

ASMS 2010 Posters/Sessions Related to SIMION

Session: MP28, Ion Sources: ESI **Time Slot/Poster:** 609, Monday, Poster Hall

Improving and Coupling Electrospray Ion Funnel Interface to Ion Mobility-Mass Spectrometry;
Junho Jeon; Chaminda M. Gamage; David H. Russell; Texas A&M University, College Station, TX

Session: MP30, Ion Activation/Dissociation: General **Time Slot/Poster:** 647, Monday, Poster Hall

Investigation of fast unimolecular dissociation reactions using surface-induced dissociation implemented in a modified commercial MALDI-TOF; Sung Hwan Yoon; Mowei Zhou; Arpad Somogyi; Chaminda M. Gamage; Vicki H. Wysocki; University of Arizona, Tucson, AZ

Session: MP31, Instrumentation: FTMS **Time Slot/Poster:** 651, Monday, Poster Hall

Design Considerations for External Ion Injection FT-ICR MS at 21 Tesla; Steven C. Beu¹; Christopher L. Hendrickson²; Alan G. Marshall³; ¹S C Beu Consulting, Austin, TX; ²National High Magnetic Field Laboratory, Tallahassee, FL; ³Ion Cyclotron Resonance Prog, Tallahassee, FL

Session: MP31, Instrumentation: FTMS **Time Slot/Poster:** 653, Monday, Poster Hall

Characterization of axial motion frequency analyses in harmonized cylindrical Penning traps as potential mass spectrometry method; Eugene Nikolaev¹; Ivan Boldin¹; Pavel Ryumin¹; Igor Popov²; ¹Institute for Energy Problems of Chemical Physics, Moscow, RUSSIAN FEDERATION; ²Russian Academy of Sci, Moscow, RUSSIAN FEDERATION

Session: MP31, Instrumentation: FTMS **Time Slot/Poster:** 655, Monday, Poster Hall

Injection of Externally-Generated Low Mass Ions into High Magnetic Field in Q/FT-ICR Instruments: SIMION Simulations and Experimental Observations; Behrooz Zekavat; Touradj Solouki; University of Maine, Orono, ME

Session: MP31, Instrumentation: FTMS **Time Slot/Poster:** 657, Monday, Poster Hall

Effects of ion introduction in the FT ICR cell on frequency shifts, mass accuracy, and resolution; Andriy Kharchenko; Ron M.A. Heeren; FOM Institute for Atomic and Molecular Physics, Amsterdam, NETHERLANDS

Session: MP31, Instrumentation: FTMS **Time Slot/Poster:** 658, Monday, Poster Hall

Investigation of collision cross section effects on ion motion in ICR cell under influence of bath gas and quadrupolar excitation; Alexander Misharin¹; Alexander Popov²; Vladimir Doroshenko¹; ¹MassTech, Inc., Columbia, MD; ²MSU, Moscow, Russia

Session: TP29, Ion Mobility I **Time Slot/Poster:** 650, Tuesday, Poster Hall

A Periodic-focusing DC-only Ion Funnel for a Cryogenic Ion Mobility- Mass Spectrometer ; Joshua Silveira¹; Chaminda M. Gamage¹; Jody May²; David H. Russell¹; ¹Texas A&M University, College Station, TX; ²Vanderbilt University, Nashville, TN

Session: TP30, Instrumentation: TOF **Time Slot/Poster:** 671, Tuesday, Poster Hall

Doughnut Multi-reflecting Time-of-Flight Mass Spectrometer; Vyacheslav Shchepunov¹; Alexander Berdnikov²; Hideaki Izumi¹; Roger Giles¹; Nicolay Gall²; ¹Shimadzu Research Laboratory, Manchester, United Kingdom; ²Institute for Analytical Instrumentation of RAS, St. Petersburg, Russia

Session: TP30, Instrumentation: TOF **Time Slot/Poster:** 682, Tuesday, Poster Hall

A Serpentine Extraction Ion Source for a Laser Desorption Postionization Microprobe Imaging MS; Jerry F. Moore¹; Gerald Gasper²; Artem Akhmetov²; Luke Hanley²; ¹MassThink LLC, Naperville, IL; ²University of Illinois at Chicago, Chemistry, Chicago, IL

Session: WP23, Homeland Security **Time Slot/Poster:** 506, Wednesday, Poster Hall

Investigation using SIMION on the implementation of a cubic ion trap as an ionization chamber on a GC/LIT; Sarah Vitcher^{1,2}; Claude Beaugrand³; Laurens Dudragne²; Roberta Collino²; Jean-Claude Tabet¹; ¹University Paris VI (UPMC), Paris Cedex 05, FRANCE; ²THALES SECURITY SOLUTIONS & SYSTEMS, Vélizy-Villacoublay, FRANCE; ³ALPHA-MOS, Toulouse, FRANCE

Session: WP28, Ion Sources: API **Time Slot/Poster:** 606, Wednesday, Poster Hall
Modular computational toolset for atmospheric pressure ionization method development: SIMION meets FEM; Walter Wissdorf¹; Larissa Pohler¹; Thorsten Pöhler²; Herwart Hönen²; Klaus J. Brockmann¹; Thorsten Benter²
¹University of Wuppertal, Wuppertal, Germany; ²RWTH Aachen, Aachen, Germany

Session: WP31, Instrumentation: New Concepts I **Time Slot/Poster:** 679, Wednesday, Poster Hall
Optimization of the Electrodynamic Ion Funnel for Enhanced Low Mass Transmission: Influence of Funnel Operational Pressure on Ion Transmission; Paul Momoh; Michael Ugarov ; Mark Werlich; Tom Knotts; Alex Mordehai; Agilent Technologies, Santa Clara, CA

Session: ThOC am, Recent Developments in Ion Mobility MS **Time Slot/Poster:** 09:10, Thursday, Ballroom BDF
A Novel, Modular Ion Mobility Drift Cell; Ryan Blase ; Chaminda M. Gamage; Joshua Silveira; David H. Russell; Texas A&M University, College Station , TX

Session: ThOD pm, Novel Developments in Instrumentation **Time Slot/Poster:** 3:30, Thursday, Room 155
Development of a portable mass spectrometer for operation at 1 Torr; Glen Jackson; Ohio University, Athens, OH

Session: ThP23, Computer Analysis **Time Slot/Poster:** 530, Thursday, Poster Hall
Numerical simulation of ion dynamics in collision multipole ion guides; Victor Laiko¹; Craig M. Whitehouse²;
¹Perkin Elmer, Inc., Branford, CT; ²PerkinElmer, Branford, CT

Session: ThP23, Computer Analysis **Time Slot/Poster:** 532, Thursday, Poster Hall
Accelerated Trajectory Simulations for SIMION with a Beowulf Cluster; Peter Williams; Agilent Laboratories, Santa Clara , CA

Session: ThP27, Instrumentation: New Concepts II **Time Slot/Poster:** 630, Thursday, Poster Hall
Development of Tripole-Multipole Rotational Ion Mobility Mass Spectrometer by Ion Simulations; Takanori Harada; Tsutomu Masujima; Hiroshima Univ. BioMed., Hiroshima, JAPAN

Session: ThP28, Instrumentation Quadrupoles and Traps **Time Slot/Poster:** 644, Thursday, Poster Hall
A tightly curved collision cell with high MSMS efficiency; Felician Muntean; Varian Inc., Walnut Creek, CA

Session: ThP28, Instrumentation Quadrupoles and Traps **Time Slot/Poster:** 646, Thursday, Poster Hall
A new linear quadrupole ion trap with axial ejection; David Langridge; Jason L Wildgoose; Waters Corporation, Manchester, UNITED KINGDOM

Session: ThP28, Instrumentation Quadrupoles and Traps **Time Slot/Poster:** 655, Thursday, Poster Hall
A Digital Linear Ion Trap based on Ceramic Printed Circuit Boards; Mu Hui ; GongYu Jiang; Tao Lin; XiaoHui Yang; JunSheng Zhang; Li Ding; Shimadzu Research Laboratory (Shanghai), Shanghai , CHINA

Session: ThP28, Instrumentation Quadrupoles and Traps **Time Slot/Poster:** 657, Thursday, Poster Hall
Short-Pulse Ion Extraction from a Quadruple Ion Trap into a Time-of-Flight Mass Spectrometer for Trapped Ion Cloud Diagnostics; Beni B. Dangi; Nicholas A. Sassin; Kent M. Ervin; University of Nevada, Reno, Reno, NV

Session: ThP28, Instrumentation Quadrupoles and Traps **Time Slot/Poster:** 661, Thursday, Poster Hall
Kinetic energies of ions ejected radially from LIT at high q; Viatcheslav V. Kovtoun; Thermo Fisher Scientific, San Jose, CA

Session: ThP28, Instrumentation Quadrupoles and Traps **Time Slot/Poster:** 662, Thursday, Poster Hall
Optimization of Multipole Components in a Planar Paul Trap; Zhiping Zhang; Ying Peng; Hannah Quist; Junting Wang; Brett J. Hansen; Aaron R. Hawkins; Daniel E. Austin; Brigham Young University, Provo, UT

Session: ThP28, Instrumentation Quadrupoles and Traps **Time Slot/Poster:** 663, Thursday, Poster Hall
Miniaturization of an axially focusing linear ion trap for mass spectrometry; Gareth Dobson¹; Christie Enke²;
¹SRI International, Menlo Park, CA; ²University of New Mexico, Albuquerque, New Mexico

ASMS 2010 Posters/Sessions, SIMION - Full Abstracts

Session: MP28, Ion Sources: ESI **Time Slot/Poster:** 609, Monday, Poster Hall

Improving and Coupling Electrospray Ion Funnel Interface to Ion Mobility-Mass Spectrometry

Junho Jeon; Chaminda M. Gamage; David H. Russell

Texas A&M University, College Station, TX

Novel Aspect

An replaceable electrospray ion source with an IF interface coupled to a commercial qTOF for high sensitivity ion-mobility experiments

Introduction

The increased ion transmission afforded by electrodynamic ion funnels (IF) is of critical importance when coupling ESI to IM-MS. In an effort to adapt an ESI-ion mobility source to a commercial q-TOF instrument (Sciex QSTAR®) we have critically evaluated the designed an EIF, i.e. fluid dynamics and ion motions in the interface region, to optimize ion transmission into the next ion optics or vacuum region. The optimization of the IF interface must include establishing the working pressures and DC E-fields for each component as well optimization of the RF power/frequency. The design of the system as well as performance of the IF interface will be discussed.

