Simulations of electrode misalignment effect in two-plate linear ion trap

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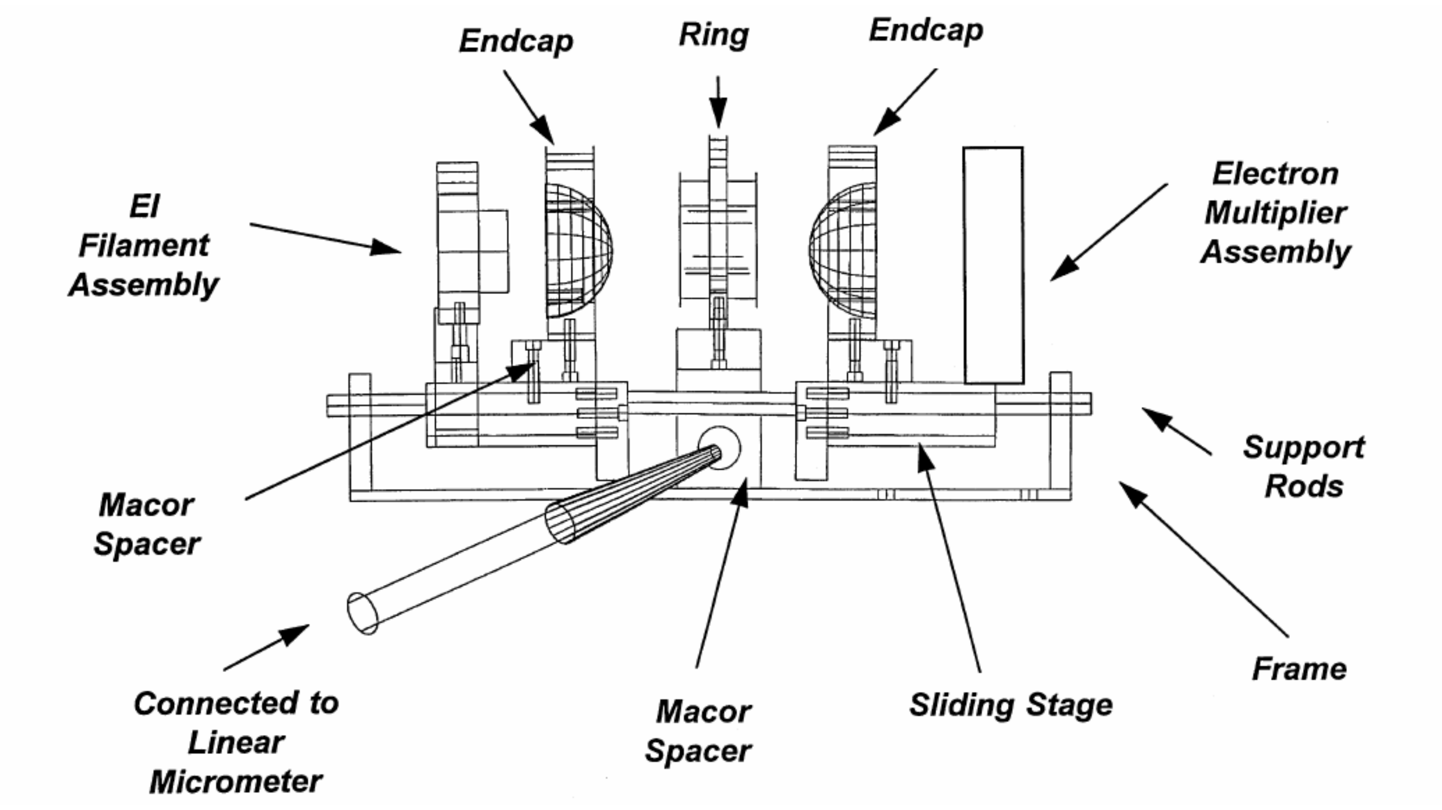
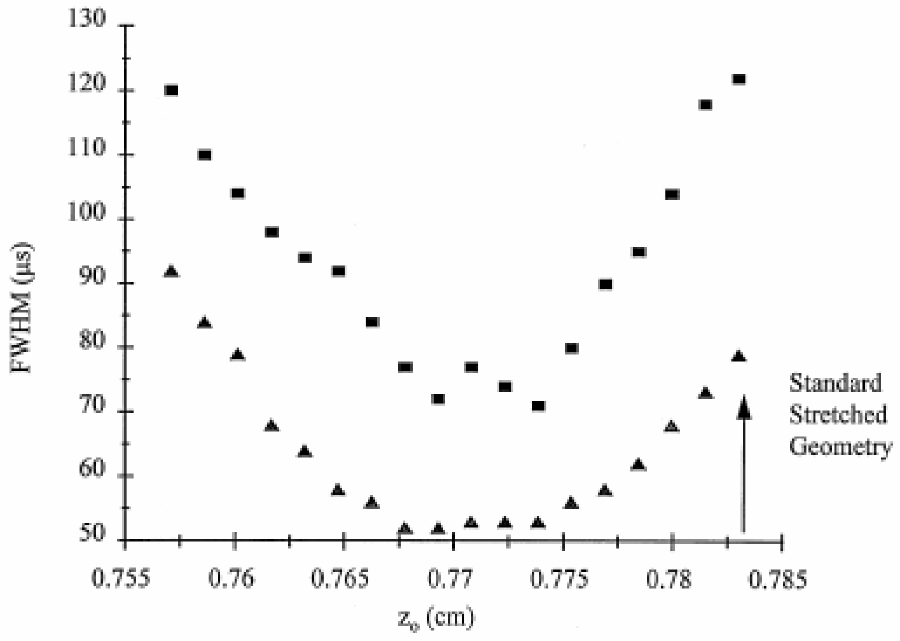
HEMS

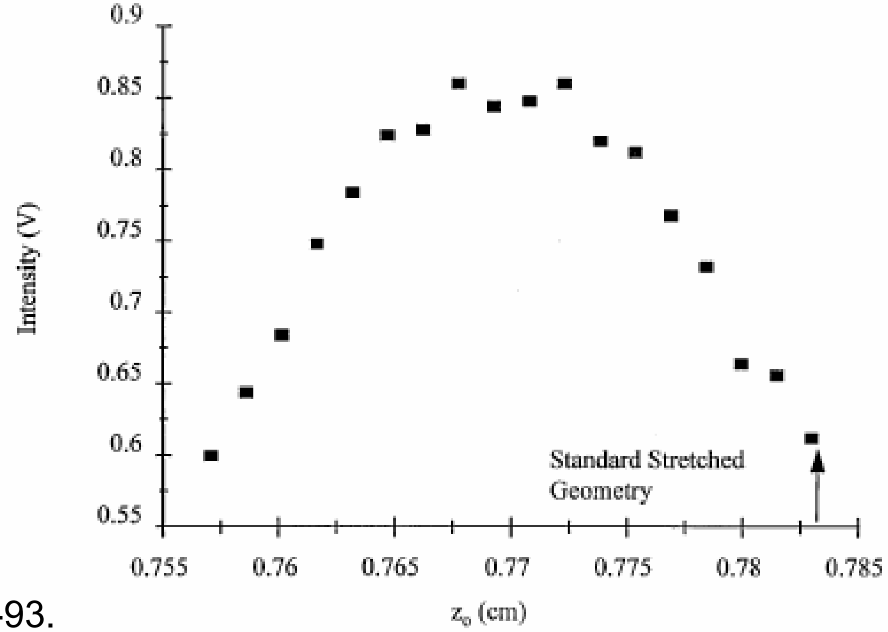
Outline

- Misalignments in ion trap
- Simulation
  - Treatment of Ge layer
  - Parameters
  - Data analysis
- Angular displacements
- Linear displacements
- Higher-order fields with Y displacement (plate spacing)
- The independence of six degrees of freedom
- Experiment
- Conclusions

