Focusing Properties of Ideal Reflectrons

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Overview

- We considered the theoretical model of the ideal reflectrons for which the time of flight is independent of the initial energy using a mathematical derivation.
- We have produced a model of the ideal reflectrons and investigated their temporal and spatial focusing properties.
- We show experimental data showing the properties using a harmonic ideal reflectron.

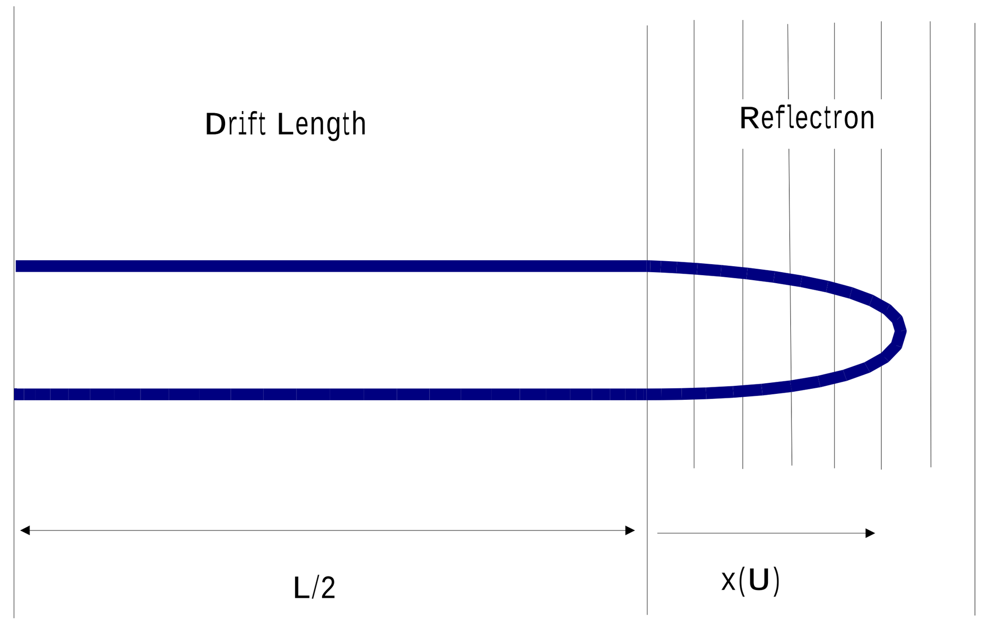
Theoretical Model

The analysis of fragment ions in MALDI post source decay can be observed using a timed ion gate and a reflectron. The reflectron separates the fragment and parent ions by mass. An ideal reflectron allows the collection of the entire mass range of the PSD spectra due to the large energy bandwidth. A theoretical consideration of this produces the following problem :-

An ion of mass *M*, charge *q* and energy $q\varepsilon$ flies through a field free region of length *L* and is repelled inside a reflectron with potential *U(x)*. For an ideal reflectron the time of flight, *T* must be independent of the initial energy (for the energy range $q\varepsilon_1$ to $q\varepsilon_2$).

This gives the equation :-

$$\left(\frac{m}{2q}\right)^{1/2}\left[\frac{L}{\varepsilon^{1/2}}+2\int_0^{\varepsilon}\frac{dU}{(\varepsilon-U)^{1/2}\frac{dU}{dx}}\right]=T=\text{constant}$$



- **$L = 0$ Harmonic Reflectron** where $U(x) = ax^2$ gives T independent of the initial energy and gives the full energy bandwidth from 0 to ε.
- **General Solution** in terms of the inverse function x(U) can be found by multiplying both sides by $d\varepsilon/[(V-\varepsilon)^{1/2}]$ and integrating for ε from ε_1 to ε_2 (Ref 1).

$$\pi\cdot x(U)=k\cdot L\cdot\left(\frac{U-\varepsilon_1}{\varepsilon_1}\right)^{1/2}-L\cdot\arctan\left(\frac{U-\varepsilon_1}{\varepsilon_1}\right)^{1/2}-2\cdot\int_0^{\varepsilon_1}\frac{dx}{dV}\cdot\arctan\left(\frac{U-\varepsilon_1}{\varepsilon_1-V}\right)^{1/2}dV$$

The integral on the right hand side means that the potential distribution is arbitrary while $U < \varepsilon_1$. The simplest solution for this is a potential step (a small gap with a constant field) which would give the general solution with a gap thickness d.

