Influence of an ion trap geometry on its trapping efficiency

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Abstract

In this work we have studied the influence of holes in the radiofrequency ring of an ion Paul trap on its trapping efficiency using simulations with the Simion software. Different geometry of the trap holes were considered and the results of the simulation are compared and analyzed in this paper.

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Contents

1 Introduction

Mass spectrometry, the science and technology of gaseous ions, has as its basis the measurement of the mass-to-charge (m/z) ratio of ions [1]. All atomic and molecular ions are, in principle, accessible by mass spectrometry, making it a universal method for chemical analysis. The simulated radiofrequency (RF) ion trap, nowadays often referred to as Paul trap, in honor to the inventor and Nobel laureate Wolfang Paul, is part of a tandem mass spectrometer. The main purpose of the Paul-trap is to increase target density to allow for studies of radiation with gas-phase ionic biomolecules [2]. The whole setup is portable and can thus be interfaced with external ionizing radiation sources. It can be interfaced with photon beamlines of third generation synchrotron facilities, such as BESSY II in Berlin and PETRA III in Hamburg, as well as free-electron laser beamlines.

In our group we study characteristics and structure of the biomolecules, where they occur and what they do. knowing the structures and the changes occurring in them is an important way to understand the function of biomolecules and therefore their role in the life cycle. One approach to reach this task is to determine their structure, as single molecules or assembled into aggregates. Small angle X-ray scattering is the most important method for this purpose. Therefore, it is important to know the influence of the trap holes on the trapped gas phase biomolecules.

At first, we need to increase the size of the hole in the trap. Why do we need this? It will influence on the fields in the trap. We want the bigger hole, such that when we radiate with photons, the light which scattered on the molecules can come out. It will be the first experiment on the gas phase, instead of diffraction of crystal structures.

In this report, the main features of the Paul trap and simulations with the SIMION software are discussed.

2 Experimental part

The experimental setup is presented in the Fig. 1. Gas-phase molecular ions are produced by an electrospray ionization source (ESI) and stored in an ion trap. As shown in Fig.1, the electrosprayed ions enter the first vacuum section of the setup through a small capillary tube. After being transported and phase-space compressed in an ion funnel and an RF-only octopole ion guide, only the ions with a selected m/z ratio (where m is the mass in a.m.u. and z is the charge state of the ions) are transported through a quadrupole mass filter. Then the mass-filtered ions reach the entrance of the RF ion trap with an electrostatic lens system. A helium buffer gas is introduced into the trap to cool down the kinetic energy of the ions and enhance the trapping effiency. The content of the trap is then extracted into a time-of-flight mass spectrometer and recorded on a micro channel plate (MCP) detector.

2.1 RF-ion trap

The radio frequency Paul trap is a type of ion trap that uses dynamic electric fields to trap charged particles. The trap is also called "radio frequency" trap because the switching rate of the oscillating electric field.

