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Ion-optical design of a high-performance multiple-reflection time-of-flight mass spectrometer and isobar separator

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ABSTRACT

The ion-optical design of a multiple reflection time-of-flight mass spectrometer and isobar separator (MR-TOF-MS) is presented. The MR-TOF-MS has been developed for the research with exotic nuclides at accelerator facilities and has been designed to provide a mass resolving power (FWHM) exceeding 300,000 and a mass accuracy of down to 10^{-7}. High-performance axially symmetric four-electrode gridless ion mirrors have been developed and optimized for the device. In addition, the MR-TOF-MS comprises several further novel ion-optical elements such as an isochronous post-analyzer reflector and an energy bunching and deceleration system for ion injection into an accumulation trap. The device has been built and commissioned and shows superb performance characteristics in accordance with the design criteria.

1. Introduction

Among the many methods of mass spectrometry only time-of-flight mass spectrometers (TOF-MS) allow for the broadband investigation of fast processes with characteristic measurement times in the millisecond range. They are also capable of achieving very high transmission efficiencies. In principle, TOF-MS are therefore ideal mass spectrometers for the research with exotic nuclides, since these nuclides can be very short-lived (half-live much shorter than a second) and are typically produced in extremely small quantities (down to yields of one ion per week). Nevertheless, conventional TOF-MS were not of interest in nuclear physics until recently, because the mass resolving power of singly-reflecting devices is limited to a few ten thousand. During the last decade, however, remarkable progress was achieved in the development of multiple-reflection [1–4] and multiple-turn [5,6] TOF mass spectrometers, some of which demonstrated a mass resolving power in excess of 100,000. This progress gives access to two particularly important applications in nuclear physics: (i) The direct high-precision mass measurement of short lived exotic nuclei, for which an accuracy of better than 10^{-6} is required [7–9]. (ii) The separation of rare exotic nuclides produced, e.g. in nuclear fission or spallation reactions, from abundant isobaric contaminants in order to deliver a purified ion beam for further investigations by different experimental techniques, thus enabling e.g. mass-selected decay spectroscopy.

We have proposed [10,11] to use an MR-TOF-MS for both, accurate mass measurements and, in conjunction with a Bradbury–Nielsen gate [12,13], as isobar separator, and demonstrated spatial separation of isobars in such a device for the first time [14,4]. Mass separation is performed in a multiple-reflection TOF analyzer based on two axially symmetric gridless electrostatic reflectors (ion mirrors). Ion bunches separated in time are directed either to a TOF detector for mass measurement or to an ion gate for selecting a required nuclide. The results of first experiments revealed high performance of the instrument. In particular a mass resolving power of 100,000 (FWHM) and of 35,000 at 10% of the peak height with excellent peak shapes were achieved [15,4,16]. The device served as proof-of-principle for experiments with exotic nuclei at the GSI Helmholtzzentrum für Schwerionenforschung (GSI, Darmstadt) and in the future at the Facility for Antiproton and Ion Research (FAIR). Similar projects are pursued at the RI-beam factory RIBF at RIKEN [17,18] and at ISOLDE/CERN in Geneva

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[19,20], and first direct mass measurements of short-lived nuclides have been performed [21–23].

Here, the ion-optical design of a next-generation, high-performance MR-TOF-MS is presented. It was proposed in [4], developed, built and commissioned. The technical implementation of the device and its experimental performance is described in detail in [24,1,25]. The present paper is devoted to a detailed description of the ion-optical solutions implemented in this mass spectrometer and separator.

2. Choice of the mass analyzer configuration

The TOF analyzer developed in this work should be able to perform three functions: (i) Broadband mass measurements with medium resolution ($m/\Delta m > 1000$ at FWHM), (ii) precise mass measurement of exotic short lived isotopes with lifetimes of the order of milliseconds with the accuracy on the level of 10^{-7}, and (iii) separation of isobaric exotic nuclides that differ in mass by 10^{-5} or more. Reliable isolation of ion species, which differ in abundance by two orders of magnitude, requires, depending on peak shape, a mass resolving power that is larger by a factor of two to three than that needed for resolution at FWHM level. Hence a mass resolving power of about $m/\Delta m$ = 300,000 at FWHM level is required. This mass resolving power also provides a possibility to measure the position of the centroid of a mass peak of just 8 ions with a precision of 5×10^{-7}. The mass resolving power of 300,000 thus can be considered as the goal value for a multiple-reflection TOF mass analyzer used in nuclear physics. However, an even higher mass resolving power will allow achieving a given mass precision with a smaller number of ions. The fastest selection of longitudinally separated short ion bunches can be performed using a Bradbury-Nielsen gate [12,13]. Since the typical time scale of ion separation by a Bradbury–Nielsen gate is about 10 ns, it is reasonable to form and fly ion bunches of a similar time width Δt. The mass resolving power of a TOF-MS is given by $m/\Delta m = t/(2\Delta t)$. Therefore a flight time t of about 6 ms is required to obtain a mass resolving power of 300,000. Ion bunches with such a time duration can be created by extracting trapped ions using pulsed electric fields of relatively low strength, which results in a moderate ion energy spread of $\delta = 3\ldots4\,\%$. Ion storage between injections into the analyzer is optimally performed in a radiofrequency (RF) ion trap. Among RF traps, a linear ion trap (LIT) with axial ion ejection into the mass analyzer possesses the simplest geometry and perfectly matches the spatial and energy spread that can be accepted by the TOF analyzer. The storage time of several milliseconds allows using a LIT filled with a buffer gas (typically He) at a low pressure of $\sim 10^{-3}$ mbar for collisional cooling of the ions, shrinking the size of the trapped ion bunch and thus reducing the energy and time spreads of the ejected ion bunches.

