Efficiently Transporting Ions From Viscous Flow to Ultra-High Vacuum with Minimal Loss

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Extrel Core Mass Spectrometers

Abstract

A conical octupole ion guide is used for the collisional focusing of ions at near-atmospheric pressures via orifice ion extraction from laminar flow. Efficient ion extraction afforded by this method is useful for achieving lower detection limits, fewer vacuum pumping requirements, and decreased process time in deposition experiments. Collisional focusing in RF multi-pole ion optics has previously been limited to high vacuum because of the high potentials required to achieve tight focusing. This limitation has been overcome by reducing the inscribed radius along the length of the optic. The effect of reducing the radius by half is suggested as having similar focusing consequences as quadrupling the peak-to-peak RF potential.

Introduction

Sources used to produce ions also produce neutrally charged "debris" comprised primarily of unionized analyte and process materials used in ion production or preparation. It is often necessary to separate ionic species from the neutral debris after ion production to provide low pressure or clean conditions. Differential pumping is a commonly used method of removing ions from neutral debris. It is achieved when two or more separately pumped chambers are connected by a small orifice thru which ions from the first chamber are focused using electric or magnetic fields. Because the ions respond differently than the neutrals to the electrostatic fields, the neutrals are not actively focused through an orifice and thus the ions are concentrated. The practice of focusing ions through a differentially pumped orifice is complicated by the fact that ions are scattered by neutral species present. Therefore it is difficult to tightly focus ions at pressures where the mean free path is less than the distance traveled by the ion or when the ions are entrained in a moving neutral gas. The purpose of a collisional focusing conical multi-pole is to allow the focusing of ions in such an environment.

Increasing the efficiency of ion extraction increases the sensitivity of a mass spectrometer, allowing for a faster, more exact analysis of trace components in addition to reducing the amount of maintenance required to keep an instrument clean and functional.

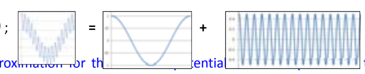
RF Multi-Pole Theory

The theory described here is the work of others and is here only to explain how and why a conical octupole can be used for collisional focusing at near-atmospheric pressures.

1. Gerlich, D. *State-Selected and State-to-State Ion-Molecule Reaction Dynamics, Advances in Chemical Physics Series,* Vol. 82, Wiley:New York, 1992, pp. 1 – 176.
2. M.A. Rottgen *et al., Review of Scientific Instruments* ***2006,*** *77,* 013302.
3. Douglas, D. J., French, J. B. Collisional Focusing Effects in Radio Frequency Quadrupoles, *J. Am. Chem. Soc.* **1992,** 3, 398.

An analytical equation has been provided by previous researchers[1,2] for calculating the "effective potential" created by a RF multi-pole. The path of a charged particle in a Radio Frequency Multi-pole can be separated, using "the adiabatic approximation" into two terms $R_0(t)$, the smooth drift term, and $R_1(t)$ is the rapidly oscillating motion at the RF frequency. The trajectories, as graphed, are not rigorously correct because the amplitude of the R_1 oscillation is directly radially dependant. The theory accounts for this, the figure does not.

$r(t) = R_0(t) + R_1(t)$;



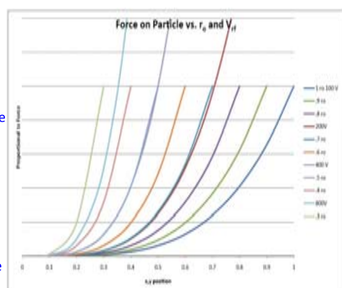
M.A. Rottgen *et al.* adapted an approx… for th… ential … the that of D. Gerlich[1] for an n-pole optic and showed it to be phenomenologically correct.[2] The effective potential is a static potential that can be used to solve for R_0:

$$\Phi_{eff} \approx \frac{4}{k^8 z^8}\frac{q^2 V_{rf}^2}{m(2\pi f)^2}\left[r^6 + \frac{r^8}{z^2}\cos^2(4\theta)\right]$$

where $k = \tan\alpha = rz^{-1}$, V_{rf} is the peak-to-peak RF amplitude, and $r = (x/r_0, y/r_0)$. Thus the resulting force on the particle is approximately:

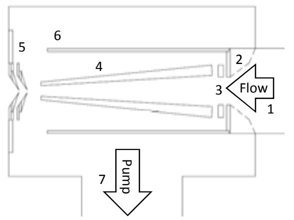
$$ma_{eff} = -q\nabla\Phi_{eff} V_{rf}^2 r^4$$

By plotting the equation of force proportionality vs. the pertinent variables we can see that a similar potential well can be created by doubling the peak-to- peak RF potential or reducing the radius to 70% of the original diameter. Quadrupling the Voltage is similar to halving the original diameter.



Design

The conical octupole design of M.A. Rottgen *et al.* was used to develop a phase space compressing focusing optic. The optic was required to increase the extraction efficiency of a fast-flow reactor to reduce process time in cluster deposition experiments.

