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A low energy ion beam facility for mass spectrometer calibration: First results

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The exploration of habitable environments around the gas giants in the Solar System is of major interest in upcoming planetary missions. Exactly this theme is addressed by the Jupiter Icy Moons Explorer (JUICE) mission of the European Space Agency (ESA), which will characterise Ganymede, Europa, and Callisto as planetary objects and potential habitats. The NIM, Neutral gas and Ion Mass spectrometer, is part of the PEP experiment and will be used to measure the chemical composition of the exospheres of the icy Jovian moons. We designed and developed a calibration facility (SATANS, Supersonic cATion and ANion Source), especially for use with the NIM instrument. In a first step, we established a low energy ion beam for positive ions in the range of 0.01–30 eV. Then we conducted beam velocity calibrations with a velocity uncertainty <5%, which provided exact settings and formulas for the cation beam velocity of different gas mixtures in the range of 1–15 km/s. In addition, first results are obtained by using the NIM prototype for direct ion beam measurements under realistic JUICE mission conditions, i.e., for velocities from 1 up to 7 km/s and even more. *Published by AIP Publishing.*
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I. INTRODUCTION

JUpiter **IC**y moons **E**xplorer (**JUICE**) is a space mission, which will explore the Jupiter system as a miniature Solar System in its own right. As an L-class mission of the European Space Agency (ESA), the JUICE will investigate and characterise Jupiter's Galilean moons Ganymede, Europa, and Callisto, which are believed to harbour subsurface oceans, as planetary objects and potential habitats.[1,2] The JUICE mission is planned to be launched in 2022 with a transfer time of approximately 8 years, resulting in an arrival at Jupiter in 2030.[2] The current trajectory of the JUICE spacecraft foresees a flyby velocity of 4 km/s at Europa, other moon flybys are in the range of 1 up to 7 km/s and orbital velocity in Ganymede orbits is around 2 km/s.

The **P**article **E**nvironment **P**ackage (**PEP**), carried by the JUICE, combines remote global imaging with *in situ* measurements to study the moons' atmospheres, magnetospheric plasma environments at the locations of the moons, and the plasma interactions with the moons. One PEP goal is to determine global surface composition and chemistry, especially as related to habitability.[3] The **NIM**, **N**eutral gas and **I**on **M**ass spectrometer, is part of the PEP suite and will be used to measure the chemical composition of the regular atmosphere produced by sublimation, energetic particle bombardment, and photon interaction with the surface of the icy Jovian moons.[4,5] The NIM measurements include volatile species, contributions from non-ice material on the surface, and the isotopic composition of major species. In addition, the NIM will also measure the ion composition of the ionospheres by direct ion measurement.

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The NIM instrument is designed to operate in three different modes (see Ref. 6 for more details):

- the thermal mode (th-mode), where the neutral gas is decelerated from the spacecraft velocity down to thermal energies by an equilibrium sphere and passed on into the ion source in thermal state, which is to be ionised and stored until the subsequent extraction through the ion-optics to the detector. This mode (also referred to as the closed source in the literature) is used for neutral gas measurements at any mission phase, mainly during Europa torus crossing and all other flybys.
- The neutral mode (n-mode), where the neutral gas enters directly into the ion source with the speed given by the flyby speed of the spacecraft, is ionised, extracted, and subsequently guided through the ion-optics to the detector. This mode (also referred to as the open source in the literature) is used for neutral gas measurements close to the moons, mainly during closest approach at flyby or in the orbit phase.
- The ion mode (i-mode), where thermal ions from the ambient plasma enter the ion source (open source entrance) with the speed relative to the spacecraft and are directly guided through the ion-optics to the detector. This mode is used for thermal ion measurements of ionospheric ions close to the moons, mainly in the orbit phase or near the closest approach during flyby.

