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Investigation of ion interactions and space charge effects in a time of flight ion trap resonator

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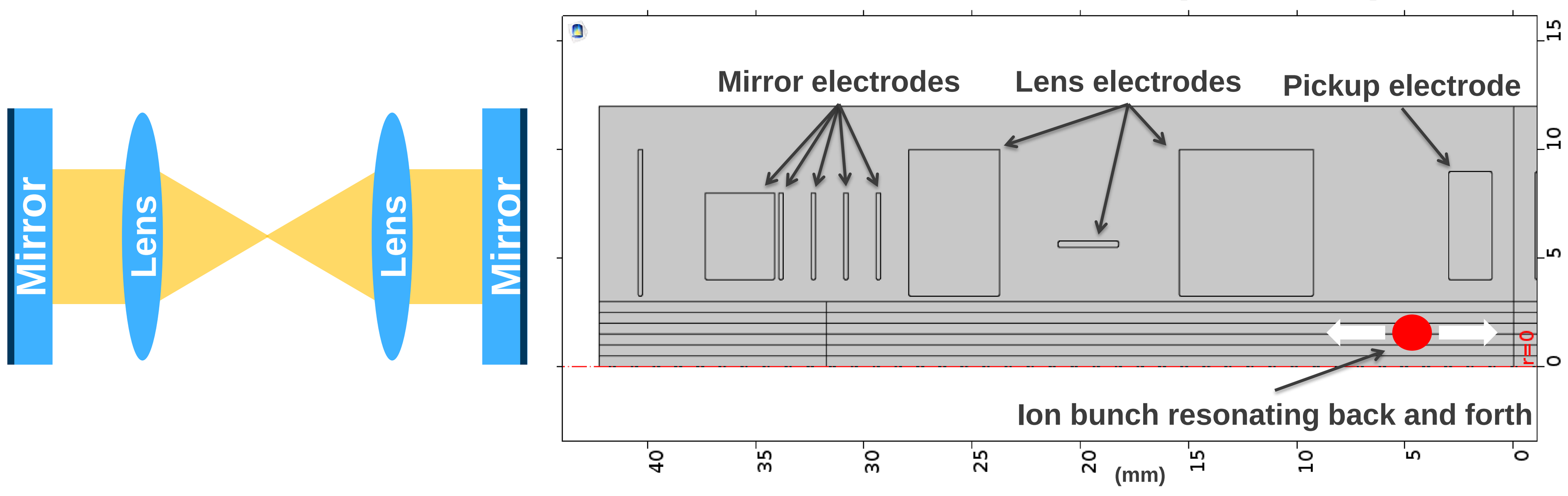
An ion trap resonator, typically used for mass spectrometry, as introduced by Zajfman et al. [1], uses a pair of opposite facing electrostatic mirrors and lenses to capture ions resonating between them. The electrostatic mirrors reflect the injected ions in the trap, while the lenses focus the ions and create a stable bunch with low ion diffusion. An interesting phenomenon that is observed in this resonator, if certain criteria are met [2], is the existence of a synchronized and low diffusion state of the ions due to ion-ion coulomb interactions. In this study a smaller version of the trap is built in 2D axisymmetric geometry. Simulations are done using COMSOL 5.1. Diffusion rates are optimized, coulomb interactions are investigated and space charge effects are compared with experimental results.

1. Trap configuration

The trap can be represented using analogy between optical lenses and mirrors; the photons (ions) are reflected back by the mirrors at each end of the trap. They are focussed by the lenses to compensate for the divergence of the beam.

Half of the 2D model of the device and the different electrodes (left-side)



The electrostatic mirrors reflect the injected ions in the trap, while the lenses focus the ions and create a stable bunch with low ion diffusion.

2. Performed simulations

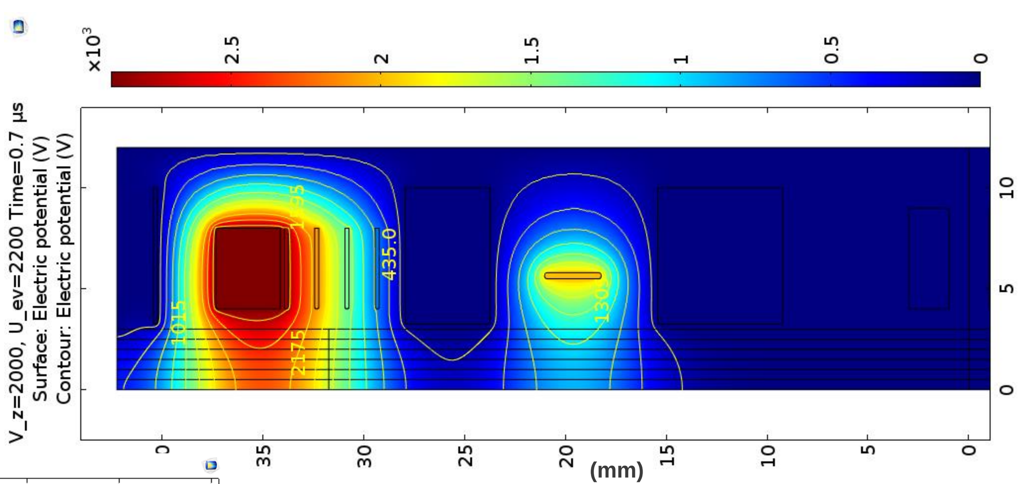
Simulations are done using the AC/DC Electric Circuit "cir", Electrostatics "es", Charged Particle Tracing "cpt", and Electric Particle Field Interactions "epfi" modules.