Paul ion trap

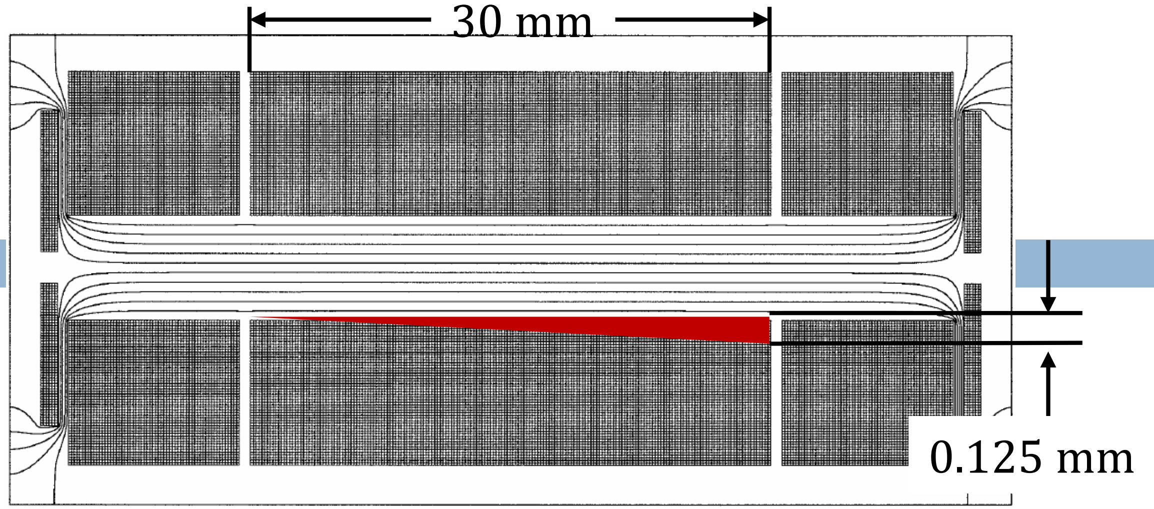


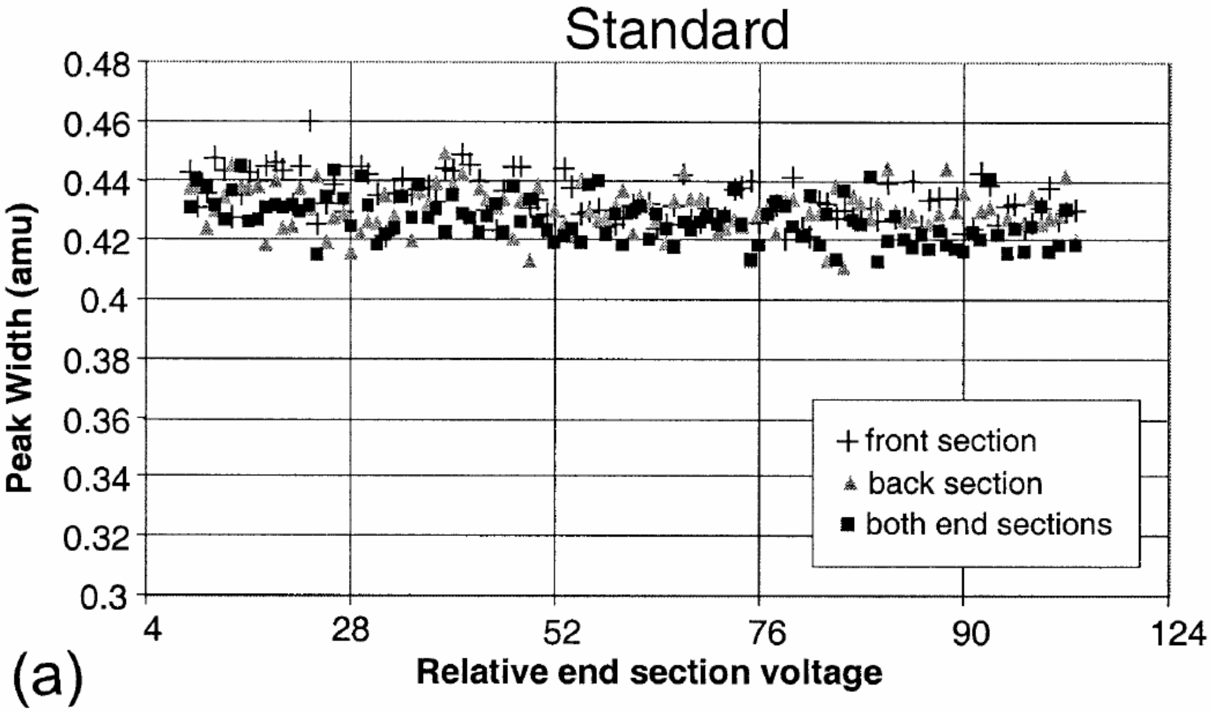


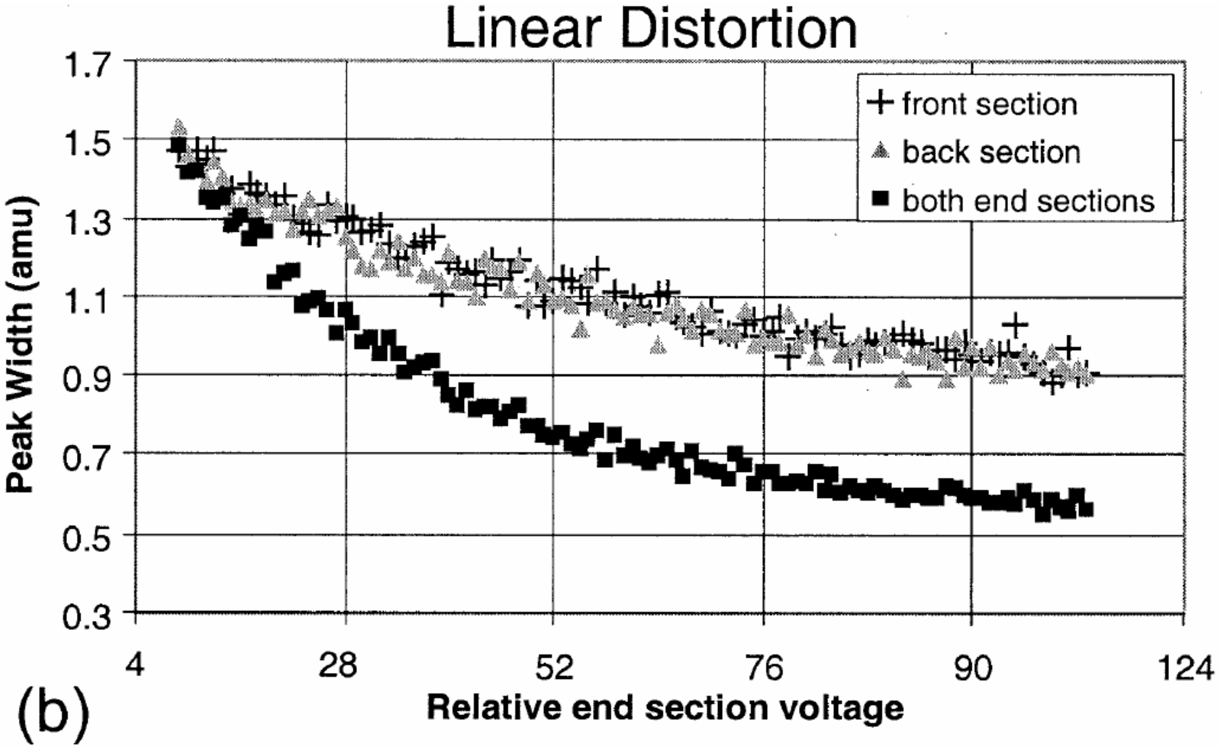


Gill, L. A.; Amy, J. W.; Vaughn, W. E.; Cooks, R. G., Int J Mass Spectrom 1999, 188 (1-2), 87-93.

Linear ion trap



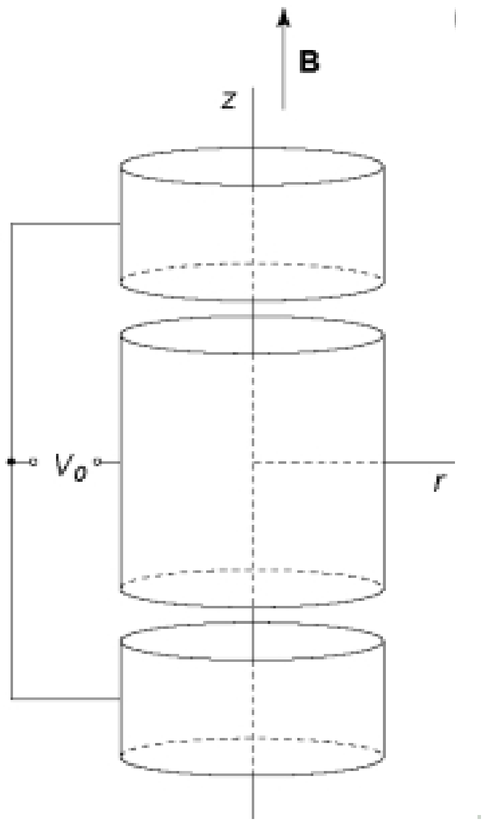


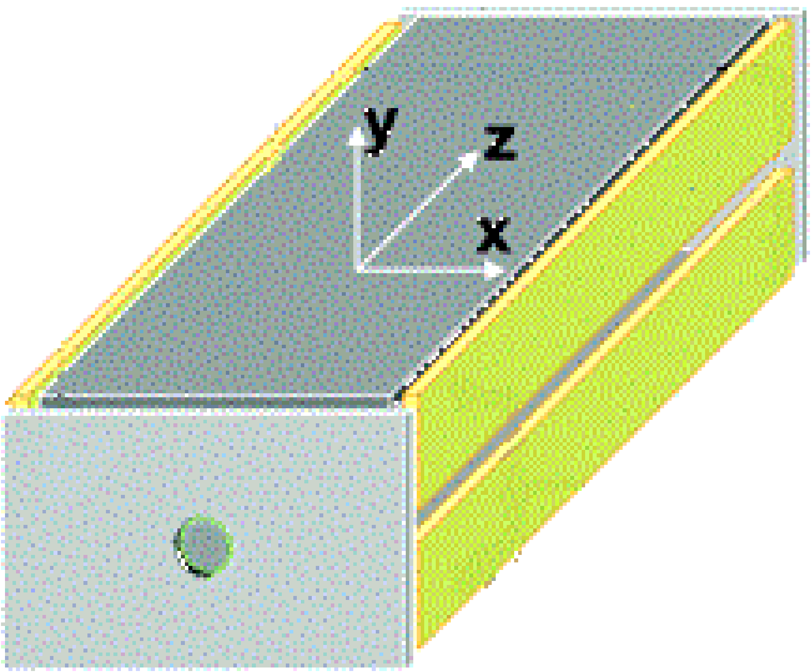


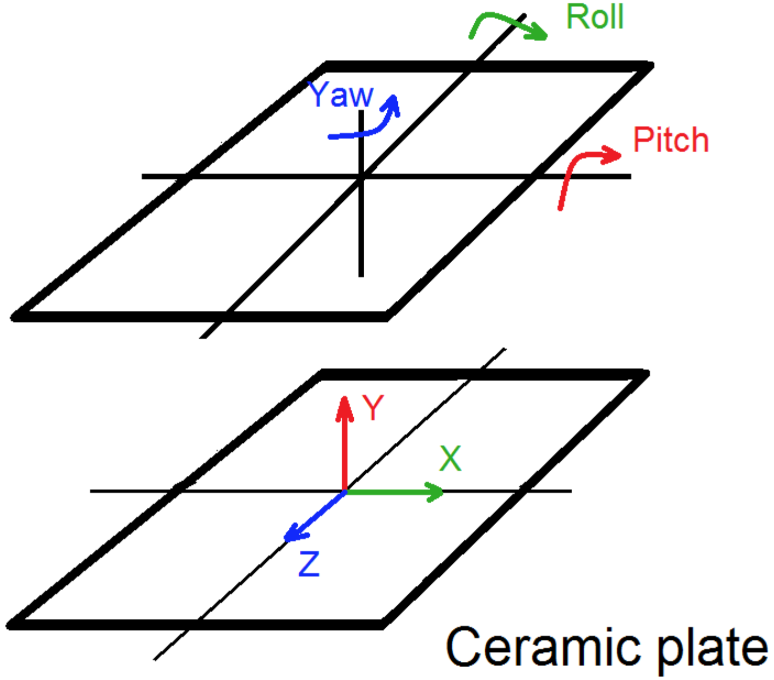
Resolution reduced to 30 % when Pitch angle = 0.24°