So far, different test tools and facilities are used to test the different parts and modes of the NIM prototype. Thereof, the request for a dedicated calibration facility for the NIM instrument arises, also with regard to the flight model calibrations of the NIM. The aim of this calibration facility, called **SATANS** (**S**upersonic c**AT**ion and **AN**ion **S**ource), is to test and calibrate the NIM instrument in all modes, the th-mode, n-mode, and i-mode, respectively, with respect to all JUICE mission requirements. This means the SATANS has to provide a low energy ion beam for positive ions in the range of 0.01–30 eV. Furthermore, the SATANS has to provide a neutral gas beam for different gas mixtures with velocities in the range of 1–7 km/s later on. In addition, a very narrow velocity distribution is requested with the SATANS, representing a realistic flyby scenario of the mission.

A number of methods for accurate and precise measurements of particle velocities can be found in the literature. Typically, molecular beam techniques such as mechanical velocity selectors, laser based technique of the diffraction of particles from nano-sized grating, and time-of-flight (TOF) analysis are applied.[7–10] The precision of the velocity measurements delivered by these methods is frequently better than 1% which is usually required in the experimental investigations of physical constants such as cross sections, polarisabilities, dipole moments in elastic and reactive particle collisions, and thermodynamic properties of the gas expansion.[11–14]

For the purpose of our applications, in addition to neutral particles, ions of atoms and molecules are of relevance. In this work, we describe the method of the ion production, ion velocity calibration using the TOF method, and ion sensitive detection system for the analysis of slow ion beams.

II. OVERVIEW OF THE SYSTEM

The design and development of SATANS is first concentrated on the production of a positively charged ion beam in the requested velocity range 1–7 km/s, which is to test the i-mode of the NIM prototype. The operation of NIM prototype in th-mode and n-mode has already been tested successfully with another in-house calibration facility for neutral gas beams.[6] The technical scheme of SATANS to provide a positively charged ion beam is illustrated in Fig. 1, together with a timing diagram of the different units.

In the first ultra-high vacuum (UHV) compartment a discharge unit (4) ionises a neutral gas packet, which is released from a pulsed spring valve (3) at the gas inlet. A short high-voltage pulse is used to perform a discharge between the ground and discharge electrodes of the gas packet. This generates a short plasma cloud pulse, which travels subsequently with the remaining neutral gas through the skimmer (5) to the second UHV compartment due to the applied pressure of about 1–5 bars. There, an acceleration unit (6) allows the pulsed acceleration of the ion bunch, which passes the skimmer (5), to the desired velocity with subsequent focusing of the ion beam. To calibrate the velocity of the generated ion beam, a third UHV compartment is added, separated by a translation stage (7). The third UHV compartment contains an ion detector (8), which can be moved along the x-axis by the translation stage. Exact velocity calibration can then be achieved by several TOF measurements at different distances. This calibration method is adopted from Ref. 14. In operation mode of SATANS, the third UHV compartment is removed and the UHV chamber with the NIM prototype installed is attached in exchange.

The discharge unit and acceleration unit are illustrated in Fig. 2 in more detail. In Fig. 2(a), a mechanical schematic of the discharge unit is shown, with the discharge electrode (1) and the counter electrode on zero-potential (2) in gray. The electrodes are made of stainless steel, and the envelope of the electrodes (body) is made out of macor® ceramic material (3) including separation plates between the pulsed gas valve and the discharge electrode, as well as between both electrodes, respectively. The sizes of the discharge assembly parts used in this study are optimised to avoid discharging between the valve body and the discharge electrode and tested for the best signal intensity and stability (separation and openings of the electrode plates) (e.g., Ref. 15). The gas packet travels through a thin channel of 1 mm diameter and expands between the electrodes to 5 mm diameter [see panel (a) of Fig. 2]. With exact timing, a high voltage (HV) pulse of 800–1000 V is applied on the discharge electrode to ignite the discharge and generate the ions. At a distance of 3 mm from the discharge electrode, the counter electrode with 3 mm hole diameter and expanding exit is kept at zero-potential.

