Simulations of Electrode Misalignment Effects in Two-plate Linear Ion Traps

Qinghao Wu, Yuan Tian, Ailin Li, Daniel E. Austin

Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT 84602, United States

Corresponding author Daniel E. Austin, email austin@chem.byu.edu

Abstract

Electrode misalignments in linear ion traps have a strong effect on performance but are hard to fully test in experiments due to limitations of mechanical accuracy and the large number of degrees of freedom in traps with multiple electrodes. Alignment in a linear ion trap made of two patterned plates involves only six degrees of freedom, facilitating a complete study of the impact of each degree of freedom on performance. In this study, a model in SIMION for the two-plate linear ion trap was compiled. Based on this model, misalignments in all six degrees of freedom were studied with respect to the resolving power and ion detection efficiency. Pitch angle and Y-axis (plate spacing) misalignments have more impact on the resolving power compared with the other four degrees of freedom: yaw, roll, X and Z. The study also shows that the X (shear) misalignment significantly impacts the ion detection efficiency. Simulations of traps with multiple simultaneous misalignments show that each degree of freedom contributes independently to the overall performance. These results provide helpful guidance in the design and fabrication process of two-plate linear ion traps as well as other types of linear ion traps.

Keywords: Quadrupole ion trap, simulation, geometry optimization, electrode misalignment, electrode spacing, misalignment tolerance

1. Introduction

Quadrupole ion traps have become one of the most common mass analyzers due to strong sensitivity, compact size, relatively high working pressure and the unique capability to perform multi-stage tandem mass analysis (MS^n). The traditional method to produce the ion trap is to generate an electric field using hyperbolic-curved electrodes. Satisfactory performance can also be obtained using simplified electrode geometries (planar, cylindrical), which are particularly useful in efforts to miniaturize ion traps. For instance, the cylindrical ion trap, derived from the hyperbolic (Paul) ion trap, has shown good performance in portable mass spectrometers [1-12]. With unit mass/charge resolution, the sensitivity extends to the low-ppb level when the trap is coupled to a membrane introduction EI system [9]. Compared with the quadrupole ion trap, the linear ion trap (LIT) has higher trapping capacity and trapping efficiency for external ions and thus has higher sensitivity [13]. Versions of the LIT with simplified electrode geometry have been developed in the last decade [14-21]. The rectilinear ion trap, one of the most extensively studied variations of the LIT, was adopted in a benchtop miniaturized mass spectrometer system and achieved a resolution of $\Delta m/z = 0.6$ Th (full width at half-maximum) and a mass range of up to m/z 900 [22]. As another example, a toroidal trap with cylindrical and planar electrodes was demonstrated by Taylor and Austin [23].

Our lab has previously introduced a way of forming a quadrupole trapping field using lithographically patterned electrodes on two ceramic plates. Aluminum electrodes were precisely deposited on the plates using standard photomask lithography. To prevent the charge build-up on the ceramic plate, a thin germanium (Ge) layer was applied. By designing the electrode geometry and applying the proper radio frequency (RF) amplitude on each electrode, several different types of ion traps have been successfully demonstrated, including a planar Paul trap [24], the halo ion trap [25-27], the coaxial ion trap [28], and more recently a linear ion trap [29, 30].

Misalignment of electrodes in ion traps is one of the major factors that affect the performance. In the two-plate linear ion trap, there are only six degrees of freedom for misalignment. Considering one plate fixed, the other has three translational and three rotational degrees of freedom. This allows us to study the relationships between the performance (resolving power and ion detection efficiency) and each of the degrees of freedom. All other types of ion traps involve more than two independently movable pieces, and have too many degrees of freedom of positioning to work experimentally, and represent a more challenging problem in simulations. For instance, the cylindrical ion trap and rectilinear ion trap have 12 and 30 degrees of freedom, respectively. Several degrees of freedom, which are believed to be the major factors to their performance, have been studied both in experiment and simulation. For instance, the electrode geometry of the quadrupole (3D) ion trap in the z dimension was studied and an optimized “stretched” geometry was found [31]. In the LIT, the axial linear distortion and twist distortion have been shown to have great influence on performance [13]. Yuzhuo et al. reported on a simulation study comparing the geometry deviation effects on three different types of linear ion traps and found that the resolving power is more sensitive to displacements in certain degrees of freedom [32].