Methods

A new ESI-IF interface for ion mobility is designed based on optimized SIMION ion trajectories. The home-built ESI source consists of an X-Y-Z adjustable stage for a pulled heated capillary and 39-lens element IF (3cm x 3cm x 5cm) for ion injections through a 1 mm orifice into a differentially pumped region which houses an Einzel lens to focus the ions into the IMS drift tube. For the initial studies the interface is installed directly on to the q-TOF instrument (QSTAR®) in place of the original Ion Spray® source. The ion current was measured right after the orifice plate of the IF. The IMS drift cell can be inserted between the IF interface and q-TOF for ion mobility experiments.

Preliminary Data

The new IF has larger dimensions to help stable ion flows inside the IF and increase RF collisional focusing effect. Ion current after the interface shows about 0.7 nA which is more than 100 times larger than before. The results of simulations are consistent with experimental data that the collisional RF ion focusing effect is valid from 0.1 torr to 5 torr with nitrogen at 500 kHz and 35 Vpp. The first 15 electrical lens having constant i.d. of 25.4 mm increased desolvation and dispersion of the gas flow. Since the IF interface is driven by a self-oscillation RF power supply (Ardara Tech), the operating frequency is changed by adding capacitors in series to it and the intrinsic capacitance of the IF (1000 pF) is adjusted to 500 pF and 330 pF which result in the variation of ion current responses. The DC potential gradient across the IF is 21 V/cm at working condition. Radial ion confinement by RF fields is obvious when no RF voltage is turned off and the ion current decreases by a factor of 30 on average. This confirms that the IF works as our simulation results. Coupling the IF to QSTAR involves matching pressure drop from the IF to Q0 region since Q0 is working with RF only at 10 mtorr. Differential pumping and Einzel lens to focus ions into the Q0 quadrupole acceptance region were tested to achieve higher ion transmission but it would be better by shortening the gap between the orifice plate of the IF and Q0 without the ion optics in this pressure region. To test this idea, the modification of the interface is under way. The inserting mobility cell is also being developed and tested so that ESI-IMS with IF interface will be tested shortly.

Session: MP30, Ion Activation/Dissociation: General **Time Slot/Poster:** 647, Monday, Poster Hall

Investigation of fast unimolecular dissociation reactions using surface-induced dissociation implemented in a modified commercial MALDI-TOF.

Sung Hwan Yoon; Mowei Zhou; Arpad Somogyi; Chaminda M. Gamage; Vicki H. Wysocki
University of Arizona, Tucson, AZ

Novel Aspect

A commercial MALDI-TOF instrument was modified with a home-built SID set-up to improve studies on fast dissociation kinetics/mechanisms.

Introduction

Previously a bench-top MALDI-TOF instrument (Bruker Proflex) with surface-induced dissociation (SID) capability was used to investigate fast dissociation kinetics. Combined with silicon nanoparticle assisted laser desorption ionization (SPALDI), small molecules such as $N(CH_3)_4^+$, $N(CD_3)_4^+$, and substituted benzylpyridinium ions were successfully studied without matrix interference. Recently the SID set-up was inserted into another commercial MALDI-TOF instrument (Bruker Reflex III) with modifications to the design. This commercial instrument has better ion optics to guide ion beams more efficiently and is equipped with a 2GHz digitizer which allows measurement of nanosecond order dissociation reactions. With these advantages, the modified commercial MALDI-SID-TOF can provide higher performance for fast dissociation reaction studies.

Methods

The previous SID set-up was placed after reflectron electrodes. In the Reflex III, however, there is no available space after the reflectron electrodes, so the SID set-up replaced the reflectron. A new ground electrode was added to the SID set-up and a ring electrode in front of the surface works as an electrical lens to guide precursor and fragment ions. $N(CH_3)_4^+$, $N(CD_3)_4^+$, substituted benzyl-pyridinium ions, $C60^+$ and $C70^+$ were used to test the SID performance. SID experiments employed fluorinated and hydrogenated self-assembled monolayers (SAM) on gold surfaces. SPALDI was used for pre-ionized samples. 30nm silicon particles were oxidized with HNO_3 and then derivatized with (heptadecafluoro-1,1,2,2-tetrahydrodecyl)dimethylchlorosilane (C10). Laser desorption ionization (LDI) was used for $C60$ and $C70$.

Preliminary Data

Pre-ionized samples, such as $N(CH_3)_4^+$ and substituted benzyl-pyridinium ions are easily laser desorbed, and adding derivatized silicon nanoparticles enables desorption at even lower laser intensity. Simion simulations were performed to predict the flight paths of different ions and to estimate optimum voltage conditions. For flight time measurements a voltage of 0.5 kV higher than the acceleration potential at the source was applied to turn precursor ions towards the detector without colliding with the surface. A variety of ions – ranging from small ions such as Na^+ to small protein ions such as insulin – returned to the detector at expected flight times. SID experiments were carried out by lowering surface voltage relative to the ion acceleration voltage. SID of $N(CH_3)_4^+$ and $N(CD_3)_4^+$ was successfully reproduced in the modified Reflex III. Fast statistical unimolecular dissociations of substituted benzyl-pyridinium ions, $C60^+$ and $C70^+$ have been studied both experimentally and computationally. With the assistance of silicon nanoparticles, substituted benzyl-pyridinium ions were generated with less in-source fragmentation than MALDI and followed the same trends reported by the Vertes group. In parallel with the previous $N(CH_3)_4^+$ results and works done by various research groups, $C60^+$ and $C70^+$ showed various fragmentation pathways with increasing collision energy and different reaction paths dominate at different collision energies. Odd numbers of carbon unit losses were also observed at over 400 eV surface collisions. All the dissociations were observed in a time window of a few tens of nanoseconds. Fast unimolecular dissociation kinetics of small molecules can be achieved without matrix interference in the modified commercial MALDI-SID-TOF instrument.

Design Considerations for External Ion Injection FT-ICR MS at 21 Tesla

Steven C. Beu¹; Christopher L. Hendrickson²; Alan G. Marshall³

¹S C Beu Consulting, Austin, TX; ²National High Magnetic Field Laboratory, Tallahassee, FL; ³Ion Cyclotron Resonance Prog, Tallahassee, FL

Novel Aspect

Computer simulations characterize ion loss and kinetic energy changes during multipole injection through a 21 T magnetic field gradient.

Introduction

The development of “next generation” 21 T superconducting solenoid magnets will greatly improve figures of merit for FT-ICR MS, but will also present new challenges for efficient injection of ions from external sources. Transfer of ions through the strong magnetic field gradient between source and analyzer regions is typically accomplished with multipole ion guides, and prior work has shown that these devices are subject to ion loss below an m/z threshold (1) and significant transfer of axial to radial kinetic energy for ions that successfully transit the gradient (2). In this work we use computer simulations to characterize these effects in a 21 T gradient, and investigate mitigation by terminating the multipole in a lower field region of the gradient.

Methods

Simulations were performed with SIMION (Version 8.0, Scientific Instrument Services) running on a homebuilt 3.00 GHz AMD Phenom II Quad-Core PC with 4 GB ram. Octopole and flat-electrode-quadrupole ion guides with an inscribed radius of 2.38 and 3.18 mm, respectively, were modeled with an array resolution of 0.0635 mm. Ion guide length was varied to provide an exit-end magnetic field ranging from 3 to 21 T while maintaining a constant distance of 1.25 m from entrance to magnet center. An analytical description of the three-dimensional magnetic field map of the proposed 21 T magnet under development at the National High Magnetic Field Laboratory was incorporated in the simulations by means of SIMION user programs.

Preliminary Data

Simulations of ion injection through a 21T magnetic field gradient show that susceptibility to ion loss and kinetic energy changes are consistent with parametric relationships derived in prior work at 14.5 T (1,2). Those relationships predict that the m/z threshold below which ion loss may occur, and the extent of axial to radial kinetic energy exchange, will vary directly with the “terminal” magnetic field that is defined differently for the two effects. In the relation describing kinetic energy exchange, the terminal field is the field at the end of the ion flight path to the ICR cell, typically the peak field of the magnet. This parameter is of course not easily varied by the operator and therefore only the multipole parameters can be changed to limit kinetic energy exchange. In the relation describing the m/z threshold for ion loss, the terminal field is the maximum magnetic field experienced by the ion while inside the multipole, typically the field present at the exit end of the multipole. In most instruments the multipole terminates near the ICR cell and the terminal field is again just the peak field of the magnet; however, the multipole length can be considered as a potential variable for controlling the m/z threshold for ion loss. Simulations indicate that that the multipole may be terminated at a lower field determined by the maximum ion m/z and kinetic energy. This work was supported by NSF Division of Materials Research through DMR-0654118 and the State of Florida. [1] S. C. Beu, C. L. Hendrickson, and A.G. Marshall, Proceedings of the 55th ASMS Conference on Mass Spectrometry and Allied Topics, (2007) MPD070. [2] S. C. Beu, C. L. Hendrickson, and A.G. Marshall, Proceedings of the 57th ASMS Conference on Mass Spectrometry and Allied Topics, (2009) TPK279.

