MODELING OF SPACE-CHARGE EFFECTS IN THE ORISS MRTOF DEVICE FOR APPLICATIONS TO FRIB

R. Hipple*[1], S.M. Lund[2], Physics and Astronomy Dept.,
Michigan State University, East Lansing, MI, USA
[1]Also at Niowave Inc., Lansing, MI, USA
[2]Also at Facility for Rare Isotope Beams, Michigan State University, East Lansing, MI, USA

Abstract

The Oak Ridge Isotope/Isomer Spectrometer and Separator (ORISS) is an electrostatic multiply reflecting time-of-flight (MRTOF) mass separator constructed by the University Radioactive Ion Beam Consortium (UNIRIB) and Louisiana State University. The device is now at Michigan State University for use at the Facility for Rare Isotopes and Beams (FRIB). The mass separation process is sensitive to space-charge effects due to the reflection of ions at both ends of the trap, as well as nonlinearities in the optics. In this study, we apply the time-based PIC code Warp [1] to model the effects of intense space-charge during the separation process. We find that the optics can be tuned for operation with many isochronous bounces with focusing in the presence of intense space-charge to enable separation of bunches with high particle counts. This suggests the device may be effectively utilized at FRIB as a separator, spectrograph and spectrometer to provide higher counts of particles on detectors.

INTRODUCTION

ORISS is a 1.43 m long cylindrical ion trap with electrostatic mirrors at each end whereby particles to be separated are repeatedly reflected from end to end. Fig. 1 shows a drawing of the left electrostatic mirror, the on-axis potential and axial field, and the paraxial radial field of a typical operating point. The right mirror geometry is reflection symmetric. There are 8 ring electrodes, and a conical electrostatic lens. All electrodes within each mirror, the conical lens, and the central drift region can each be independently biased. The ring electrodes have a diameter of 146 mm, axial length 32.49 mm, and are separated by thin insulating gaps (ceramic balls) with 12.7 mm diameter. The conical lenses have a smaller aperture of 50 mm and full axial length of 40.51 mm. This is the smallest aperture in the system, and therefore limits radial excursion of the particles. These conical lenses can be removed and replaced with the large-aperture variety [2].

OVERVIEW OF OPERATIONAL TUNING

To analyze the physics of of the reflections we model ORISS as an array of coaxial rings of charge. The on-axis potential of a thin ring of charge Q and radius R at axial position $z = 0$ is [3]

$$\phi(r = 0, z) = \frac{1}{4\pi\epsilon_0} \frac{Q}{\sqrt{R^2 + z^2}} \tag{1}$$

from which we can calculate the off-axis values of the electric field components E_z and E_r to 2nd order in r as [4]

$$E_z(r, z) = -\frac{\partial \phi}{\partial z} \approx -\phi' + \frac{1}{4}\phi''' r^2,$$
$$E_r(r, z) = -\frac{\partial \phi}{\partial r} \approx \frac{1}{2}\phi'' r,$$