In the present work SIMION models were used to understand the effects of misalignments in each of the six degrees of freedom in the two-plate LIT. Factors studied include both resolving power and ion detection efficiency.

2. Methods

2.1 Overview

SIMION 8.1 (Scientific Instrument Services, Inc., Ringoes, NJ) was used for model building with different displacement or misalignment in all degrees of freedom, and also for simulations of ion

trajectories in the trap. The parameters in SIMION were controlled using a modified user program. Data processing for field calculations and mass spectra analysis were performed with MATLAB (Mathworks, Natick, MA).

2.2 SIMION model

A two-plate LIT model was generated based on our previously published geometry (Figure 1) [29]. In this geometry, the LIT was formed by discrete, lithographically patterned electrodes, and each plate was coated by two thin Ge layers on the facing sides. In the model, the two Ge layers were simulated by 410 independent electrodes, with an equal potential difference between all sets of neighboring electrodes. The width of each electrode was set to be one grid unit (0.025 mm). Potentials were assigned during simulations using the fast proportional array technique. This technique allows the potential on each electrode to be assigned by an array in a *.pa+ file. The advantages of this technique is that no extra memory is required. More details are illustrated in Additional Fast Proportional Scaling Solutions in SIMION 8.1 Supplemental Documentation. In addition, a model without the Ge layer was simulated to compare with the Ge-covered model.

2.3 Field calculations

To understand the influence of the Ge layer on the electric field, we compared the differences in potential and higher-order electric field between the two models. The potential and electric field along the Y axis (the ejection direction) was obtained from SIMION by flying 10000 sequential neutral particles along the Y axis and recording the electric field when they initialized. To show the nonlinear contributions, an extrapolation of the central linear region was calculated and subtracted from the

calculated field. The higher-order electric field contributions were obtained by fitting the potential data using a 25th order polynomial [23, 33-35].

The Ge layer is intended to prevent charge build-up on the otherwise bare ceramic, and it also provides a smooth potential gradient between electrodes. In real devices, the thickness of the Ge layer has some effect on the RF amplitude applied to each electrode. When a capacitive voltage divider is used to establish RF amplitudes, the resistance of the Ge layer must be factored into the overall circuit. However, there was no need to consider this effect in the present work; the simulations assumed ideal values for the RF amplitude applied to each electrode. It is difficult in SIMION to model the effect of a bare dielectric material, so the simulations without germanium assume empty space between the electrodes. In a real device, the potential on bare ceramic would be difficult to determine and may be influenced by charge build-up.

2.4 User programs

The user programs for this study were modified from the examples provided with SIMION 8.1. The user programs controlled all the parameters in the model, including the geometry, static voltages, RF frequency and amplitude, scanning rate, and pressure. All the mass spectra were obtained under the parameters of initial trapping amplitude of 600 V (0-p), RF frequency of 2 MHz, time step of 20 ns, mass-to-charge ratio of 150 Th, and scanning rate of 26.7 kTh/s. The user programs were executed with a random distribution of the ion's initial position near the trapping center. Each ion had an initial energy of 0.04 eV in a random direction. The hard-sphere collision model was incorporated in the user programs, and collision conditions were 0.5 Pa (3.7 mTorr) with helium (4 amu) as background gas.

Boundary ejection is a basic operation mode for the two-plate linear ion trap as only RF voltages are required. The ions were first trapped and collisionally cooled under trapping RF voltages and then

were scanned out with increasing RF amplitude. The mass spectra acquired in boundary ejection reflect the intrinsic properties of the ion trap, therefore, they were used in this study for evaluating the adequacy of the electric fields under misalignment conditions. The commonly used AC resonant ejection is affected by factors such as the AC frequency, AC amplitude and phase difference, which involve more variables and reduce the reliability of the simulation [36].

2.5 Mass spectra analysis

Ion parameters, including the position, time of flight and ejection voltages, were recorded in a text file by SIMION. Ions that passed through the slit (width = 0.7 mm) among the initial 2000 ions were considered to be detected and were used to simulate a mass spectrum. Resolving power was determined from spectra using Gaussian fitting in MATLAB. For a spectrum with 1600 detected ions, the relative standard deviation for the resolving power calculation is around 5%. The scan speed in this study was approximately 26.7 kTh/s in order to complete all simulations in a reasonable amount of time. The resolving power is affected by scan mode and several other factors, such as scan speed, pressure, etc.; although the scan speed in the present simulations is somewhat higher than has been reported in experiments designed to optimize resolution, this scan speed is adequate for the objective of this study, which is to observe trends related to electrode alignment.