Characterization of axial motion frequency analyses in harmonized cylindrical Penning traps as potential mass spectrometry method

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Novel Aspect

Cylindrical Penning trap is invented with large volume of effective hyperbolic field, permitting mass analyses through axial frequency measurements

Introduction

Determination of ion masses by measuring frequencies of their oscillations in quadratic potential is an old idea used for many years in Penning traps and recently implemented on Kingdon type traps in Orbitrap type devices. Such measurements are possible only in traps with quadratic dependence of potential on axial coordinate, which hyperbolic and Kingdon traps provides. Hyperbolic trap is not convenient for FT ICR because of relatively small volume of harmonic field in comparison to the whole dimensions of the trap. This factor causes pure sensitivity and large space charge effects together with construction inconveniences. The new methods of electric field harmonization offered recently [1] could make possible implementation of this methodology on moderate magnetic field cylindrical Penning traps

Methods

The investigated measuring cell is practically a Penning type cell which is divided by a plane perpendicular to the axis into two parts for detection signal generated by axial motion (like it was done in the Orbitrap). The method used for making axial potential distribution quadratic by shaping cell electrodes is described in [1]. Magnetic field is used for averaging of electric field and trapping in radial direction. Ion cloud motion simulations were performed by computer code based on 1) Boris integration scheme for solving motion equations 2) Particle In Cell (PIC) algorithm for solving Poisson equation and calculating particle-particle interactions (N-body problem), Surface Charge Method(SCM) and SIMION for accurate precalculating of electric field (solving Laplace equation).

Preliminary Data

The concept of such type of mass analyzer was proved by numerical experiments. Ions are trapped in axial direction by harmonized trapping potential and in radial direction by magnetic field. Magnetic field should be high enough for proper averaging of the trapping field and compensating its radial component. For higher m/z ratio higher magnetic field is required to trap the particle using the same trapping potential. To “harmonize” the electric field in the whole volume of cylindrical Penning trap averaging of force experienced by ions in axial direction at every moment of axial motion is needed. This averaging is performed by cyclotron motion. Cyclotron frequency should be higher than axial motion frequency for proper averaging. Electric field distribution in the suggested Penning trap is too complicated for analytical evaluation of the extend of nonharmonicity caused by non proper averaging, so computer simulation was used. Empirical formulae was obtained as a result of these simulations which connects magnetic field needed for proper averaging with potential creating the axial electric field and ion m/z ratio. Mass resolution of such type of mass spectrometer have been evaluated. It was shown that at moderate magnetic field (around 1 T, which can be formed by permanent magnet) the resolution of around 10K could be reached. The effect of phase locking of close m/z ions have been investigated and empirical dependence of this phenomenon on m/z difference, cyclotron radius, magnetic field and the number of ions have been found. It was found that resolution obtained in numerical experiment strongly depends on accuracy of trapping field precalculation and its real limit should be investigated further. Dependence of mass resolution on the number of electrodes was also investigated. 1. Ivan Boldin ; Eugene Nikolaev, Harmonization of electric field in FT ICR cell. The new approaches abstract 293

Injection of Externally-Generated Low Mass Ions into High Magnetic Field in Q/FT-ICR Instruments: SIMION Simulations and Experimental Observations

Behrooz Zekavat; Touradj Solouki
University of Maine, Orono, ME

Novel Aspect

Theoretical/practical aspects of problems associated with injecting low-mass ions into strong magnetic fields in external ion source Q/FT-ICR are discussed.

Introduction

We are interested in utilizing a 9.4 tesla GC/FT-ICR MS to characterize complex samples that contain small molecules. Our instrument is equipped with a quadrupole ion guide (QIG) coupled to a home-built external EI/CI ion source. Previously, we showed that externally generated ions with $m/z > 28$ can be guided/trapped in the ICR cell by applying higher (> 2.5 MHz) frequency waveforms on QIG [1]. To better understand and address the challenges associated with guiding small mass ions into a strong magnetic field, we have used SIMION calculations to examine trajectories of small ions in a QIG, placed in an experimentally measured magnetic field gradient. [1] B. Zekavat; J. E. Szulejko; D. LaBrecque; T. Solouki, 57th ASMS Conference on Mass Spectrometry and Allied Topics, 2009, Philadelphia, PA.

Methods

SIMION 8 (SIS, Inc., NJ) was running on a 2.5 GHz Pentium 4 PC with 1.25 GB RAM (Dell, Inc., TX). The mass spectrometric system including external ion source, QIG, and ICR cell was created by writing a single geometry file in SIMION. To adjust/apply RF frequency, RF amplitude, and DC voltages on ion source, QIG, and ICR cell, LUA user programming was used. Fast Fourier transform (FFT) of ion trajectory coordinates (X and Y) were performed using MATLAB 7 (The MathWorks, Inc., MA). The magnetic field gradient of 9.4 tesla superconducting magnet (Cryomagnetics, Inc., TN) was measured using a gaussmeter (F.W. Bell, Inc., FL). Ion current measurements were performed using a multimeter (Tektronix, Inc., OR).

Preliminary Data

The ion trajectory simulations suggest that the primary cause of ion loss in QIG and in the presence of magnetic field is the ion excitation. Applying different RF frequencies on QIG introduces different mass cut-off (MC). At constant RF amplitude, increasing the RF frequency decreases MC. For examples, increasing the RF frequency (100 Vpp) from 1.0 MHz to 6.5 MHz decreases the mass cut-off from $m/z \sim 420$ to $m/z \sim 44$. On the other hand, increasing the RF amplitude at constant RF frequency increases MC. For example, increasing the amplitude of 6.5 MHz RF frequency from 100 Vpp to 600 Vpp increases MC from $m/z \sim 44$ to $m/z \sim 64$. Based on the onset of ejection magnetic field (B_{eject}) values as a function of RF angular frequencies (ω), a linear relationship was found between B_{eject} and ω . We also established a linear relationship between MC and B_{eject} in QIG when a constant RF frequency is applied. FFT analysis of ion trajectories in QIG and in the presence of magnetic field reveals the existence of four frequencies: fundamental resonance frequency (FRF), modulated applied RF frequency (i.e., $RF \pm FRF$), and ion excitation frequency (IEF). For experimental comparisons, ion currents (from a constant leak of acetone to external ion source) on quadrupole trapping plate (QTP) and filament trapping plate (FTP) of the ICR cell were measured. With 5.2 MHz RF on QIG, the ion currents on FTP and QTP were: a) ~ 3.0 nA and ~ 0.0 nA (for ICR cell/QIG positioned inside the magnet) and b) 0.0 nA and ~ 35 nA (ICR cell/QIG positioned outside the magnet), respectively. These measurements suggest that only a small portion of guided ion can be transferred to the ICR cell when a magnetic field is present around QIG.

Session: MP31, Instrumentation: FTMS **Time Slot/Poster Number:** 657, Monday, Poster Hall

Effects of ion introduction in the FT ICR cell on frequency shifts, mass accuracy, and resolution

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Novel Aspect

Effects of cloud shape and velocity distribution on ion clusters fragmentation and forming chaotic ion trajectories at injection explored.

Introduction

Study of deviations from the expected cyclotron frequency has been of constant interest in FTICR-MS as the desire to reduce mass errors to the sub-ppm range. These shifts are due to the interplay of space charge and image-charge interactions. First, ion species get on different orbital radii with subsequent loss of coherence as a result of their individual trajectories becoming increasingly complex. Second, ion clusters increase in relative volume of their convex shells and fragment forming multiple energy clusters. The purpose of this work is to extend recent research on space charge/image charge effects by exploring causes of ion dynamics leading to frequency shifts and signal decay which are initialized at ions' injection in the cell.

Methods

The particle in cell supercomputer simulation schema was used for accounting the space charge effect via solution of Poisson equation in cylindrical cell geometry showcased with sidekick ion optics calculated both in Simion and via the capacitance matrix method for reducing software artifacts. The simulated transients were analyzed in variable windows via the harmonic inversion method accompanied by a discussion of Fourier transform versus harmonic inversion family methods. Samples: 10000-500000 ions of 132.9054-150.0 Da at 7-15T.

Preliminary Data

Temporally, concurrent action of several factors result in ion species' getting on different orbital radii with subsequent loss of coherence as a result of ions' individual trajectories becoming increasingly complex. Topologically, the space-charge effect and image charge interaction [1] cause fragmentation of ion clusters observed as increased relative volume of their convex shells, formation of multiple energy clusters of ions. It was recently observed and confirmed computationally that the major reason of ion species ending up on time-locally stable different orbital radii at detection is due to the space-charge effect between ion species of like sign [2]. However, space charge effect is not a one-time discrete interaction but rather a repetitive continuous evolution of ion clouds excited by the energy of RF excitation field. This evolution is determined by energy distribution of ions within their clouds damped by z-oscillations of ion clusters of specific ion specie. We observe that these factors in turn are significantly depending on injection-phase parameters like ion cloud shape, velocity distribution, and cloud rotation. References: 1. D.W. Mitchell, R.D. Smith. Cyclotron Motion of 2 Coulombically Interacting Ion Clouds with Implications to Fourier-Transform Ion-Cyclotron Resonance Mass-Spectrometry. / *Phy. Rev. E*, 1995, 52, p. 4366–4386. 2. F.E. Leach, A. Kharchenko, R.M.A. Heeren, E. Nikolaev, J. Amster. Comparison of particle-in-cell simulations with experimentally observed frequency shifts between ions of the same mass-to-charge in Fourier transform ion cyclotron resonance mass spectrometry. / *Journal of American Society of Mass Spectrometry*, 2010, vol. 21, no. 2, p. 203–208.

Investigation of collision cross section effects on ion motion in ICR cell under influence of bath gas and quadrupolar excitation

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Novel Aspect

A novel experimental scheme to perform ion mobility separations in an ICR cell is proposed and demonstrated in simulations.

