ION OPTICAL CALCULATIONS OF HIGH RESOLUTION ANALYZING MAGNET SYSTEM FOR HEAVY MOLECULAR IONS AT KACST

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Abstract

At the King Abdulaziz City for Science and Technology KACST, a beam line injector is being constructed to provide the multi-purpose low-energy, ELectrostAtic Storage Ring (ELASR), with the required high-quality ion beams. The injector is being equipped with a 90° high resolution mass analyzing selector magnet system and a new ECR ion source. The magnet system was designed to provide a singly-charged ion beam of kinetic energy up to 50 keV and ion mass up to 1500 amu with the mass resolution of $\Delta m/m = 1/1500$. In this paper, the ion-optical calculations, the determination of the required momentum resolution and the actual analyzing magnet system parameters will be discussed. The simulation of the beam envelop along the the injector and through the magnet will be presented.

INTRODUCTION

The ELectrostAtic Storage Ring (ELASR) facility is being built at the King Abdulaziz City for Science and Technology (KACST), in Riyadh, Saudi Arabia [1]. The Ring is designed to store ion beams at fixed-energy up to 50 keV/q for the purpose of atomic, biophysics and molecular physics applications. A highly flexible injector was developed to provide the ring with the required ion species [2]. It injector was mainly designed to possess a flexible injection system for different applications and planned research programs. The injector consists of ~ 3.3 m inline electrostatic ion optics to steer, shape and focus the beam as being transported to the 90° high resolution mass analyzing selector magnet. The analyzing magnet is followed by a matching section, which consists of a single quadrupole triplet for beam emittance adaptation before the beam is finally injected to the ring.

The high resolution mass analyzing magnet was manufactured in 2014 [2,4], and currently is being constructed at KACST. The magnet was design mainly to achieve a proper beam selection as well as an adequate transmission of a high quality macro-molecular ion beam. Equidistant entrance and exit slits are combined with the magnet analyzing arrangement to sustain the required magnet system specifications, namely a mass resolution fixed to $\Delta m/m = 1/1500$. The main parameters of the system are chosen to fulfill a maximum magnetic field of 1.25 T, which are 1 m central trajectory radius, 90° bending angle and 50 mm magnet gap.

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ION-OPTICAL CALCULATIONS

The process of matrix multiplication is normally used to simplify the transportation of charged particle through electric or magnetic elements along the beam line. The particle's coordinates, at an initial position with respect to the curvilinear coordinate system, are described in a trajectory vector as $X_0 = (x_0, x_0', y_0, y_0', \delta_0)$. Similarly, at some position 1 along the central trajectory, the particle's coordinates are then $X_1 = (x_1, x_1', y_1, y_1', \delta_1)$. This approach enable us to calculate a particle's coordinates at position 1 if X_0 and the linear transport matrix R are known. The multiplication is performed as following:

$$X_1 = RX_0 \tag{1}$$

The matrix R provides a very good first order approximation to the ion-optical transformation that the charged particles undertake between positions 0 and 1. Ion optical calculations for an analyzing magnet or spectrometer system can be performed by defining the position at the entrance slit 0 and selection the position at exit slit 1. It corresponds to the conjugate object and image and can be explicitly written as follows:

$$\begin{pmatrix} x_1 \\ x_1' \\ y_1 \\ y_1' \\ \delta_1 \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} & 0 & 0 & R_{15} & \\ R_{12} & R_{22} & 0 & 0 & R_{16} & \\ 0 & 0 & 0 & R_{33} & R_{34} & 0 \\ 0 & 0 & R_{43} & R_{44} & 0 & \\ 0 & 0 & 0 & 0 & 1 & \end{pmatrix} \begin{pmatrix} x_0 \\ x_0' \\ y_0 \\ y_0' \\ \delta_0 \end{pmatrix}$$

The condition $R_{01} = 0$ provides a focus in the horizontal plane between particle's position at entrance and exit slit. The analyzing magnet system is shown in Fig.1 for the nominal case where the slit apertures are chosen to be 1 mm wide in the horizontal plane, the bend angle to be 90°, and the radius of curvature of the magnet to be 1 m. Since the particle is not accelerated through the magnet section, the momentum deviation of the particle from the central trajectory is not changing, which gives $\delta_1 = \delta_0 = \delta$.