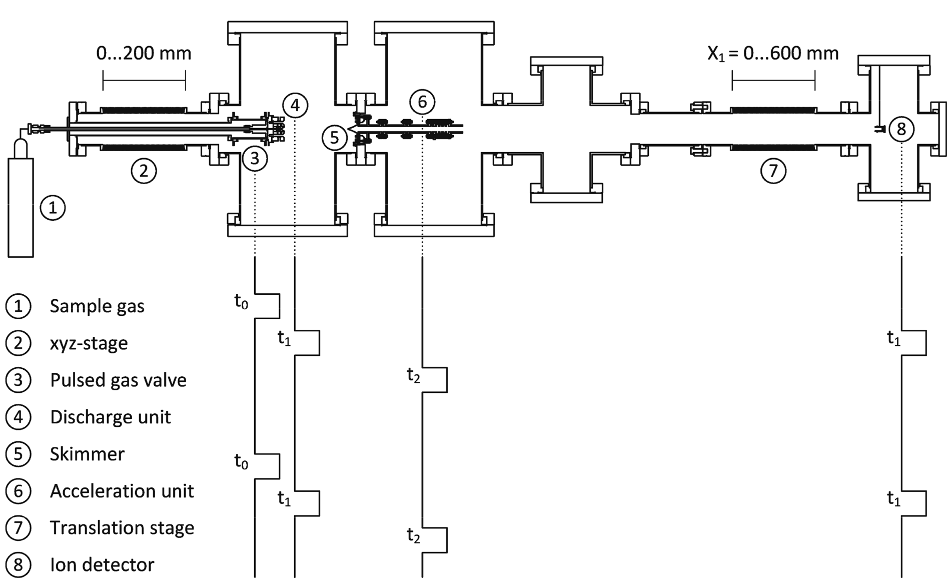

FIG. 1. Technical scheme of SATANS with trigger timing of the different units.

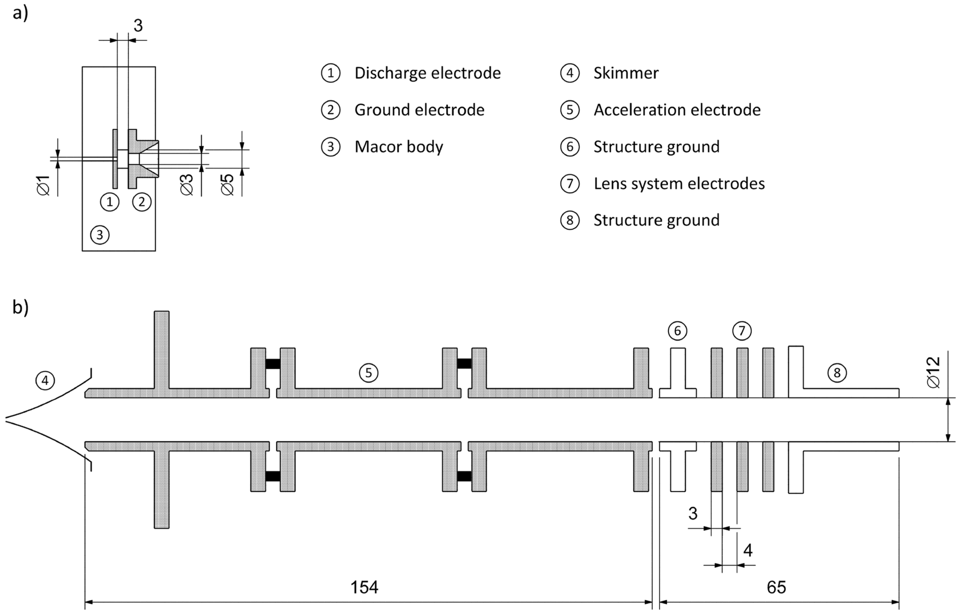

FIG. 2. (a) Mechanical design of the discharge unit, with the discharge electrodes in gray. (b) Ion-optical design of the acceleration unit with corresponding acceleration electrodes and lens system electrodes in gray.

For the production of positively charged ions, the discharge unit is charged by a custom-made power supply allowing the application of up to +3 kV voltage pulses with the pulse duration from 1 μs up to a few hundreds of μs. The pulse duration can be tuned by the external pulse generator.

In Fig. 2(b), a mechanical schematic of the acceleration unit with corresponding acceleration electrodes (5) and lens system electrodes (7) is presented. The acceleration unit is placed into the beamline directly after the skimmer (4). To obtain a voltage free drift region, the lens system electrodes (7) are surrounded by electrodes kept on zero-potential (6) and (8).