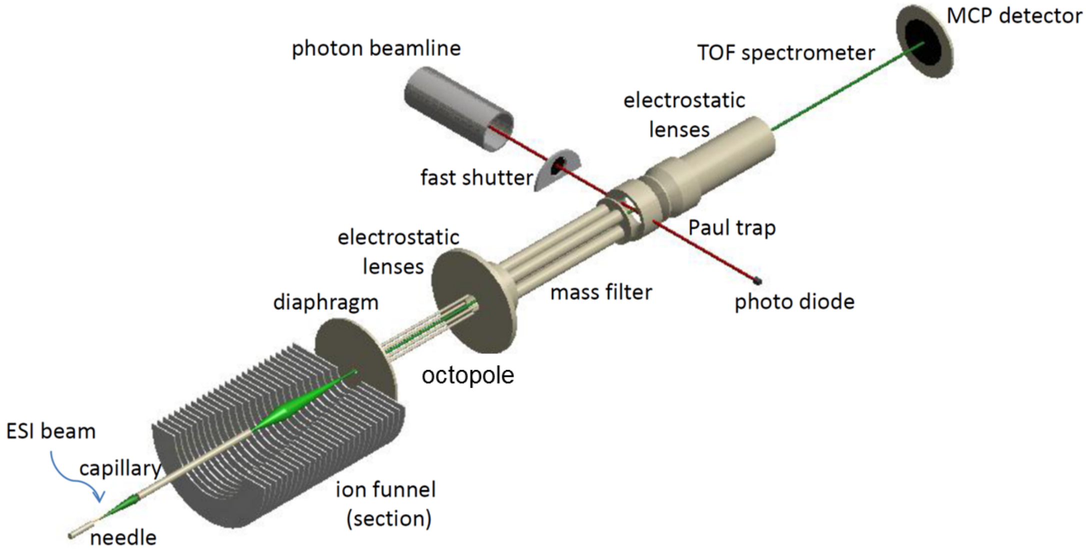

Figure 1: Experimental setup

The quadrupole is the simplest electric field geometry used in such traps. The electric fields are generated from electric potentials on metal electrodes. The ion trap consists of three electrodes with hyperbolic surfaces, the central ring electrode, and two adjacent end-cap electrodes. The picture of the assembly shows how the electrodes are aligned and isolated using ceramic spacers and posts. The device is radially symmetrical, as shown in Fig. 2 and in Fig. 3.

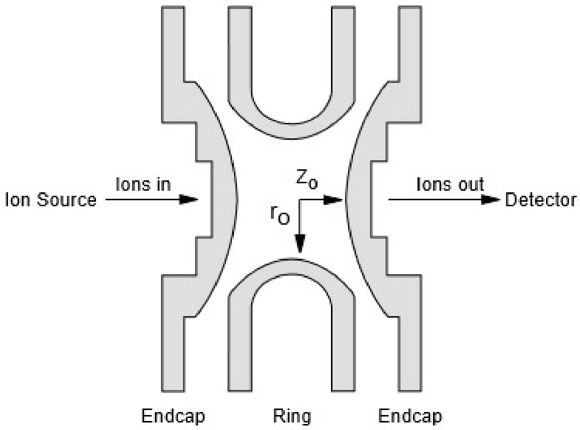

Figure 2: Schematic view of the ion trap

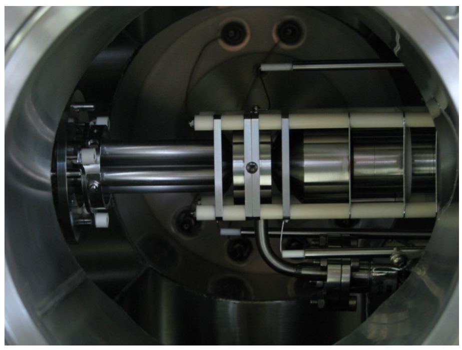

Figure 3: Picture of the Paul trap inside setup

A three-dimensional radio-frequency field is created in the quadrupole ion trap, which holds the ions. In the trap, the radio frequency voltage for the capture and retention of ions is applied between the end and ring electrodes. Paul traps confine charged particles without applying any magnetic fields. Radio frequency ion traps do this by forming a potential with a saddle point (which confines the particle in all but one direction), and then changing the unstable direction by applying a sinusoidal potential to the the electrodes, as shown in Fig.

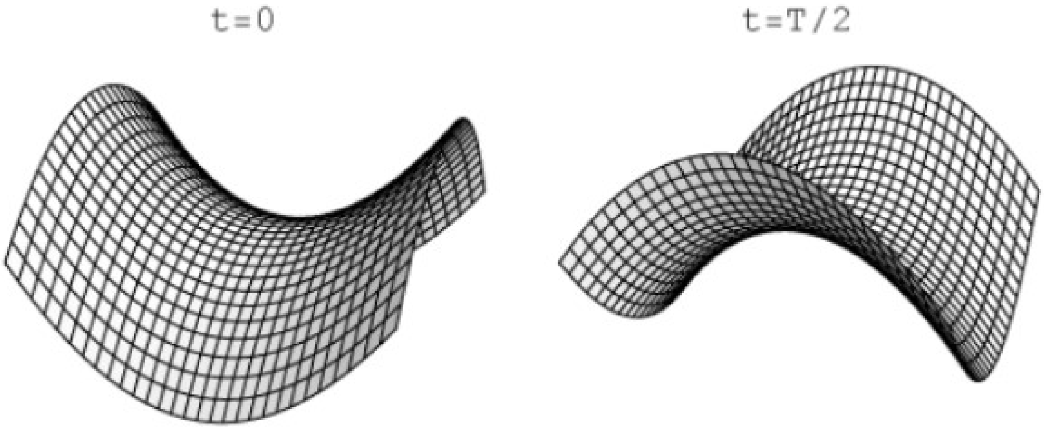

Figure 4: The potential with a saddle point

In the figure the particle is first confined in the left-right direction, and in the second half of the period becomes confined in the perpendicular direction. So, the particle is always confined in one direction and unstable in the other direction, and theses stable and unstable directions are interchanging constantly with a high enough frequency to prevent the particle from escaping. So, the only critical feature of a confining potential is having a saddle point. There is no restriction on the shape of the electrodes as long as they form a potential with a saddle point.