Introduction

The level of sample complexity in glycomics is extremely high. Analysis of stereochemical saccharide variants requires utilization of tandem MS with rapid structure-sensitive separation techniques for their identification. The scheme of analysis in which ion isolation for each stage of the MS_n analysis is performed based on either ion mobility or m/z or both would be a universal and rapid way of carbohydrate (including their stereoisomers) analysis. The idea of performing IM separation of products at each step of the MS_n oligosaccharide analysis was proposed by Hill's group [1]. In this work we discuss a new implementation of the ion mobility technique which can make this analysis scheme possible. The scheme can also provide means for selective manipulations with mobility-separated protein conformations.

Methods

We propose to perform ion mobility separations using "sideband ion cooling" technique (termed "quadrupolar axialization" in FT-ICR) in a dual ICR cell arrangement. Sideband ion cooling is utilized for (ultra)high resolution ion m/z-based separations in atomic physics. It involves utilization of the quadrupolar excitation on the "unperturbed" ion cyclotron frequency in the presence of a bath gas which generally leads to the interconversion between the ion cyclotron and magnetron motions. Equations of the ion motion during the sideband cooling process contain cross section Ω of the ion-neutral collisions as a parameter. Hence, ions with the same m/z but different collision cross sections will have different trajectories that lead to their (position and energy) separation according to the cross section values.

Preliminary Data

SIMION model was created to investigate the ion mobility –based separation processes inside an ICR cell. A number of simulations were also performed using three-dimensional particle-in-cell code PIC3D developed at MSU. Motion of two small ion groups (40-250 ions) having different collision cross sections was simulated. In one set of simulations, ions initially occupied a magnetron orbit with $R_m=5\text{mm}$ in a hyperbolic ICR cell of 20mm diameter placed in a 5T magnetic field. "Stepwise" scheme for quadrupolar excitation in the presence of bath gas (He at 7.5×10^{-5} and 7.5×10^{-6} Torr was tested so far) was chosen to avoid excessive excitation of the ion internal energy in a real experiment. Timing parameters and amplitude of the quadrupolar excitation were varied to provide maximum separation of the mean radial coordinates and mean translational energies between ion groups. Standard deviations of these variables within each ion group were monitored. The difference in the ion radial positions and energies acquired during separation process will be manifested in the different efficiencies of their transfer between compartments of the ICR cell, and/or different rates of the ion loss on the cell side electrodes (ion "evaporation" process), and/or different times and positions of the ion arrival to a (MCP) detector positioned behind the ICR cell in a real experiment. As shown by one of the initial simulations, ions with 5% difference of the collision cross section have 4 times different rate constants of the "evaporation" process. Time dependencies of the ion radial coordinates and kinetic energies will be presented for different collision cross section differences between the ion groups, bath gas types and pressures, amplitudes of the quadrupolar excitation, detuning from the resonance cyclotron frequency, and other parameters. Design of the experimental setup to test the proposed ion mobility separation scheme is under way. [1] Dwivedi, J. Am. Soc. Mass Spectrom-2007-18-1163.

Session: TP29, Ion Mobility I **Time Slot/Poster Number:** 650, Tuesday, Poster Hall

A Periodic-focusing DC-only Ion Funnel for a Cryogenic Ion Mobility- Mass Spectrometer

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Novel Aspect

The PDC IF can transmit and focus spatially diffuse ions using a few ring electrodes and DC voltage.

Introduction

Sensitivity is the most sacrificed figure-of-merit in high resolution ion mobility-mass spectrometry (IM-MS), owing to the necessary transfer of the ion packet from the drift cell, through a conductance limiting aperture, into the mass analyzer. To improve ion transmission in the interface region, we developed a periodic-focusing DC-only ion funnel (PDC IF) designed to collect and focus divergent ions from a uniform field cryogenic drift cell into a time-of-flight mass spectrometer without a significant concomitant decrease in resolution. The initial studies indicate that the PDC IF is a very simple yet efficient device that can also be used in other applications including ambient pressure ionization source interfaces where ion transmission from high pressure regions into the mass spectrometer is critical.

Methods

The instrument features a MALDI source, a quadrupole mass spectrometer for m/z selection of ions prior to injection into a uniform field variable temperature (325-78 K) drift cell, followed by an orthogonal time-of-flight mass spectrometer. PDC IF designs for the IM-MS interface region were evaluated using ion trajectories for C_{60}^{++} ions (720 m/z) modeled with SIMION 8.0 modified to include ion/neutral elastic collisions between 1-5 torr. A uniform electric field was established in the drift cell and PDC IF by applying an independently varied linear potential drop across each region.

Preliminary Data

The PDC IF is a novel design derived from the periodic focusing ion guide developed by our laboratory [1]. The design utilizes the periodic high and low field effects created by the electrode geometry in order to spatially focus and defocus ions. The device bears resemblance to a DC-only ring ion guide, however, the application of a simple DC voltage gradient across the PDC IF generates the periodic focusing effect superimposed on an axial electric field to assist ion transmission. Our initial studies indicate that transmission through the PDC IF is strongly dependent on the electrode geometry—specifically, electrode thickness, spacing, and inner diameter. Similar to the DC-only ring ion guide, the effective RF in the PDC IF creates an effective potential that radially confines ions, the magnitude of which is controlled by the inner diameter of the electrodes and the axial electric field. Several PDC IF designs were evaluated in terms of ion transmission and mobility resolution. The simulation results indicate that the PDC IF can easily be adapted toward applications that require high ion transmission or high IM resolution based on the electrode geometry. For our application, maintaining high resolution with a modest gain in transmission is preferable. The simulation results at cryogenic temperature show that a small PDC IF constructed from only three electrodes can transmit ~58% of an ion packet through a 30 cm drift cell with a resolution ~68; additional transmission and resolution increases can be achieved as the axial electric field strength is increased. These findings indicate a substantial improvement in ion transmission through our cryogenic IM-MS interface which typically yields ~2% transmission at room temperature. [1] Gillig, K. J.; Ruotolo, B. T.; Stone, E. G.; Russell, D. H. *Int. J. Mass Spectrom.* 239, 2004, 43-49.

Session: TP30, Instrumentation: TOF **Time Slot/Poster Number:** 671, Tuesday, Poster Hall

Doughnut Multi-reflecting Time-of-Flight Mass Spectrometer

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Novel Aspect

The novel MR TOF mass spectrometer based on a transaxial mirror is described. It features compact size, high mass resolving power and transmission and wide mass range.

Introduction

Multi-reflecting and multi-turn time-of-flight mass spectrometers are proven to provide high mass resolving powers m/dm in the approximate range of 40,000-200,000 for the systems with open trajectories after Verentchikov and Satoh and 100,000-1,000,000 for those with closed trajectories after Wollnik, Toyoda, Furuhashi and Plass. The systems with open trajectories are most suitable to mass spectrometry applications as they retain full mass range at high transmission efficiency and a compact size. A novel multi-reflecting TOF with open trajectories is described in this work. It is based on a gridless transaxial mirror consisting of concentric ring electrodes. Results of ion-optics simulation studies are presented.

Methods

The spectrometer comprises an ion storage device, the gridless transaxial mirror, a detector and interfaces connecting the mirror with the ion storage device and the detector. Ions extracted from the ion storage pass through the injection interface, the mirror, the extraction interface and are registered with the detector. While within the mirror, ions move along star-like jig-saw trajectories. Trajectories of injected (extracted) ions can approximately lay in the plane of the mirror. The system has been numerically simulated and optimized using SIMION 8 and in house simulation software.

Preliminary Data

The Doughnut spectrometer has been simulated for ions from an ion trap in the mass range 500-5000 Da with the extraction energy of 5keV. The geometry and potential of the transaxial ion mirror were optimized to provide isochronicity of ions' motion in the longitudinal direction and focusing in both the transversal planes. It is shown, in particular, that m/dm (fwhm) are at least not worse than 40,000 in the specified mass range of ions.

A Serpentine Extraction Ion Source for a Laser Desorption Postionization Microprobe Imaging MS

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Novel Aspect

Serpentine ion path cleanly separates desorbed ions from postionized molecules and enables high resolution imaging MS.

Introduction

Smaller length scales in imaging MS require dramatically increased instrument sensitivity. Postionization of desorbed neutrals is one method for increasing sensitivity[1]. Creating an ion source that can extract ions created in the large postionization laser volume is a challenge, as is eliminating background due to direct ions, while maintaining mass resolution. We introduce a method for achieving these aims with a cuboid geometry source, where the desorption axis is perpendicular to the TOF. The ions follow a serpentine trajectory through the cuboid and into an offset lens before being injected into a two-stage reflectron TOF. This allows for complete separation of the desorbed ions from the postionized signal and for exquisite refocusing of the large, uncooled ion source volume.

Methods

A microprobe-mode imaging laser desorption postionization MS (LDPI-MS) has been constructed [2]. A 349 nm laser with a ~20 μm focus was used for desorption, while postionization was accomplished with a 157 nm laser with 8 mm diameter above the sample. Along with the sample plate, a cuboid source was formed with four other electrodes, allowing for pulsed extraction and steering through a serpentine path into a conventional Einzel lens followed by a two-stage reflectron TOF. SIMION 8.0.4 was used to model this inherently asymmetric set of optics in full 3D. Cu and Mo TEM grids were used to establish the spatial resolution, and various crystalline samples established the empirical sensitivity and mass resolution of the instrument.

Preliminary Data

The entire instrument was modeled in a single full 3D potential array (PA) with 0.5 mm resolution, eliminating artifacts due to discontinuities. Nine non-ground applied potentials were used along with 36 resistively referenced electrodes, primarily reflectron rings. Full refinement of the PA on an i7 workstation typically took 1 hour. Sets of ions flown through the model show clearly the effective separation of ions originating from the surface from those of principal interest originating in the 157 nm laser volume ranging from 2-10 mm above the surface. A variety of samples were used to optimize the LDPI and test its capabilities in measuring refractory and soft materials simultaneously and to perform microprobe imaging. As in the simulation, complete separation of direct ions and the postionized neutrals is achieved. Measurement of the TEM grids gave a spatial resolution of 12 microns, limited by the desorption laser focus. N-pyrenyl maleimide, sexithiophene, and fullerenes were detected with high efficiency and reasonable mass resolution (1500 m/dm). These experimental results corresponded reasonably well to the SIMION model, and the model was used to find further refinements on the empirically optimized instrument settings. Optimization of desorption laser power was also found to allow repetitive sampling for high efficiency. [1] L. Hanley and R. Zimmermann, *Anal. Chem.* 81 (2009) 4174. [2] A. Akhmetov et al., *J. Mass Spectrom.* in press 45 (2010). (210)

Investigation using SIMION on the implementation of a cubic ion trap as an ionization chamber on a GC/LIT
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Novel Aspect

The cubic ion trap acting as an ion source is the novel element of this apparatus.