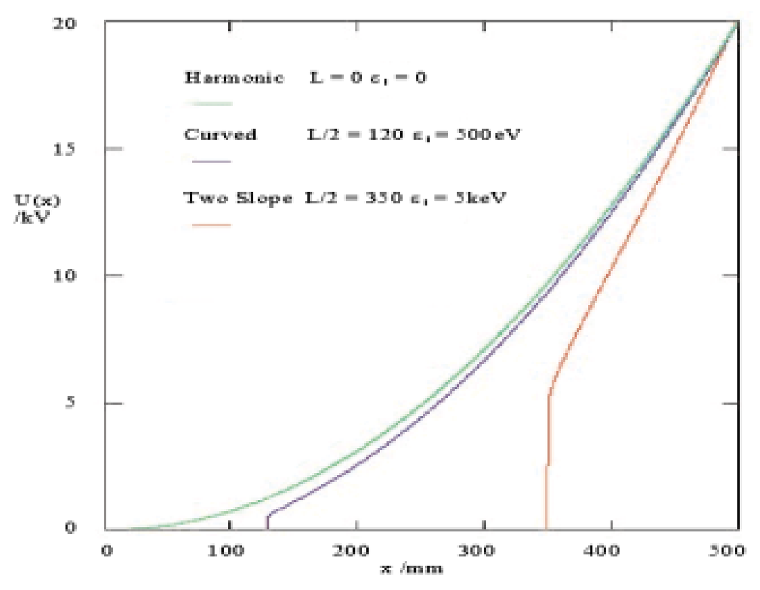
$$\pi\cdot x(U)=(k\cdot L-2\cdot d)\cdot\left(\frac{U-\varepsilon_1}{\varepsilon_1}\right)^{1/2}+\pi\cdot d\cdot\left(\frac{U-\varepsilon_1}{\varepsilon_1}\right)-\left(L+\frac{2\cdot d\cdot U}{\varepsilon_1}\right)\cdot\arctan\left(\frac{U-\varepsilon_1}{\varepsilon_1}\right)^{1/2}$$

The constant k represents the ratio of the time of flight of an ion of energy $q\varepsilon_1$ in the drift region to that of the time of flight in the drift region and step region this gives for the step case $k \geq (L+4d) / L$.

Three cases

The three case considered give an overall size of the drift length and reflectron length at 20kV (L/2 + x(20kV)) of 500mm.

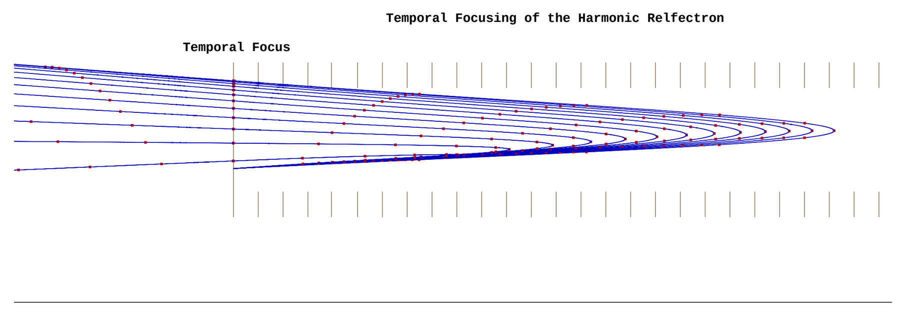
- Harmonic L = 0 $\varepsilon_1 = 0$
- Curved L/2 =120 mm $\varepsilon_1 = 500$V
- Two Slope L/2 = 350 mm $\varepsilon_1 = 5$kV



