Miniature Ion Trap Technology for Portable Mass Spectrometry Applications

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Introduction

The instrument of choice for RGA applications traditionally has in many cases been the quadrupole mass spectrometer (QMS). However, in recent years, miniature quadrupole ion traps (QIT) have become commercially available and are currently attracting considerable interest. QIT instruments offer some advantages over their QMS counterparts. In particular since the operating pressures are higher for certain applications the vacuum demand may be reduced and this in turn can lead to smaller, more portable systems. However, there are some disadvantages, e.g. instrument sensitivity and/or resolution. Essentially the QMS is a device with a strong two-dimensional symmetry whereas the ion trap is a truly three dimensional instrument which means that computer modelling can be more challenging. This work outlines a novel method of manufacture using rapid manufacturing techniques for linear ion traps (LITs) and presents some recent results obtained using a portable ion trap MS system.

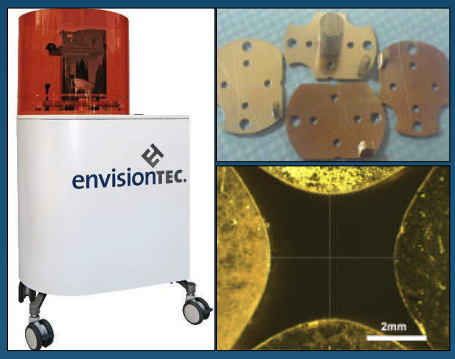

Figure 1: The EnvisionTec Perfactory and typical gold coated components used in previous experiments.

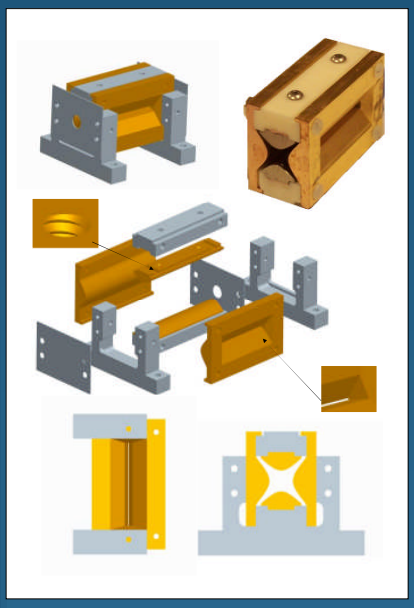

Figure 2: DLP LIT prototype with CAD model and exploded assembly.

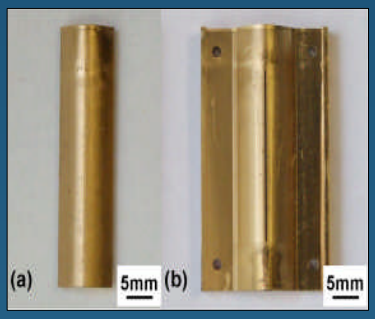

Figure 3: Photographs of the DLP LIT components showing gold coated individual electrodes (**a**) *y* electrode, (**b**) *x* electrode.

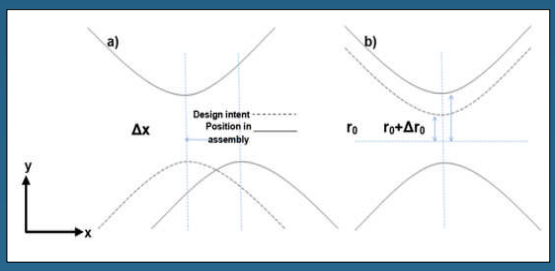

Figure 4: Design drawing for DLP LIT electrode positioning in assembly.

Design and Manufacture

Electrodes featuring a hyperbolic profile are well understood to result in an ideal electrical field profile for ion traps. To achieve this, 3D models where created which included hyperbolic surfaces arrived at through calculation. The designs and assemblies were commonly subject to change so a flexible manufacturing method was required. Digital Light Processing (DLP) presents itself as excellent method for producing short run bespoke components for instrument manufacture. Although the polymer components manufactured in this way are not conductive a gold coating was applied to correct this and sufficient conductivity was displayed for use as a none current carrying electrode. Alignment on assembly is still an issue and is the subject of further investigation.

Modelling

Numerical simulations using boundary-element method were done to predict the performance of the ion trap. From these sources it was possible to evaluate the effect of stretching LIT *x*-electrodes to compensate for loss of linearity for higher order electric fields when ion ejection slits are included.