Schwartz, J. C.; Senko, M. W.; Syka, J. E. P., J Am Soc Mass Spectr 2002, 13 (6), 659-669

Degrees of freedom





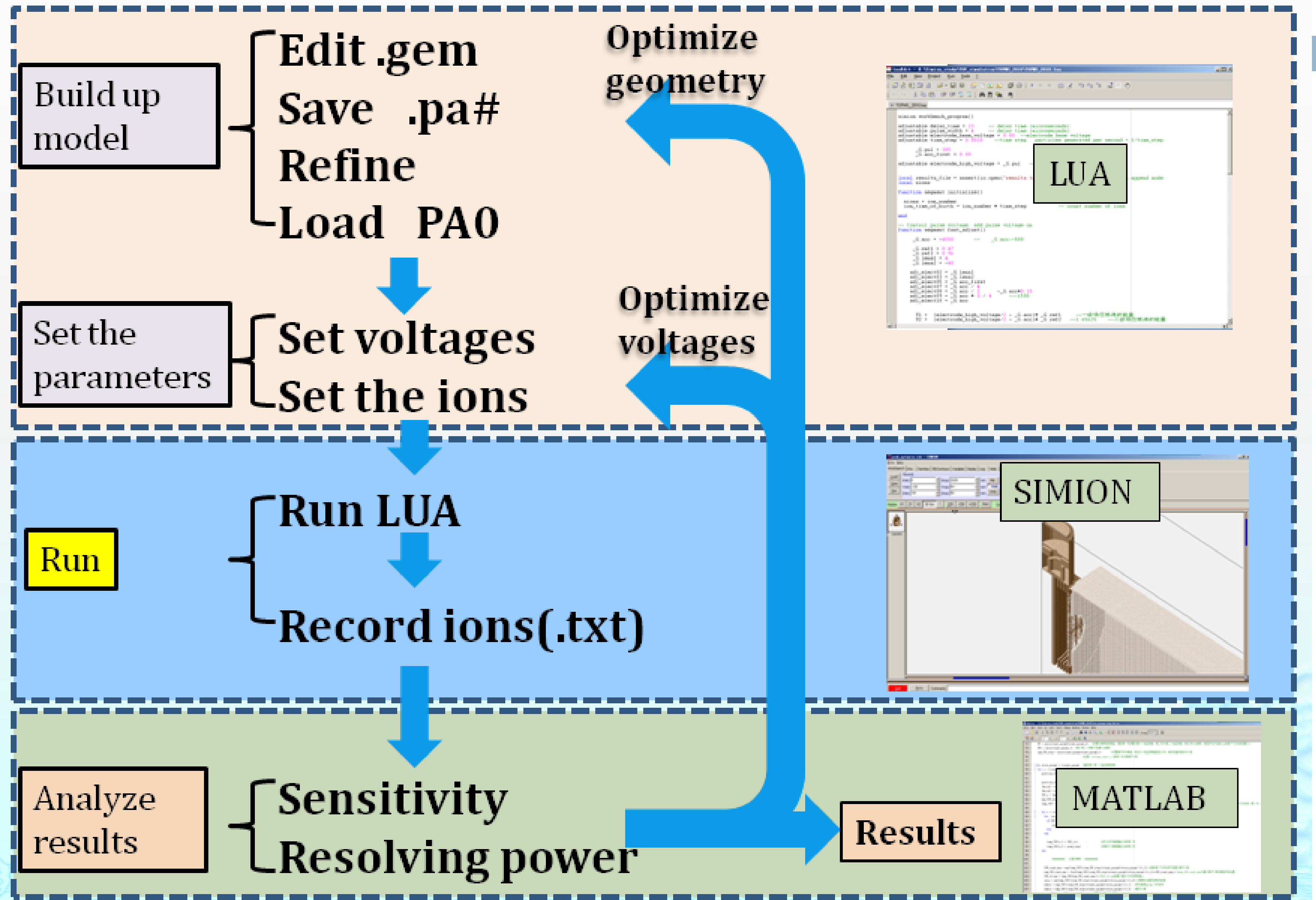


Cylindrical ion trap
12 (6)