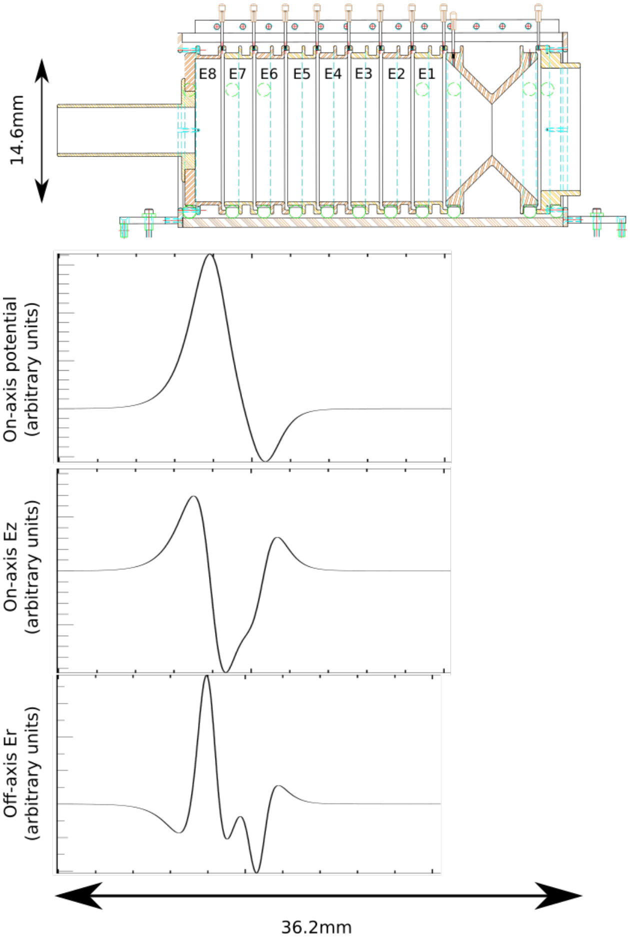

Figure 1: ORISS showing the mechanical structure and relevant electrostatic fields (Mechanical drawing courtesy LSU).

---

* hipple@msu.edu

giving after some algebra

$$E_z \approx \frac{Q}{4\pi\epsilon_0}\left\{\frac{z}{(R^2+z^2)^{3/2}} + \frac{1}{4}\left[\frac{9z-15z^3}{(R^2+z^2)^{5/2}}\right]r^2\right\},$$
$$E_r \approx -\frac{Q}{8\pi\epsilon_0}\left(\frac{1}{(R^2+z^2)^{3/2}} - \frac{3z^2}{(R^2+z^2)^{5/2}}\right)r.$$

The paraxial E_r field component is plotted in Fig. 2. The second order variation of E_z on axis in z gives rise to a linear field gradient that can provide focusing.

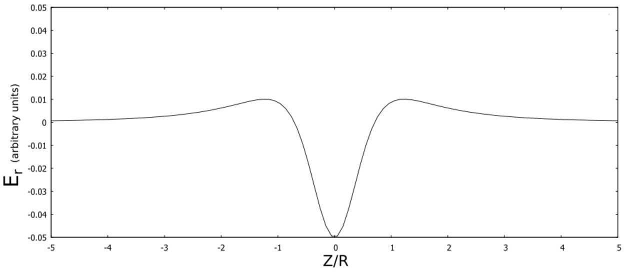

Figure 2: Paraxial radial field E_r showing focusing region near the plane of the ring at $z = 0$.

We can take advantage of the radial focusing region if the turning point of the orbit is close enough to the ring. The energy of the approaching particle must be high enough to enter the focusing region, but not so high that it is overfocused and exits the system. Between these two limits, we find stable orbits between two rings of charge. However, for a given energy within this range, there is a limit on the transverse acceptance. From Eq. (2), $E_r(r) \propto r$, whereas $E_z(r) \propto r^2$. Hence the axial field of the mirror will always eventually dominate the transverse field at large enough r. To make additional progress, we must introduce separate focusing elements to allow simultaneous tuning for transverse and energy-isochronous focusing. Adjacent rings can be biased for isochronous tuning and focusing simultaneously using different potential rings to form an einzel type lens [4].

The principle of time of flight mass spectrometry depends critically on the initial ion kinetic energies being identical. This is due to the requirement that any difference in velocity between two ions should be due to the mass difference of the ions to translate into mass correlated time of flight differences over many bounces in the trap. Since there will always be some initial distribution of energies $\Delta\mathcal{E}$, the device should be designed such that ions of the same mass with slightly different initial kinetic energies have isochronous orbit transits. Since an ion with a higher kinetic energy will have a higher velocity, this requires that the higher energy particles travel slightly longer paths into the reflecting mirror. This leads to a condition of energy isochrony. An analysis of the required conditions can be found in [5].

PARTICLE-IN-CELL (PIC) SIMULATIONS

We model ORISS with the Warp particle-in-cell (PIC) code [1]. Warp is a time based code with a variety of r-z and 3D Poisson solvers that is well suited for modeling the device. Detailed representations of biased conductors (subgrid) are loaded onto the spatial mesh and an multigrid method field solver is applied with mesh refinement capability which allows fine gridding near the turning points to resolve space-charge forces at stagnation points. Mesh resolutions were tested for adaquacy.