A three-dimensional representation of an ion trajectory in the ion trap, as shown in Fig. 5, has the general appearance of a Lissajous curve or figure-of-eight composed of two fundamental frequency components of the secular motion [3].

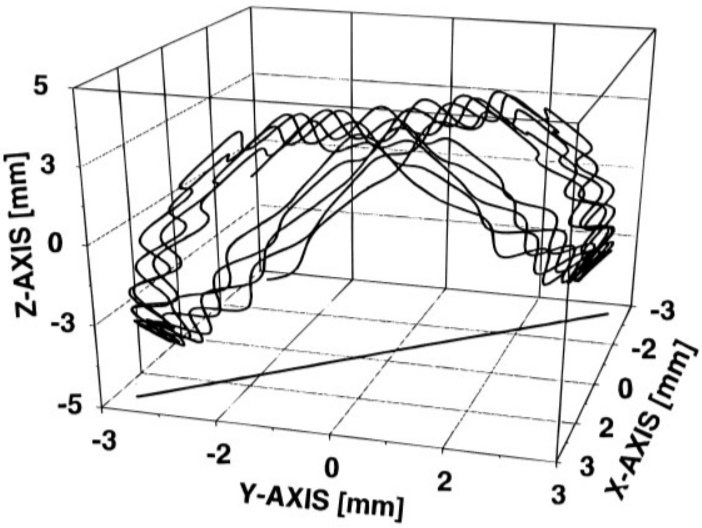

Figure 5: Trajectory of a trapped ion

As shown in the Fig. 3, the ring electrode has four holes used for the injection of the He gas in the trap and to allow the photon beam going through the trap for irradiating the trapped ions.

3 SIMION 8.1

We have used the program SIMION for simulations. Ion and Electron Optics Simulation Package (SIMION) was developed in 1973 by Don McGilvery, and in 1986 David A. Dahl developed it for the PC [4]. SIMION is a software package primarily used to calculate electric fields and the trajectories of charged particles in those fields when given a configuration of electrodes with voltages and particle initial conditions, including optional RF (quasistatic), magnetic field, and collisional effects.

In SIMION, electrode shapes can be custom made by entering them into a potential array (.pa of .pa#) file. When entering the electrode shape manually, the user must first define the dimensions of the array in grid units (gu) and whether the array will have planar and/or cylindrical symmetry. When creating a .pa# file, electrodes can be given different numbers that can refine the array.

Also, the user can control the number of particles as well as the mass, charge, initial position, initial velocity, and the start time of the particle. As the field is recalculated at each time step, a particles position and velocity are also recalculated with the effects of the electric field. The user can also control if another particle is simulated after the current particle splats on an electrode surface or array boundary.

For outputting data, the user may select variables for data output by using either the graphical user interface (gui) or the user program. The gui can be used to record data for the flight time, mass, charge, position, velocity, and acceleration of the particle as well as the electric potential and field that the particle experiences. The user program can also be used to record this data as well as any of the variables used in the user program and other reserved variables. The recorded data can either be saved in the same location as the simulation file or in another location.

3.1 Geometry

In the first case, we have used a symmetric geometry with respect to location of electrodes and size of the holes, as shown in Fig. 6. Then we have increased one of the four holes, as seen in Fig. 7. Results of such simulations are mainly sketches of trajectories for investigated cases (green lines) and small red dots are place where the ions splat.

Simulations included the following: observing the parameters affecting trapping and keeping of an ion cloud in the center of the trap.

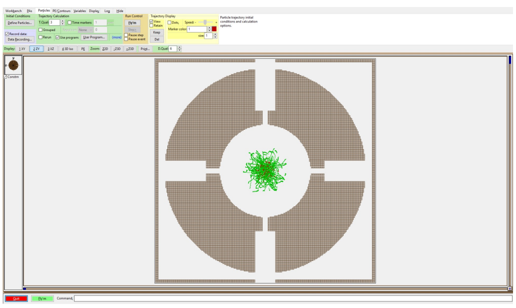

Figure 6: Example using SIMION with symmetric holes in the ring electrode

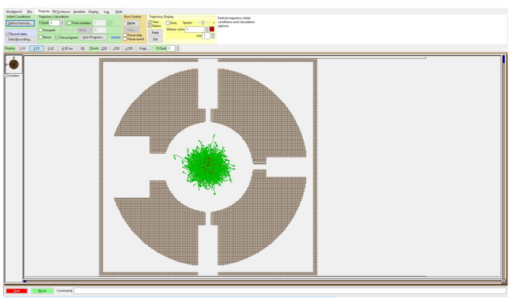

Figure 7: Example using SIMION with asymmetric holes in the ring electrode

In the Fig. 8 we can see 3D view of the Paul trap in SIMION, where the end-cap electrodes are displayed in yellow and the central ring electrode in green.

