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Abstract

A novel method comprising two sub-procedures—global search and local refinement—has been developed and presented for the design of a multiple-reflection time-of-flight (MRTOF) mass analyzer. Utilizing this method, a distinct type of MRTOF mass analyzer, wherein each mirror consists of five cylindrical electrodes, has been designed for isobaric separation at the Lanzhou Penning Trap (LPT). The optimal potential parameters for the electrodes have been obtained, achieving a maximal resolving power of 1.3x105 with a total time-of-flight of 6.5 ms for the 40Ar1+ ion species. Simulations demonstrate that the inaccuracy of the potentials applied to the mirror electrodes must be less than 50 ppm, and preferably 20 ppm.

Full Text

Preamble

Designing a multi-reflection time-of-flight mass analyzer for LPT
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Abstract

A new method comprising two sub-procedures—global search and local refinement—has been developed for designing a multiple-reflection time-of-flight (MRTOF) mass analyzer. Using this approach, we have designed a novel MRTOF mass analyzer featuring mirrors composed of five cylindrical electrodes each, intended for isobaric separation at the Lanzhou Penning Trap (LPT). The optimal electrode potentials have been determined, achieving a maximum

resolving power of 1.3$×10^{5}$ with a total time-of-flight of 6.5 ms for $^{40}Ar^{1+}$ ions. Simulations indicate that the potentials applied to the mirror electrodes must be stable to within 50 ppm, or preferably 20 ppm.

Keywords: Time-of-flight mass spectrometer, Multiple-reflection, Mass measurement, Isobar separation, Exotic nuclei

1. Introduction

The multi-reflection time-of-flight mass spectrometer (MRTOF-MS) was first proposed by Wollnik [1] more than 25 years ago. This device, developed in recent years for mass spectrometry and isobaric separation, operates with ion bunches having kinetic energies ranging from a few hundred electron-volts to a few kilo-electron-volts. By extending the flight path through multiple reflections between electrostatic ion mirrors, the MRTOF-MS overcomes the resolving power limitations of conventional time-of-flight mass spectrometers (TOF-MS) while retaining unique advantages: extremely short measurement times, a large mass range, very high sensitivity, and non-scanning operation. These capabilities address the challenges of mass spectrometry at current and future accelerator facilities for exotic nuclei research, making the technique suitable for studying very exotic nuclei with extremely low production yields and purities as well as very short half-lives.

Plaß et al. [2] reviewed MRTOF-MS developments for short-lived nuclei research and various instrumental implementations. Based on the potential distribution along the optical axis, existing analyzers can be categorized into two types: asymmetric and symmetric. The asymmetric type was implemented at Oak Ridge National Lab. [3] and RIKEN [4], while the symmetric design has been adopted by many other research groups worldwide. The configuration described in Ref. [5], featuring mirrors made of eight cylindrical electrodes, was derived for the ISOLTRAP experiments [6] at ISOLDE/CERN and achieved significant success in mass measurements [7, 8] and isobaric separation. A duplicate of this design may be operated at RAON/RISP [9]. An advanced coaxial four-electrode design has been implemented for the LEB of the Super-FRS at FAIR [10], for TITAN [11], and for MLL-TRAP [12]. Additionally, MRTOF-MS systems are being implemented at ANL [13] and IGISOL [14].

The Lanzhou Penning Trap (LPT) [15] is an ion trap facility currently under construction at the Institute of Modern Physics, Chinese Academy of Sciences. We plan to build an MRTOF-MS for isobaric separation for the LPT. Since the number of electrodes affects the potential smoothing along the optical axis and determines the number of power supplies—and thus the overall cost—we have designed a new MRTOF mass analyzer configuration in which each mirror consists of five cylindrical electrodes. This paper focuses exclusively on the design and optimization of our MRTOF mass analyzer and its corresponding results; ion injection and ejection are not considered.

2. Design of the MRTOF Mass Analyzer

The MRTOF mass analyzer under design, shown in Fig. 1 [Figure 1: see original paper], comprises two identical electrostatic mirrors (each consisting of four electrodes) combined with two einzel lenses and a drift tube. Ions from an upstream RFQ cooler/buncher enter the analyzer when the potentials on the mirror electrodes are switched down. Subsequently, the mirror-electrode potentials are reactivated, and the ions travel hundreds of revolutions between the two mirrors, becoming separated by their mass-to-charge ratio during oscillation. Ions of interest are released from the analyzer by switching down the mirror-electrode potentials and then arrive at a time-focus plane, where either an MCP detector for mass measurements or a Bradbury-Nielsen gate [16] for isobaric separation is deployed.

All electrodes in this analyzer have a cylindrical shape, with a total length of 708 mm and an inner diameter of 60 mm. The mirror electrodes M1–M4 have lengths of 20, 16, 26, and 26 mm, respectively, while the lens electrode L is 46 mm long. Electrode M1 features a smaller aperture of 30 mm diameter at its outer end for electric shielding from adjacent components. The intermediate drift tube has a length of 400 mm (optimized later) with reduced apertures of 30 mm diameter at each end to shield the drift region from the electric fields of the lens electrode. The distance between adjacent electrodes is 4 mm. The time-focus plane, where an MCP detector or Bradbury-Nielsen gate can be placed, is located 255 mm after the analyzer.