SPACE CHARGE EFFECTS

FRIB will be a CW SRF linac with high 400kW power. Rare isotopes will be separated by a multistage fragment separator and be transported to a variety of systems including an RF cooler buncher in which up to 10^8 ions will be trapped and cooled. These bunches will be the input for ORISS. Because space charge gives an energy spread to the particles, we require Δz to be independent of ΔE, the energy deviation, at the end of a full orbit. To operate with space charge, we need to find a potential configuration that is both energy isochronous and point-to-point focusing.

We require a kinetic energy for the particles that is energy-isochronous. This is found by testing a range of reference energies and then launching bunches with a ±5% spread of energies about each of these reference energies. The objective is to find a reference energy that results in a longitudinal focal point at the midpoint of the system. As can be seen from Fig. 3, all particles in a range about this central energy return approximately to a focus at the midpoint ($t = 22\,\mu$s). The second criterion to be met was transverse parallel to point focusing. A parallel set of rays must be focused to a point at the center of the device (Fig. 4). To confirm that these conditions are sufficient to separate particles of differing mass, a bunch containing equal parts of $^{238}U^+$ and $^{237}Np^+$ were launched through the system. Successful separation of this bunch by mass after only 5 reflections is illustrated by Fig. 5.

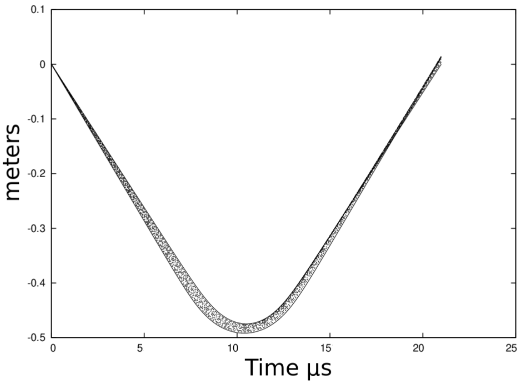

Figure 3: Optimal energy focusing.

TUNING FOR MASS SEPARATION AT HIGH SPACE-CHARGE INTENSITY

In ths manner electrode settings were found that worked all the way up to $n = 10^6$ particles, but the time it took to

ISBN: 978-3-95450-223-3 ISSN: 2673-7000 doi:10.18429/JACoW-NAPAC2019-WEPLS10

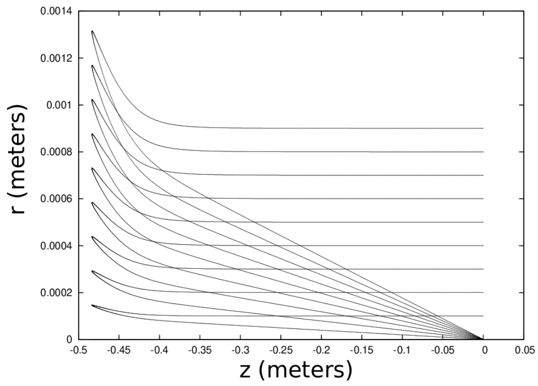

Figure 4: Trajectory of a particle revealing both focusing and defocusing of a ring of charge. $z = 0$ m is the center of the device, $z = -0.6$ m is the location of the mirror.

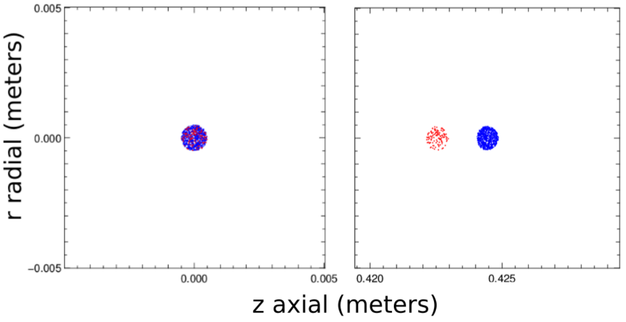

Figure 5: Initial configuration and after several reflections.