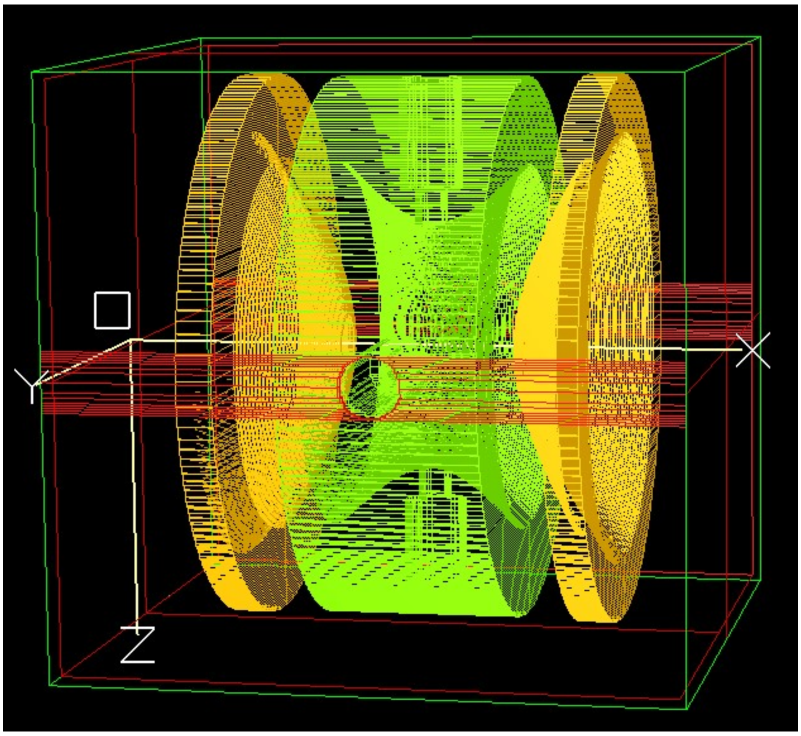

Figure 8: 3D view of the Paul trap

Besides defining the geometry of the electrodes, it is necessary to describe the parameters of the experiment. Such as frequency, temperature, pressure and mass of the gas. These parameters are shown in the table 1.

Table 1: Parameters of the experiment

Parameter	Value
RF-frequency	1 (MHz)
RF-voltage	700 (V)
Gas pressure	$10^{-}4$ (mbar)
Temperature	300 (K)
Mass of cooling gas particles	4 (u)

3.2 Simulation results

As a result of simulation of symmetric geometry, particle distributions from the coordinates in the ion trap were obtained. The results of the simulations for geometries with large and small radii are given below, in the Fig. 9 and in the Fig. 10. As shown in the picture, black square denotes the hole with radii 11 and 5, red circle denotes thr hole with radii 33 and 15, blue triangle denotes the hole with radii 55 and 25. The distributions have the form of a Gaussian and as can be seen from the

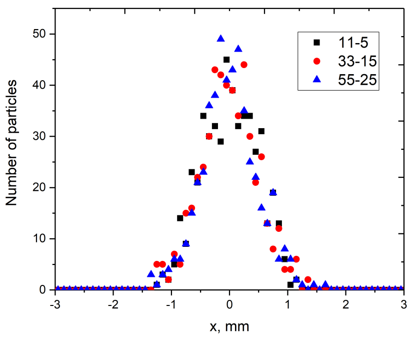

Figure 9: The distribution of the number of particles along the x coordinate (symmetric geometry)

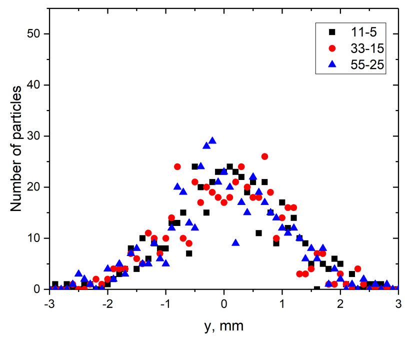

Figure 10: The distribution of the number of particles along the y coordinate (symmetric geometry)

these pictures the distribution on y is two times larger than x, because of the shape of the potential well.