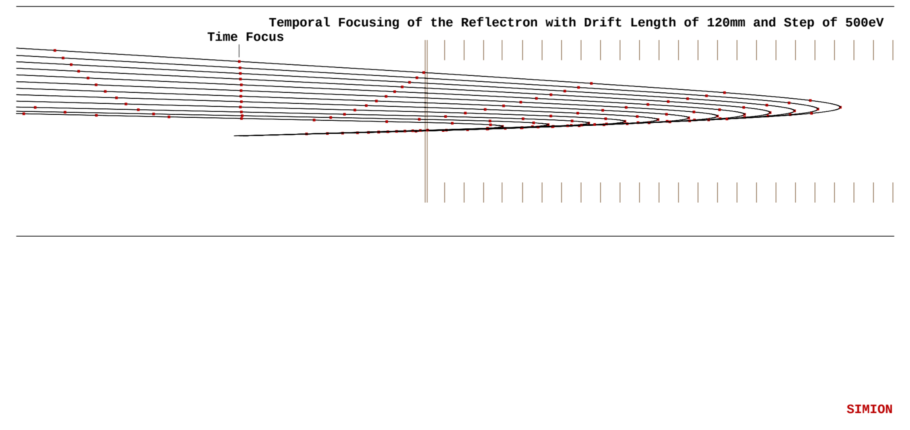
Focusing Properties

1) Temporal

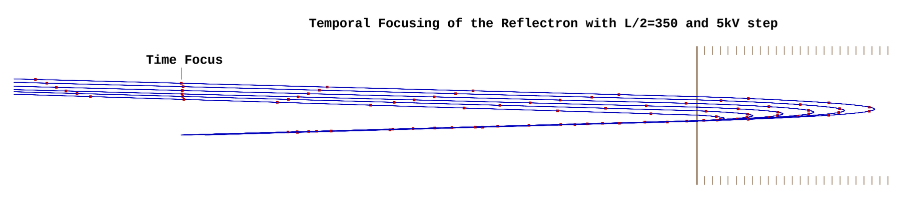
A model of the temporal focusing for the three cases is shown using the SIMION 6 program.



Temporal focus plane at exit of reflectron.
Most defocusing case.



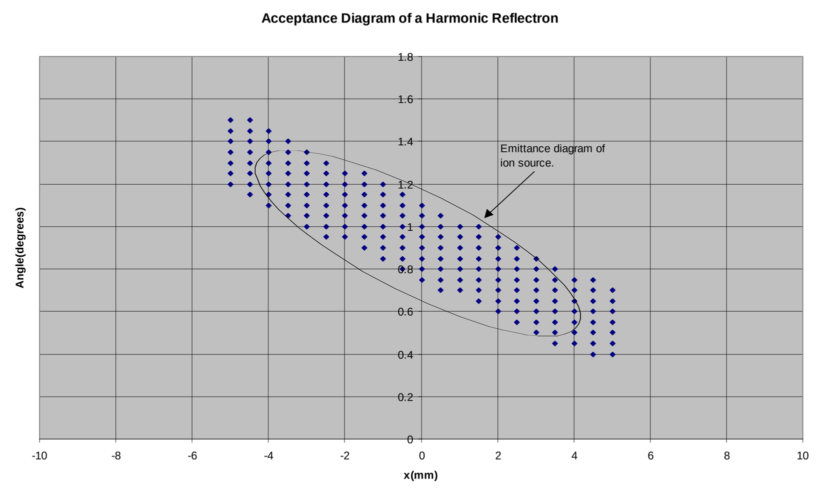
Temporal focus plane at L/2 = 120mm.



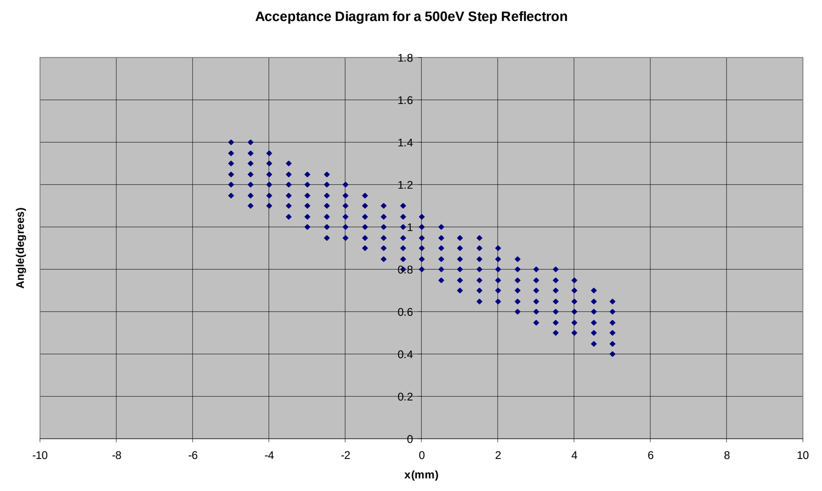
Temporal focus plane at L/2 = 350.
Least defocusing case.

