltages.



Enlarged part of the PMMA rod, taken by scanning electron microscope (SEM). The surface roughness of the DLP rods is 1.5 μm. Evaporative gold coating technique was used.

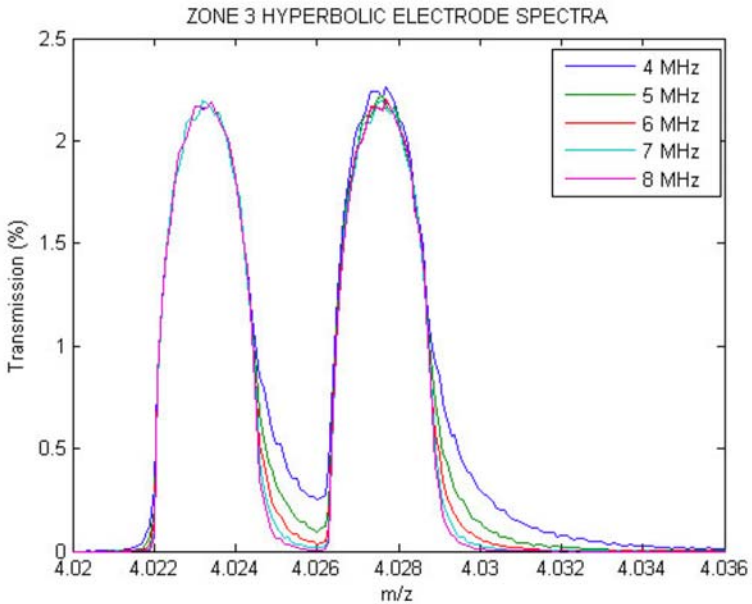
Fabrication – DLP QMF assembly

Cross section of the DLP QMF prototype with r_0 = 2mm showing the assembly and electrode alignment. Rod displacement is 5% of r_0. The length of the rods is 50mm and the length of the housing is 40mm.



Cross section of the DLP QMF prototype with r_0 = 0.9mm showing the assembly and electrode alignment. Rod displacement is 5% of r_0. The length of the rods is 50mm and the length of the housing is 40mm.