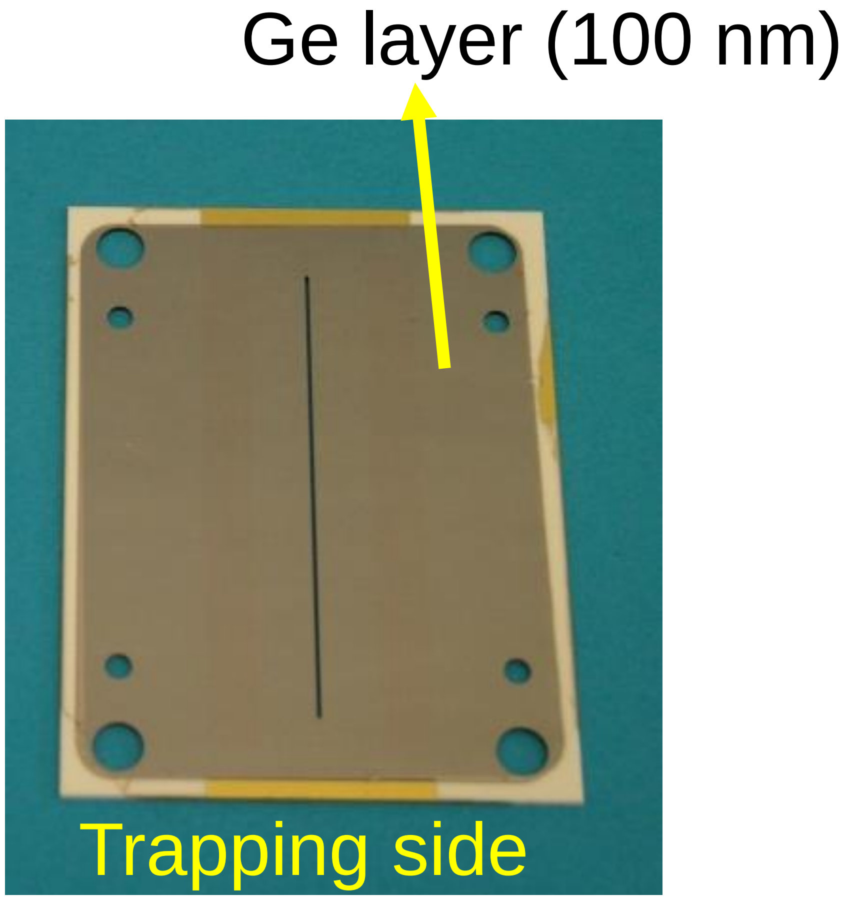
Rectilinear ion trap
30

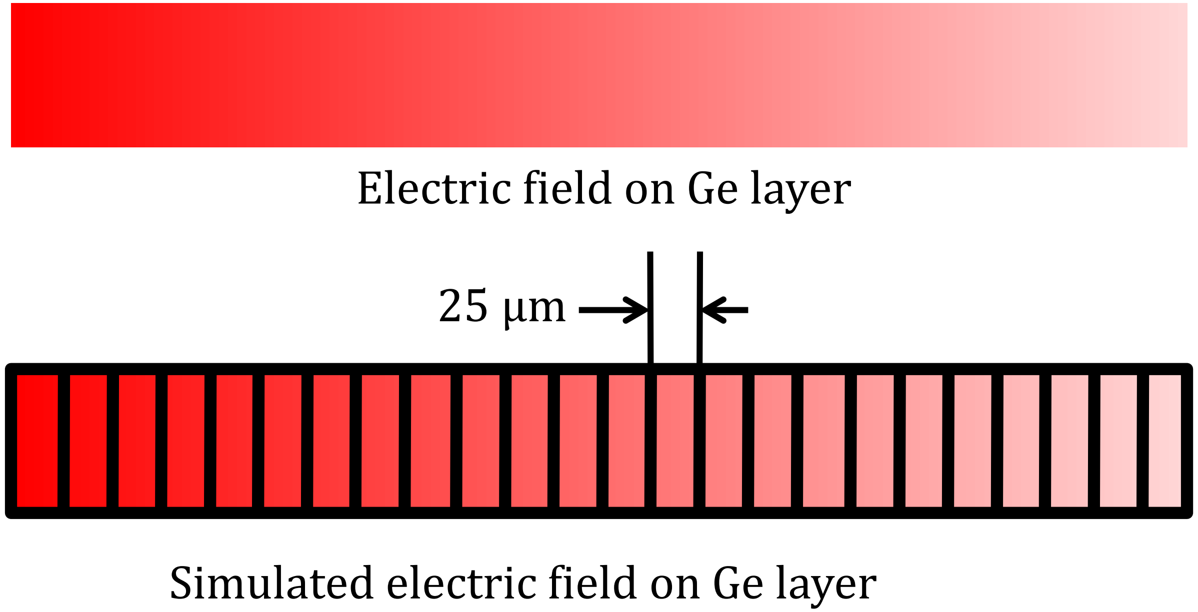
two-plate linear ion trap
6

General simulation procedure



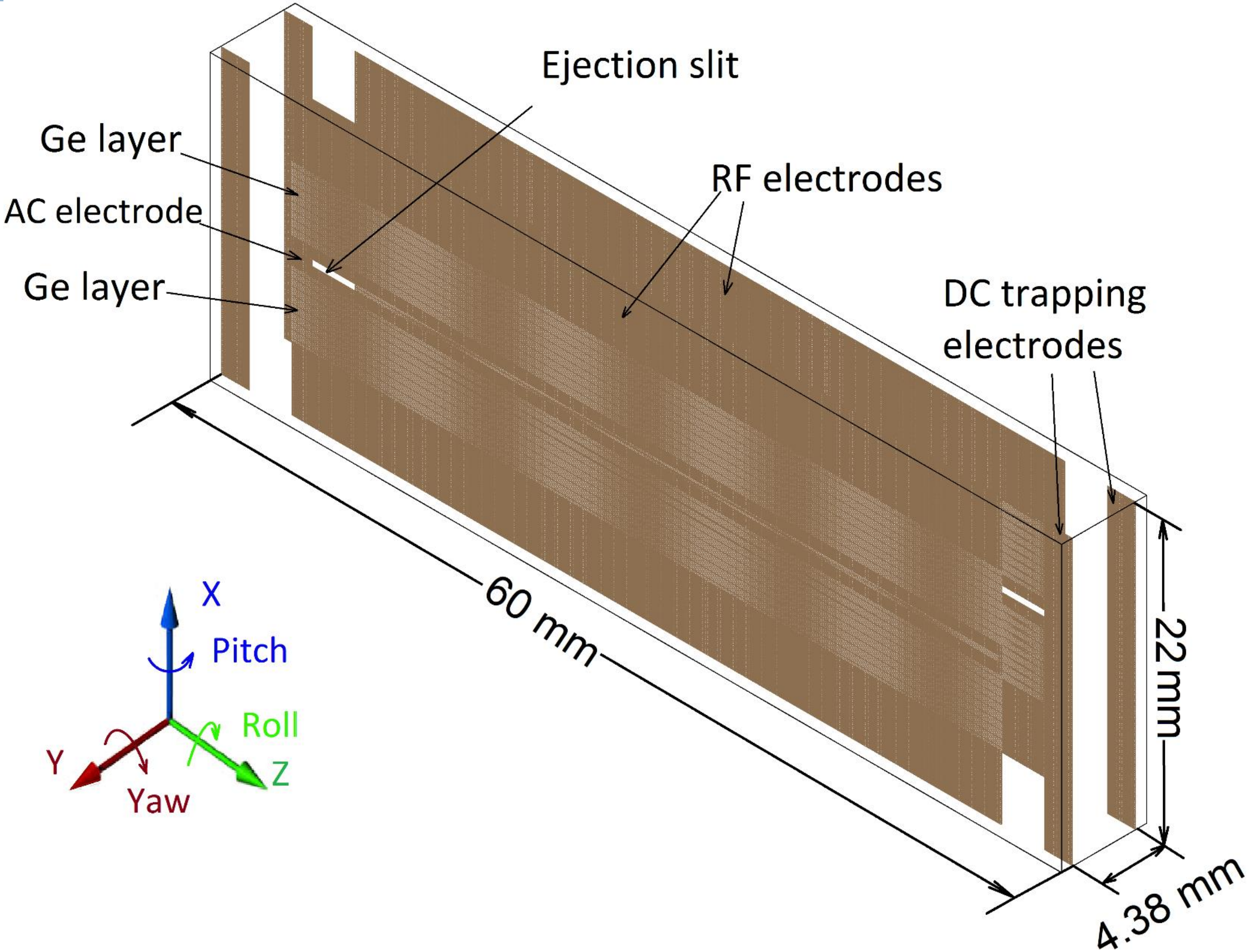
Simulation of Ge layer



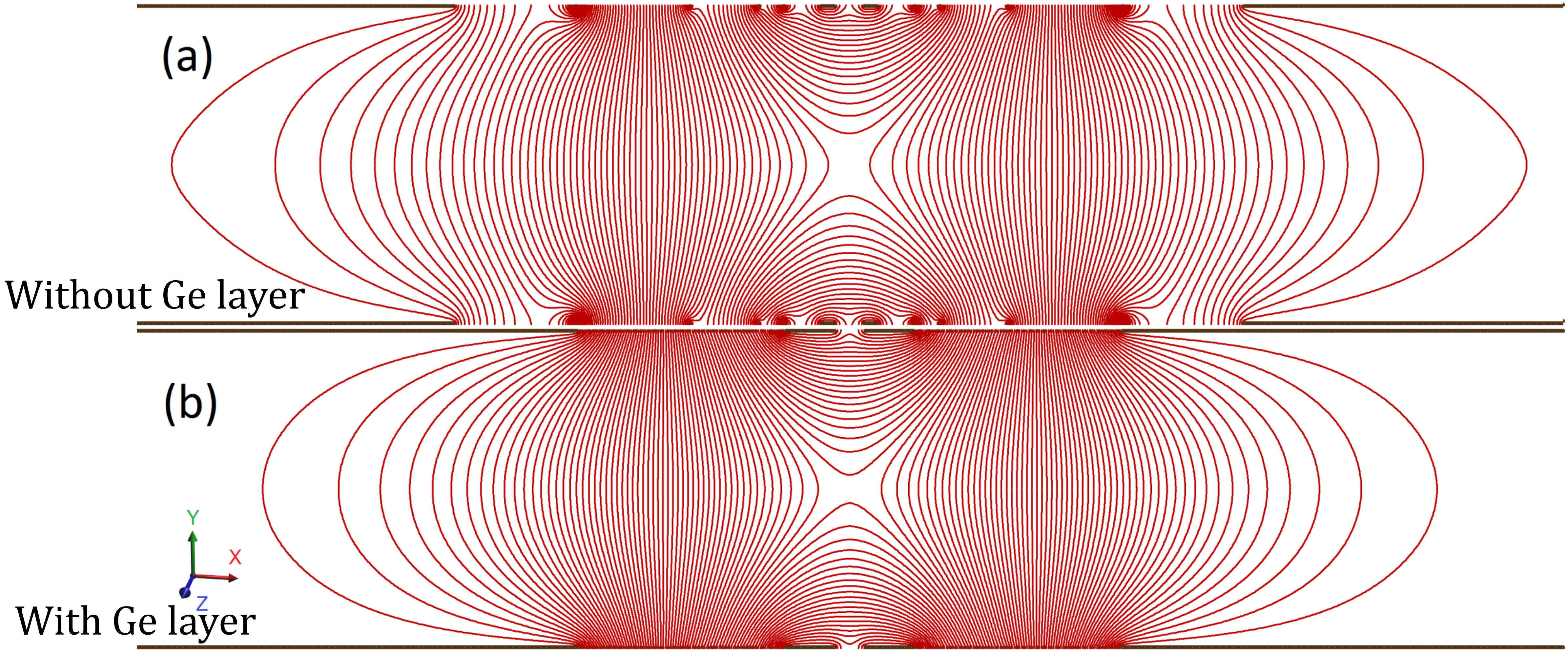


- Voltages on each electrode are assigned separately
- Fast proportional array in SIMION
- The width of the electrode is 25 μm
- Over 200 electrodes are used for simulating one Ge layer

