Metrological Characterization of the Fourier Transform Ion Trap Mass Spectrometer (FTMS)

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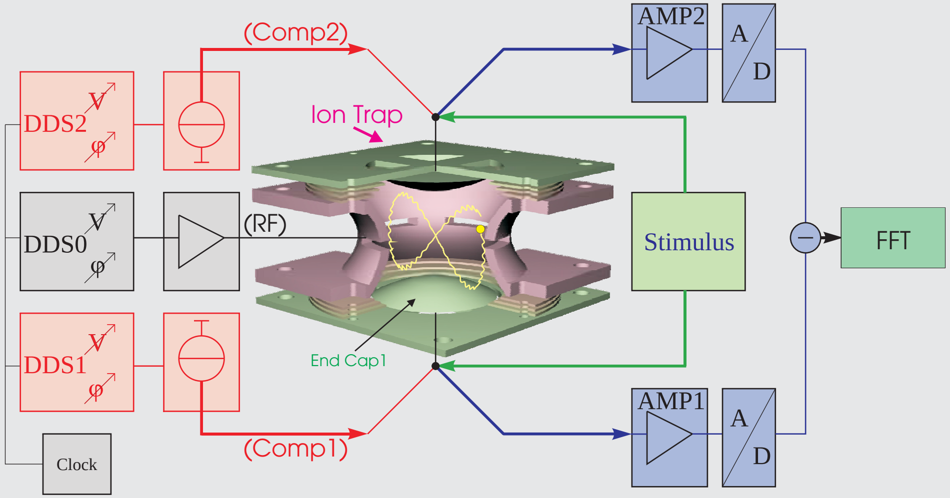
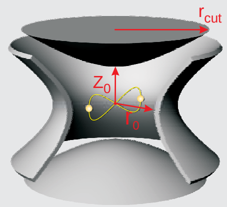
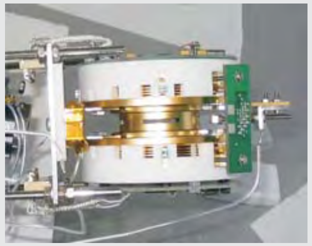
Goals of study: Characterization of important parameters like transient signal amplitude, mass resolution, sensitivity, signal-to-noise ratio, mass line distortion

Block-Diagram of the Ion Trap Electronic



Instrumentation data and test conditions





trap dimension:	60x60x40 mm^3
core radius r_0:	15 mm
half core height z_0:	$\sqrt{2} \times r_0$ = 21.2 mm
cutoff-radius r_{CUT}:	30 mm
equivalent noise level:	5 Ions
residual pressure:	8 x 10-8 mbar
RF-HV Storage field:	
- Frequency	1 MHz
- Amplitude	270 ... 400 Vpp
excitation Level (stimulation energy):	1 Vµs ... 30 Vµs
laser-ionization:	
- lasertype	Argon fluoride excimer laser
- wavelength	193 nm
- energy per pulse	100 µJ
- repetition rate	100 Hz
- pulses per ionization	50 ... 700
sample gas:	Nitrogen monoxide (NO)

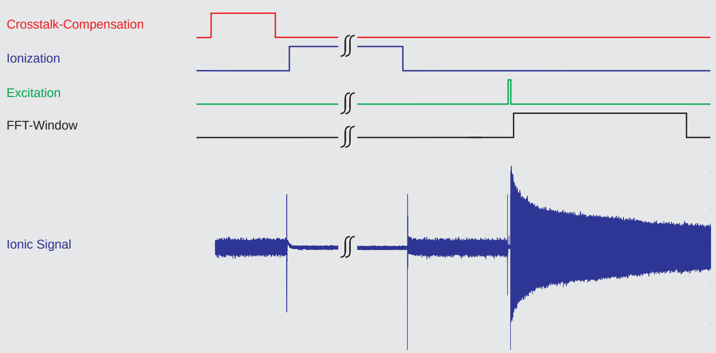
Introduction

Within the last years new solutions with special designs of the electrical ion trap (Paul trap) in combination with sophisticated techniques to compensate the crosstalk signal were published which allow for mass spectroscopy of stored ions by Fourier Transform analysis of the influence charge with high signal-to-noise ratio.

Applied Methods

- Definite test conditions by nitrogen monoxide sample gas (only one massline in spectrum)
- Measuring of transient signals and calculation of frequency spectra by Fourier Transform
- Soft ionization (low kinetic energy) by laser ionization of nitrogen monoxide within the trap

Measurement Timing Diagram



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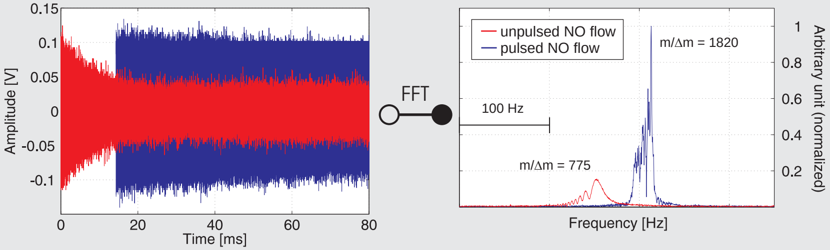
(FTMS)