HEMS application: H2 and Helium isotope identification : 1 - 6.2 Da

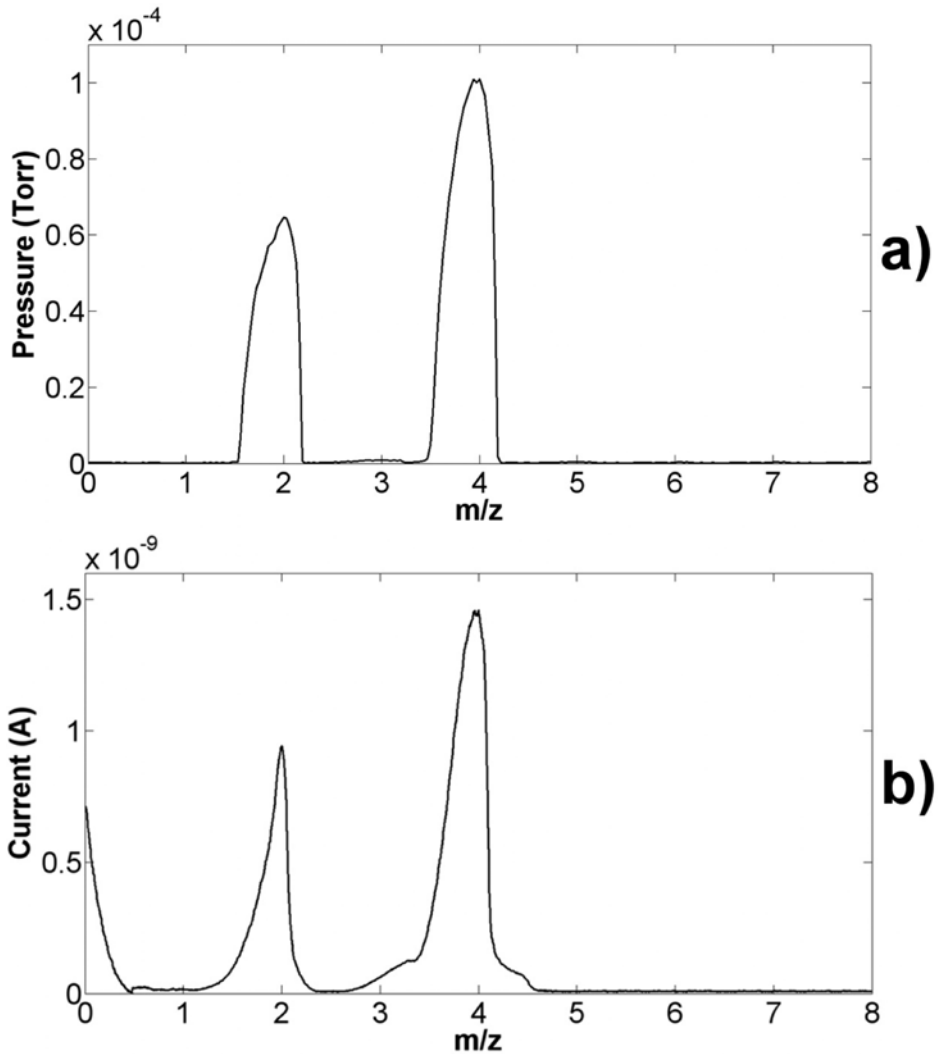


Variation of mass spectra with frequency for a hyperbolic electrode QMF (L = 300 mm, r0 = 2.76 mm, Ei = 15 eV, , ion source radius = 0.276 mm) for HT^+ and D_2^+ ions with equal abundance.

Simulations show that the use of hyperbolic electrodes in conjunction with operation in stability zone 3 provides resolutions > 1000 which exceeds the minimum required performance criteria for process control applications

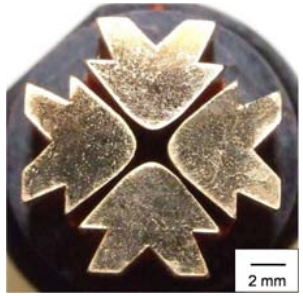
Funded by AWE (UK)

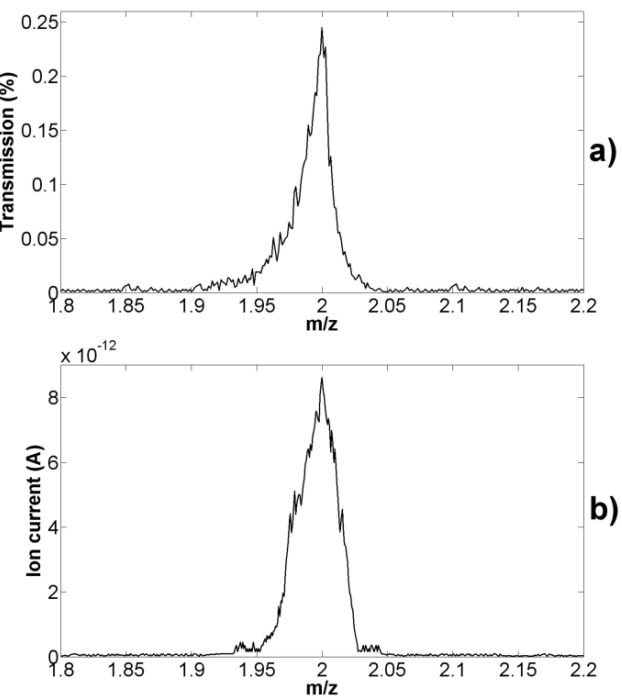
DLP RGA with hyperbolic electrodes: 1 - 6.2 Da



Experimental mass spectra for $H_2/D_2/He$ gas mixture: showing spectrum obtained from the commercial MKS QMS with circular electrodes (**a**) and spectrum obtained from the hyperbolic DLP QMF (**b**).