The particle distributions along the coordinates for traps with large radius have also been approximated by the Gauss function, the parameters are given in the table 2.

Table 2: Parameters by approximation the Gaussian function

The radius of large aperture	The radius of small aperture	Half-width	Amplitude
11	5	1.2507	51.83314
22	10	1.01243	49.5432
33	15	1.11358	49.2653
44	20	1.18587	50.44933
55	25	1.02182	48.07212
110	50	1.1137	48.93456

Next it was interesting to transform the value of the small aperture from mm to angular degrees. Knowing the relevant parameters, such as the length from the center to the hole, the radius of the hole, as seen in Fig. 11, we can easily calculate the angle by using the formula $tg(\alpha) = r/L$. The table 3 shows the corresponding values.

Table 3: Values of small hole size and angles

The radius of the small aperture	The angle
5	13°
10	25°
15	37°
20	48°

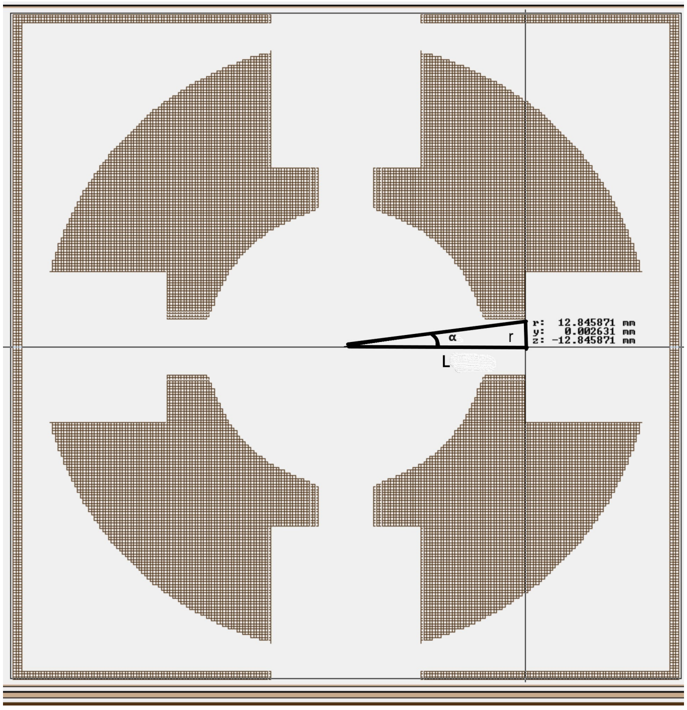

Figure 11: Example of calculating the angle

After this, an asymmetric geometry was created, in which one of the four holes was larger. Using this geometry, we obtained the distributions, as shown in Fig. 12 and Fig. 13. In these pictures black square denotes the three holes with radii 11 and 5 and one hole with radii 22 and 10, red circle denotes the three holes with radii 11 and 5 and one hole with radii 33 and 15, blue triangle denotes the three holes with radii 11 and 5 and one hole with radii 55 and 25.

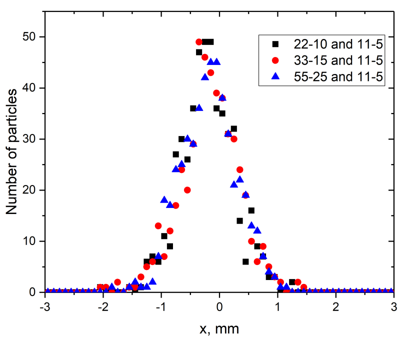

Figure 12: The distribution of the number of particles along the x coordinate (asymmetric geometry)

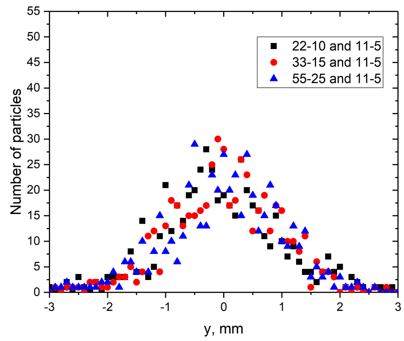

Figure 13: The distribution of the number of particles along the y coordinate (asymmetric geometry)

4 Conclusions

Our results show that even large holes in the RF ring of the Paul trap doesn't significantly affect the ion cloud dimension in the trap. Such modification could then be achieve experimentally to perform Small Angle X-ray Scattering on trapped biomolecules.

5 Acknowledgements

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