3. Results and discussion

3.1. The influence of Ge layer on potential and higher-order fields

Fig. 2 shows the isopotential contours of the two-plate LIT both with a Ge layer (Fig. 2a) and without a Ge layer (Fig. 2b). A clear difference was observed in the isopotential contours between

electrodes on the same plate. Without the Ge layer, the potential between electrodes shows permeation from neighboring electrodes. On the other hand, when Ge layer is present, a uniform electric field results on the plate surface. The potential midway between the two electrodes is slightly different when the Ge layer is present than it is without a germanium layer.

Fig. 3 shows the higher-order fields obtained from these two models. Although only a slight difference on the center isopotential contours is observed in Fig. 2, the difference in the higher-order field components is significant. The electric field in the model without the Ge layer was optimized as reported previously [35], and shows the classic pattern of positive higher-order terms. However, it clearly deviates from this pattern if the effects of the Ge layer are considered, resulting in reduced performance. It is believed that this electric field could be corrected by optimizing the voltage distribution on the electrodes [34, 35].

3.2 Effects of angular displacements

Fig. 4 (a) shows how the resolving power changes with increased angular displacements (pitch, yaw and roll). Because all of these angular displacements are symmetric, the displacements in only one direction are shown. Among the three angular displacements, the resolving power is more sensitive to the pitch. A pitch angle within 0.05 degrees of ideal alignment is suggested to avoid severe deterioration of resolving power. This value is on the same order as the smallest misalignment that can be simulated in SIMION using the array size and scaling that were used in this study. Yaw angle error has roughly an order of magnitude smaller influence on the resolving power, while the roll error has a negligible effect on the resolving power if the error is less than 3 degrees.

The simulated ion detection efficiencies (IDEs) corresponding to these angular displacement are shown in Fig. 4 (b). The IDE is calculated by dividing the number of ions passing through the slit by the initial number of ions. This figure shows that the IDE is almost the same for pitch and roll displacement,

but is reduced with yaw displacement as the extremities of the slits are no longer directly under or over the trapping center.

3.3 Tolerance to linear displacements

Fig. 5 (a) shows the relationship between the resolving power and linear displacements along the X, Y, and Z axes. Due to symmetry, only one direction was used for X and Z linear displacement. For displacement in the Y direction, both closer and farther plate spacing were studied, as these should produce different electric fields and show different effects. Therefore, the Y axial displacement was scanned from -1.15 mm to 1.275 mm with our previously-published plate spacing (4.38 mm) representing zero displacement. Among all three linear displacements, the resolving power is dominated by displacement in the Y direction. The resolving power increased from 65 to 119 when the plate distance was increased from 3.23 to 4.08 mm, and reduced to 72 when the plate spacing was increased from 4.08 to 5.655 mm. A higher resolving power in 4.08 mm plate spacing indicates that this distance shows the best electric field of the device. The other two displacements, X and Z linear displacements, do not show a significant influence on the resolving power within the range of motion studied. Note, however, that the uncertainty in the resolving power error increased when the IDE was reduced during simulations of X axis displacement.

Fig. 5 (b) shows the IDE versus the three linear displacements. As the increased displacement along the X axis moves the slit away from the trapping center, the fraction of detected ions are dramatically reduced. A misalignment of less than 3 mm in the Z axis has no significant change on the IDE. The IDE trend in Y displacement is different from the above displacements: the IDE increases steadily to 0.94 when the displacement increases from -1.15 to 0.45 mm (plate spacing from 3.23 to

4.82 mm), and reduces to 0.79 when the plate displacement increases from 0.45 to 1.2 mm (plate spacing from 4.82 to 5.58 mm).