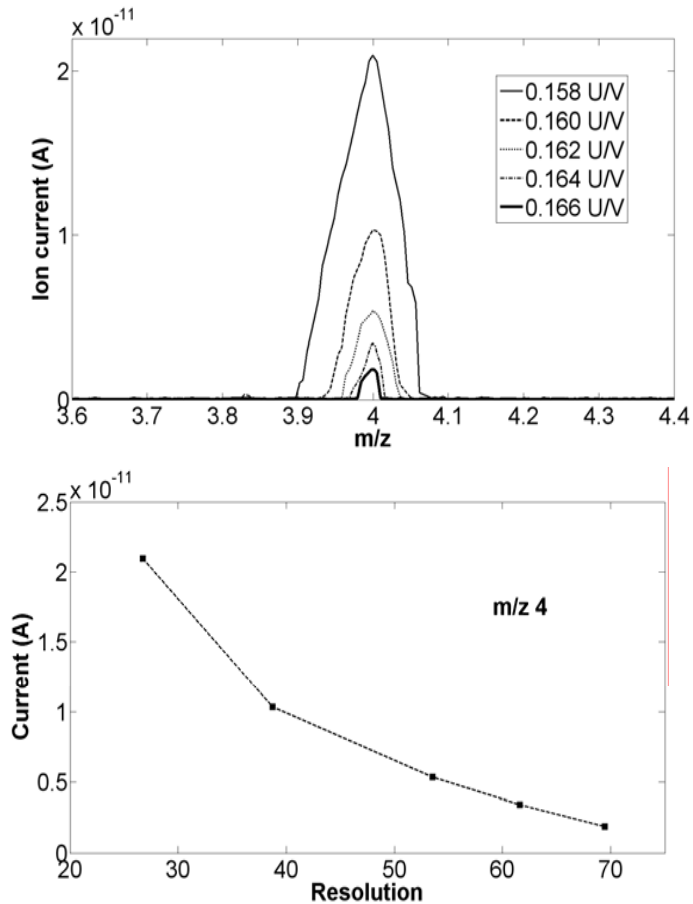
DLP RGA with hyperbolic electrodes





Left: Mass peaks for $^{2}H^{+}$ ions for the hyperbolic DLP QMF: showing (**a**) simulated mass spectral peak, and (**b**) experimental mass spectral peak

Right: Experimental optimisation of the hyperbolic DLP QMF spectra:
Upper: optimisation of $^{4}He^{+}$ ion spectra by altering the ion source cage extraction voltage (ion energy) and U/V ratio
Lower: experimental variation of ion peak current with instrument resolution



B.Brkić, N.France, A. T. Clare, C.J. Sutcliffe, P.R. Chalker, and S. Taylor
'Development of Quadrupole Mass Spectrometers using Rapid Prototyping' J. ASMS (2009)