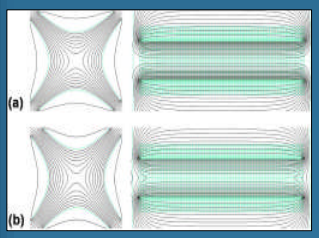

Figure 5: Equipotential contours in *xy* plane (left) and *zy* plane (right) for (**a**) DLP LIT with $r_{0x} = r_{0y} = 2.526$ mm and (**b**) DLP LIT with $r_{0x} = 3$ mm and $r_{0y} = 2.526$ mm.

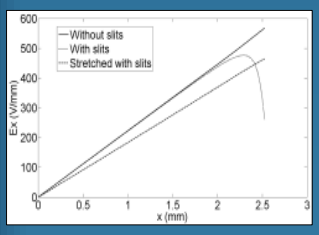

Figure 6: Electric field variations in *x* direction from the center of the DLP LIT to the electrode edge with 716 V_{p-p} rf amplitude. Variations were done with original $r_{0x} = 2.526$ mm.

x-electrodes	Electrode Spacing (mm)		Secular frequencies (kHz)	
	r_{0x}	r_{0y}	$\omega_{x,y}/2\pi$	$\omega_z/2\pi$
Without slits	2.526	2.526	495	0.79
Including slits	2.526	2.526	491	0.78
Stretched including slits	3	2.526	348	0.70

Table 1: Numerical results for radial (*x,y*) and axial (*z*) secular frequencies for rhodamine B (*m/z* = 443) ions within DLP LIT.

Experiments

The DLP ion trap was subjected to testing post manufacture at Purdue University. These experiments were intended to evaluate the mass range detectable and characterise the resolution of the instrument. Typical spectra of analytes of interest were also collected.

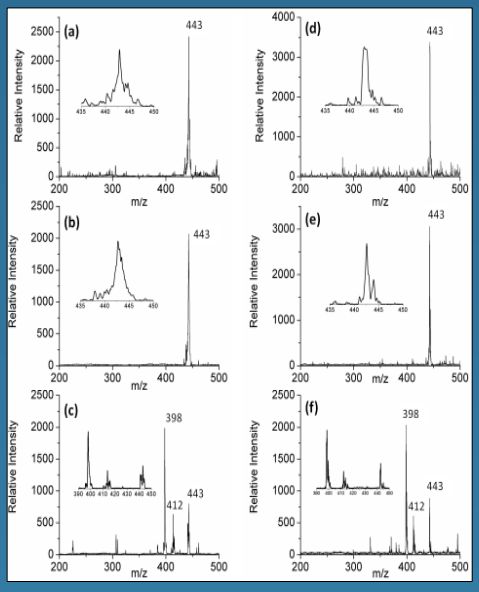

Figure 7: Mass spectra of rhodamine B collected using the DLP LIT (**a**,**b**,**c**) and spectra obtained using a conventional RIT built by Purdue University operating under identical conditions (**d**,**e**,**f**). The rf voltage corresponding to *m/z* 443 was 717 V_{p-p} for DLP LIT and 2280 V_{p-p} for RIT.

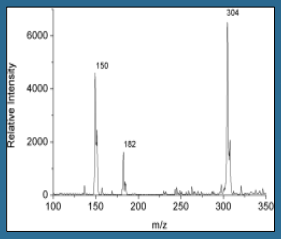

Figure 8: Mass spectrum for 5 ppm mixture of cocaine and methamphetamine. Protonated methamphetamine and cocaine are observed at *m/z* 150 and 304. The peak at *m/z* 182 corresponds to a fragment of cocaine.

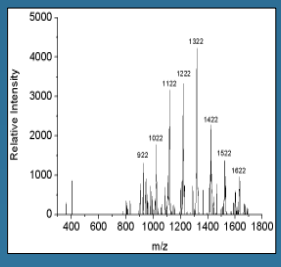

Figure 9: Mass spectrum of Ultramark obtained from Mini 10 and the DLP LIT. The drive parameters include rf amplitude of approximately 2670 V_{p-p} and rf frequency of 990 KHz.

Conclusions

The use of DLP LIT can be suitable in field (harsh environment) applications where a high mass range is required and work is ongoing to address this issue. The DLP technique has been found to be particularly suitable for realization of mass analyzers with hyperbolic or other non circular geometry electrodes and is capable of accurate features sizes in the sub-millimeter range.

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