simulate $n > 10^6$ particles began to increase dramatically. At this point we switched to macroparticles. Using 10^6 particles with a macroparticle weight of 100 reaches the goal of 10^8 particles. As we reach a focusing electrode settings 10 kV, the optics are such that the beam will stay radially confined over many turns, even with a high degree of space charge. This result demonstrates that if the optics are tuned in such a way that energy isochrony is maintained, and first order optics with space-charge are kept from expanding beyond the limits of the system, then separation can occur even in the presence of intense space-charge. However, it must be emphasized that this process is sensitive to the optics. Figures 6 and 7 show a similar run with non-optimal optical settings. The quality of the movie is slightly improved; more tracer particles are used.

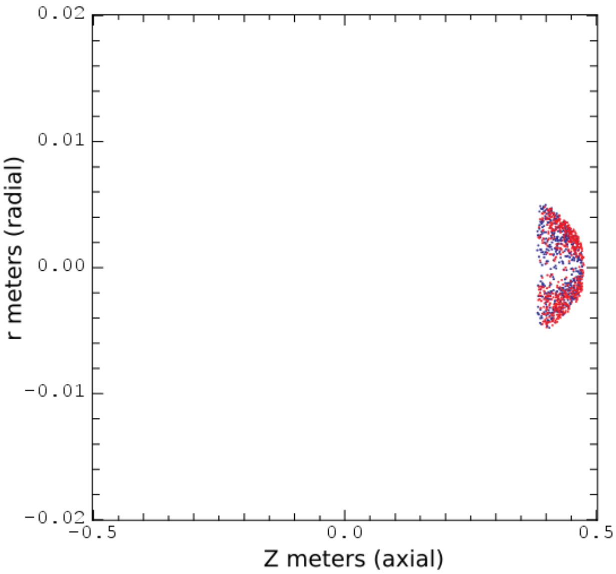

Figure 6: Bunch reaches the turning point, but the optics has distorted the shape of the bunch.

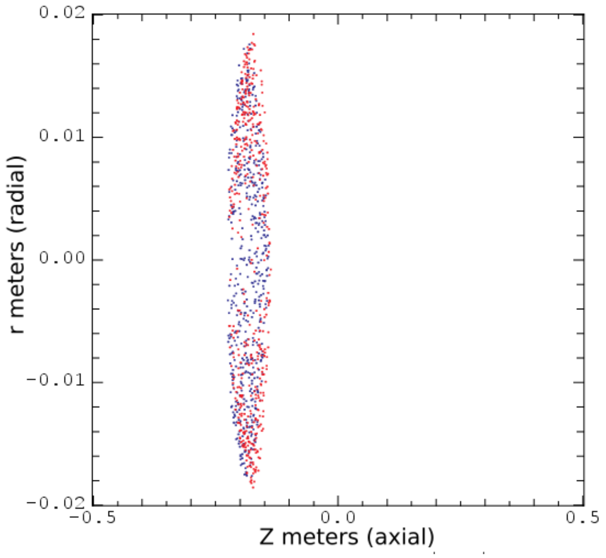

Figure 7: In an untuned system with space charge, the particles do not separate.

CONCLUSION

An operating point for ORISS capable of containing a beam up to 10^8 particles was found empirically. A development cycle evolved, comprised of increasing the particle counts, increasing the electrode biases, and maintaining energy isochrony and parallel to point focusing.

It was discovered that unless these criteria were adhered to, the nonlinearities induced by space charge overwhelmed the longitudinal separation of particles by mass alone. The transverse and longitudinal optics must be tuned to keep these nonlinearities in check in order that mass separation can be achieved.

REFERENCES

[1] Warp, `http://warp.lbl.gov`

[2] Ken Carter, private communication.

[3] Jackson, J. D. *Classical Electrodynamics,* 2nd ed., New York: J. Wiley, 1975.

[4] Martin Reiser, *Theory and Design of Charged Particle Beams,* 2nd Edition, Wiley-VCH, 2008.

[5] Hipple, Robert. Ph.D. Thesis, Michigan State University, 2019.