Linear Ion Trap using DLP

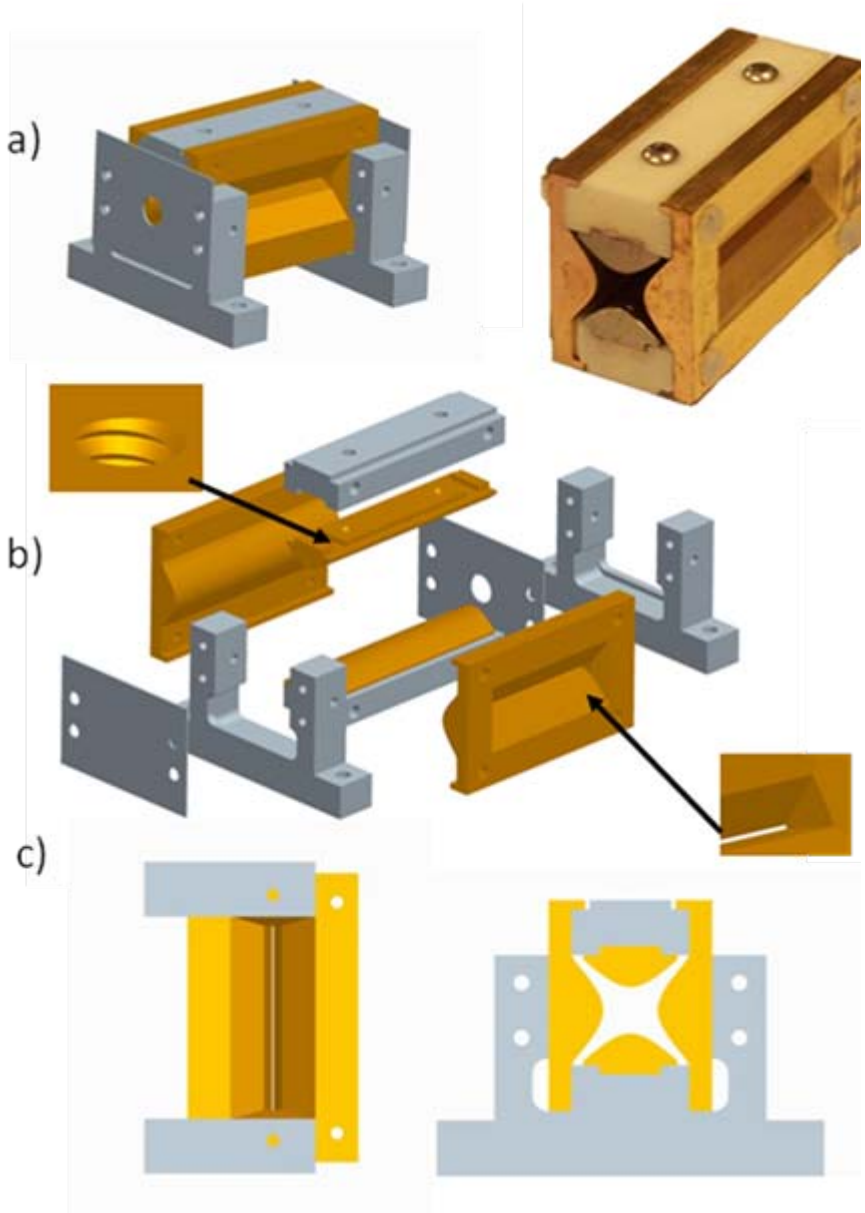
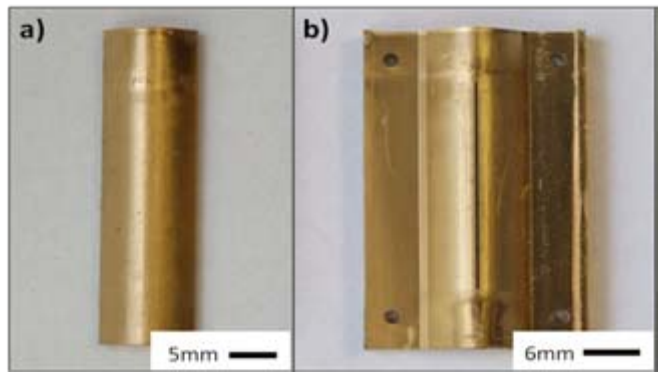
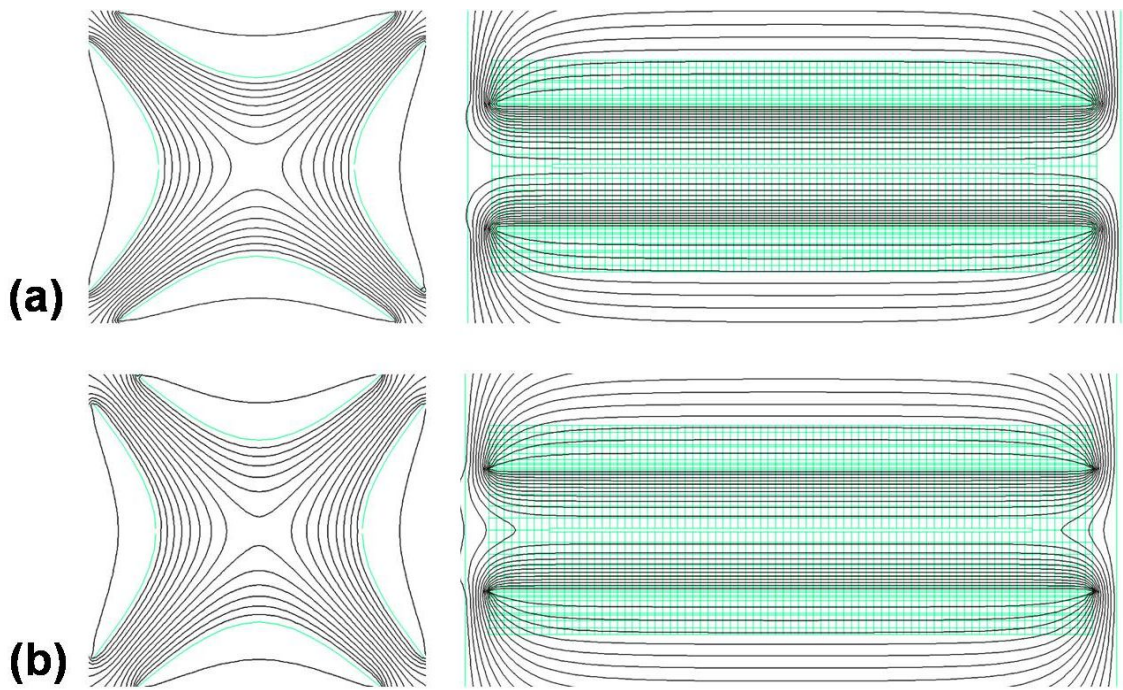


Figure (left) DLP Linear Ion Trap model and picture
a)CAD model and actual prototype of the LIT
b)Exploded assembly of LIT showing threaded hole and ion entrance/extract details
c)LIT electrode profile

Figure (below) Photographs of the DLP LIT components showing gold coated individual electrodes (a) y electrodes (b) x electrodes.