Introduction

Electronic ionization is the oldest method used for analyzing volatile molecules by GC/MS. Large data banks have been established and regarded as standards in the field. It is by far the most reliable method for the analysis of chemical warfare agents, however molecular ions are often absent. In GC/MS, the separated gaseous molecules (intact or devitalized) introduced into the source either interact with the electron beam or are self-ionized without reduced sensitivity. The aim of this work is to focus on a renewed source concept whereby an ionization cubic cell located prior to the LIT is used. Besides, gated trapping is performed to accumulate selected ions to be transferred to the LIT where reagents are introduced for specific ion-molecule reactions.

Methods

In view of testing the trapping efficiency in this system, simulations using SIMION 8 have been undertaken. The design comprises four parallel planar electrodes defining the cubic trap, four parallel circular rods defining the LIT, both sandwiched between two square electrodes. The geometry has been designed with a scale factor of 0.2 mm per gu. The electrodes of the cubic traps are ~4 mm apart and ~8 mm long. Those of the LIT define a r/r_0 ratio ~ 1.13 and are ~8 cm long whereas the dimension of the end electrodes are 8 mm by 8 mm. Ions are stored and manipulated in the traps by using DC and RF electric fields in a series of timed events.

Preliminary Data

A home-made program was written to simulate the ion trajectories through the different systems. Gating the front electrode to 10 V and maintaining the LIT float voltage ~ 10 V creates a potential trapping well in the x-direction in which ions are stored and in the y-direction, ions are trapped by the RF field generated by the parallel planar electrodes. The residence time of the ions in the cubic trap is ~10 ms, time after which the float voltage of the LIT is reduced to 0 V to allow the ions to reach the linear trap. Simultaneously, the float voltage of the cubic trap is increased to 10 V to avoid the ions from going back into the cubic trap. A light bath gas, helium, is used to translationally cool ions along the central axis of the traps to ensure ion transfer between the two ion traps through the holes drilled in the electrodes. Thus, the movement of the ions is a back-and-forth movement along the axis of the LIT. The geometry of the cubic trap has been optimized by varying the space between the planar electrodes as well as the radius of the holes drilled in the pair of electrodes perpendicular to the x-axis. The reaction time has also been varied in order to determine the time limit within which a large percent of the ions can be transferred through the hole of the electrode to the LIT. Moreover, great care has been taken for the injection of electrons in the cubic trap, which is wholly determined by the phase of the RF voltage applied to the electrodes of the cubic trap to increase the ionization efficiency. The results obtained from the simulations are promising and show the feasibility of the implementation of the cubic trap on a GC/MS

Session: WP28, Ion Sources: API **Time Slot/Poster:** 606, Wednesday, Poster Hall

Modular computational toolset for atmospheric pressure ionization method development: SIMION meets FEM
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Novel Aspect

Modular toolset for ion trajectory and ion distribution simulations which incorporate fluid dynamical driving forces and chemical reaction dynamics

Introduction

The calculation of ion trajectories using computational methods in collision free environments is a powerful tool for the development of ion optical devices, or even entire mass analyzers. In this regard, SIMION has been used over the past decades and has reached a mature state. However, trajectory calculations elevated pressures remain a challenge, due to the high collision frequency. Thus, the numerical simulation of the fluid dynamic conditions in the device geometry is required. We are presenting a toolset which uses the output of fluid dynamical simulations as input parameters for ion trajectory and ion distribution calculations. The computational results are compared with experimental data.

Methods

The FEM Package Comsol Multiphysics was used for fluid dynamical, ion distribution and chemical kinetics simulations. These simulations were performed on a Dell Precision T7500 workstation. Large scale fluid dynamical simulations of an AP ion source were performed with the Ansys CFX12.0 program package running on a Sun X2200 cluster computer system. Ion trajectories were calculated with SIMION8 using the Statistical Diffusion (SDS) Approach. The interface layer for the data exchange between the used software packages was custom designed using multiple programming languages (Java, Lua, Matlab). Experimental data were acquired using a home-built laminar flow atmospheric pressure ion source, as described in a separate contribution. Ions were generated in a corona discharge.

Preliminary Data

The primary goal of these research efforts is a reliable simulation of ion trajectories, ion concentration, and ion reaction kinetics in the presence of complex fluid dynamical gradients at or near atmospheric pressure. The ultimate idea is to simulate the behavior of entire atmospheric pressure ion (API) sources including the MS transfer region. To our knowledge, in the past such attempts were mainly based on trial-and-error.

The initial validation process of the computational approach calls for a well defined, controllable environment, which is accurately described by fluid dynamical calculations with the finite element method. Such an environment is represented by laminar flow API sources.

The initial results of the simulations clearly demonstrate the validity of the approach. The arrival time of temporally and spatially well defined ion packets, generated in the experiments upstream via laser ionization, is reproduced. Trends in the ions current density recorded at the flow tube exit as function of the position and electrical potential of a corona needle tip positioned in the center of the flow tube are also supported by the calculations.

Currently we are exploring the application of the developed toolset for geometries resulting in more complex fluid force gradients and under more complex chemical conditions. Both the calculations as well as the experimental verification of the computational results are far more demanding. Preliminary results will be presented.

Session: WP31, Instrumentation: New Concepts I **Time Slot/Poster:** 679, Wednesday, Poster Hall

Optimization of the Electrodynamic Ion Funnel for Enhanced Low Mass Transmission: Influence of Funnel Operational Pressure on Ion Transmission

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Novel Aspect

The absolute intensity of low mass ions through the dual ion funnel was increased 7X without increasing the pressure downstream.

Introduction

The use of the electrodynamic ion funnel as a replacement of the skimmer has profoundly improved the transmission of ions from atmospheric pressure conditions to the sub-vacuum interiors of the mass spectrometer. In addition, the implementation of a dual ion funnel configuration permits the use of transmission interfaces with high gas-throughputs. Much has been done by D. Smith et al. to improve the overall transmission of low mass ions, for example, reducing the distance between plates (d), installation of the jet-disruptor, increasing the exit orifice radius (p) and more. We report optimization to the dual ion funnel resulting in a 7X increase in low mass ion transmission over the standard (p/d= 1.0) ion funnel configuration.

Methods

The dependence of ion transmission on the funnel operating pressure was investigated using an Agilent 6460 QQQ equipped with a thermal gradient focusing Electrospray source and modified with the dual ion funnel. SIMION simulations were performed as well. The Agilent tuning mix (118, 322, 622,922, 1522, and 2122 Da) was used in all experiments.

Preliminary Data

Results monitoring the dependence of the relative intensity, I_{xi} , where $I_{xa} = I_a / \Sigma(I_a, I_b, I_c, \dots, I_n)$ of the 118 Da ion on the ion funnel pressure showed transmission of this ion decreased 6 folds when the pressure was increased from 3.0 to 27.0 Torr. This behavior was not observed for larger ions. Ion collision with buffer gas is generally accepted as a transmission enhancing process in most RF devices but our observations point to collision-induced "ion scattering" as a major impediment to the transmission of low mass-high mobility ions through the ion funnel. The degree of "ion scattering" increased with increasing pressure. "Ion scattering" impair transmission by increasing the phase-space and secular amplitudes of the ions especially in the decelerating fields near the funnel exit orifice. This experiment suggests that low mass ion loss occurs predominately in the high pressure ion funnel (HPIF) where the operational pressure is between 10 and 20 Torr. Consequently, measures to improve low mass ion transmission should be informed by the operational pressure of the funnel and need not be applied monolithically to both funnels as they operate at distinctly different pressures. Guided by this observation, the p/d ratio of the high pressure funnel was increased from 1.0 to 1.9. This resulted in a 7 fold signal gain for the 118 Da ions. Similar changes in p/d ratio to the low pressure funnel (≈ 2 Torr) showed negligible gains. As a result, the high pressure funnel p/d ratio was increased and the low pressure funnel ratio remained at 1.0 resulting in significantly improved low mass transmission without affecting the vacuum downstream of the MS.

A Novel, Modular Ion Mobility Drift Cell
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Novel Aspect

The modular drift cell allows drift tube ion mobility spectrometry to be introduced to a variety of commercial mass spectrometers.

Introduction

Ion mobility spectrometry is a powerful gas-phase separation technique that has been coupled with mass spectrometry for fast, high-throughput orthogonal separations yielding both ion structure and mass information. Ion mobility-mass spectrometry (IM-MS) offers analytical utility by its distinct separation of different chemical families in conformation space. The availability of ion mobility spectrometers in commercial instrumentation is limited. In order to address this, we designed a modular ion mobility drift cell that can be coupled to a variety of commercial mass spectrometers. One distinct advantage of the simplistic design of the modular drift cell is that it allows the facile coupling to tandem mass spectrometers capable of activation and dissociation of precursor ions for further structural investigation.

Methods

The modular drift cell consists of three major components: drift cell electrodes, compression flanges, and an alumina tube to establish a vacuum seal from the drift cell interior and atmosphere. The alumina tube used allows for a stacked ring electrode design with electrodes of up to 51-millimeter outer diameter. The number of electrodes and electrode geometries can be easily varied to establish a desired drift length. The compression flanges are designed from Delrin, an insulating material, mitigating the chances of electrical breakdown. The flange design contains gas inlet ports, electrical feedthroughs, and a 6" Con-flat for mating with different ion sources and instrumental platforms. The modules can also be coupled together to create a multi-section variable length drift cell.