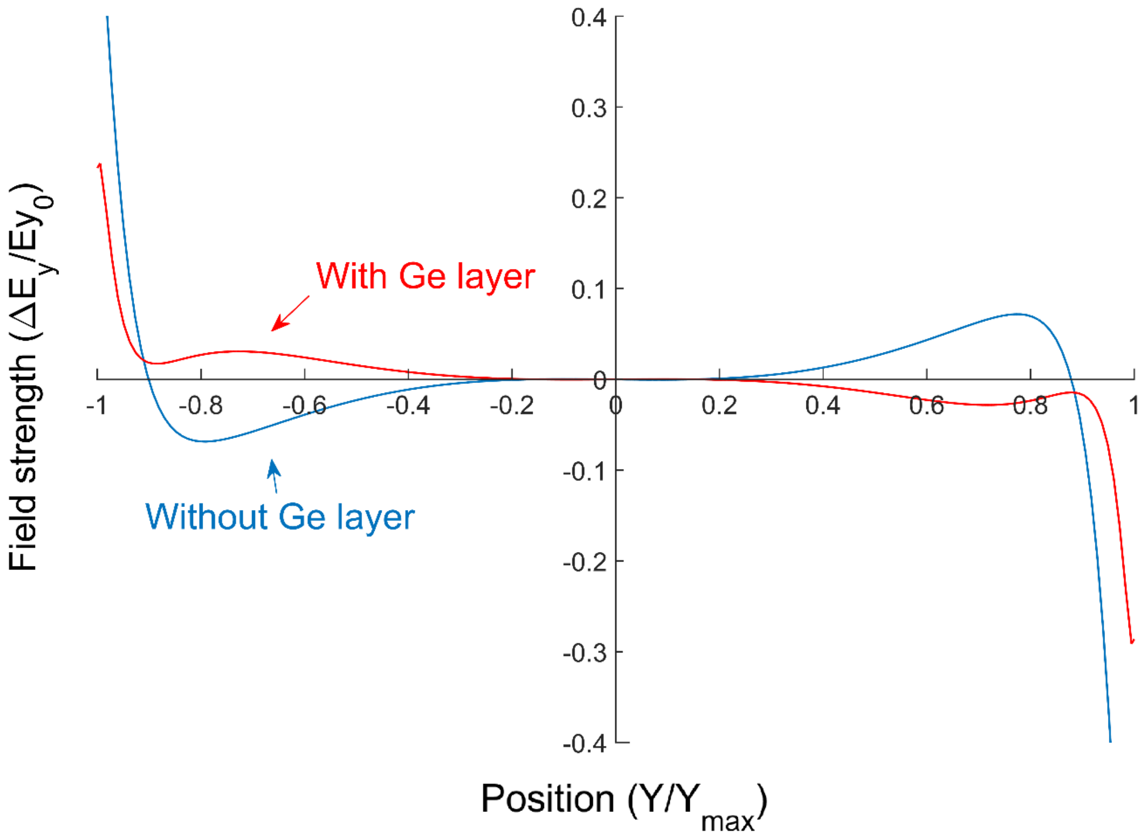
Model building



The impact of Ge layer to the electric field



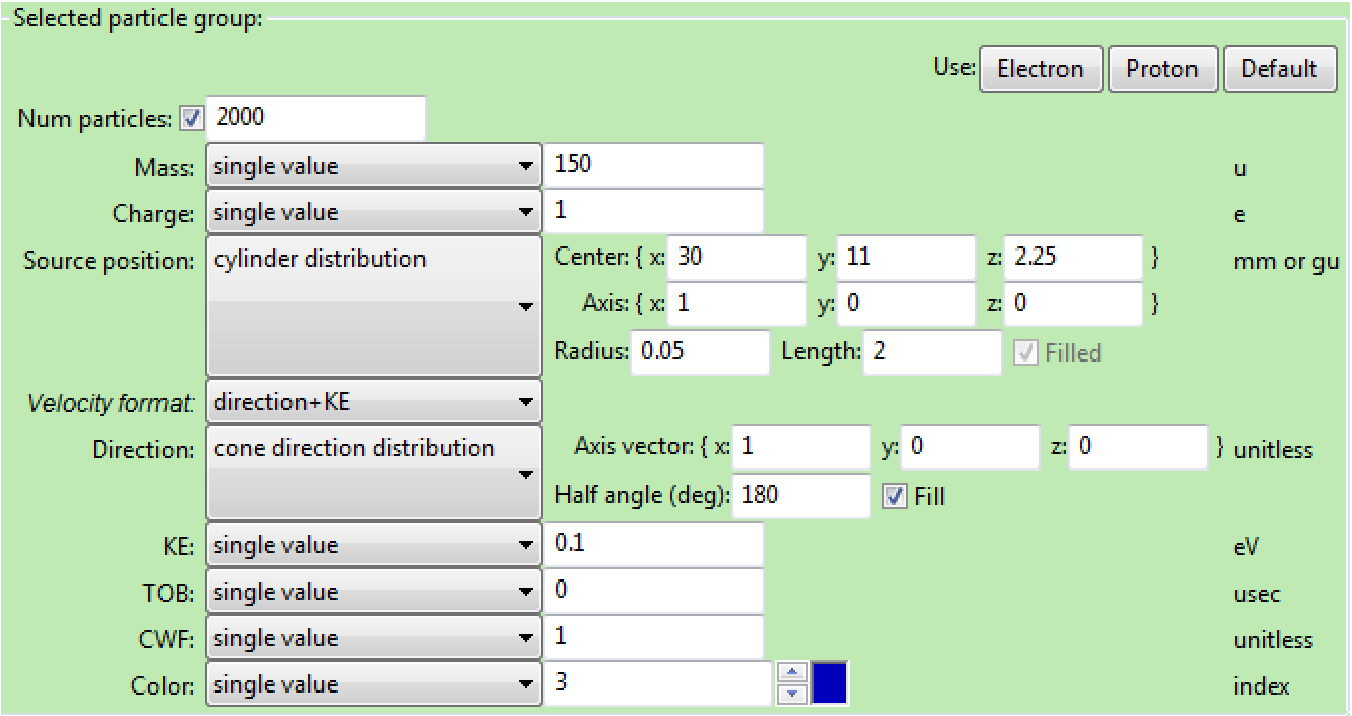
Higher-order field



The non-linear contribution in the model with Ge layer (red) clearly deviated from model without Ge layer (blue).

Simulation parameters

- Ω = 2 MHz
- Trapping voltages (0-p) = 600 V
- Endbar voltages = 15 V
- Scan speed = 26.7 kTh/s
- Pressure = 4 mTorr Helium
- Time step = 20 ns



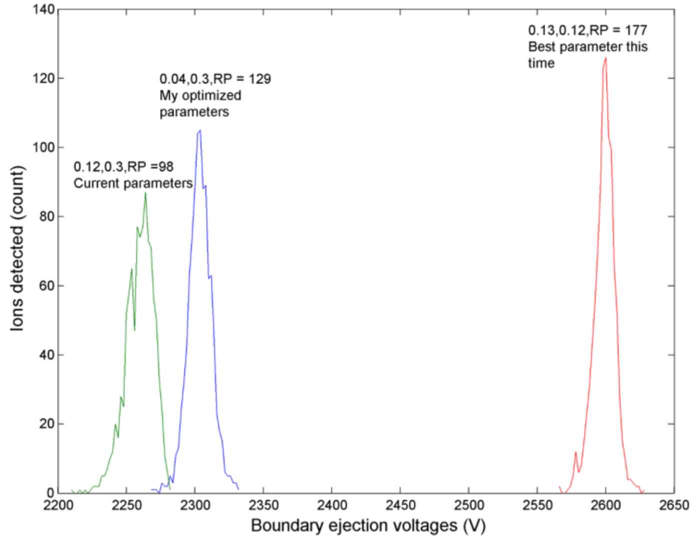
Data analysis

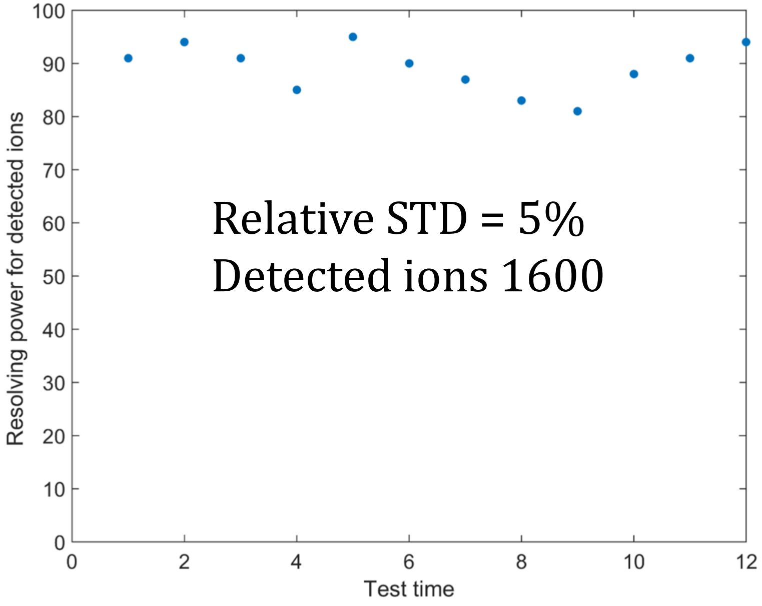
Saved Data

Mass spectra

Performance

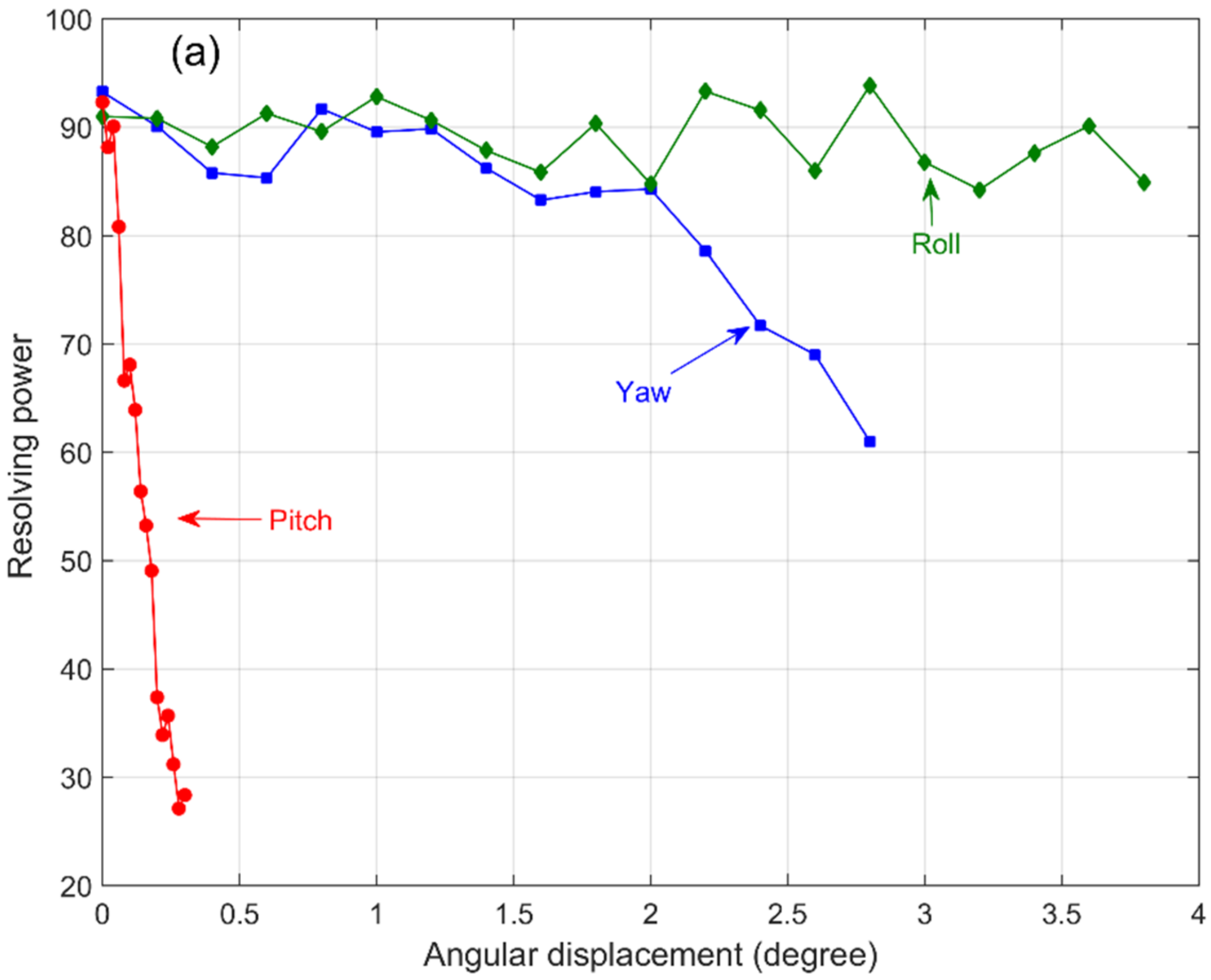
- Resolution
- Ion detection efficiency (IDE)