Decay time: pulsed vs. unpulsed NO flow



Results of parameter

Linear dependency between stimulation energy and transient amplitude up to kick-out limit

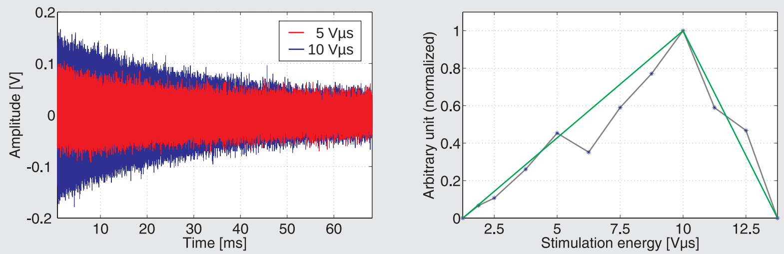
Pulsed testgas injection leads to longer transients, higher mass resolution and improved SNR

Low pressure leads to less generated ions, but leads also to less space charges and therefore to higher mass resolution

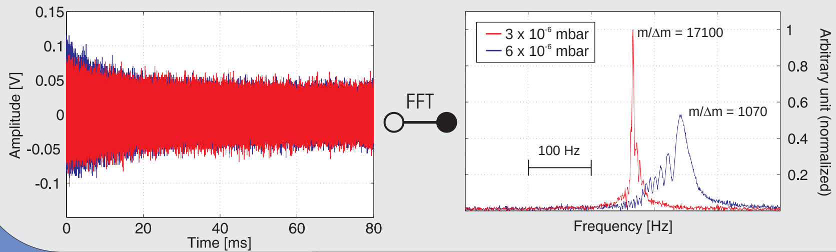
High linearity between RF amplitude and ion frequency:

$f_{ION} = (\sqrt{2} * e) / (4 * \pi^2 * f_{RF} * m * m_z * r^2) * U_{RF} = k * U_{RF}$

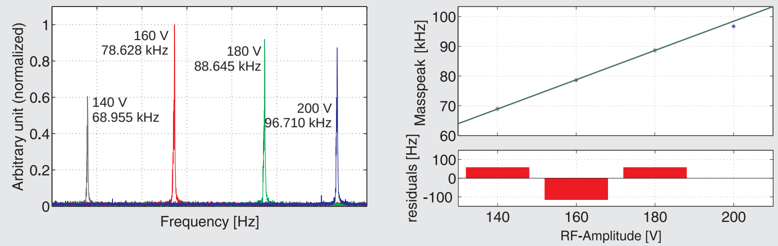
Ion stimulation



Decay time: different unpulsed NO flow



Mass peak shift by storage field amplitude shift



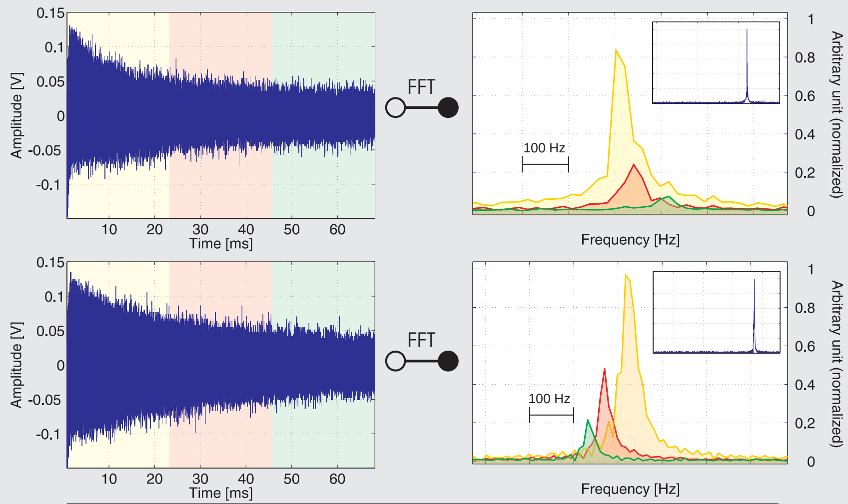
Discussion

- Ion transients will be up to 20 time longer if the sample gas flow is pulsed, because of less collisions betweens ions and neutral molecules. As a result of longer ion transients the FFT-window can be longer and mass resolution will be increased.
- Using low sample gas pressure leads to a reduction of space charge effects. The resulting mass peaks will be more sharp and the mass resolution will be increased. Mass resolution > 10^4 can be archieved.
- The transient signal amplitude varies proportional to the stimulation energy up to a maximum when the ions hit onto the end cap electrodes. If this happens, most of the ions will be neutralized and the ion signal amplitude decreases fast.
- There is high linearity between ion frequency and RF storage field amplitude with a slope of 492 Hz per 1 V amplitude shift. Short time variations of the amplitude decrease the mass resolution, long time variations the mass accuracy.
- During an ion signal transient the ion frequency ist not constant. This may be caused by space charges, which affect the storage field.

Outlook

- For further investigations an external ion source with an ion transfer optic will provide reproducable conditions for more complex meareuments.

Space charge and surface charge effects



There is a frequency shift of the masspeak during ion oscillation, because of space and surface charges