3.4 Higher-order field with linear displacement in Y

Table 1. Multipole expansion coefficients for different plate distances. The results from model without Ge layer were also shown in the table.

geometry	quadrupole	octopole		dodecapole		
plate spacing (mm)	A2	A4	A4/A2 (%)	A6	A6/A2 (%)	(A4+A6)/A2 (%)
3.48	-57.97	1.013	-1.747	-9.604	16.57	14.82
3.78	-55.09	0.6781	-1.231	-7.583	13.77	12.53
4.08	-52.10	0.395	-0.7581	-5.777	11.09	10.33
4.38	-49.10	0.1474	-0.3002	-4.246	8.647	8.347
4.68	-46.14	-0.0409	0.0886	-3.109	6.738	6.826
4.38 (without Ge layer)	-46.02	-1.161	2.524	0.2707	-0.5882	1.936

The higher-order terms of the trapping field are predictive of the performance of the trap. Due to the large impact of Y displacement on performance, the higher-order components along the Y axis for each of the different geometries were examined. Fig. 6 shows the normalized higher-order fields for five different plate distances. The calculated coefficients for even terms are listed in Table 1.

Fig. 6 shows that the electric field can be optimized to some extent simply by changing the plate spacing, analogous to the electrode stretch in quadrupole ion traps. The octopole term increases from -1.747% to -0.0886% as the plate spacing increases from 3.48 to 4.68 mm. The variation in the dodecapole is greater. Previous studies have shown that proper compensation of the higher-order field can improve the resolving power. A rough criterion called the “ -10% compensation” rule was proposed by Wu et al. during optimization of the electric field of cylindrical ion trap [11]. The criterion suggests that the sum of octopole and dodecapole components should be -10% of the quadrupole component. However, we observed that the resolution is best in the planar LIT with a different combination of higher-order terms: the best resolution exists with -0.7581% octopole and 11.09% dodecapole, for a total of $+10.33\%$. These results are similar to those observed experimentally by Zhang using a quadrupole ion trap made using lithographically patterned plates—in that case the best resolution was observed with 0% octopole and $+8\%$ dodecapole [35]. In the present results the IDE and the resolving power are maximized at different electric field configurations, so a trade-off may be needed for best overall performance.

3.5 The combination of degrees of freedom

All six degrees of freedom were studied independently in the above simulations. However, in a real ion trap, misalignments involving two or more degrees of freedom always exist. If the six degrees of freedom are independent, the resolving power and the IDE in combined degrees of freedom could be estimated using Equation 1:

$$\frac{U_c}{U_0} = \frac{U_X}{U_0} * \frac{U_Y}{U_0} * \frac{U_Z}{U_0} * \frac{U_{pitch}}{U_0} * \frac{U_{yaw}}{U_0} * \frac{U_{roll}}{U_0} \quad (1)$$

where

U_c is the resolving power (R) or IDE (E) for combined displacements of six degrees of freedom; U_0 is the resolving power or IDE with no displacement; U_x , U_y , U_z , U_{pitch} , U_{yaw} , and U_{roll} are independent resolving power or IDE under X, Y, Z, pitch, yaw, and roll displacement, respectively.

As Y, pitch and yaw displacements dominate resolving power and IDE, they were used to test the validity of Equation 1. The resolving power and IDE were studied using simulations where the trap had misalignments along two degrees of freedom, and these results were compared with the values estimated from Equation 1. The results are shown in Table 2. For the resolving power, the values for all experiments match to within the range of the error of the individual measurements. The values for resolving power are slightly higher in the combined simulation, but the difference is not statistically significant. The IDE in the tested results and the estimated results matched very well. Peak height is proportional to the resolving power and the IDE, and thus can also be estimated based on Equation 1. These results demonstrate that Equation 1 is valid for the three dominant displacements; therefore, in a real ion trap with these three combined misalignments, each misalignment can be tuned without the interference of the other two displacements.

Table 2. Resolving power (R) and IDE (E) verification in three instances. In the calculation, each value and its standard deviation in resolving power and peak area were calculated from five mass spectra with 2000 initial ions. For this simulation only, the zero displacement in Y-axis is changed from the 4.38 mm (our previously-published geometry) to 4.08 mm (the best geometry in the present simulations).