The mass resolving power R is defined as mass m divided by the difference between neighboring distinguishable masses Δm, and is related to the time-of-flight TOF and temporal width ΔTOF by $R = m/\Delta m = TOF/(2\Delta TOF)$, where the overall spread ΔTOF is the full-width-at-half-maximum (FWHM) of the time-of-flight peak. The ΔTOF value depends on both the initial bunch width and the time-of-flight aberration from the start point to the time-focus plane.

3. Optimization Procedure

To determine optimal parameters for the structure shown in Fig. 1, an optimization strategy is required. Ref. [17] describes a procedure for potential parameter optimization using a Nelder-Mead simplex algorithm [18] within the SIMION code [19], where the ion trajectory must first satisfy the point-to-parallel/parallel-to-point focusing condition for highest trajectory stability. However, we believe this approach may not necessarily find the optimal parameter sets. The point-to-parallel/parallel-to-point focusing condition is easily satisfied, and numerous parameter sets meeting this condition can be found even in a small parameter space. Searching a larger space is time-consuming, and it is difficult to ascertain whether the best starting point has been found within limited time.

Therefore, we employ an alternative procedure consisting of two sub-procedures:

global search and local refinement. In our approach, ion trajectories are calculated in SIMION using our specified user program, while parameter variation via the Nelder-Mead simplex algorithm is performed in a separate optimization program coded by us. This procedure offers two advantages: (1) the best parameters can be found with certainty because we search all possibilities in the entire parameter space; (2) the optimization program does not require modification if the MRTOF mass analyzer structure is changed. This enables us to find optimal parameters not only for the analyzer itself but also for the complete MRTOF-MS including additional elements such as einzel lenses for beam injection and ejection.

The procedure details are as follows. First, a model is created in SIMION according to the MRTOF-MS configuration, enabling calculation of the average and deviation of the TOF and resolving power. Second, for the global search, the possible potential for each electrode is estimated based on beam optics knowledge, and variation ranges are deliberately set, creating a potential matrix with dimensions equal to the number of parameters to be optimized. This matrix serves as the initial parameter sets for the search. All initial parameter sets are input into SIMION, ion trajectories are calculated for the same species, and a few sets with relatively high resolving power for a specified number of revolutions are selected. Third, for local refinement, all parameters in these selected sets are varied using the Nelder-Mead simplex algorithm and input into SIMION again. The peak width of the same species is measured and used as the objective function to be minimized. After approaching a local minimum of the TOF surface within a certain radius, these optimized parameters are multiplied by random numbers close to 1 and the optimization is restarted. This procedure yields numerous local minima, from which the best are chosen as the optimal parameter sets.

4. Results and Discussion

To calculate the mass resolving power as a function of the number of revolutions, we considered the following initial beam conditions. The beam consists of 100 ions (unless specified otherwise) of $^{40}Ar^{1+}$ with an average kinetic energy of 1.5 keV and a bunch width of 20 ns (FWHM) at the analyzer center. In the middle plane between the ion mirrors, the ion beam coordinates x and y (orthogonal to the optical axis z), the angles $\alpha = dx/dz$ and $\beta = dy/dz$ relative to the axis z, and the energy K are approximately represented by Gaussian distributions with standard deviations $\sigma = \sigma = 1$ mm, $\sigma = \sigma = 1.5$ mrad, and $\sigma = 8.5$ eV.

4.1. Optimization of Potential Distribution and Drift-Tube Length

Considering the symmetric design of our MRTOF analyzer and practical potential control through power supplies during experiments, we selected the potentials applied to the four mirror electrodes and one lens electrode as optimization

parameters—five in total. The potential on the inner drift tube was fixed at 0 V for all calculations.

In the global search step, we considered 6$×6×5×6×$6 = 6480 potential combinations as initial parameter sets and ultimately selected only the best five sets for further local refinement. Using the Nelder-Mead simplex algorithm, all parameters were varied to obtain numerous local minima, and the parameter set yielding the smallest TOF peak width was chosen as optimal.

To achieve very high resolving power, we also optimized the drift-tube length while fixing all other parameters, thereby optimizing the flight times in both the drift tube and mirrors. Fig. 2 [Figure 2: see original paper] shows the calculated mass resolving power as a function of drift-tube length. The highest resolving power is achieved when the drift tube is 398–402 mm long, and we selected 400 mm as our optimal value.

With the drift-tube length fixed at 400 mm, we optimized the potentials for different numbers of revolutions and determined the maximum achievable resolving power, shown in Fig. 3 [Figure 3: see original paper]. As the number of revolutions increases up to 400, the maximum resolving power increases steadily, but the slope of this increase declines. This suggests that achieving higher mass resolving power requires ions to travel longer distances in the MRTOF analyzer. Due to computational constraints, we did not continue optimization beyond 400 revolutions.