2) Spatial

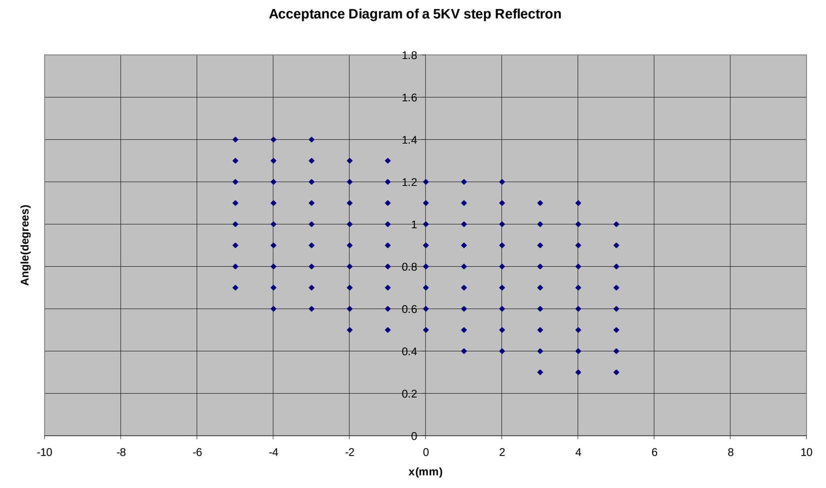
The spatial acceptance phase diagrams of the three cases along with a magnetic sector instrument were used with a 5mm radius off axis entrance aperture along with a 10mm radius detector. The harmonic case is shown with a typical emmitance of a MALDI ion source.