The acceleration pulse of the order of U_{ap} = −10 V is applied on the three connected tubes right after the skimmer [see (5) in Fig. 2], when the ion bunch enters this region. Thereof, the ions are accelerated over the duration of the acceleration pulse within the acceleration electrodes and subsequently focused by the ion-optical lens [see (7) in Fig. 2] at the end of the unit. The acceleration pulse has to be applied exactly when the ion packet is inside the acceleration tube. Thereby, a short voltage pulse is needed, which changes the energy of the ions (adding more energy for acceleration) before leaving the acceleration tube. Similar principle of operation is also described in Ref. 16, but for decelerating an anion beam. The exit of the acceleration unit is kept at zero-potential, to guarantee a field free drift path for the ions up to the ion detector, i.e., the NIM prototype entrance.

To produce the requested positively charged ion beam by the SATANS, the correct timing of the individual units is of crucial importance. Therefore, the timing diagram of SATANS for generating a cation beam is displayed in Fig. 1. First (at t_0 in Fig. 1), the spring valve at the gas inlet has to be opened for about t_{open} = 250 μs to introduce the gas packet into the UHV chamber. Next (at t_1 in Fig. 1), the discharge HV pulse (typically U_{dis} = 850 V) has to be applied for t_{dp} = 4 μs with a delay of typically $t_{dis} = t_1 - t_0$ = 800 μs, with respect to the valve opening pulse. Then (at t_2 in Fig. 1), the acceleration pulse is applied, according to the desired ion beam velocity. Typical values are $t_{acc} = t_2 - t_1$ = 6 μs with a pulse width of t_{ap} = 9 μs for a beam velocity of about 7 km/s at a corresponding acceleration pulse voltage of U_{ap} = −10 V (see Table II for exact values). Meanwhile (at t_1 in Fig. 1), the data acquisition system has to be triggered. The recorded TOF from the ion detector depends on the setting of the translation stage, i.e., the position of the detector with respect to the x-axis and the ion beam velocity. Values between t_{TOF} = 100–400 μs have been observed during calibration. In general, a repetition frequency of 100 Hz is used, i.e., 10 ms from one ion packet to the next one.

To perform measurements with the NIM prototype in the i-mode at the SATANS, the last UHV compartment has to be removed and replaced with the UHV chamber with the NIM prototype installed. A photograph of SATANS, showing the whole setup with the attached UHV chamber and installed NIM prototype is illustrated in Fig. 3.

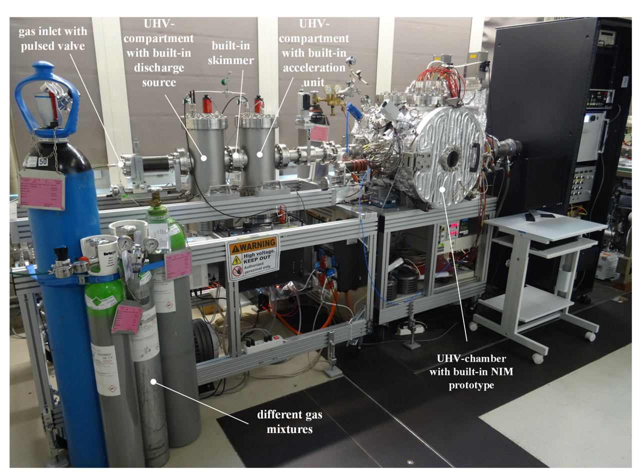

FIG. 3. Photograph of SATANS with attached UHV camber with the NIM prototype installed.

TABLE I. Neutral gas velocity calibration results, obtained from the n-mode measurements with the NIM prototype at the SATANS, compared with theoretical v_{gas} from Eq. (1). The coupling delay t_{drift} is tuned to the maximum signal at the NIM (in the n-mode) and consequently used to estimate the TOF of the neutral gas packet from the opening valve up to the entrance of the NIM prototype.