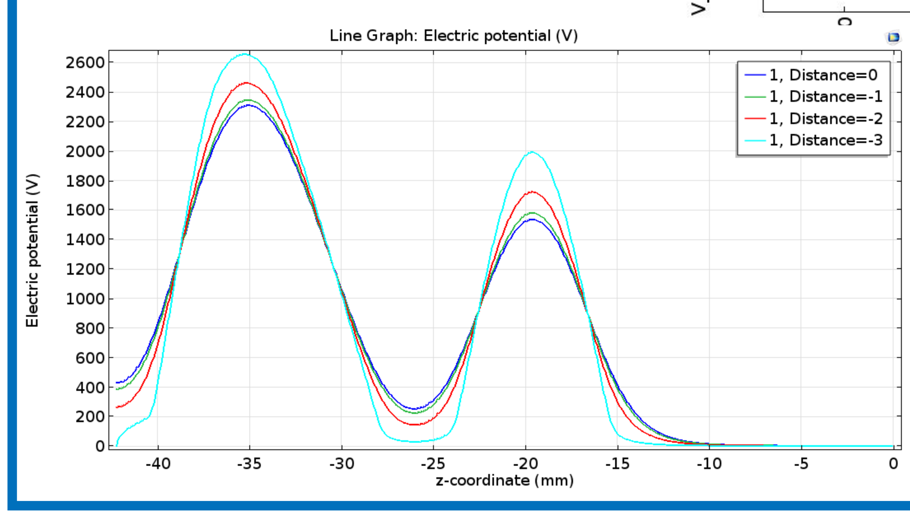
Simulations are used iteratively to optimize the lens and mirror voltages that in turn maximize the ion flight stability-criteria and also provide information on the focal point of the lenses.

Multi-physics "epfi" option simulates the space charge effects that induce voltages on the pickup electrodes. The pickup electrodes are connected to the ground via resistors that are simulated using "cir" module.

3. Trap field optimization

Mirror-electrodes of the trap create a uniform field with parallel potential contour lines.





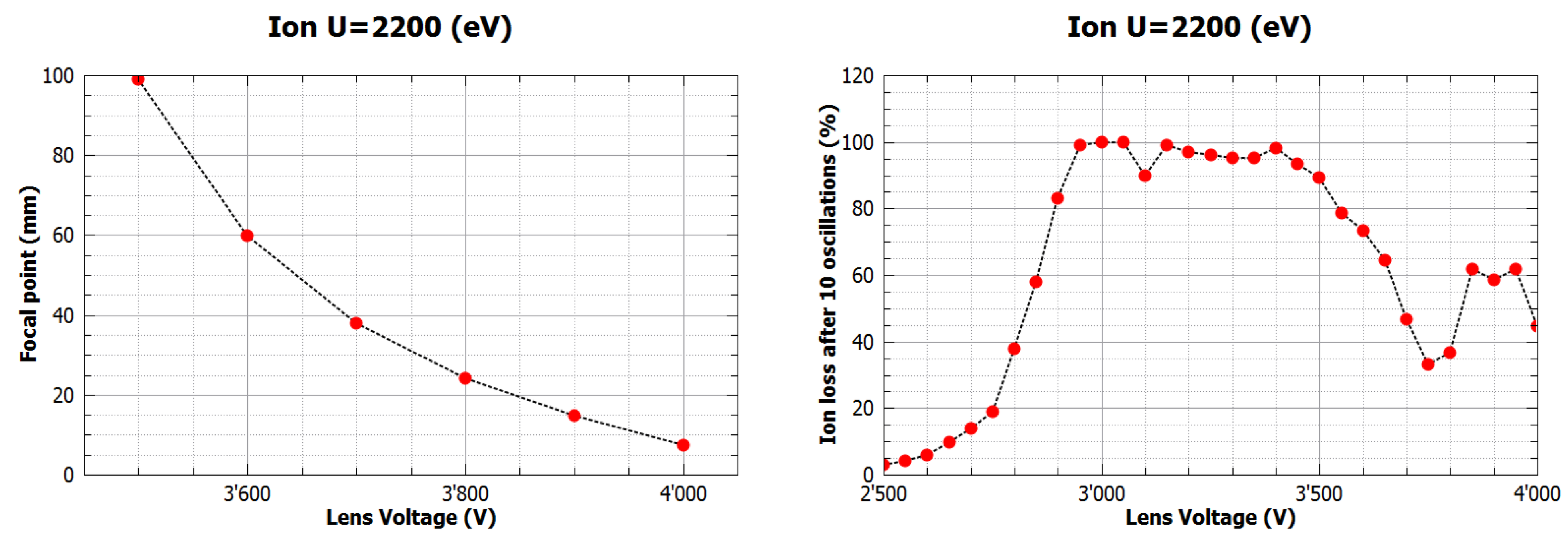
Axial variation of potential at different radii:

The mirror and lens voltage slopes are optimized to concentrate diverging ions.

