XVII IMEKO World Congress Metrology in the 3rd Millennium June 22–27, 2003, Dubrovnik, Croatia

Ion Optical Design and Experimental Results of an Experiment to Accumulate a Weighable Mass of Ions

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Abstract –. A still unsolved problem in the field of metrology is the definition of the SI unit kg in terms of universal physical constants as it was done for the other fundamental SI units. One possibility is to accumulate ions up to a weighable mass [1]. Then the atomic mass unit can be determined by measuring the total charge and mass of the accumulated ions. This article describes the ion optical properties of an existing experiment for ion accumulation at the PTB. Results of the ion optical calculations are used for experimental settings to measure mass spectra of a mixed xenon gold ion beam.

Keywords: ion optic, ion beam, mass spectroscopy.

1. Experimental Set Up

In order to accumulate a weighable mass in a manageable time heavy ions have to be created preferably with only one stable isotope within mA currents. Therefore, the experiment can be accomplished using gold ions produced with a CHORDIS ion source in the sputter version or with bismuth ions from an oven version [2].

The gold ion beam is established using argon or xenon as working gas and are finally extracted with 18 kV out of the ion source. The ion beam is now focussed with a quadrupole triplet lens to a double focussing 90 degree dipole magnet. Behind the quadrupole triplet the focus can be controlled using different kinds of beam monitors. By means of the magnet the ion beam is separated according a chosen mass to charge ratio. Finally the ions hit the collector where they are decelerated to eV energies in order to keep sputtering effects as small as possible. The collector can be connected directly to an equal armed beam balance to determine the collected mass of the ions.

2. Ion Optic

For the ion optical calculations the computer program MIRKO [3] was used. Ion optical elements are presented by 6×6 matrices. Higher order effects like chromatic and geometrical aberrations as well as space charge effects can be taken into account. The numerical results can be dis-

played in terms of single particle tracks, beam envelopes or in a Monte Carlo representation.

The ion optic was investigated assuming a given emittance provided by the CHORDIS ion source, which is in the order of $20 - 100 \pi$ mm mrad. Also, the relative distances of the optical elements were fixed according the real experimental set up. A whole bunch of calculations was done exploring the different possible modes of the quadrupole triplet. These modes are shown in Figure 1.



Fig. 1. Image properties which can be realized with a symmetric quadrupole triplet. The figure shows a triplet with two focussing quadrupoles in *x*-direction (outer quadrupoles) and one quadrupole focussing in *y*-direction (central quadrupole).

In each figure selected trajectories are presented except the last picture in the right corner showing the envelope.

The modes were obtained by a fit to match a default image at the backend. The optic is shown in terms of particle trajectories separated in x- (above the optical axes) and ydirection (below the optical axes). An exception is the matched mode, which means the same envelope at the front and the back part of the triplet. These features are illustrated by plotting the envelopes in x and y.

The telescopic image can be realized either in x- or ydirection. For our purposes only those optical images are relevant which provide a focus in front of the dipole magnet. In these cases the mass resolution of the magnet is good enough to achieve a clean ion beam at the collectors place. Therefore, the most common application of the triplet is in the point to point focussing mode. Particles ideally starting from one point of the optical axes will then be focussed behind the triplet at one point. This condition is fulfilled when the matrix elements (x|x') and (y|y') of the transport matrix are zero, which means that there is no dependence of the positions of a particle from his angle with respect to the optical axes.

Another possibility to get a focus is the parallel to point focussing mode. In this case parallel incident tracks will be focussed at a certain point of the optical axes behind the triplet. This mode can be realized if the matrix elements (x|x) and (y|y) are zero, which means that there is no correlation between the object and the image of the object.



Fig. 2. Ion optic of the experimental set up with the point to point focussing mode (left) and parallel to point mode (right). The upper pictures show the envelopes starting with a phase space of 100 π mm mrad, the pictures below show selected trajectories. The divergence of the starting rays is around 1,5 degree.

The two modes, which are useful for the ion accumulation experiment are plotted for the whole set up in Figure 2. The pictures show in the upper part the envelopes and in the lower part two selected trajectories. The part above the optical axes represent the x-direction, the part below the ydirection. It should be noted at this point, that parallel incident rays which are quite far from the optical axes have a focussing point which is apart from the beam waist. The occurrence of such rays is more academic, since in practise the beam is restricted through the aperture hole of the ion source.