Gas mixture	Measured t_{drift} (μs)	Calculated v_n (km/s)	Theoretical v_{gas} (km/s)
99% Ar and 1% C_2H_2	2400 ± 500	0.65 ± 0.14	0.606 (for pure Ar)
97% Ar and 3% N_2	2300 ± 500	0.68 ± 0.15	0.606 (for pure Ar)
100% N_2	1700 ± 500	0.92 ± 0.27	0.857 (for pure N_2)
99.4% He and 0.6% toluene	850 ± 150	1.85 ± 0.33	1.916 (for pure He)

The measurement cycle at the NIM prototype has to be synchronised with the SATANS ion pulse cycle so that the NIM measurement starts when the ion bunch arrives at the entrance of the NIM prototype. This means that the ion extraction pulse of NIM has to be synchronised to the discharge pulse of SATANS, with a corresponding delay of t_{acq}, which compensates the TOF of the ion bunch up to the entrance of the NIM prototype. Typically, t_{acq} = 1'080 μs, depending on the ion beam velocity and the mass of the used gas mixture (99% Ar and 1% C_2H_2 mixture at 7 km/s for this example). The ion extraction pulse duration of the NIM prototype is kept at 1.4 μs for all measurements in the i-mode at the SATANS. The data acquisition system of the NIM prototype is triggered together with the ion extraction pulse. This time, the TOF recorded by the NIM prototype can be transformed into mass-per-charge scale and the corresponding mass spectra are obtained. In general, again a repetition frequency of 100 Hz is used, i.e., 10 ms from one ion packet to the next one, which means a measurement time of 500 s for spectra containing 50 000 accumulated waveforms, since the NIM has to be coupled to the SATANS cycle.

III. RESULTS

A. Neutral-beam calibrations

Neutral gas velocity calibration has been conducted, with the NIM prototype and SATANS in the so-called measurement mode. This means that the NIM is operated in the n-mode and the measurement cycle is synchronised with the opening of the gas valve at the SATANS. Thereby, the coupling delay t_{drift} from the valve opening pulse of SATANS to the NIM extraction pulse is tuned to the maximum signal at the NIM and consequently used to estimate the TOF of the neutral gas packet from the opening valve up to the entrance of the NIM prototype. The distance from the opening valve of SATANS to the entrance of NIM prototype has been determined as d_{NIM} = (1570 ± 30) mm. The neutral gas beam velocity is then estimated as $v_n = d_{NIM}/t_{drift}$.

Table I lists the obtained neutral gas calibration results v_n, together with the theoretical gas beam speed v_{gas}. It is stated in Ref. 17 that the free jet expansion into a vacuum converts about 95% of the thermal energy into a directed motion of the beam and the beam speed v_{gas} can be calculated for the isentropic expansion of perfect gas from a reservoir. For the supersonic regime, i.e., $v_{gas} > 0.4$ km/s, this reduces to

$$v_{gas} = \sqrt{\frac{\gamma \cdot k_B \cdot T}{m} \cdot \frac{2}{\gamma - 1}}, \tag{1}$$

where k_B is the Boltzmann constant, T is the nozzle temperature, γ is the heat capacity ratio, and m is the mean molecular mass of the beam.[9]

A temperature of 80 °C has been taken into account for T since the spring valve gets quite hot at the used repetition frequency of 100 Hz (the outside of the gas inlet gets about 45 °C and maximum operating temperature of the valve is stated to be 100 °C). It can be seen from the listed results that the measured neutral gas velocities v_n are in good agreement with the theoretical v_{gas} from Eq. (1).

B. Ion-beam calibrations

Concerning the cation beam, an exact velocity calibration can then be achieved, by several TOF measurements at different distances, as has been shown in Ref. 14. An example of such a calibration, with the SATANS in the calibration mode, is given in Fig. 4. The analysis of ion beam velocity calibration measurements is exemplarily shown and explained for the case of an ion beam resulting from a gas mixture of