4. Ion focusing and diffusion

Focal point of the lens is estimated using an average operation on the radial particle positions.

Diffusion at each voltage configuration is estimated by loss of ion energy in the trap after several oscillations.

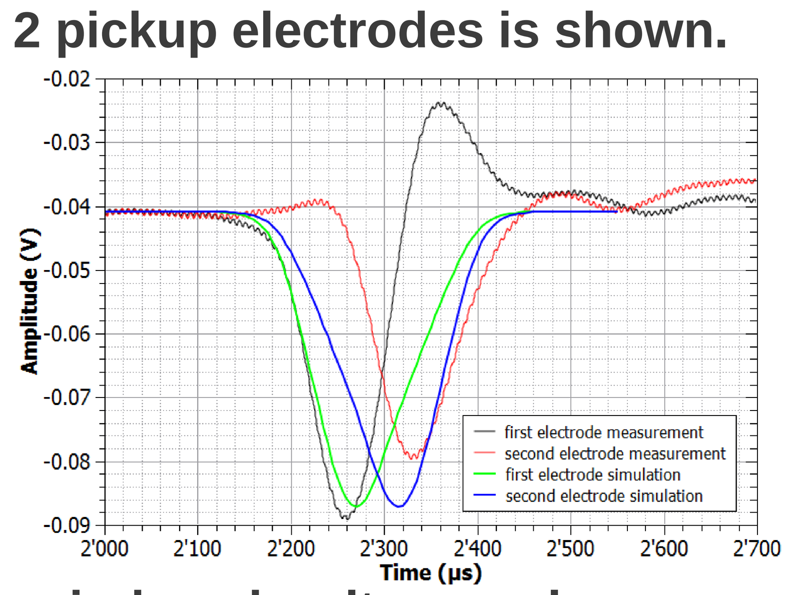


5. Space charge effects

Simulation of induced voltages in 2 pickup electrodes is shown.

In experimental results, the offset in the responses of the two electrodes is removed.

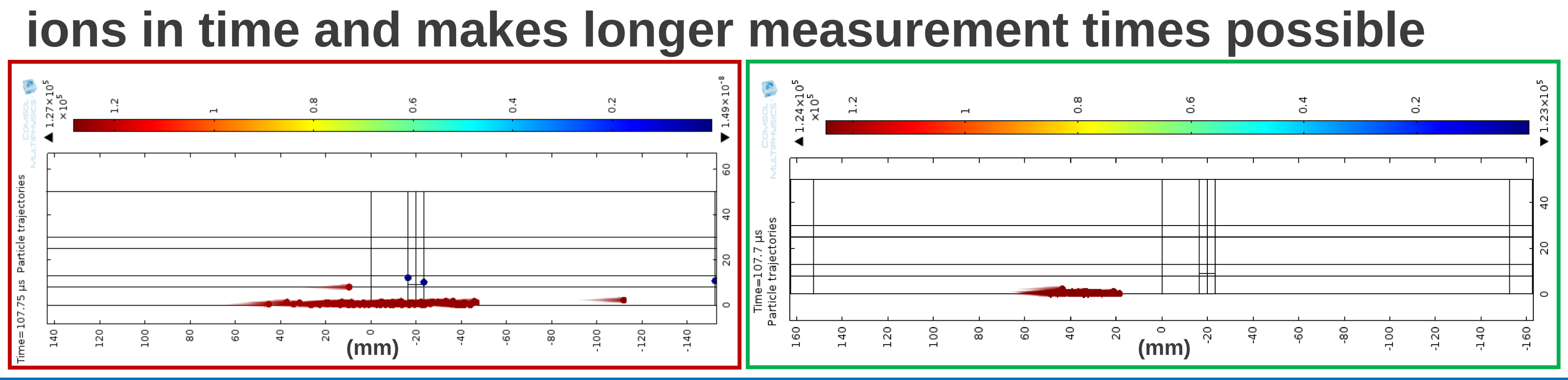
The simulation data is scaled and aligned with experimental pulses.



The simulated time periods of the induced voltage pulses on the electrodes agree well with the experimental results.

6. Ion synchronization

The results of simulations of ions with and without coulomb-force interactions in the Zajfman trap [1]: The synchronization due to Coulomb forces between ions (right) limits the spread of ions in time and makes longer measurement times possible



7. Conclusion

The simulations define the stabilization criterion of ion trajectories by optimization of the electrode configurations. Induced flight-time voltages on the electrodes agree well with the experimental results. The capability of modelling ion interactions is also demonstrated.

8. References

[1] D. Zajfman et. al, "Electrostatic bottle for long-time storage of fast ion beams," *Phys. Rev. A*, vol. 55, no. 3, pp. R1577–R1580, Mar. 1997.

[2] H. B. Pedersen et al, "Diffusion and synchronization in an ion-trap resonator," *Phys. Rev. A*, vol. 65, no. 4, p. 042704, Mar. 2002.

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