Nuclear Instruments and Methods in Physics Research B 361 (2015) 311–316

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Computer simulations for a deceleration and radio frequency quadrupole instrument for accelerator ion beams

J.A. Eliades *, J.K. Kim, J.H. Song, B.Y. Yu

Korea Institute of Science and Technology (KIST), Hwarang-ro 14-gil 5, Seongbuk-gu, Seoul 136-791, Republic of Korea

ARTICLE INFO

Article history:
Received 28 November 2014
Received in revised form 14 August 2015
Accepted 16 August 2015
Available online 1 September 2015

Keywords:
Radio-frequency quadrupole (RFQ)
Accelerator mass spectrometry (AMS)
Deceleration
Ion cooling
Negative ion

ABSTRACT

Radio-frequency quadrupole (RFQ) technology incorporated into the low energy ion beam line of an accelerator system can greatly broaden the range of applications and facilitate unique experimental capabilities. However, ten's of keV kinetic energy negative ion beams with large emittances and energy spreads must first be decelerated down to <100 eV for ion–gas interactions, placing special demands on the deceleration optics and RFQ design. A system with large analyte transmission in the presence of gas has so far proven challenging. Presented are computer simulations using SIMION 8.1 for an ion deceleration and RFQ ion guide instrument design. Code included user-defined gas pressure gradients and threshold energies for ion–gas collisional losses. Results suggest a 3 mm diameter, 35 keV $^{36}Cl^-$ ion beam with 8 eV full-width half maximum Gaussian energy spread and 35 mrad angular divergence can be efficiently decelerated and then cooled in He gas, with a maximum pressure of 7 mTorr, to 2 eV within 450 mm in the RFQs. Vacuum transmissions were 100%. Ion energy distributions at initial RFQ capture are shown to be much larger than the average value expected from the deceleration potential and this appears to be a general result arising from kinetic energy gain in the RFQ field. In these simulations, a potential for deceleration to 25 eV resulted in a 30 eV average energy distribution with a small fraction of ions >70 eV.

1. Introduction

Since the late 1990's, radio-frequency quadrupole (RFQ) instruments have been incorporated into the low energy lines of accelerator systems for ion cooling in radioactive ion beam analyses [1–5] and isobar suppression for rare isotope analyses by accelerator mass spectrometry (AMS) [6–10]. Recently, application to novel ion-gas reaction studies with AMS has also been reported [11,12]. While these are not fundamentally new RFQ technology applications [13–16], RFQ-accelerator systems facilitate unique analytical capabilities. They also present new design challenges.

Typical AMS ion sputter sources produce large currents of negative ions at ten's of keV kinetic energies with relatively large emittances and energy spreads [17–21]. Large, stable and predictable transmission of the ion beam after deceleration to <100 eV during interactions with gases in RFQs has thus far proven difficult [1,6,8,11,12]. However, negligible drop in transmission with rising gas pressure has been demonstrated for ions of significantly greater mass than the initial collision gas when reaction cross sections were small [8,11,22,23]. For ion–gas reaction applications, it is further desired to have a narrow and well-defined energy spread upon entering the RFQ gas reaction cell, and be able to maintain ion energy within a range appropriate for the desired reactions. Such can be achieved with an initial RFQ gas cooling cell and then a second RFQ reaction cell based on segmented RFQs.

Presented here are computer simulations for an RFQ instrument that is currently under construction for incorporation into the recently commissioned 6 MV AMS facility at Korea Institute of Science and Technology (KIST) [24]. It will be located between a low energy analyzing magnet and the accelerator, similar to a configuration described in [11]. The RFQ system is intended to be versatile, with sections that can function as separate cooling regions, ion-gas reaction regions, a single RFQ collision cell, or allow full transmission of an AMS ion beam when the RFQ instrument is not in use.

Simulations were meant to provide conservative assessments of the deceleration matching optics and initial RFQ cooling region proposed for KIST, and to provide general insights into the capture of an accelerator ion beam by RFQs after deceleration. As a test case of interest to the AMS community, $^{36}Cl^-$ deceleration and cooling

* Corresponding author.
E-mail addresses: j.eliades@alum.utoronto.ca, jae@kist.re.kr (J.A. Eliades).

http://dx.doi.org/10.1016/j.nimb.2015.08.032
0168-583X/

in He gas is discussed. Although ^{36}Cl analysis is already possible with a 6 MV AMS system, it has proven difficult to achieve large Cl^- transmission in prototype gas RFQ–AMS systems [6,8] and work related to other ions is sparse in the literature for comparison. In particular, the simulated ion beam energy spread and size is monitored over the initial RFQ capture and cooling process.

2. Computer simulation methods for initial ion deceleration and cooling

The simulation package SIMION 8.1 [25] was used with a 64 bit Intel Xeon 2.4 GHz CPU, 8 GB RAM computer. Because of memory demands, work was split into multiple simulations by saving the final ion time of flight (TOF), velocity, position and kinetic energy (*KE*) values of one simulation to generate a SIMION ".Fly2" file for the initial ion trajectory values of the next simulation. All simulations used a "grid unit per millimeter" (gu/mm) scale of 6 gu/mm (except for an Einzel lens, discussed below), "T.Qual" (SIMION "trajectory quality") value of 300, frequency f = 1.9 MHz and a 0-peak RF voltage of V_{0p} = 380 V with a maximum simulation time step of 0.01/f. Electrode segments were enclosed in conducting tubes with end caps used to define reference potentials (Fig. 1), and simulations were conducted one ion at a time ("fired individually" in SIMION jargon).