Preliminary Data

The first prototype modular drift cell is 36.2 centimeters in length with an electrode geometry of 51-millimeter (mm) outer diameter, 8-mm inner diameter, 6.35-mm electrode thickness, and 6.35-mm spacing between electrodes. This electrode geometry is employed owing to its periodic-focusing field geometry which increases ion transmission through the drift cell. The geometry has been used previously in our laboratory on a 1.25 meter high-resolution IM-oTOF-MS. A small MALDI ion source equipped with a DC only ion funnel was designed and adapted to the IM drift tube. This device focuses the MALDI produced ions and enhances ion transfer to the ion mobility cell. SIMION simulations were performed to optimize the performance of the ion source with the modular drift cell. A 1-mm aperture is placed at the drift cell exit followed by a small electrode acting as a Faraday collector. Each ion impact event and drift time is recorded. Preliminary simulations show ion transmissions approaching 50 percent with a mobility resolution, $t/\Delta t_{fwhm}$, of 60. Ion transmission can be increased by employing a periodic-focusing DC-only ion funnel (PDC-IF) at the mobility exit rather than the aperture plate. The PDC-IF design possibilities are extensive as the number of electrodes and subsequent decreasing electrode inner diameters can be varied to change the angle and focusing properties of the funnel. Multiple designs will be tested in order to increase sensitivity albeit without a great expense in mobility resolution. The simulations will be a guide for optimum construction of the modular drift cell for its future coupling to the SE-Sciex API Pulsar Q-STAR. The instrumental set-up would allow for a variety of experiments including high resolution TOF analyses of mobility separated ions and trapping and enriching low abundance ions of interest, or mobility selected conformers, for activation and dissociation via CID.

Development of a portable mass spectrometer for operation at 1 Torr

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Novel Aspect

Mass operating at 1 Torr and with waveforms less than 50 Vpp offers unprecedented prospects for portability

Introduction

In the early 1960s, a mass filter was built and tested by Eiber, which was shown to be capable of resolving O-, O₂⁺, and O₃⁻ ions in an oxygen plasma at ~1 Torr. Eiber's filter accomplished this mass separation with a sinusoidal waveform of less than 5 Vpp! This demonstration remains the highest-pressure mass (not mobility) spectrometer tested to date. The immediate goals of this project are to reconstruct the mass filter using modern machining methods and to test/establish the mass filtration capabilities of the device using modern electronics and data-handling techniques. The long-term goals include assimilation of the filter into a complete, miniaturized mass spectrometer system with data interpretation mechanisms that could enable its use in a portable format.

Methods

Two different approaches have been used to reproduce the micro-positioned electrodes required for the Loeb-Eiber mass filter. One uses a laser-etched polyimide support through which 75 micrometer nitinol wires of cylindrical cross-section were wound to obtain a Bradbury-Nielsen-like array of wires. A second approach uses SOI-MEMS to create 25 micrometer 'wires' with square cross-sections. Simulations indicate that either wire geometry (square wires or round wires) will provide effective mass filtering on the scale of the wires. At 1 Torr, the mass filtering of ions is still less than the mean free path, which is the most unique feature of this device.

Preliminary Data

A significant number of SIMION simulations have been performed to understand the effects of ion kinetic energy and operating parameters. Simulations of mass filtering of fragment ions of perfluorotributylamine (PFTBA) show that the unexpected result that mass calibration is not quite linearly-related to the filter amplitude. As expected, the mass resolution is found to be highly dependant on the kinetic energy of the ions from the ion source and on the filtering frequency and amplitude. Simulations also verify that operation with a square instead of a sinusoidal wave is also effective. A prototype vacuum system including ion source, optics and faraday collector for operation over the vacuum range 5 Torr -1 x 10⁻⁵ Torr has been constructed, but no new data has been obtained at the time of abstract submission We will present a detailed explanation of the device, the originally-acquired data collected by Eiber, and our latest simulation and experimental results.

Numerical simulation of ion dynamics in collision multipole ion guides

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Novel Aspect

Energy/radial ion distribution of ions in collision ion guides is calculated. Collision ion guides maximum ion capacity is estimated.

Introduction

Multipole ion guide is the necessary part of atmospheric interface of any mass spectrometer equipped with atmospheric ion sources. Typically installed in millitorr region after the skimmer, the ion guide is used for the reduction of translational energy spread, collimation of the ion beam, storage of ions and transmission of ions into the mass analyzer. The objective of the present study is to calculate both the radial and temperature distributions of the ions cooled by the collisions. Another goal is to calculate the maximum capacity of the ion guide limited by the space charge of the ion cloud. The knowledge of ion dynamics provides the basis for designing ion guides of high ion transmission with well-characterized exit beam properties.

Methods

For the 2D calculation of the guide electric field and ion trajectories SIMION v.8 software was used. To increase the calculation speed, the electrostatic field was modulated and scaled as $A \cdot \cos(Wt)$ instead of using slower “fast adjust” technique. A hardsphere collision model was used for the calculations of random ion-neutral molecule collisions. To simplify the calculation of histograms, fixed time-step of the motion integration was chosen. After calculation of ion evolution over t_1 , the radius and translational ion temperature histograms were calculated until time t_2 . Similar histograms were calculated for two times smaller time steps, different initial ion position and energy, to validate the method convergence.

Preliminary Data

The ion radius histogram shows that the probability to find an ion at the axis is close to zero. For a hexapole of 4mm inscribed diameter; 2mm road diameter; 4MHz 800V RF, nitrogen pressure 40mTorr, 300oK, the 500Da ion population has the maximum at 0.28mm and drops to zero at 0.55mm. At 50oK, the maximum is 0.18mm, while at 500oK it is 0.32mm. If RF voltage is 400V, the maximum is 0.38mm. The distribution is nearly the same for mass range 100-1000Da. Lower frequency corresponds to smaller radius: 0.18mm at 2MHz and 0.35mm at 6MHz. The distribution is nearly independent of pressure of 20-80mTorr. The distribution of ion translational energy depends on the buffer gas temperature. At 300oK, the average ion temperature is above 600oK with a long tail above 1500oK. Ions of high translational energy are colliding with room temperature nitrogen, and the probability of energy transfer into molecular bond vibration is low. This provides a possible explanation of the absence of ion thermo decomposition. Energy distribution is almost independent of voltage, frequency, ion mass and pressure. The maximum capacity of an ion guide is important parameter both for storage and transmission modes. A large number of ions create a repulsive force that increases the size of an ion cloud. If the guide is filled almost to the capacity, an addition of one more “test” ions result in the unstable motion that takes place at radii close to inscribed radius of the ion guide. The electric field there is independent on unknown space charge distribution and is $\sim 1/r$. The trajectory of the “test” ion is calculated while the ion population per unit length is increasing, until the ion ejection. The final population gives the estimate for the ion guide capacity.

Accelerated Trajectory Simulations for SIMION with a Beowulf Cluster

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Novel Aspect

By accelerating SIMION computations by several orders of magnitude, we have made the computationally-intensive problem of design optimization more practical.

Introduction

The commercial ion optics tool SIMION(TM) is a common workhorse for the design of ion optics for mass spectrometers (MS). SIMION calculates electrostatic or radio-frequency (RF) electric fields given a set of electrodes with prescribed voltages, and it calculates trajectories of ions through the resultant field. In principle, SIMION can be used as a front end in which field solutions or ion trajectories are calculated by a separate program. We take advantage of this feature to perform field and trajectory solutions separately using a custom-developed parallel software code. Our code allows us substantial speedup in trajectory simulations over what can typically be attained using SIMION alone on a standalone Windows desktop computer.

Methods

Our code is written in Python and MPI-parallelized Fortran 2003 and has been run on our 128-core Beowulf cluster. It calculates ion trajectories, given field solutions provided in SIMION format and initial ion conditions provided separately. Results presented here do not include mutual Coulombic repulsion of ions (i.e. space charge), but our code is designed to allow the inclusion of this effect. Without space charge effects, calculating multiple trajectories is easier to parallelize. We implement a master-slave model in which the master maintains a queue of trajectory initial conditions (ICs) and distributes these ICs to waiting slaves. Full trajectories can be stored, but typically the user specifies a limited number of parameters to be returned from each trajectory integration.

Preliminary Data

Our code running on our cluster demonstrates substantial speedup over SIMION running on a typical desktop Windows PC. Our worst-case scenario uses methods for electric field interpolation that mirror those of SIMION, and fourth-order Runge-Kutta integration with time steps very conservatively designed to undercut SIMION time steps for a given quality factor. This results in a speedup of 50x. We have also implemented different interpolation schemes and integration methods which substantially improve on this figure. These methods are described in detail below. As a demonstration of the utility of this speedup, we optimize a Wiley-McLaren TOF with Mamyrin reflectron, with fixed geometry and five independent parameters for the prescribed voltages. Optimization is performed using a modified Nelder-Mead downhill simplex optimization algorithm similar to the optimization algorithm provided by SIMION. Optimization is performed first in 1D and then in 2D axisymmetry with fringing fields. The use of our code accelerates optimization by two orders of magnitude, potentially making optimization substantially less daunting of a task.

Development of Tripole-Multipole Rotational Ion Mobility Mass Spectrometer by Ion Simulations

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Novel Aspect

The combination of tripole and multipole for ion mobility mass spectrometry showed a large ion separation capability in short length.

Introduction

The generation of a large difference in the drift time of ions is important for the ion separation with an ion mobility mass spectrometer (IMMS). We have developed a new ion optics, tripole, and the tripole shows a long ion flight distance in short electrodes due to the rotational ion trajectory in it. In this work, we constructed the tripole rotational IMMS (RIMMS) by the combination of the tripole and IMMS. In addition, the tripole-multipole RIMMS was developed by the multipole insertions in the tripole RIMMS. For these RIMMS, we investigated the capabilities for ion separations and the effects of the multipole insertions by ion simulations.