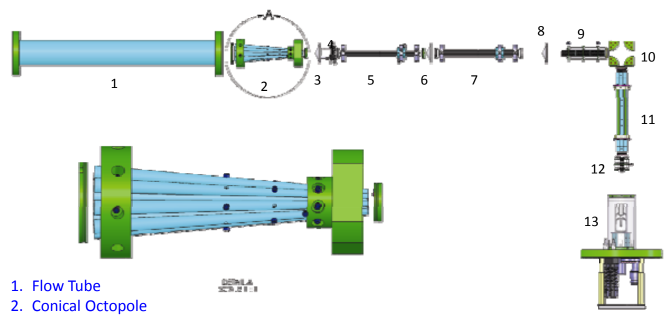


1) Clusters are produced upstream in a laser vaporization source and enter in a laminar stream of Helium.
2) An adapter directs the ion/gas mixture into the acceptance region of the optic.
3) An acceptance lens is used to direct ions into the optic. A slightly repulsive potential results in maximum ion transmission.
4) Eight poles are used to form a conical octupole.
5) A complex orifice is used for extraction an optic. The second lens is not for differential pumping. It is held at or near ground to shape the extraction field.
6) The optic is held in a vented can to maintain velocity along the length of the optic.
7) A trapped rotary vein pump fitted with a mechanical booster is used to pump the apparatus.

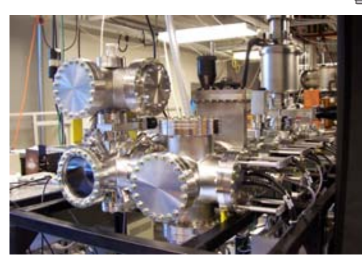
Entrance

Exit

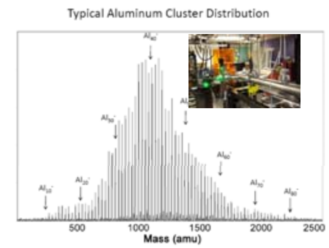
Implementation

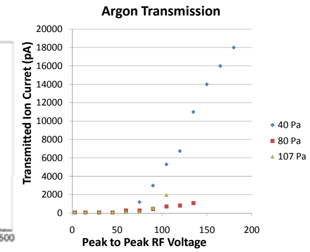


1. Flow Tube
2. Conical Octupole
3. 2mm Orifice
4. Lens Assembly
5. Standard Octupole
6. 3 mm Orifice
7. Standard Octupole
8. 5 mm Orifice
9. Einzel Lens Assembly
10. Quadrupole Bender
11. Quadrupole Mass Filter
12. Einzel Lens Assembly
13. Conversion Dynode/Channel Electron Multiplier Assembly



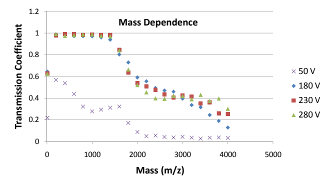
Experimental Data



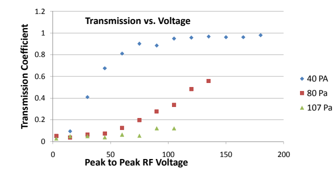


Simion® Trajectory Calculations

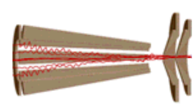
The Ion trajectories were calculated using Simion 8. The RF field is modeled using the SIMION Lua workbench program for octupole simulation (D .Manura-2007-09). The Collisions are modeled using the hard-sphere collision workbench program (REVISION-4-2007-02). Ions are started at a random position on a disk outside the acceptance region. The drift velocity of the carrier gas (adjustable parameter) in the x direction was estimated to be 1000 m/s. 490 ions are flown . The location of Ion "splats" are counted, and a transmission coefficient is calculated. The Transmission Coefficient is equal to the number of ions transmitted divided by the number of ions flown.



The reduced transmission at higher masses can be rationalized from the mass dependence of the effective potential.



The calculated transmission curves generally match the measurements. Deviations at lower RF Voltage are suspected to arise from non-ideal flow trajectories.



Exemplary Ion Trajectory

Ion trajectory of a 35 amu ion. Lens voltages used are the actual voltage used to obtain maximum throughput in the functioning instrument.

Conclusions

A novel approach for efficiently transporting ions from viscous flow to ultra-high vacuum while achieving minimal loss has been developed. This is accomplished using a conical octupole ion guide to collisionally focus ions at near-atmospheric pressures through an extracting orifice. Further differential pumping is then utilized to achieve a final pressure < 1 X 10^{-9} Torr. It is shown using established RF multi-pole theory that a conical octupole achieves the same focusing effect as would be had from increasing the peak-to-peak RF amplitude. The backing gas velocity and pressure is important for the successful transport of ions through the complex extraction orifice. Experimental data supports the validity of Simion® trajectory simulations. It is shown that the conical octopole and extraction region allow very low loss.

Acknowledgments

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