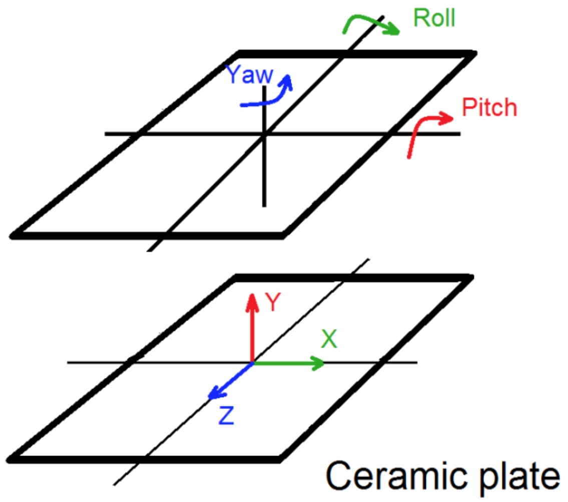




Errors for resolution calculation

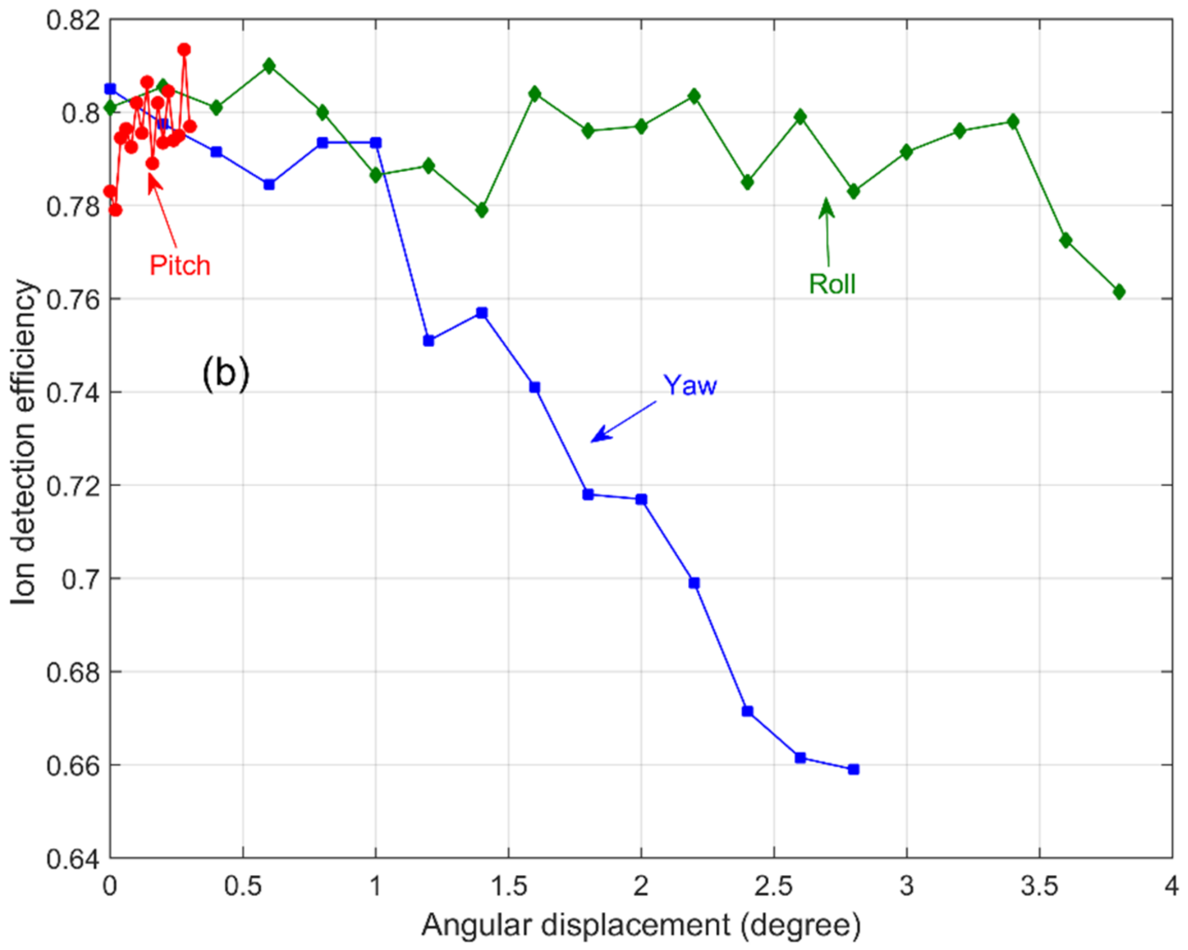
Resolution in angular displacements

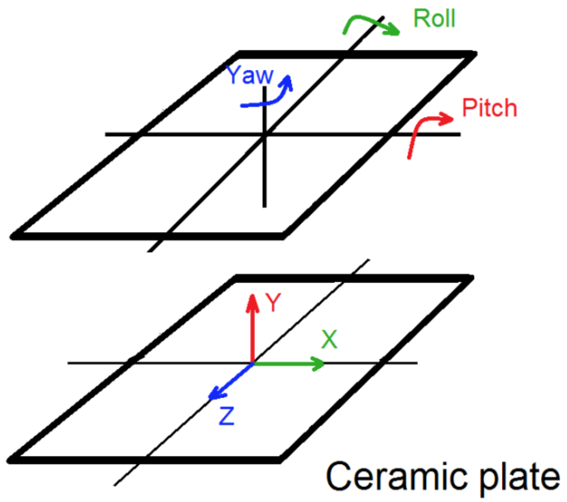




- Pitch displacement is dominated
- Yaw displacement has one order less impact as pitch
- Roll displacement almost have no impact on resolution.

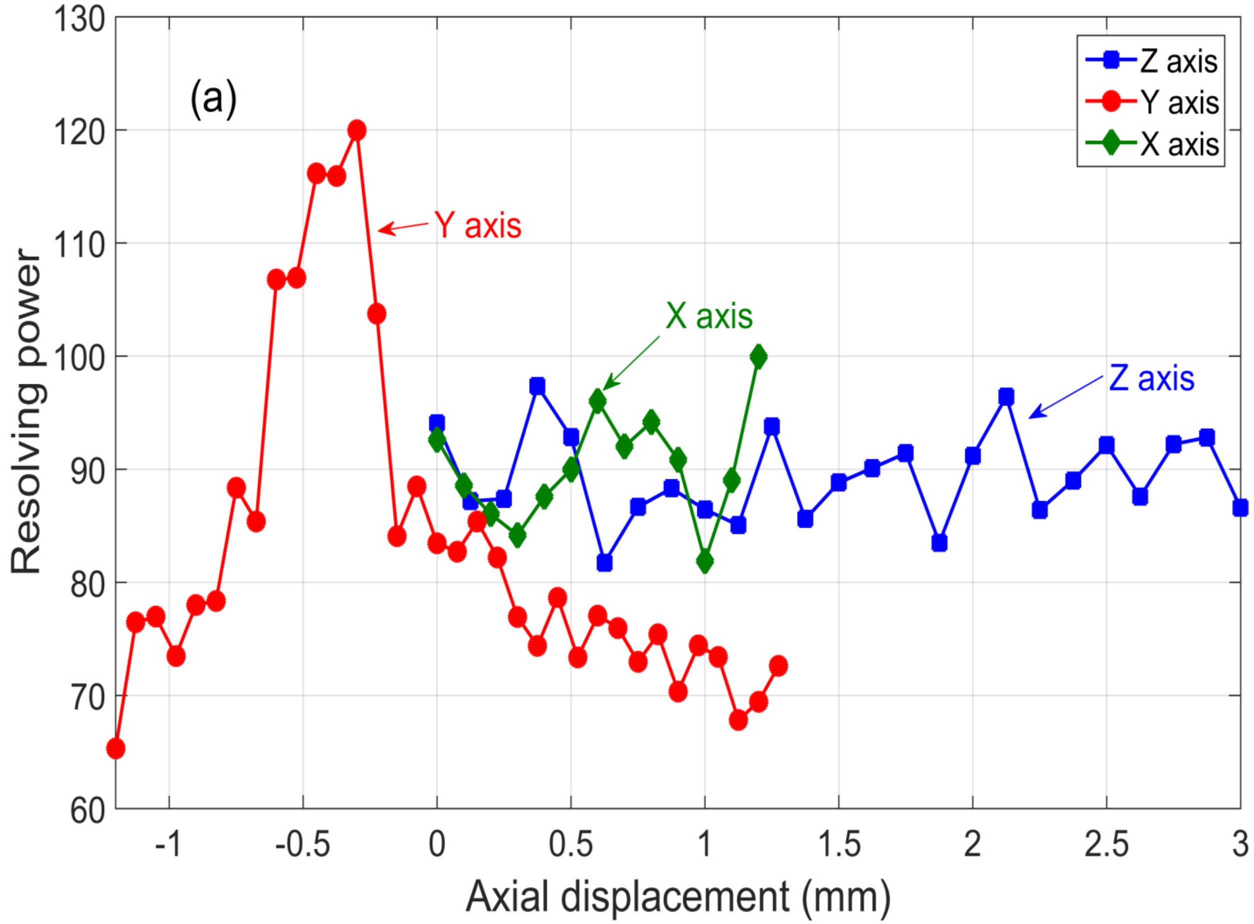
Ion detection efficiency (IDE) in angular displacements

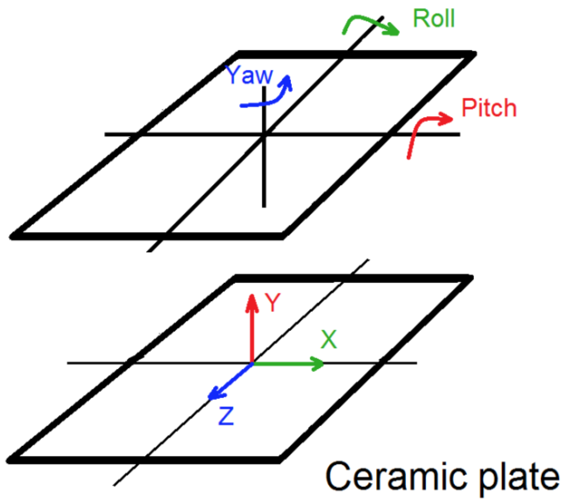




- Pitch displacement does not show significant impact on the IDE in the range 0 to 0.3 degree
- Yaw displacement can reduce the IDE
- Roll has little influence on the IDE