Methods

The drift tube used in this work has a length of 99.6 mm. The ring electrodes with an internal diameter of 21.6 mm and a thick of 1.2 mm were placed at 2.4 mm intervals in the drift tube. RF voltages of tripoles and multipoles were 125 V and over 125 V, respectively. The frequency of 0.4 MHz was applied to all electrodes. The phase differences between in-plane adjacent electrodes and between front electrodes were 120 degree and 0 degree, respectively. The drift tube contains He gas at a pressure of 0.5 Torr. The drift time was simulated for ions with m/z 200 to 1000. The simulations were performed by SIMION 8.0 software.

Preliminary Data

Our simulations indicated that smaller m/z ions flew with longer drift time in the tripole RIMMS, which is an opposite trend to a typical IMMS. The comparison of drift time for ions with different charge states, $z = 1$ and 2 at m/z 275, showed a time difference of about 300 μs . For the separation of variously-sized ions, a flight of an m/z 250 ion with a collision cross section of 95 \AA^2 and 105 \AA^2 gave average drift time of 450.4 μs and 487.5 μs , respectively. The tripole RIMMS has a large ion separation capability, considering short drift tube length. We also investigated the effects of multipole insertions on the ion separation. In the case of the drift tube placed a tripole and a hexapole alternately, as with the tripole RIMMS, longer drift time was obtained for smaller m/z ions. The introduction of the foregoing m/z 250 ions in the tripole-hexapole RIMMS resulted in an average drift time difference of 35.1 μs , which was similar to that obtained by the tripole RIMMS (37.1 μs). In contrast, the hexapole insertion enabled to measure the drift time of lower m/z ions which could not be estimated by the tripole RIMMS. The RF voltage was another possible factor for enhancing the ion separation capability as ion flight was controlled by the change in the RF voltage of hexapoles. However, little difference in the drift time was obtained by the increase in the voltage from 125 V to 500 V. The RF voltage is less effective in the ion separation in the RIMMS.

A tightly curved collision cell with high MSMS efficiency

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Novel Aspect

A solution for making tightly curved collision cells with efficient performance at higher energies for a wide mass range

Introduction

RF multipole collision cells are ion guides filled with a neutral gas and are used to perform the function of MSMS in tandem mass spectrometers, particularly in triple quadrupole mass spectrometers. A curved collision cell is one where the ion flight path is curved rather than straight such that there is no line-of-sight between the ion entrance of the collision cell and the ion exit. Curved collision cells have the advantage of providing a line-of-sight separation of the neutral noise, large droplet noise, or photons from reaching the second mass analyzer and detector. In addition, they allow folding the ion paths of tandem mass spectrometers and enable smaller instruments.

Methods

The idea (patent pending) is to apply a deflecting DC electric field along the radial direction of a curved collision cell to compensate the radial energy of the parent ions. This radial DC field has a gradually decreasing magnitude along the ion flight path. As a result, parent ions that lose energy as they collide with gas molecules are optimized by a gradually decreasing deflecting electric field. On the other hand, the product ions, which are formed later and further down along the collision cell path have lower kinetic energy but experience a lower deflecting electric field and their transmission is also optimized.

Preliminary Data

We apply a radial DC along with the RF electric field on the collision cell. The radial DC field magnitude is a function of the kinetic energy of the parent ions, with an initial value calculated as described previously [1]: The rate of decrease of the deflecting radial field is also a function of pressure, temperature, and the collision cross section between the parent ion and gas molecule. For fixed collision cell geometry and collision gas type and pressure, we can use an exponentially decreasing deflecting field to provide good transmission for a wide range of parent and product ions. Preliminary results of ion trajectory simulations using the SIMION package consider a Patent pending partially segmented curved RF collision cell with radial DC field applied on the outer, segmented pair of rods, with gradually decreasing magnitude. As an example, for a curved collision cell with rods of square cross section, r_0 3 mm, curvature radius 60 mm, and at a collision energy of 100eV, the optimum initial radial DC deflection voltage is 16.8 V. The DC voltages applied on the subsequent outer segments are 30% less than on each previous segment. For a MSMS transition 800 \rightarrow 100 Da at 100eV with Ar at 0.25 Pa, ions are nicely contained and guided along the curved path for a q-parameter of 0.04 for the parent and 0.3 for the product ion. Despite the relatively high energy, low q, and the tightly curved path, the simulated CID efficiency is \sim 30%, about 6x better than in the absence of the radial deflecting DC field. References: [1] Felician Muntean and Urs Steiner, "Curved ion guide and related methods", US Patent application 20090294663, Varian Inc. 2009.

A new linear quadrupole ion trap with axial ejection.
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Novel Aspect

A novel geometry linear ion trap with mass-selective axial ion ejection at low ion exit energies.

Introduction

Linear quadrupole ion traps are viable either as stand-alone mass analysers, or incorporated into hybrid instruments. The linear ion path afforded by axial ejection is particularly suited to hybrid geometries, however it is desirable that the LIT can still be operated in conventional ion-guide and quadrupole analyser modes. Here we present theoretical and experimental results from a new design of quadrupole-LIT with mass-selective axial ejection that requires no geometrical modifications to a standard quadrupole, thus normal quadrupole modes of operation are not compromised. Unlike existing methods, ejection is not due to coupling with RF fringing fields, hence the low axial kinetic energy of ejected ions, which is advantageous for coupling to further analysers in a hybrid instrument.

Methods

The device was implemented in the third quadrupole of a triple quadrupole geometry instrument. No physical changes were made to the quadrupole assembly, the existing post-filter was used to apply the axial barrier. The electronics were modified to allow a supplemental AC voltage for dipolar excitation, and to allow the various barrier voltages to be controlled appropriately. A bleed valve was used to control the gas pressure in the LIT. Simulations of the device were performed using SIMION 8. In addition to initial feasibility tests, this allowed the calculation of ion exit kinetic energies, and enabled comparison to other LIT geometries.

Preliminary Data

Experimental data has been obtained for various modes of operation of the device. In a slow 'zoom-scan' mode high mass resolutions have been demonstrated (>20k). The effect of scan speed has been examined. A comparison of daughter ion spectra between the trap mode of operation and the conventional scanning quadrupole mode show an improvement in sensitivity of greater than 2 orders of magnitude. Manipulation of the trapping voltages allows an estimate of the trapping and extraction efficiencies, and the overall transmission efficiency. The limited control of experimental voltages and gas pressures means that significant improvements could be made to the experimental configuration of the instrument. SIMION calculations demonstrate significantly higher transmission efficiencies are possible. Theoretical calculations of the exit energies confirm the low energy nature of the ejected ions. In contrast existing methods, which rely on the interaction of the ions with an RF fringing field to eject the ions, result in high exit energy ions.

A Digital Linear Ion Trap based on Ceramic Printed Circuit Boards
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Novel Aspect

A new linear ion trap fabrication method used for making ceramic PCB ion trap which is tested with digital driving waveforms.

Introduction

A linear ion trap (LIT) can be made in various forms, eg, with four hyperbolic rods, four planar metal plates (RIT) or the one made of printed circuit boards (PCBs). The PCBs linear ion trap may lead to the low cost production and allows field adjustment after production, while enjoys the common advantage of larger charge capacity. Considering ceramic plates have much higher mechanical strength than epoxy resin PCBs, a ceramic PCB ion trap was designed and its fabrication process was investigated. The ion trap analyzer, including ion detector has been optimized using SIMION 8.0 and experimentally tested with an ESI source.

Methods

The electrodes on the surface of ceramic were divided into 3 parts, middle, side and ground, made by coating the ceramic with thick film of silver. RF potential on side-electrodes is certain percentage of that on middle-electrodes, so that quadrupole field was formed inside of ceramic trap and adjusted through high order field variation. A Burle Channeltron with 6.8mm id, is used as detector. In order to obtain higher detection efficiency, the ion detector was designed to enable strong focusing for the ejected ions. Screen-printing and masked spray were respectively used for metal layer electrodes fabrication. High voltage high frequency switches are used to generate digital waveform for driving the trap and resonance ejection was used in mass scans.

Preliminary Data

In simulation work, driven by digital square waveforms, we have obtained resolutions over 5000 under 1588Th/s and over 7000 under 159Th/s, with detection efficiency of 47% and 22%, respectively. In experiment, the ceramic LIT was operated under digital waveforms. With the prototypes made with grooved ceramic substrate structure and silver sintering metallization, we reached the sensitivity of Limit of Detection of reserpine/ESI: 0.1119pg/uL with S/N ratio 241 in full scan MS mode and 67 in full scan MS-MS mode. With the latest configuration, the MS can be run from below 18Th to a high mass end of 5900Th and the mass range for MSMS (precursor: human insulin 2+ 2908Th) reaches 3425Th. Mass resolution of 6000 at scan speed of 500Th/s and resolutin 5000 at 2000Th/s, by using Fibiuropeptide A+ 2H₂⁺ (766.6Th) under +/- 300V digital waves, has been obtained. The relation between resolution and corresponding potential division percentage was investigated and compared with the simulation results. The peak intensity as well as the dynamic range has also been studied. Other experiments, such as sensitivity test and MS-MS with peptide sample have also been operated.

Short-Pulse Ion Extraction from a Quadrupole Ion Trap into a Time-of-Flight Mass Spectrometer for Trapped Ion Cloud Diagnostics

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Novel Aspect

Short-pulse extraction provides a narrow energy spread and a convenient diagnostic for the size of the trapped ion cloud.

Introduction

The combination of a quadrupole ion trap (QIT) with a time-of-flight (TOF) mass analyzer is desirable in many tandem mass spectrometry applications. However, the non-parallel field inside the QIT distorts the ion extraction for TOF-MS or for reaction kinetics experiments using the extracted ion packet. We investigate the extraction pulse type and timing via simulations and experiments. Wiley-McLaren spatial focusing can be used in a linear TOF instrument to obtain best resolution at the expense of broad energy spread of ions. We report a new short-pulse extraction mode that minimizes the energy spread. This mode is shown to be useful for diagnosis of ion cloud size and distribution inside the QIT.