As compared to life science applications, in which ion analysis is typically performed in a very wide mass range, short-lived exotic isotopes created in nuclear reactions, such as fission, fragmentation or spallation, can typically be (pre-)separated by a magnetic separator. Thus, high-resolution mass measurements in a TOF analyzer are often performed within a relatively narrow relative mass range, which allows using the closed type of a multiple-reflection TOF mass analyzer, in which ions perform repetitive motion along a cyclic ion path. The simplest closed mass analyzer is formed by two coaxial ion mirrors, between which ions are reflected back and forth. The coaxial geometry has an advantage of cancelling out first order TOF aberrations with respect to the spatial spread of the ion bunches due to the straight optic axis. This configuration of the analyzer with ion injection and ejection through the cap electrodes of pulsed switched ion mirrors was chosen for the considered mass spectrometer and separator. Technical limitations of the high voltage switches used for the fast and precise changing of the mirror electrodes restricts the values of the potentials of the cap electrodes. For this reason, the nominal kinetic energy K_0 of ions in the drift space between the mirrors was chosen not to exceed 1500 eV.

3. General layout of the mass spectrometer and separator

The mass spectrometer and isobar separator (Fig. 1) includes an injection linear ion trap, a coaxial multiple-reflection TOF mass analyzer, a post-analyzer reflector, a Bradbury–Nielsen gate for ion separation, which can be replaced by an ion detector for direct mass measurement, an energy buncher and a deceleration system for injecting the separated ions into an accumulation linear ion trap.

The injection LIT forms short ion bunches, which are maximally compressed in length at a position of a primary time focus located somewhere between the LIT and the exit mirror of the analyzer. Ions are injected into the analyzer through the hole in the cap electrode of the entrance mirror. During the process of injection, some electrode potentials of the entrance mirror are switched to lower values, and after injection they are raised back to lock the ions inside the analyzer. Each mirror is tuned such that a time focus in the analyzer is re-translated to the same point after each full turn of the ions in the analyzer (i.e. after each two reflections from ion mirrors).

The ion ejection from the multiple-reflection analyzer is performed through a hole in the exit ion mirror opposite to the entrance mirror by switching some electrode potentials of this mirror to lower values. Ions leaving the analyzer are reflected by 180° in a post-analyzer reflector [4,1]. This reflector translates the primary time focus to the position of the Bradbury–Nielsen gate or to the position of the ion detector. Since the intermediate time foci after each full turn in the multiple reflection TOF analyzer are located at the same point, the overall flight distance is then isochronous. Furthermore, all voltages in the system are independent of the number of turns. Hence no voltage retuning has to be performed when changing the resolving power and mass range of the system.

The ions of interest, separated from contaminants by the Bradbury–Nielsen gate, are trapped in an accumulation gas-filled linear ion trap, cooled there and transferred to experiments downstream of the device. For efficient trapping, the ions should be slowed down to kinetic energies of less than 10 eV. It is not possible to achieve such retarding without prior reduction of the ion energy spread, which typically amounts to up to $K_0 \times \delta \approx 60$ eV. Reduction of the ion energy spread is performed by a dynamic energy buncher based on a pulsed retarding electric field [4,1].

A detailed description of the design of the ion-optical elements of the separator is given in the following.

4. Ion injection into the multiple-reflection time-of-flight analyzer

Ion injection into the multiple-reflection TOF analyzer is performed from a linear RF ion trap (LIT) filled with a buffer gas (He) at a pressure about 10^{-3} mbar. Ions are delivered to this trap from a multi-stage trapping and cooling system [26,24,25]. RF voltages of up to 300 V_{pp} at a frequency of about 2 MHz are applied to four cylindrical electrodes with a length of 4 mm and a field diameter of 4 mm. The ions are confined to a sub-millimeter length bunch in the axial direction by applying bias potentials of about 20 V to the apertures surrounding the trap. They are ejected from the trap by applying accelerating push and pull voltages to these apertures. The strength of the ejecting field in the trap amount to up to 100 V/mm, corresponding to an initial peak width as determined by the turn-around-time [27] of 4 ns for ions of mass-to-charge ratio of 100 u/e. Behind the pull electrodes the ions are further accelerated to the nominal mean kinetic energy K_0.