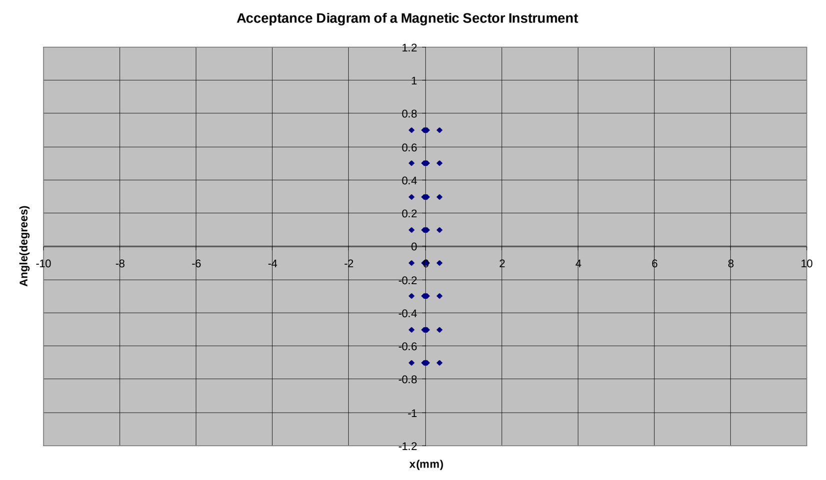
Acceptance = 3.2 mm degrees



Acceptance = 3.2mm degrees



Acceptance = 7.2 mm degrees



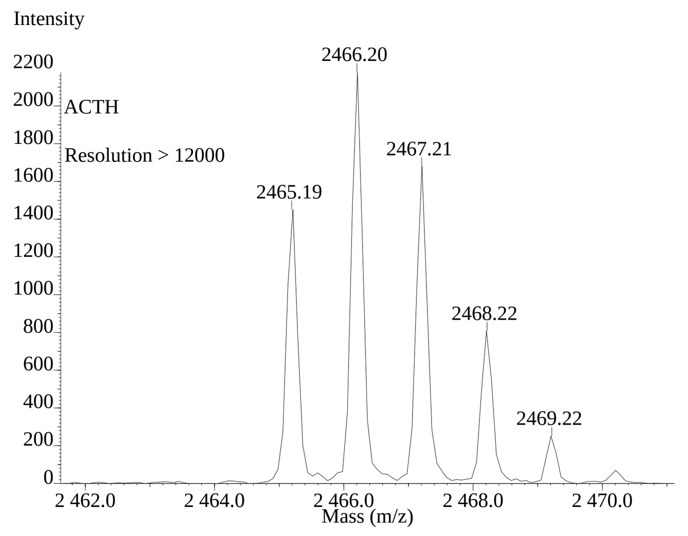
Acceptance = 1.2 mm degrees

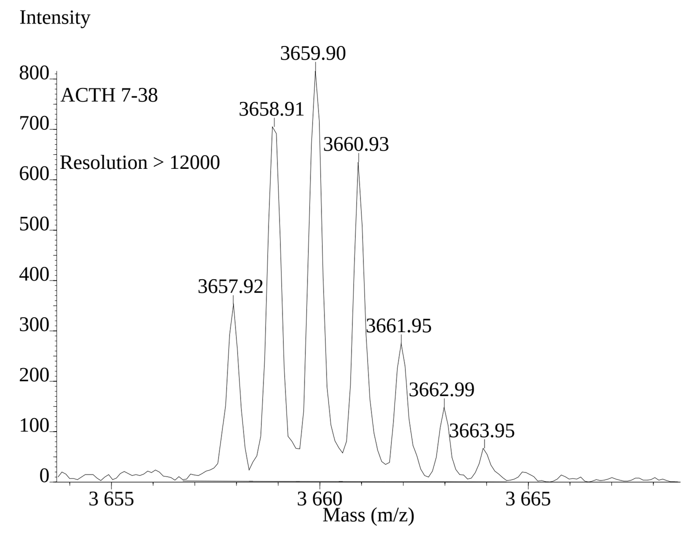
Experimental Data

Experimental data was obtained using a SAI LT3 with delayed extraction and a timed ion gate at the entrance to a harmonic reflectron.

Resolution

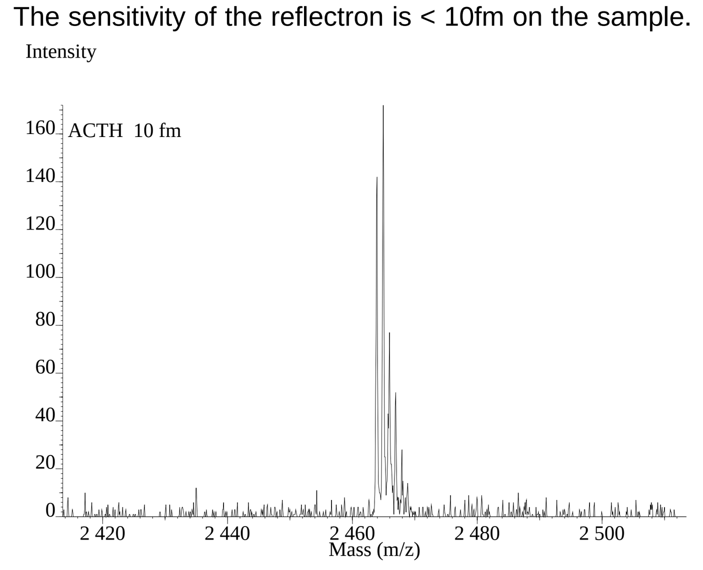
The mass resolution of the harmonic reflectron is > 12,000 and shows the temporal focusing of the reflectron.