Methods

Ions are generated externally using electrospray ionization, then trapped and thermalized in the QIT. The ions are extracted from the QIT into the linear TOF region using monopolar or bipolar pulses on the endcap(s). The extraction mode may be conventional long pulses or else short pulses that turn off before any ions exit the trap. SIMION is used to model the instrument and pulses and to simulate the times-of-flight. A separate program written in FORTRAN is utilized to account for the distribution of ion positions and velocities. The program employs a Monte-Carlo sampling of initial ion positions and velocities, with the times-of-flight obtained from SIMION. The simulated TOF peak profiles are compared with experiment.

Preliminary Data

To investigate the effect of non-parallel fields inside the QIT, simulations are performed for the actual hyperbolic geometry and for idealized parallel-plate geometries of the end-caps. Plots of TOF versus extraction amplitude provide the absolute TOF and Wiley-McLaren spatial focus conditions. Deviations from the parallel fields are especially severe for the monopolar extraction mode (ion entrance end-cap grounded) compared with bipolar extraction (equal and opposite pulses on both end-caps). Experiments under the same conditions match the simulated absolute TOF and spatial focus voltages. Two different mass ions, tetrahexyl ammonium ion ($m/z=354$) and tetraoctyl ammonium ion ($m/z=466$) yield similar peak resolutions and spatial focus conditions. The more highly curved field inside QIT in the monopolar mode focuses a larger radial portion of the ion cloud onto the detector, giving higher signal intensity compared with the bipolar mode. A second Einzel lens was added in the TOF chamber to re-focus the ions in the bipolar mode. In the long-pulse extraction mode, the ion energy spread is around 100 eV. This can be reduced to 1 eV by using the short-pulse extraction mode, for which all of the ions receive nearly the same acceleration. A narrow energy distribution is desirable for energy-resolved ion-molecule reactions using the ion packet. TOF peaks simulated for short-pulse mode reflect the broad TOF distribution indicating the absence of spatial focusing. These peaks show different shapes and widths for assumed initial Gaussian versus uniform distribution and size. Thus, the comparisons of experimental peaks with simulated peaks provide the ion-cloud size and distribution in the QIT. Experiments performed at various ion abundances yield Gaussian type distribution of ions with axial extents of 1.2 to 2.6 mm (fwhm), which are comparable to previous reports using laser photodissociation tomography methods.

Kinetic energies of ions ejected radially from LIT at high q .

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Novel Aspect

Kinetic energy distributions for ions exiting LIT under $\beta=2/3$ conditions for a variety of geometries and experimental conditions.

Introduction

Fundamental properties of resonant ion ejection have been studied both experimentally and theoretically, for 3D and 2D linear ion traps. It has been shown that kinetic energy (KE) of ions exiting the ion trap is dependent on ejection conditions, such as the q value of the resonant excitation and its amplitude, presence of slots and other sources of high order field components, collision gas type and pressure, and ion properties. It is known that low q ejection results in low energies of ejected ions. The goal of this work was to study experimentally the KE distribution at an ejection $\beta=2/3$ for various geometries and ejection conditions. Simulation of experiments was run in parallel using SIMION package.

Methods

Experiments were performed on a modified LTQ system equipped with a nano-spray ion source. Several modifications of the ion trap geometry were studied including the standard LTQ trap with a balanced RF field and an unbalanced RF field, a trap with an ideal geometry (no stretch) and with a smaller slot depth, and covering the slot with a mesh. KE were measured using a three-electrode assembly mounted in close proximity to the slot. Transmission curves were acquired by scanning a stopping potential on the middle electrode. Effects of a various factors affecting KE of ejected ions were investigated, such as geometry, phase shift between the main and auxiliary RF, resonance ejection amplitude, charge state of ions and collision gas pressure.

Preliminary Data

Compared to a 3D ion trap, use of a balanced RF in a 2D LIT results in significant modulation of ion kinetic energy while ions travel between the slot and the three-electrode lens assembly. Simulations clearly show that ion energies may enter into the several keV range because of this effect. The width of the kinetic energy distribution was shown to scale proportionally with the average energy. The effect is more pronounced for ejection conditions when ions leave the ion trap with low energies, and due to the RF phase changes significantly during slow ion travel to the area not affected by RF field, creating a whipping effect. Removal of RF voltage from slotted electrodes (only auxiliary dipole excitation voltage applied), resulted in significant, up to three-fold, reduction of both average energy and its distribution width. Further experiments were performed using a more ideal ion trap geometry: hyperbolic shape RF rods, $R_0=4.00$ mm, no stretch, slots covered with 500 lines/inch mesh. While the electric field inside the ion trap was not perfectly quadrupolar (unbalanced RF resulting in additional higher-order term), this geometry was shown to provide significantly lower kinetic energies (more than factor of 2) of exiting ions. Kinetic energies of the ions studied was typically in the range 0.04-0.2 keV. Meantime, mass resolution was degraded compared to the stretched, no-mesh geometry. Kinetic energies of ions also depend on the charge state, z , going up with z however not linearly. Distributions for $z = 1, 2$ charge states of Angiotensin II and $z = 2, 3$ of Insulin, chain B, oxidized were investigated. The phase relation between the main RF and the auxiliary voltage affects both transmission and the kinetic energy distribution.

Session: ThP28, Instrumentation Quadrupoles and Traps **Time Slot/Poster:** 662, Thursday, Poster Hall

Optimization of Multipole Components in a Planar Paul Trap

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Novel Aspect

A novel method for adjusting the multipole components in the electric field of a planar Paul trap is presented.

Introduction

Electric field plays an important role in determining the performance of an ion trap mass analyzer. The electric field of a trap includes monopole, dipole, quadrupole, and higher-order multipole components. Among them, the quadrupolar field and two other higher-order field components (octapole and dodecapole) are of critical importance. For optimizing the electric field in a conventional ion trap, the adjustment of these multipole components is generally realized by changing its geometry. This process is time consuming, and multipoles cannot be modified independently. In this study, a novel method is proposed to change the multipole components (octapole and dodecapole) inside an electric field, and the effect of the multipole components on performance of a planar Paul trap has been investigated systematically.

Methods

The electric field within the trap was analyzed by using the ion optical program SIMION, and the multipole expansion coefficients were obtained through a least-squares fit in MATLAB program. For a certain multipole component, the voltages to different rings were calculated via the SOLVER function in Microsoft Office Excel. The ions with different mass-to-charge ratios from benzene, dichloromethane, toluene and butylbenzene were used to evaluate the effect of multipole components (e.g., octapole and dodecapole) on the performance of the planar Paul trap. Also, the effect of sample concentration in the trapping region was investigated.

Preliminary Data

The contribution of the multipole components of each ring was first obtained by combination of the SIMION simulation and MATLAT calculation. Then the desired relative weights of multipoles including octapole (A_4/A_2), dodecapole (A_6/A_2) and others can be easily obtained by changing the applied voltages to different rings through the SOLVER function in Microsoft Office Excel. The change of the voltage to each ring is performed by adjusting the capacitor values attached to the ring. By using this method, the quantity and sign of the multipoles can be easily adjusted. The experimental demonstration of the effects of the octapole percentages, ranging from -8.0% to 8.0%, and dodecapole percentages, ranging from -6.0% to 12.0%, on the performance of the planar Paul trap is also presented. In addition, the results illustrate that the sample concentration inside the trapping region has a great effect on the performance of the planar Paul trap with the change of octapole and dodecapole percentages.

Miniaturization of an axially focusing linear ion trap for mass spectrometry.

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Novel Aspect

Characterization of miniaturized axially focusing linear ion traps.

Introduction

A miniature linear ion trap (MLIT) with tubular end cap lenses has been developed allowing compact ion focusing in both the axial and radial planes, this contrasts with the broader axial confinement more conventionally performed in linear ion traps. A study of methods allowing collisional focusing of ions and their ejection has been undertaken on a fabricated MLIT. The role of parameters (such as MLIT electrode shape and size) that would allow further miniaturization of the MLIT has been studied theoretically.

Methods

A MLIT has been fabricated with 15mm long quadrupole rods and tubular end cap lenses. These end cap lenses have 5mm long tubes penetrating 3mm into the quadrupole volume. A QqTOF (MDS Sciex) has been heavily modified and the MLIT has been introduced following a shortened LINACTM (MDS Sciex). The ions are transferred into the MLIT from the LINACTM where they are focused by collisional cooling with He in the radial pseudo-potential well and the axial potential well. The MLIT and different parameters on the QqTOF are controlled by a program written in LabView. Simulations have been performed using Simion 8.0.

Preliminary Data

Characterization of a fabricated MLIT

Characterization of a MLIT has been performed by modification of a QqTOF mass spectrometer. Introduction of ions into the ion trap from a LINACTM are undertaken in 20-35 μ s. Focusing of the ions in the MLIT allows ion packet sizes comparable with a 3D ion trap of less than 1mm in both the radial and axial planes. Ion ejection can be performed with narrow kinetic energy distributions of less than 1V (determined using a retarding grid).

Characterization of parameters including electrode shape and size which would allow further miniaturization

MLIT electrode shape

The change in the shape of MLIT electrodes from cylindrical to rectangular allows the possibility of the use of microfabrication techniques. The characterization of ion packet sizes and the transfer of ions between ion traps have been compared for MLITs with rectangular and cylindrical electrodes.

MLIT size

The role of the MLIT size has been studied for quadrupole electrodes lengths of 15mm to 0.15mm. The conditions allowing focusing of ion packets in the MLIT as a function of the voltages applied to the electrodes and the helium gas pressure necessary for collisional cooling have been determined. The transfer of ions between a series of ion traps has also been characterized for the sub-millimeter quadrupole electrode MLITs.