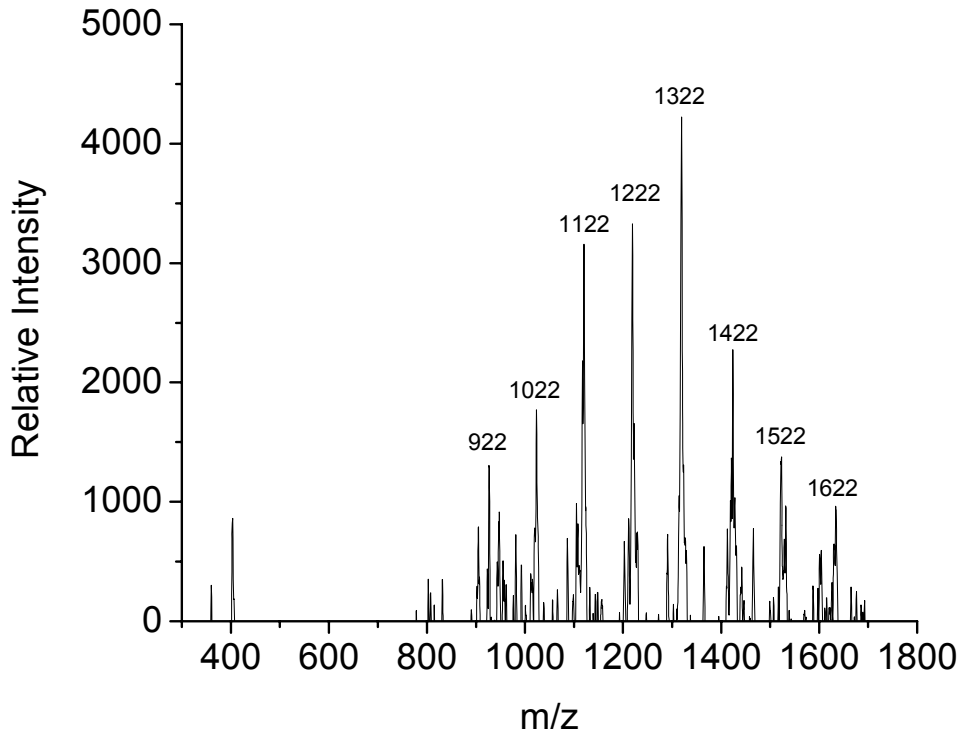


DLP LIT electrical field simulation



Trap stretching simulation: Equipotential contours in xy plane (left) and zy plane (right) for
(a) DLP LIT with r_0 = 2.526 mm and (b) DLP LIT with r_{0x}=3 mm and r_{0y}=2.526 mm

Mass spectra using the DLP LIT



Spectrum of Ultramark obtained from Mini 10 (Purdue) and the DLP trap. RF frequency 990 KHz Resonance AC frequency 360 KHz RF 2670 V_{p-p}
High mass range can be achieved with low RF voltage compared to RIT trap