Code was written in LUA language to control electrode voltages and to implement an ion–gas collision model modified from the HS1 code provided by SIMION (Rev. 5, 2008–11). Additions included reaction threshold energies, simultaneous use of multiple gases at different pressures and pressure gradients, and a trajectory terminate plane value which, if crossed, resulted in ion parameters being saved and an end to the trajectory. Reactions were assumed to take place if the center-of-mass energy during a collision exceeded the user defined threshold. Trajectories were marked at a collision and changed color dependent on the gas involved. The SIMION data recording at a plane feature (at x=, y=, z=) in the Data Recording menu can miss some ions if a trajectory time step misses the acquisition plane coordinate, whereas the trajectory terminate code captured all ions. Also, data acquisition could be stopped before ions entered regions not representative of an actual RFQ system (at the ends of each simulation split), also avoiding un-necessary calculation time.

A hard sphere He–Cl^- collision cross section of $\sigma = 3.1 \times 10^{-15}$ cm^2 was assumed as collision cross sections could not be found in the literature. However, at each collision, the ion *KE*, position, velocity and TOF were recorded so that ion beam energy spreads could be described in terms of the number of collisions. A collision event was considered to have taken place if

$$\text{RAND} \triangleright 1 - \exp\left[-v \cdot \Delta t \cdot \left(\frac{\sigma \cdot P}{K_B \cdot T}\right)\right]$$

Here, RAND is a random number generated by the SIMION random number generator, v is the ion speed, Δt is the ion time step, K_B the Boltzmann constant, and P and T are the gas pressure and temperature (273 K) respectively. Electron detachment was used for a reaction threshold with centre-of-mass energy 7 eV for Cl^- on He [26]. The initial ion beam consisted of 1000 anions of m = 36 amu with a 35 keV Gaussian energy distribution of full-width half maximum 8 eV, from a point source with a cone-half-angle divergence of 2° (±35 mrad). This was the simplest way to model a 35 keV $^{36}Cl^-$ AMS ion beam with a diameter of 3 mm (~43 mm downstream from the simulation point source position) and ±35 mrad angular spread after analysis in a magnet. SIMION ion "birth" times (the time at which an ion began a trajectory) were uniformly distributed over 0.53 µs to test RFQ acceptance over one period of the RF frequency.

Deceleration involved an Einzel lens designed to minimize chromatic and spherical aberrations while focussing ions for the deceleration optics. Deceleration lenses were static voltage electrodes that focussed the ion beam into an RFQ segment referenced to −34,975 V for ion deceleration to 25 eV on average.

The RFQs were operated as ion guides only, but a static voltage could be applied to each rod of a segment on top of the RF voltage for a potential offset between neighbouring segments (ΔV_{dc} Fig. 1) to maintain a forward field gradient. The first RFQ segment, accepting the ion beam from the static deceleration optics, was 250 mm long with gradient bars inserted between the RFQ rods, followed by eight short RFQ segments, each 25 mm in length, with a 1 mm gap between each segment. All RFQs used $2r_{rod}$ = ϕ22 mm cylindrical rods with RFQ inscribed radius r_0 = 9.58 mm.

The first simulation segment (Fig. 1) was broken into 2 SIMION "instances", merged in the simulation "workspace". The first instance modeled the Einzel lens portion using a 2 gu/mm scaling up to a ground electrode of the deceleration section where fields from the deceleration optics had negligible effects on ion trajectories. The second "instance" included the deceleration optics and 180 mm of the first RFQ segment using 6 gu/mm, and the ion trajectory limit was set at 170 mm of the RFQ length. In the second simulation, ions traversed the remaining 80 mm of the first 250 mm RFQ segment, the first 3 short RFQ segments, and 20 mm of the fourth. The remaining RFQ segments required a third simulation. The gas gradient and ion beam energy distributions at points along a simulation for maximum 7 mTorr He gas in the RFQs are shown in Fig. 2.

Data from the first simulation at 5 mm inside the first RFQ segment where ions had been captured by the RFQ fields but where fringing field effects from the deceleration optics were still significant, was used to create a .Fly2 file. At this point less than 1% of the ion beam had interacted with He. One ion had been lost during deceleration during collision with He gas, and eight other ions had each experienced one collision with He gas in the RFQs. Ions

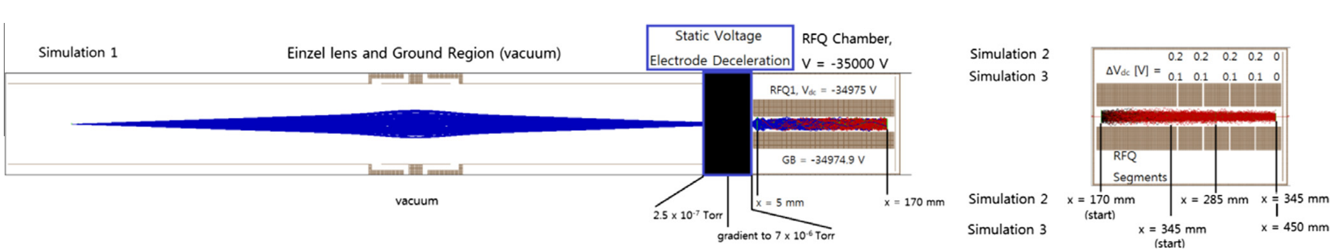

Fig. 1. Simulation workbenches for Cl^- ion beam deceleration and cooling in He gas. RFQ segment static voltage offsets are given by ΔV_{dc} and gradient bar voltages by GB. Radial coordinates are the simulation y–z coordinates, while x was in the axial direction with x = 0 defined at the start of the first RFQ segment. All other parameters are given in Section 2. Ion trajectories turned red upon collision with He gas. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)