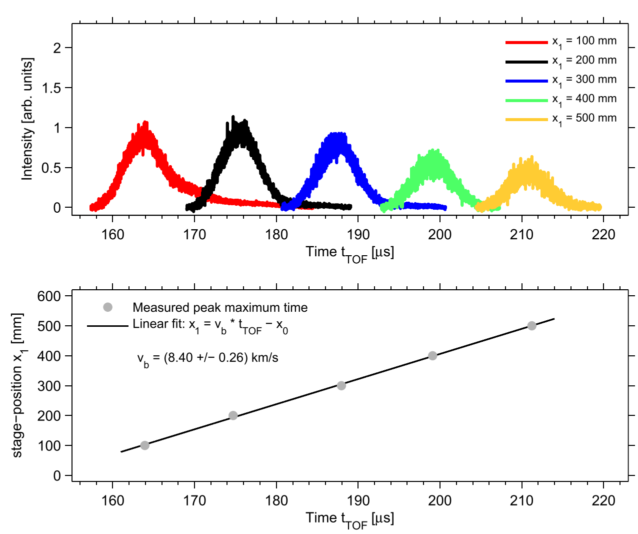

FIG. 4. Example of the analysis of ion beam velocity calibration measurements at the SATANS for the case of an ion beam resulting from a gas mixture of 99% Ar and 1% C_2H_2, at a backing pressure of 2.0 bars, with U_{ap} = −15 V, t_{ap} = 9 μs, and t_{acc} = 6 μs.

99% Ar and 1% C_2H_2, at a backing pressure of 2.0 bars. An acceleration pulse voltage of U_{ap} = −15 V was applied for t_{ap} = 9 μs with a delay of t_{acc} = 6 μs with respect to the discharge pulse. The ion beam velocity [in this case, $v_b = (8.40 \pm 0.25)$ km/s] is obtained by the linear fit of the TOF peak maxima, measured at different distances, depicted in the lower panel of Fig. 4. The corresponding TOF peaks are plotted in the upper panel of Fig. 4. To obtain good statistics, 5–6 TOF measurements were made in the range of 0–500 mm in the x-direction, by tuning the translation stage accordingly. It can be seen in Fig. 4 that the TOF peak widths are <5% of its nominal value. This means an ion beam velocity with an uncertainty <5% is reached with the SATANS and the applied calibration method.

Actually, a full set of calibration measurements and analyses have been performed for a gas mixture of 99% Ar and 1% C_2H_2, with different backing pressures (0.5–2.0 bars) and different acceleration pulse settings (U_{ap} = −5 to −50 V). Thereby, the focusing lens has been adjusted accordingly, by different voltages on lens electrode L1, U_{L1} = −20–0 V. The other lens electrodes were kept at zero-potential, U_{L2} = 0 V and U_{L3} = 0 V. All ion beam calibration measurements with corresponding settings and obtained velocity are listed in Table II.

TABLE II. Positive ion beam calibration measurements at the SATANS, with corresponding settings and obtained velocity for a gas mixture of 99% Ar and 1% C_2H_2.

Pressure (bars)	U_{ap} (V)	U_{L1} (V)	t_{acc} (μs)	t_{ap} (μs)	Calibrated v_b (km/s)
0.5	−5	−10	26	20	4.96 ± 0.10
0.5	−6	−10	20	14	5.28 ± 0.13
0.5	−8	−15	12	14	5.64 ± 0.21
0.5	−11	−20	10	10	7.25 ± 0.14
0.5	−15	0	6	9	8.52 ± 0.25
0.5	−20	0	5	9	9.61 ± 0.23
0.5	−45	0	5	8	13.35 ± 0.42
1.0	−5	−10	26	20	4.10 ± 0.04
1.0	−6	−8	20	14	5.16 ± 0.10
1.0	−8	−15	12	14	6.75 ± 0.26
1.0	−11	−20	14	10	8.30 ± 0.14
1.0	−15	0	6	9	8.63 ± 0.38
1.0	−20	0	5	9	8.77 ± 0.23
1.0	−45	0	5	8	14.28 ± 0.59
1.5	−5	−10	26	20	4.34 ± 0.06
1.5	−6	−10	20	14	5.18 ± 0.10
1.5	−8	−15	12	14	5.80 ± 0.20
1.5	−11	−20	10	10	7.33 ± 0.14
1.5	−15	0	6	9	8.68 ± 0.24
1.5	−20	0	5	9	9.76 ± 0.25
1.5	−45	0	5	8	13.60 ± 0.44
2.0	−5	−10	26	20	3.97 ± 0.09
2.0	−6	−10	20	14	5.36 ± 0.11
2.0	−8	−15	12	14	6.07 ± 0.21
2.0	−11	−20	10	10	7.37 ± 0.12
2.0	−15	0	6	9	8.40 ± 0.26
2.0	−20	0	5	9	9.79 ± 0.44
2.0	−45	0	5	8	13.21 ± 0.66