Instances	Equations being tested	Values from combined simulation	Values predicted from Eq. 1
Y = 0.3 mm	$R_{Y\&pitch} = \frac{R_Y * R_{pitch}}{R_0}$	67 ± 2	63 ± 8

pitch = 0.1°	$E_{Y\&pitch} = \frac{E_Y * E_{pitch}}{E_0}$	0.911 ± 0.003	0.932 ± 0.036
Yaw = 2°	$R_{yaw\&pitch} = \frac{R_{yaw} * R_{pitch}}{R_0}$	76 ± 2	63 ± 11
pitch = 0.1°	$E_{yaw\&pitch} = \frac{E_{yaw} * E_{pitch}}{E_0}$	0.601 ± 0.008	0.620 ± 0.033
Y = 0.3 mm	$R_{Y\&yaw} = \frac{R_Y * R_{yaw}}{R_0}$	78 ± 3	68 ± 9
yaw = 2°	$E_{Y\&yaw} = \frac{E_Y * E_{yaw}}{E_0}$	0.896 ± 0.007	0.851 ± 0.036

3.6 Misalignment effects in other types of linear ion traps

Previous results have shown that resolving power in the 2D linear ion trap with hyperbolic electrodes is sensitive to pitch misalignment [13]. The agreement between our simulation results and the experimental results is due to the similar electric field in both ion traps. The effects of misalignment observed in these simulations likely are present into other types of LITs, including the rectilinear ion trap and the conventional LIT. For example, the yaw angular misalignment of two opposing electrodes in a four-electrode, 2D linear trap may have a much smaller effect on the resolution than a misalignment of pitch; the “stretch” or spacing of opposing electrodes, which resembles the Y displacement in the two-plate ion trap, is the most important physical variable to optimize for performance.

4. Conclusions

Simulations of electrode displacement revealed the impact of each degree of freedom on the resolving power as well as the ion detection efficiency in the two-plate linear ion trap. Among angular

misalignments, resolving power is more sensitive to the pitch angle than yaw and roll angle. In plate position misalignments, displacement in Y (increasing or decreasing plate spacing) has the largest effect because the higher-order components of the trapping field are significantly changed as plate spacing changes. The results on ion detection efficiency versus each degree of freedom indicate that the ion detection efficiency is very sensitive to displacement along the X-axis (shear displacement). This study is helpful to understand the effects of different types of electrode misalignment and to minimize resolving power deterioration caused by misalignments in two-plate linear ion trap. These results also demonstrate that the electric field in planar traps is strongly affected by the presence of the applied germanium layer. In addition, the displacement effect on resolving power and peak area in three degrees of freedom (Y, pitch and yaw) are verified to be independent. Finally, the results presented in this study provide estimates for the effects of electrode misalignment in other type of linear ion traps.

Acknowledgments

The authors are grateful for funding from the National Science Foundation (United States) Chemical Measurement and Imaging Program.

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Figures

Fig. 1

Fig. 2

Fig.3

Fig. 4

Fig. 5

Fig. 6

Graph abstract figure

Figure captions

Fig. 1. SIMIOIN model for the two-plate linear ion trap. The distance between the two plates is 4.38 mm. A series of electrodes with single-grid-unit width were built between the middle AC electrode and outer RF electrodes.

Fig. 2. Isopotential contours for ion trap model without Ge layer (a) and with Ge layer (b). The trap dimensions are identical, and all differences are due to the presence or absence of the Ge layer.

Fig. 3. Non-linear contribution to the electric field along the Y-axis in models with and without the Ge layer, but identical electrode geometry. Both fields are normalized independently with respect to the maximum value for each variation (with and without germanium) and are expressed as fractions of the quadrupolar term of the potential.

Fig. 4. Resolving power (a) and ion detection efficiency (b) as a function of angular displacement of one plate with respect to the other in the two-plate LIT. The scan steps for pitch, yaw and roll displacement are 0.02, 0.2 and 0.2 degrees, respectively.

Fig. 5. The linear displacements versus resolving power (a) and ion detection efficiency (b). The distance between the two plates at zero displacement is 4.38 mm according our previously published geometry. The scan steps for X, Y and Z linear displacement are 0.1, 0.075 and 0.125 mm, respectively. When a given misalignment is varied, all other misalignments are zero.

Fig. 6. The higher-order field (sum of all terms greater than quadrupole) in designs with different Y linear displacements. The voltage applied on the outer electrode is 1000 V. The distance between the two plates (D), resolving power (RP) and ion detection efficiency (IDE) are shown for each design.

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