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A high-performance multiple-reflection time-of-flight mass spectrometer and isobar separator for the research with exotic nuclei

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ABSTRACT

A novel multiple-reflection time-of-flight mass spectrometer (MR-TOF-MS) and isobar separator for the research with exotic nuclides at low-energy rare isotope beam facilities has been developed, commissioned and characterized. It can be used (i) as broadband mass spectrometer with medium resolution, (ii) as highly accurate mass spectrometer for direct mass measurements and (iii) as high-resolution mass separator. The device features a worldwide unique combination of performance characteristics: a mass resolving power of 600,000 (FWHM), a mass measurement accuracy of $\sim 10^{-7}$, large ion capacities in excess of 10⁶ ions per second, a transmission efficiency of up to 70%, single-ion sensitivity, and cycle frequencies of up to 400 Hz have been achieved. The spatial separation of close-lying isobars with an intensity ratio of 200:1 and a binding energy difference as small as 4 MeV have been demonstrated. The MR-TOF-MS is ideally suited for experiments with rare and very short-lived nuclei at present and future in-flight, ISOL or IGISOL facilities, such as the FRS Ion-Catcher and SHIP/SHIPTRAP at GSI, TITAN at TRIUMF, IGISOL at the University of Jyväskylä and the Low-Energy Branch of the Super-FRS at FAIR.

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1. Introduction

In recent years much progress has been made in the research with exotic nuclei [1,2]. Experiments with exotic nuclei yield key information about nuclear structure and about the origin of the chemical elements in the universe. Further advances, such as closer access to nuclides along the nucleosynthesis pathways, will be achieved at next-generation accelerator facilities, which are presently under construction (such as the Facility for Antiproton and Ion Research FAIR in Darmstadt, Germany, SPIRAL2 at GANIL, France and the Facility for Rare Isotopes FRIB at Michigan State University, USA) or already in operation (RI-beam factory RIBF at RIKEN, Japan). It is difficult to produce very exotic nuclei in sufficient amounts and purity and to study their properties. Even existing facilities face serious challenges for experiments with exotic nuclei in the form of life time limitations caused by the cycle time of the experiments and the overwhelming amount of contaminants produced together with the nuclides of interest. These

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challenges will intensify at future facilities, as the primary beam intensities are increased and more exotic species can be produced.

A new approach to precision experiments with exotic nuclei is the production and in-flight separation of the nuclei and their subsequent slowing-down and thermalization in gas-filled stopping cells [3]. It enables precision experiments with ions almost at rest, including mass measurements in ion traps, high-resolution decay spectroscopy, and laser spectroscopy, while retaining the advantages of the in-flight method of fast and universal production. Alternatively, exotic nuclei can be made available with low kinetic energies at conventional ISOL or at IGISOL facilities. At all these low-energy rare isotope beam (RIB) facilities the fast, universal, sensitive and broadband identification of ions is an additional challenge, which must be met in order to efficiently perform and optimize experiments.

Time-of-flight mass spectrometry (TOF-MS) allows for fast and broadband measurements as well as for high transmission efficiency and single-ion sensitivity. It is hence an ideal tool to address these issues. However, hitherto the mass resolving power obtained by TOF-MS has been limited to a few ten thousand, which is not sufficient for the resolution of most atomic isobars. The most important limitation is the turn-around time [4] caused by the initial, viz. thermal, velocity spread of the ions prior to acceleration. It leads to different flight times even for otherwise identical

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ions, which have initially different velocity components along the direction of extraction. For a given ion temperature, the turnaround time can only be reduced by increasing the extraction field strength. However, the energy spread of the ions, and hence the extraction field strength, cannot be made arbitrarily large, otherwise chromatic aberrations would limit the quality of the energy focusing [4,5] and hence the ion optical resolving power. Furthermore, the detector bandwidth also sets a lower limit to the peak width.

A method to overcome the limitation in resolving power is to extend flight path using devices with multiple passes [6]. Assuming the time-of-flight errors due to initial conditions, Δt_0 , which include in particular the turn-around time, and the time-of-flight errors in each turn in the time-of-flight analyzer due to aberrations, Δt_a , are independent of each other, the resolving power of a multiple-pass TOF-MS is given by

$$\left(\frac{m}{\Delta m}\right) = \frac{t_0/N_a + t_a}{2\sqrt{\left(\frac{\Delta t_0}{N_a}\right)^2 + (\Delta t_a)^2}} \tag{1}$$

where t_0 is the time-of-flight from the start position to the detector without any flight path extension, t_a is the time-of-flight for a single turn in the analyzer and N_a is the number of passes in the analyzer. Clearly, in the case of a large number of passes, $N_a \rightarrow \infty$, the overall mass resolving power tends towards the ion optical resolving power $t_a/(2\Delta t_a)$, which can be made orders of magnitude larger than the resolving power achievable in single-pass TOF-MS.