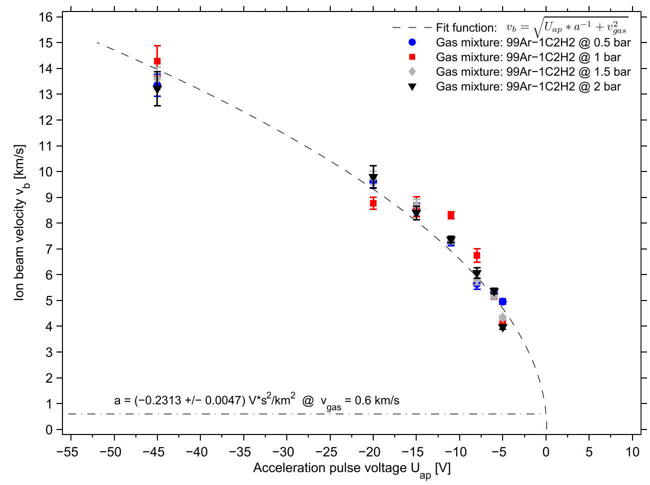

FIG. 5. SATANS ion beam calibration results for 99% Ar and 1% C_2H_2 gas with respect to acceleration pulse voltage U_{ap}, including a fit model, combining the neutral gas calibration results.

Finally, the presented ion beam calibration results are combined with the neutral gas velocity calibrations to show the consistency of the SATANS calibration processes and the thereby used settings. Therefore, the calibration results from 99% Ar and 1% C_2H_2 gas (see Table II) are depicted in Fig. 5, where the ion beam velocities are plotted as a function of the applied acceleration pulse voltage U_{ap}. In addition, a fit function for the velocities is included with an initial velocity, which corresponds to the estimated neutral gas velocity v_{gas}. This means that the fit function is based on the assumption that the initial kinetic energy of the gas is linearly increased by the energy of the applied acceleration pulse for the produced ions. Thereof, a general calibration relation between acceleration pulse voltage U_{ap} and ion beam velocity v_b can be formulated as

$$v_b = \sqrt{\frac{U_{ap}}{a} + v_{gas}^2}, \tag{2}$$

where v_{gas} is the velocity of the corresponding neutral gas mixture, which can either be measured or estimated using Eq. (1) (see Table I). Thereof, the fit parameter a is a constant depending on the gas mixture. See Fig. 5 for the exact value of the measured gas mixture.

It can be observed in Fig. 5 that the so-obtained velocities are independent of the applied backing pressure in the range of 0.5–2.0 bars, which is expected from Eq. (1).

The SATANS is still under development, but the above presented calibrations were already used to verify the performance of the NIM prototype in the i-mode against the mission requirements.

C. NIM prototype measurements

Measurements with the NIM prototype in the i-mode at the SATANS were performed using different gas mixtures according to the stand-alone calibration of the ion beams at the SATANS, presented above. After synchronising the measurement cycles of SATANS and NIM, as well as optimising the voltage sets in the i-mode of the NIM, TOF spectra of different gas mixtures were measured with NIM, each with 50 000