For each specific number of revolutions, we obtained one potential set with the highest mass resolving power. Table 1 lists the potentials optimized for 350 revolutions. Fig. 4 [Figure 4: see original paper] shows the potential distribution along the optical axis in one mirror of the analyzer, which exhibits two regions with approximately constant electric fields [20, 21], where E1 < E2. Ions turn around in the weaker constant electric field E1.

Applying the potentials from Table 1 to the electrodes, we calculated the temporal width at the detector plane as a function of the number of revolutions. Fig. 5 [Figure 5: see original paper] shows the calculated total TOF, temporal width ΔTOF, and mass resolving power R versus number of revolutions. The total time-of-flight increases almost linearly with the number of revolutions, while the initially high temporal spread decreases to a minimum of only 22 ns at 350 revolutions, where the resolving power reaches $1.1\$\times 10^{\{5\}}. The maximum resolving power of R = 1.3\times 10\{5\}\$$ is achieved at 430 laps (TOF = 6.5 ms), as the temporal spread increases more slowly than the total time-of-flight.

4.2. Effects of Potential Inaccuracy

Fig. 6 [Figure 6: see original paper] shows the relative variation of TOF and mass resolving power as functions of the relative variation of bias potentials determined by our optimization code. For TOF, the behavior from mirror elec-

trode M4 differs from other electrodes, with the largest variation originating from mirror electrode M2. The maximum achievable mass resolving power decreases as expected when electrode potentials deviate from their ideal values. Potential variations in mirror electrode M4 and lens electrode L (which form an einzel lens with the drift tube) have almost no effect on the final resolving power. Variations from mirror electrodes M1 and M2 have relatively larger effects, while variations from mirror electrode M3 have the greatest impact: the resolving power decreases by 35% from 1.1$×10^{5}$ to 7.0$×10^{4}$ for a relative potential variation of 500 ppm. Therefore, we must ensure that potentials applied to mirror electrodes M1–M3, especially M3, are stable to better than 50 ppm, or preferably 20 ppm.

4.3. Peak Shape

To accurately determine the TOF and understand the peak shape, we extracted the TOF spectra shown in Fig. 7 [Figure 7: see original paper]. In these calculations, the potentials listed in Table 1 were applied to the electrodes and beam properties remained as described previously, except that 2500 ions were used to improve statistics. The peak shape can apparently be fitted by a Gaussian function with a FWHM of 21.6 ns. This result differs from Ref. [22], where the authors reported that the TOF peak was better fitted by an exponential-Gaussian hybrid function rather than a Gaussian, suggesting that the slow-side tail might be related to higher-order optical aberrations.

5. Summary

We have presented a new method for designing a multiple-reflection time-of-flight mass analyzer comprising two sub-procedures: global search and local refinement. This method offers two key advantages: (1) the optimal parameters can be found with certainty through exhaustive search of the parameter space; (2) the optimization program requires no modification if the MRTOF analyzer structure is altered. The method also can find optimal potentials for the complete MRTOF mass spectrometer or isobar separator.

Using this new method, we have designed an MRTOF mass analyzer with each mirror consisting of five cylindrical electrodes. The optimal electrode potentials have been determined, achieving a maximum resolving power of 1.3$×10^{5}$ with a total TOF of 6.5 ms for $^{40}Ar^{1+}$ ions. Simulations show that potentials applied to mirror electrodes M1–M3, especially M3, must be stable to better than 50 ppm, or preferably 20 ppm. This analyzer, together with injection and ejection elements, will be installed on the LPT beamline for isobaric separation.

Acknowledgments

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Figure Captions

Figure 1: The geometry of the MRTOF mass analyzer under design. The time-focus plane (detector plane) is also shown.

Figure 2: Calculated mass resolving power R as a function of drift-tube length.

Figure 3: The maximum mass resolving power Rmax achieved at different

numbers of revolutions.

Figure 4: Potential distribution along the optical axis z in one mirror of the MRTOF analyzer for the mean ion kinetic energy of 1.5 keV. The position z = 0 corresponds to the midpoint between the ion mirrors. E1 and E2 denote two regions with approximately constant electric fields.

Figure 5: Calculation results of (a) TOF, (b) temporal width ΔTOF, and (c) mass resolving power R as functions of the number of revolutions.

Figure 6: Calculated relative variation of TOF (left) and mass resolving power R (right) as functions of relative variation of bias potentials as determined by the optimization code.

Figure 7: Left: Initial TOF distribution of $^{40}Ar^{1+}$ ions (m/q = 40). Right: Calculated TOF distribution after 350 laps in the MRTOF analyzer. The total ion number is 2500. The red lines show Gaussian function fits.

Table 1: Optimized potentials on the mirror electrodes and lens electrode shown in Fig. 1 for $^{40}Ar^{1+}$ ions. M1–M4: mirror electrodes 1–4 from outside to inside; L: lens electrode.

Electrode	Potential (V)
M1	-4473.1
M2	-
M3	-
M4	-
L	-

Note: Figure translations are in progress. See original paper for figures.

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