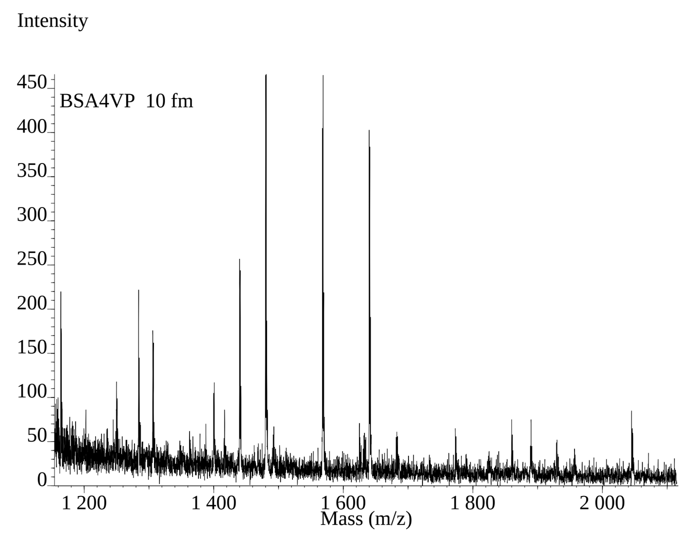




Sensitivity

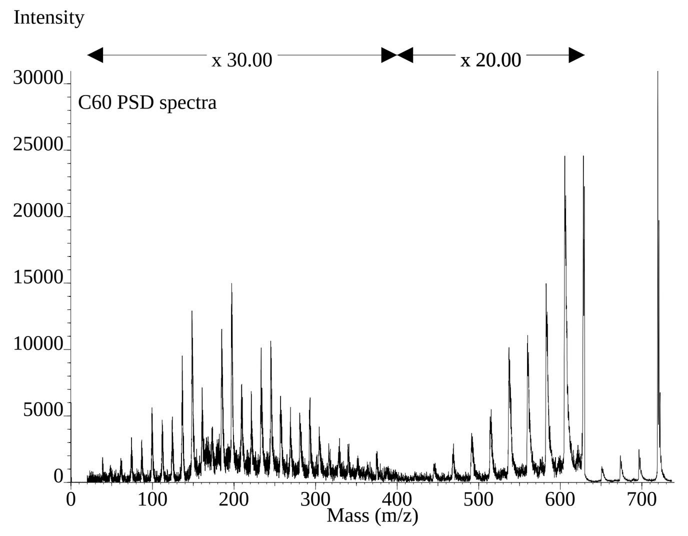
The sensitivity of the reflectron is < 10fm on the sample.

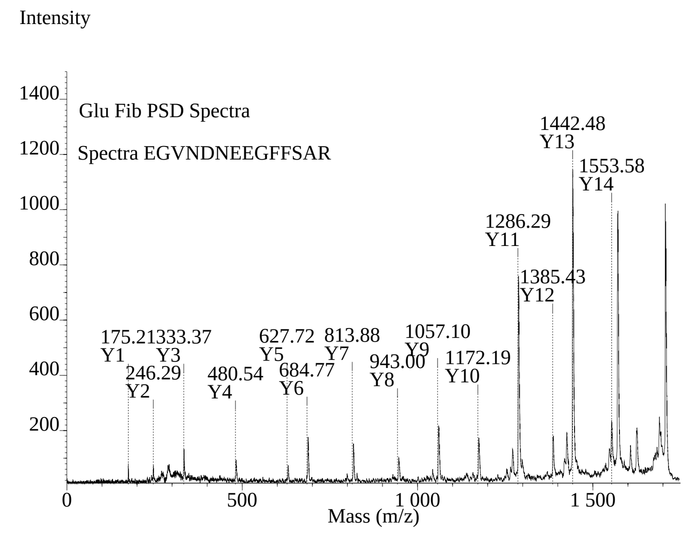




Energy Bandwidth for Fragment Ions

The carbon 60 and GluFib spectra shows the complete mass range of the PSD spectra in a single run.





Conclusion

- As the energy bandwidth of an ideal reflectron decreases from the harmonic case the spatial acceptance of the device increases.
- All ideal mirrors (other than harmonic) are characterised by a potential step to exclude ions with energy < ε_1.
- The acceptance of all reflectrons is large compared to high performance magnetic sector instruments.

References

1) G.G. Mannagadze & I.Yu. Shutyaev, *Exotic Instruments and Applications of Laser Ionization Mass Spectrometry in Space Research, Laser Ionization Mass Analysis,* Chemical Analysis Series, Vol 124,