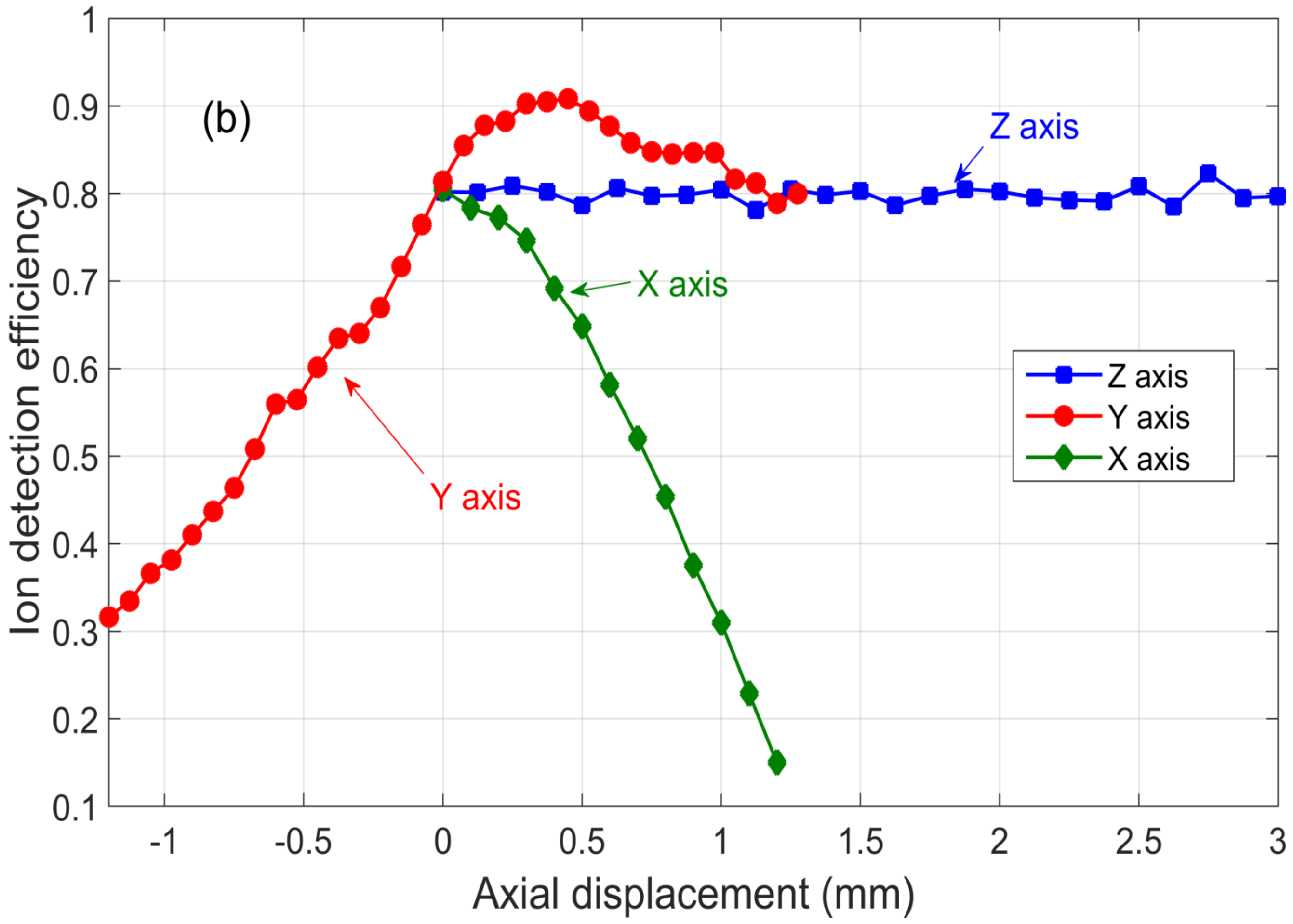
Resolution in linear displacements

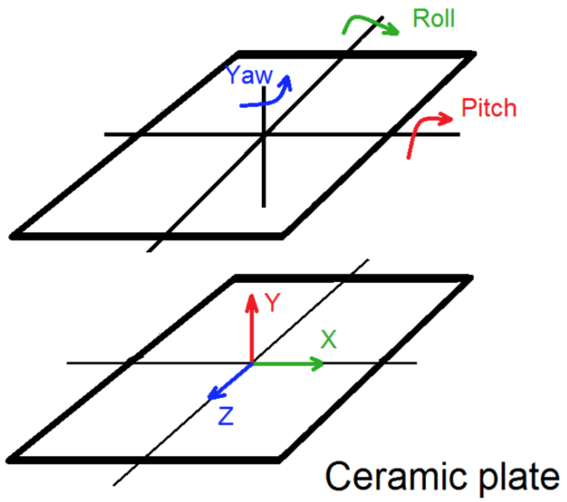




- Y displacement significantly changes the resolution
- X and Z displacements have little impact on the resolution.

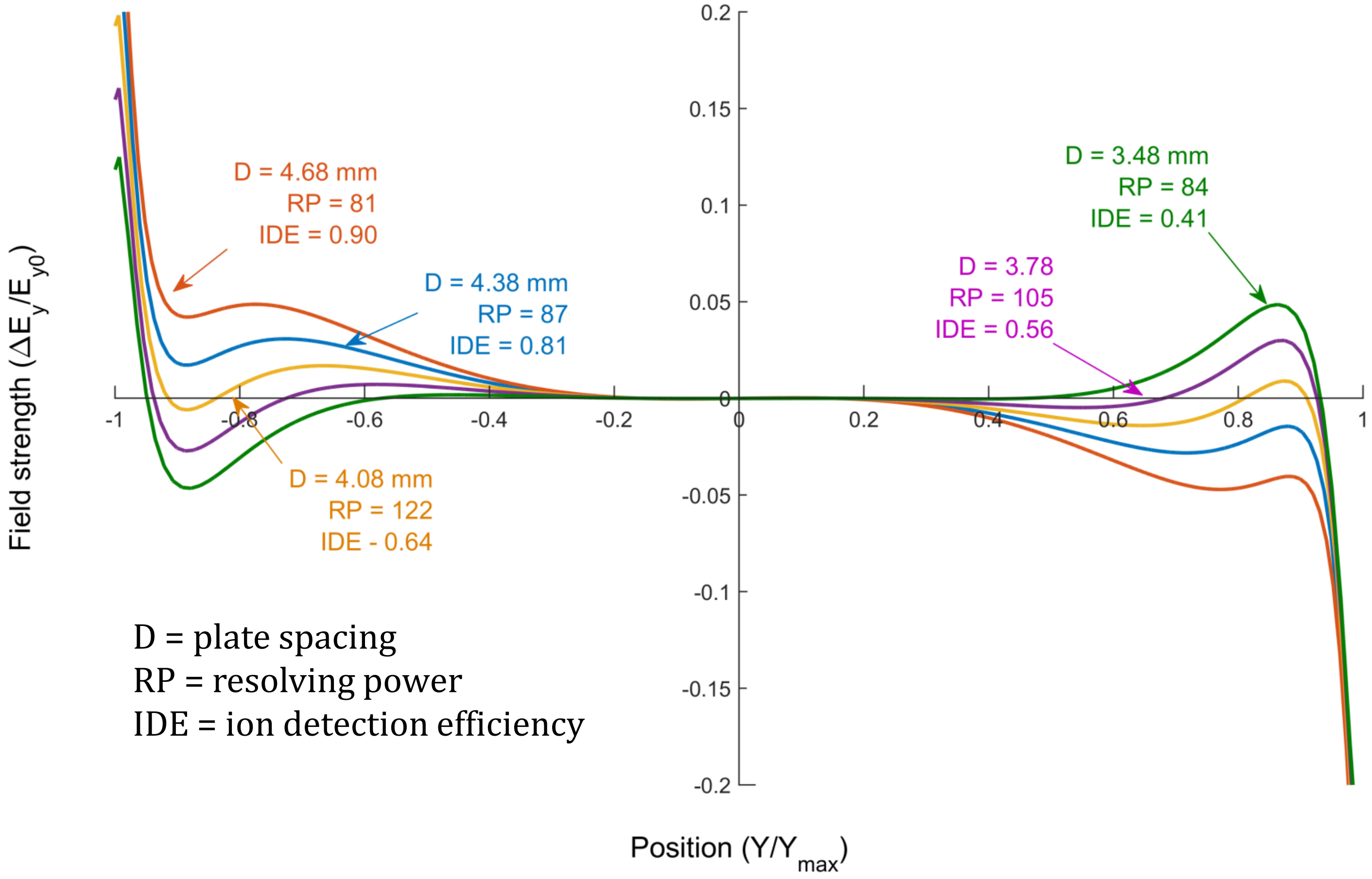
Ion detection efficiency in linear displacements





- Increase in Y displacement can increase the IDE
- X displacement significantly reduces the IDE
- Z displacement has no impact on e tIDE

Higher-order fields with Y displacement



D = plate spacing
RP = resolving power
IDE = ion detection efficiency

geometry	quadrupole	octopole		dodecapole		
distance (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 relationship between the displacements

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

- U_c is the **resolving power** or **ion detection efficiency** for combined displacements of six degrees of freedom
- U_0 is the **resolving power** or **ion detection efficiency** with no displacement
- U_X, U_Y, U_Z, U_{pitch}, U_{yaw}, and U_{roll} are independent resolving power or ion detection efficiency under X, Y, Z, pitch, yaw, and roll displacements, respectively.

If this is true, each degree of freedom can be tuned independently.