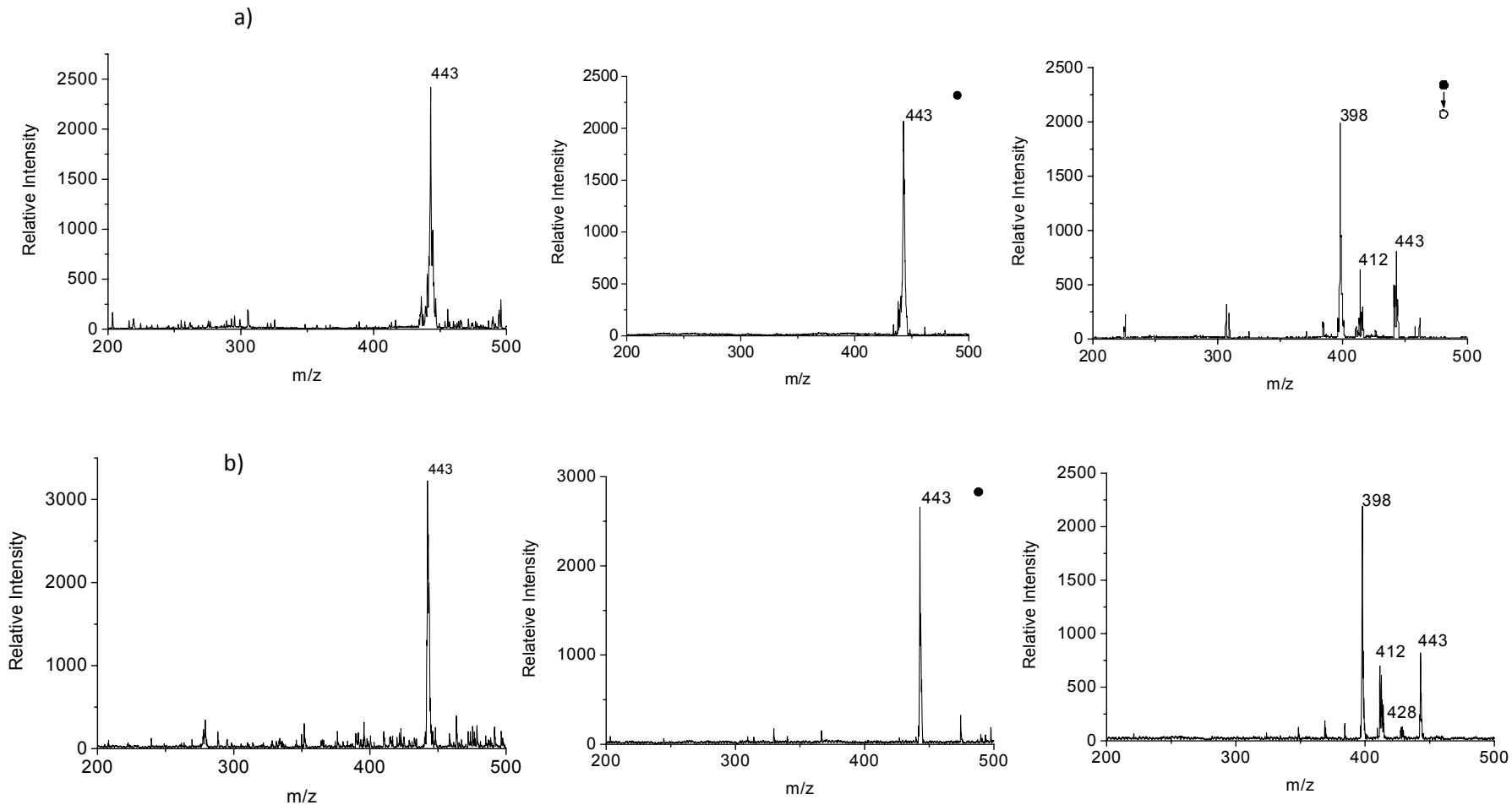