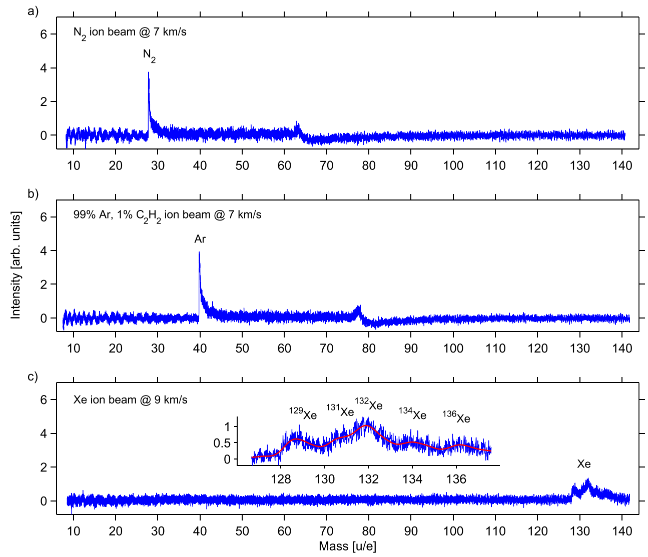

FIG. 6. Mass spectra from NIM prototype measurements at the SATANS, with 50 000 accumulated waveforms. The feature at 63 u for the N_2 ion beam and at 78 u for the Ar ion beam mixtures is an artefact from the electromagnetic interference of the discharge pulse. A mass resolution of $m/\Delta m = 120$ is obtained for the Xe isotopes in this measurement with a 9 km/s Xe ion beam.

accumulated waveforms (500 s of measurement time at 100 Hz repetition frequency). The corresponding mass spectra are depicted in Fig. 6. The 7 km/s beam velocity corresponds to the case of the fastest Ganymede flybys and represents the most challenging operation situation.

Panel (a) of Fig. 6 shows a measured mass spectrum for an ion beam of pure nitrogen gas with a beam velocity of 7 km/s. An ionised argon-acetylene gas mixture of 99% Ar and 1% C_2H_2 with a beam velocity of 7 km/s is measured and displayed in panel (b) of Fig. 6. Only the Ar mass peak is observed in the spectra. The other possible products of plasma chemistry (carbon clusters) induced by the discharge in 1% of acetylene are not observed due to too low detection limit for these species at these measurement conditions. In panel (c) of Fig. 6, a measurement from an ion beam of 9 km/s made of 100% Xe gas is shown. Concerning ion-optics, the measurement of high mass ions (m > 100 u) at the highest velocities (with respect to the JUICE mission) is the most challenging case (see the considerations about ion-optical simulations in Ref. 18). Nevertheless, it is possible for the NIM prototype to resolve the isotopes of Xe at a mass resolution of about $m/\Delta m = 100$ for this case.

The first measurements of the NIM prototype in the i-mode with the SATANS are presented in Fig. 6. A mass resolution of $m/\Delta m = 120$ is obtained for the Xe isotopes in this measurement with a 9 km/s Xe ion beam. The mass resolution obtained for the ions of various velocities were compared with SIMION® Version 8.1 ion-optical modeling results. Thereby, the NIM ion-optical elements have been simulated in 3D with SIMION® Version 8.1 and the TOF, and its dispersion of the simulated ions have been analysed for different masses, to be able to get the expected mass resolution for different masses and different velocities. Close agreement was found between modeling and measurement. This means, the i-mode of the NIM prototype could be successfully verified by these first measurements with the SATANS. In addition, the SIMION® Version 8.1 ion-optical model predicts an improvement in the mass resolution to about $m/\Delta m = 250$ for a velocity of 2 km/s, which represents the typical measurement case for Ganymede flybys and orbits during the JUICE mission.

IV. SUMMARY

A new calibration facility SATANS has been designed for NIM performance tests and calibration. In the current experiments, we could successfully accomplish the measurements for neutral gas and positively charged ions. The conducted calibrations have provided exact settings and formulas for the cation beam velocity of different gas mixtures in the range of 1–15 km/s, which corresponds to particle energies of about 0.01–30 eV. With the applied calibration method, an uncertainty <5% is reached for the ion beam velocity. Moreover, first results using the i-mode of the NIM prototype are very encouraging; it has been shown that ion beam measurements are possible under realistic JUICE mission conditions in the range of 1–7 km/s and even more. The mass resolution of the different velocities was compared with the SIMION® Version 8.1 ion-optical modeling and very close agreement to the experimental values was found. Further tests are planned for the analysis of the negatively charged species. Also improvements of the setup will be made to increase ion production and ion transport efficiencies.

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