Multiple-pass devices have been proposed in multiple-turn 30 31 configurations with sector fields [7] and in multiple-reflection 32 configurations with electrostatic ion mirrors [8,9]. The use of a 33 multiple-reflection time-of-flight mass spectrometer (MR-TOF-34 MS) [6] for direct mass measurements of very short-lived, exotic 35 nuclei has been proposed more than a decade ago [10]. First 36 implementations of an MR-TOF-MS at the Justus-Liebig-University 37 Gießen (Germany) and at RIKEN (Japan) yielded mass resolving 38 powers of up to 65,000 [11–13]. The mass spectra obtained with 39 these devices were however characterized by strong tails, limiting 40 the application to separation of ion species with similar abun-41 dance. We have overcome this limitation by employing an 42 advanced coaxial four-electrode design [14,15]. Even for uncooled 43 ion populations with the emittance of an electron impact ion 44 source excellent peak shapes characterized by a mass resolving 45 power of 100,000 at FWHM and 35,000 at 10% height of the peak 46 were achieved in a very compact MR-TOF-MS prototype at Justus-47 Liebig-University Gießen [16,14,17]. An MR-TOF-MS can not only 48 be used to perform mass measurements, but it can also be 49 employed as a mass separator. We have proposed to use an MR-50 TOF-MS in conjunction with a Bradbury-Nielsen Gate [18,19] as 51 isobar separator [20,21], and we have demonstrated the spatial 52 separation of isobars in an MR-TOF-MS for the first time [22,14]. 53 Furthermore, we have proposed to employ an MR-TOF-MS for 54 diagnostics purposes at rare isotope facilities [14,23]. Our device 55 served as proof-of-principle for future MR-TOF-MS experiments 56 with exotic nuclei at the GSI Helmholtzzentrum für Schwerionen-57 forschung GSI, Darmstadt (Germany) and the Facility for Antipro-58 ton and Ion Research (FAIR). Similar projects are pursued at the RI-59 beam factory RIBF at RIKEN (Japan) [24,25] and at ISOLDE/CERN in 60 Geneva [26,27], and first direct mass measurements of short-lived 61 nuclides have been performed [28,29].

Here, a next-generation device is presented, which reaches an
unprecedented performance level for MR-TOF-MS. It has been
developed for experiments at SHIP/SHIPTRAP [30], the FRS Ion
Catcher [31] at GSI and at the Low-Energy Branch (LEB) [32] of the
Super-FRS at FAIR. Based on the technology of this MR-TOF-MS, an

MR-TOF isobar separator for the TITAN experiment at the ISAC67facility at TRIUMF (Vancouver, Canada) [33] has been constructed68and commissioned at the Justus-Liebig-University Gießen and is69being installed at the TITAN facility. A duplicate of the MR-TOF-MS70for GSI and FAIR is being built for MLLTRAP [34].71

72 The MR-TOF-MS includes several novel components and 73 extends existing approaches in several important points [14,6]. (i) It has an advanced ion optical layout with a simple, yet ion 74 optically advantageous time-of-flight analyzer and an additional 75 post-analyzer reflector. The combination of these two elements 76 yields a flexible high-performance mass spectrometer, which is 77 easy to optimize and to operate and which can be switched 78 79 instantaneously between modi with different resolving power. (ii) A novel triple-stage injection trap enables efficient ion accu-80 mulation, fast cooling and ejection of the ions without significant 81 collisional reheating. Application of a rectangular radiofrequency 82 (RF) voltage allows for a shift of the potential of the ions and 83 turning off the RF voltage during ejection, which removes detri-84 mental mass-dependent time-of-flight variations. (iii) The MR-85 TOF-MS can be used for broadband measurements at medium 86 resolution, for high-resolution mass measurements, and as an 87 88 isobar separator, transmitting an arbitrary combination of ions of 89 interest, while constantly monitoring the ions to be removed. (iv) A novel dynamic energy buncher enables efficient recapturing 90 of the selected ions, which can then be accumulated and trans-91 mitted to experiments downstream of the device. (v) The MR-TOF-92 MS has a compact, mobile setup. Due to the shift of the ion 93 potential in the injection trap its operation is independent of the 94 entrance potential of the incoming ions. It can thus be used easily 95 with only minor modifications at different accelerator facilities, 96 and setup times are a few hours only. 97

Prior to its construction, the MR-TOF-MS was designed using extensive simulations using the programs SIMION [35] and ITSIM [36,37]. The general design of the device and its operation modes have been introduced in [14]. For an in-depth description of the setup of the MR-TOF-MS, its operation and the performance characteristics see [38]; its ion optical design is presented in [15].

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2. Setup

2.1. Overview

109 The setup of the MR-TOF-MS is shown schematically in Fig. 1. 110 Ions are introduced into the mass spectrometer through straight 111 and curved radiofrequency quadrupole (RFQ) ion guides [21]. In 112 the injection trap system the ions are accumulated, cooled by 113 collisions with the buffer gas and injected as bunches into the 114 time-of-flight analyzer. In the analyzer the ions are trapped and 115 travel back and forth between the two reflectors of the analyzer 116 for a selectable number of turns. Then they are ejected, pass 117 through the post-analyzer reflector and alternatively (i) impinge 118 on an isochronous secondary electron multiplier for measurement 119 of their time-of-flight (mass measurement mode) or (ii) pass 120 121 through a Bradbury-Nielsen Gate (BNG) [18,19], in which con-122 taminant ions can be deflected and only the ions of choice are transmitted (mass separator mode). The mass resolving power is 123 determined by the number of turns in the time-of-flight analyzer 124 (see Eq. (1)). Without reflections in the analyzer (pass-through 125 mode) a medium mass resolving power (several thousands) is 126 obtained; with hundreds of turns in the analyzer (multiple-turn 127 mode) a mass resolving power of several 10⁵ is achieved. In the 128 future, the energy spread of the selected ions will be reduced in an 129 130 energy buncher [14], such that the ions can be recaptured 131 efficiently in an RFQ and trap system and delivered to experiments 132 downstream of the device. The re-accumulation serves to

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