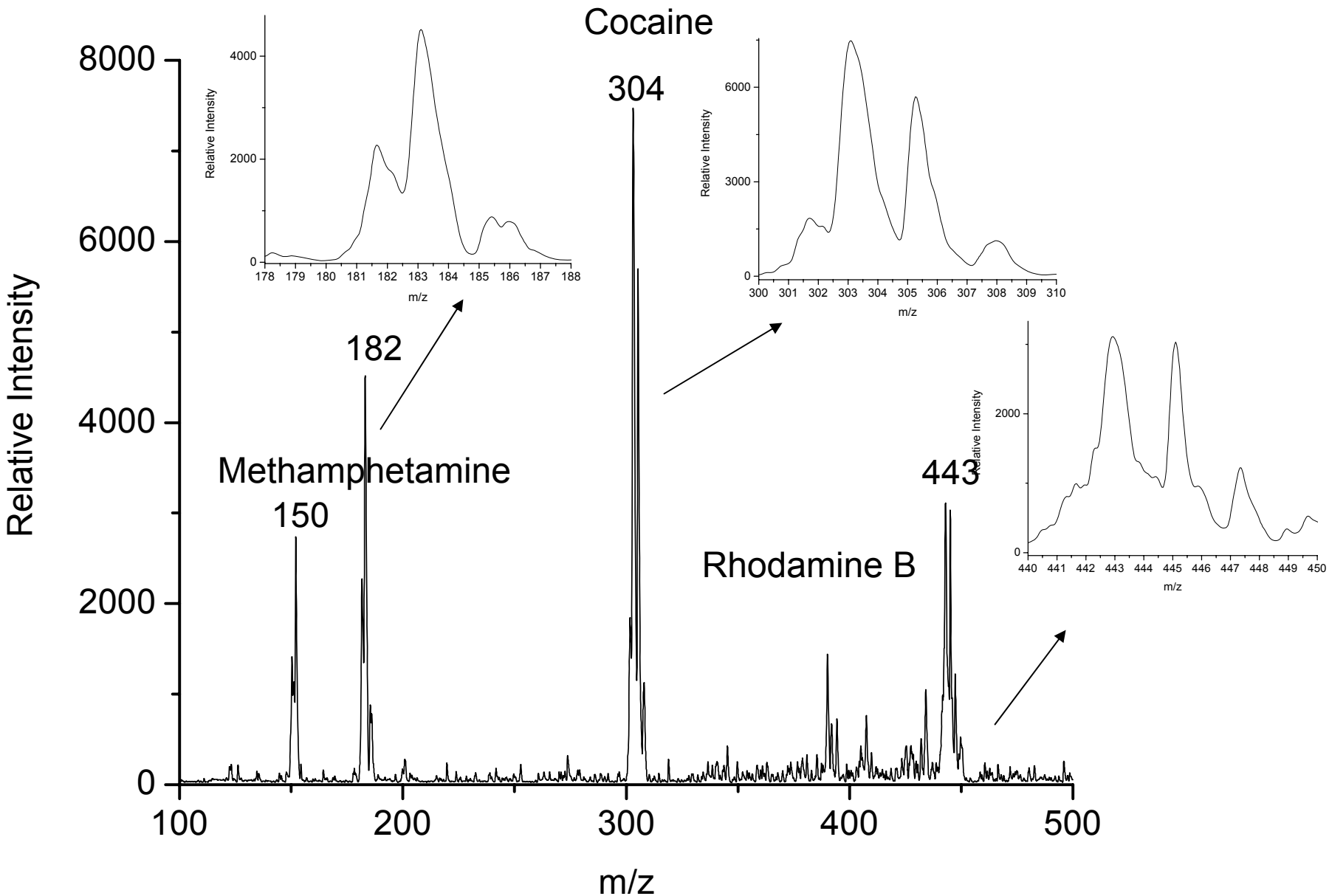