In order to optimize the two modes the influence of the middle focus position between the quadrupole triplet and the dipole magnet was investigated. For this purpose the emittance of the ion source was chosen in such a way that the envelopes have the maximum extension which is possible within the given apertures. To achieve the maximum transmission it is essentially to choose a setting where the transmitted emittance can be as high as possible.

The curves in Figure 3 were obtained by varying the focus between the quadrupole triplet and the dipole magnet by 50 mm.



Fig. 3. The maximum emittance as a function of the focus between the triplet and the dipole magnet, which can be used for the experiment. The calculations are shown for the two modes, point to point (upper viewgraph) and parallel to point (lower viewgraph).

focus distance from QT (mm)

1400

200

400

600

For each point the maximum emittance was calculated, which can transmit through the experimental set up. The upper viewgraph shows the conditions using a point to point mode, while the lower one presents the parallel to point image. The three graphs show the emittance in x-direction (triangles), the emittance in y-direction (circles) and the product of both divided by 100 (squares).

For the point to point mode (upper viewgraph) a sharp maximum of the emittance can be seen passing the system at a focus of 650 mm behind the triplet lense. This behaviour is caused by the x-emittance which has the same shape. The yemittance shows a sharp increase up to the maximum of the *x*-emittance and then they stays more or less constant.

In contrast, the parallel to point focussing mode (lower viewgraph) of the quadrupole triplet has no such sharp optimum, but a single maximum which is approximately only half of the magnitude of the point to point mode. A further difference is the more moderate decrease of the emittance if the middle focus point comes closer to the dipole.

3. Experiments

In order to verify the ion optical calculations a mass analysis of the beam was performed using the experiment in the point to point focussing mode. The CHORDIS ion source in the sputter version was used with a gold electrode and natural xenon gas, since it shows a better sputter efficiency for gold compared for instance to argon. The extraction voltage was 18 kV.

The measurement of the mass spectra (see figure 4) was done by stepwise varying the magnetic fields of the quadrupole triplet lense and the dipole according to a given mass to charge ratio. An aperture of a 1 cm hole was mounted in front of the dipole magnet to achieve a reasonable mass resolution. Behind the magnet the beam current was measured using a single wire with a thickness of 1 mm. The resolution ($A/\Delta A$, where A is the atomic mass) obtained for a singly charged xenon ion was about 400.

The total current of the ion beam can be obtained by the integration of the current over the whole mass spectrum which leads to a value of 20,5 μ A. The integration of the gold peak gives a current for gold of 0,26 μ A, which is 1,3 % of the total beam current.

In the measured mass spectrum 7 of the 9 stable xenon isotopes can be observed. The mass spectrum shows three groups of isotopes. The first group around the mass to charge ratio of 65 are doubly charged ions which were extracted from the ion source. The second group around 130 are singly charged extracted ions.



Fig. 4. Experimental mass spectra of a mixed ion beam of xenon and gold. There are three groups of xenon isotopes, singly charged xenon isotopes, doubly charged xenon and xenon ions which have changed there charge from $2+ \rightarrow 1+$. The small picture in the upper right corner shows a zoomed region of the xenon ions. Here one can see the clear distinction of neighbouring Xe-isotopes due to the excellent mass resolution.

Doubly charged ions which picked up one electron during their flight from the ion source to the dipole magnet are to be seen in the third group. These ions have in contrast to the other singly charged ions twice the energy and occur therefore at twice the mass to charge ratio of about 260. The fact that all three groups have nearly the same abundance pattern is a strong evidence for a charge transition from $2+ \rightarrow 1+$ in the 3rd group. This is not unusual because of the presence of electrons steaming from rest gas ionisations in the beam line. A surprising result is that the amount of ions which have changed their charge state from $2+ \rightarrow 1+$ is in the order of 10 % relative to the total amount of originally extracted 2+ ions.

4. Conclusions

In this article ion optical calculations for an experiment with the aim to accumulate ions up to a weighable mass were presented. It turned out that beside other ion optical modes of the used quadrupole triplet the point to point focussing mode is the best choice. This mode provides an optimum setting for maximum transmission.

Experimental results using the point to point focussing mode show the opportunity to measure high resolved mass spectra with the present apparatus. It was possible to analyse the isotopic composition of the mixed xenon/gold beam.

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