Pitch and Y displacement

$$\frac{U_{Y\&pitch}}{U_0} = \frac{U_Y}{U_0} * \frac{U_{pitch}}{U_0}$$

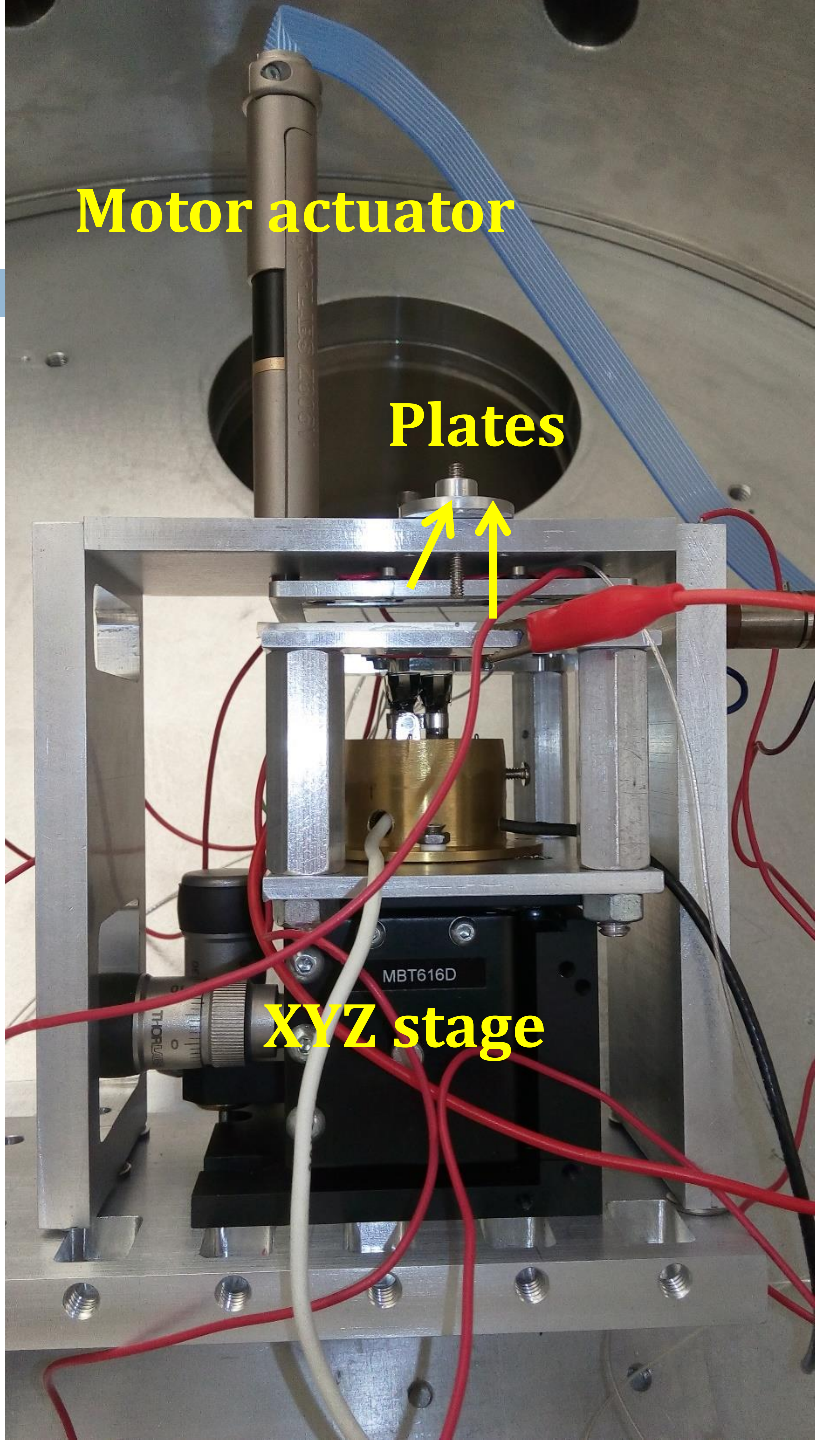
Y = 0.3 mm, pitch = 0.1°

- $\frac{R_{Y\&pitch}}{R_0} = 0.56 \pm 0.03$
- $\frac{R_Y}{R_0} * \frac{R_{pitch}}{R_0} = 0.52 \pm 0.03$
- Difference = 7%

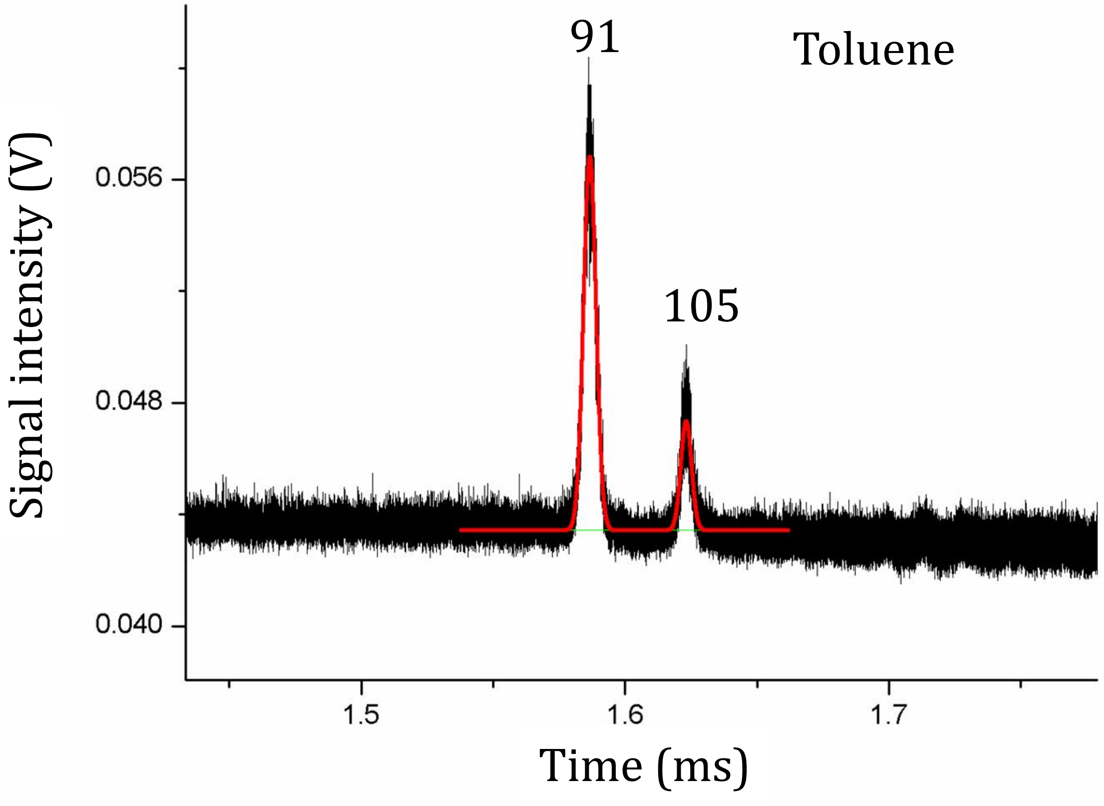
- $\frac{IDE_{Y\&pitch}}{IDE_0} = 1.25$
- $\frac{IDE_Y}{IDE_0} * \frac{IDE_{pitch}}{IDE_0} = 1.19$
- Difference = 5%

Experiments

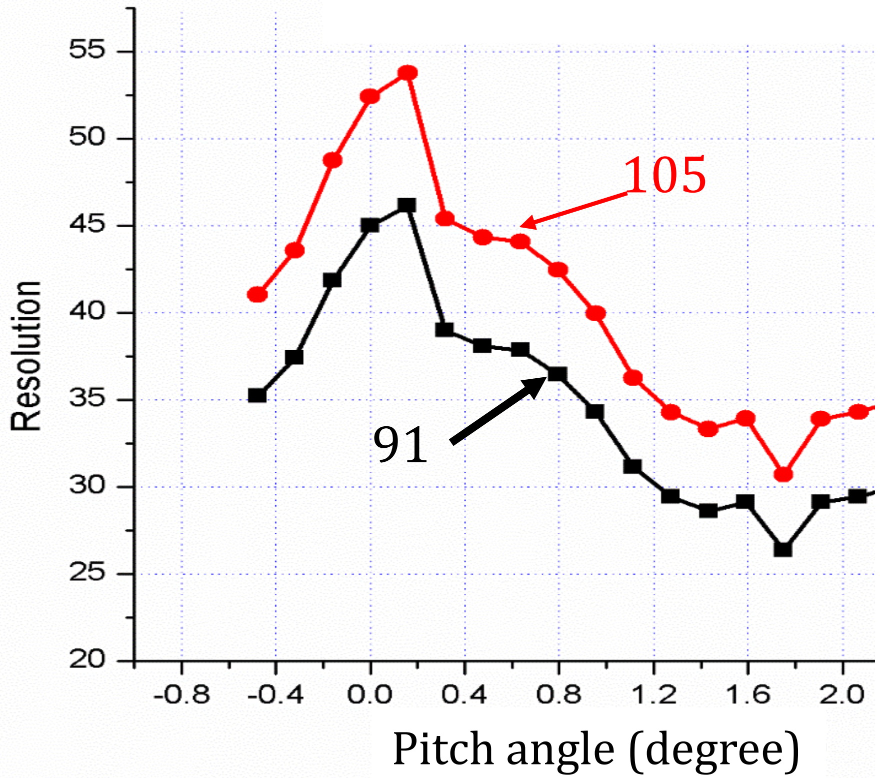
- Assembled the plates in a geometry adjustable platform
  - A strong signal was observed
  - Pitch displacement was tested
- Poor reproduction due to the manually tunable XYZ stage
- The manually tunable XYZ stage is being replaced by a motor actuator driving XYZ stage



Preliminary results



Mass spectrum



The resolution vs. pitch displacement

Conclusions

- The Ge layer plays an important role in shaping the electric field, especially the higher-order field.
- Resolution is sensitive to pitch and Y displacement (plate spacing)
- Ion detection efficiency is sensitive to X displacement (shear displacement)
- The impact to the performance from six degrees of freedom are independent
- This study provides estimates for the effects of electrode misalignments in two-plate ion trap as well as other type of linear ion traps

Acknowledgement

Dr. Daniel Austin

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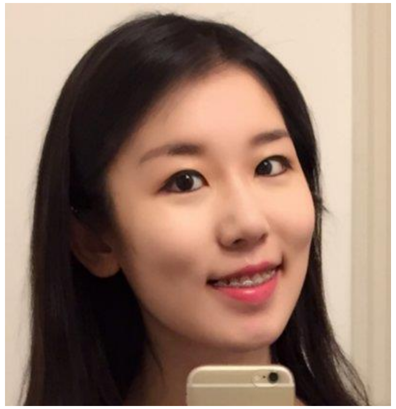

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