Figure (a) Mass spectra of 10 ppm Rhodamine sample collected using the DLP LIT (Vptp at 443) = 717V
(b) Mass spectra of Rhodamine collected using a conventional RIT operating under identical conditions (Vptp at 443 = 2280 V)


Cocaine
304
182
Methamphetamine
150
Rhodamine B
443
Relative Intensity
m/z
8000
6000
4000
2000
0
100
200
300
400
500
Relative Intensity
m/z
4000
2000
0
178 179 180 181 182 183 184 185 186 187 188
Relative Intensity
m/z
6000
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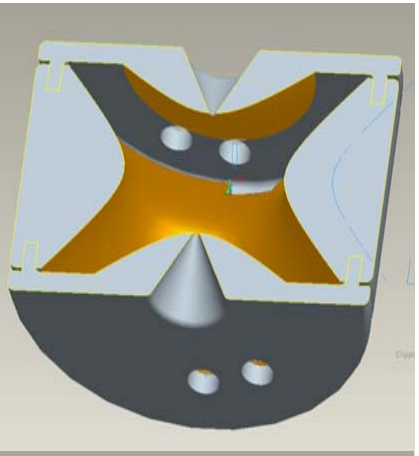
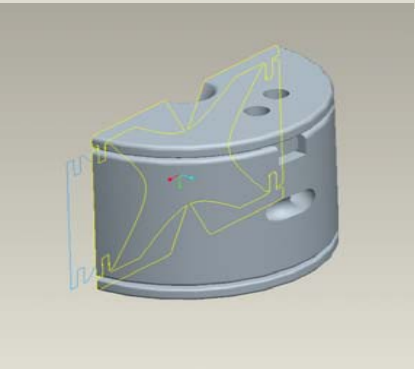
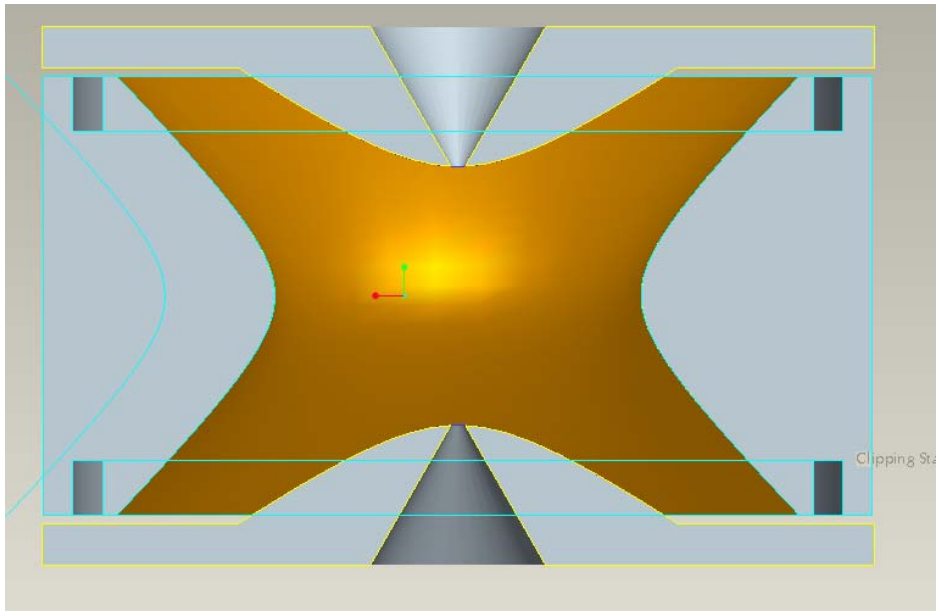
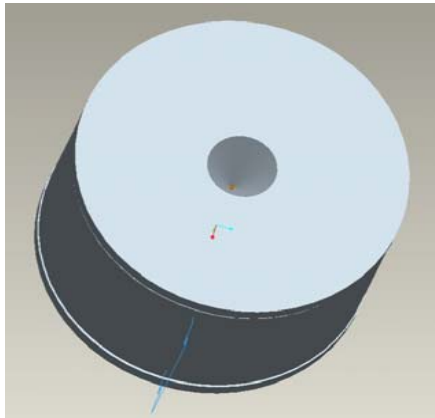
Relative Intensity
m/z
2000
0
440 441 442 443 444 445 446 447 448 449 450

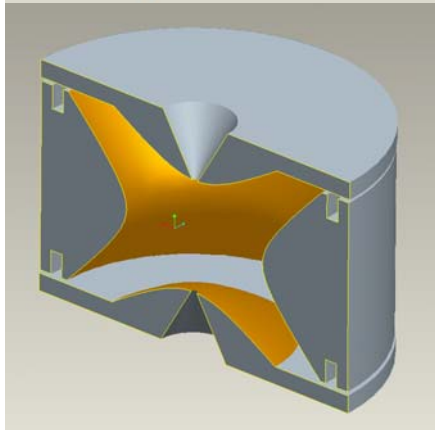
Paul trap using DLP











200um apertures

R0 = 1mm

Miniature QMF and LIT using LBMT...

Conclusions and future work

- Hyperbolic electrodes offer better resolution, sensitivity and are more tolerant to manufacturing tolerances than their circular (or other) counterparts.
- Digital light processing (DLP) is a low cost, light weight, rapid manufacturing technique suitable for realisation of devices with complex geometries.
- Compared to other rapid prototyping techniques the DLP offers significantly smaller feature size that allows higher degree of accuracy.
- A miniature hyperbolic quadrupole mass filter (QMF) and Linear Ion Trap (LIT) have been fabricated using DLP.The DLP QMF was incorporated into portable residual gas analyzer and used to obtain spectra in the 1-6 Da mass range.
- The LIT was incorporated into the Mini 11 portable mass spectrometer system (at Purdue) and experimental mass spectra were obtained for methamphetamine (m/z=150), cocaine (m/z =182,304) and rhodamine B (m/z = 443) with a resolution of 250.
- Spectra obtained for the DLP LIT occur at a much lower RF voltage than a rectilinear ion trap of similar size, due to the hyperbolic electrode geometry.
- DLP also has the potential to produce a fully integrated mass spectrometer with a single mass analyser or with array of analysers.
- Future work will be focused on realisation of mass analysers and other mass spectrometer components at the micro scale for harsh environment applications