In order to define the limiting specifications of the system, the matrix can be broken down for the horizontal plane where the condition $R_{01} = 0$ is valid, and this gives :

$$x_2 = R_{11}x_1 + R_{15}\delta \tag{2}$$

Since we are considering all particles that end up on the central trajectory at slit 1, so that $x_1 = 0$, then; $0 = R_{11}x_1 + R_{15}\delta$, and $-R_{15}\delta = R_{11}x_1$, which finally gives;

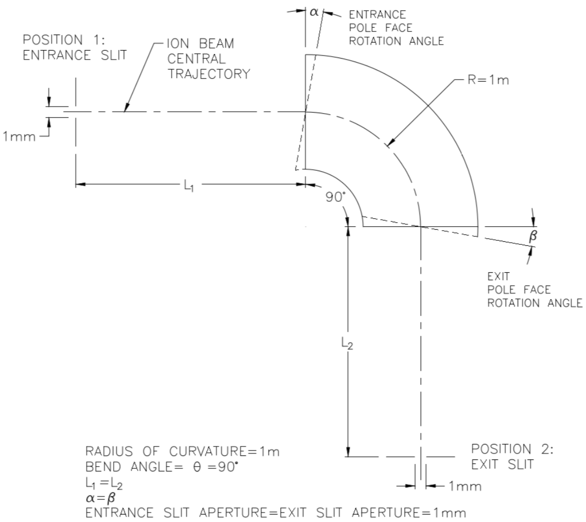

Figure 1: The analyzing magnet system

$$\delta = -R_{11}x_1/R_{15} \tag{3}$$

All particles of momenta p, where p is the momentum of interest, which is chosen to be analyzed or selected by the magnet, satisfy:

$$\delta = (p - p_0)/p_0 = R_{11}x_1/R_{15} \tag{4}$$

The momentum resolution for the magnet system will be given by the ratio R_{11}/R_{15}, which is equivalent to mass resolution $\Delta m/m$ chosen to be 1/1500. Therefore, in Fig. 1 the drift lengths L_1 and L_2 and the pole face rotation angles α and β can be adjusted in order to meet the required mass and momentum resolution. The specification for the magnet analyzer is to resolve molecular "particles" with mass difference of 1 *amu* out of 1500 *amu*. This is because a molecule with plus or minus a single hydrogen atom can behave significantly different in chemical and/or biological reactions and processes, and the analyzing system must be able to distinguish ionized molecules with a difference in mass of plus or minus a single hydrogen atom attached. Using the equation for particle momentum (eq.5), the momentum for M_{1500} and M_{1499} are calculated for kinetic Energy of the molecular "Particles" to be 50 keV by [3] :

$$p = T\sqrt{\frac{1}{c^2} + \frac{2M}{T}} \tag{5}$$

where p is the momentum (MeV/c), T is the particle kinetic energy (MeV), M is the particle mass (MeV/c^2). Then, δ_{1amu} is computed which gives $\delta_{1amu} = 1/3000$.

ANALYZING MAGNET SYSTEM PARAMETERS

Using the Beamline Simulator software, the analyzing magnet system parameters (entrance drift L_1, exit drift L_2, entrance pole face rotation α, and exit pole face rotation β) are adjusted to achieve $R_{12} = 0$. It will only be possible to achieve $R_{12} \sim 0$, with realizable pole edge angle precision, but it will be nearly zero within a small tolerance. The spacing between the entrance slit and the analyzer magnet, and between the analyzer magnet and the exit slit, both were set at $L_1 = 1500mm$. The analyzer magnet parameters that were used to achieve the R matrix values are the effective length of 1570.8 *mm*, angle bend of 90° and entrance and exit pole face angle is 18.43487°. The entrance and exit slits are set with a horizontal opening of 1 *mm*. A view of bottom half of magnet iron and the UHV vacuum box with conflate flanges are shown in Fig. 2. The final design of the mass resolution 1/1500 analyzing magnet system is displayed in Fig. 3. Currently, the magnet is placed on its stand in the beam line and the related cooling system is being constructed. Some other lab preparation services are ongoing.

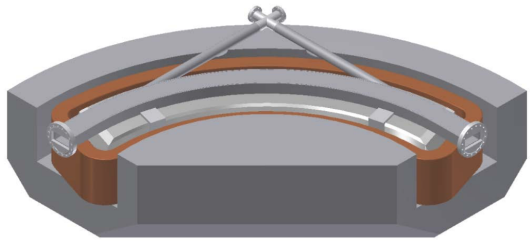

Figure 2: View of bottom half of magnet iron and the UHV vacuum box with conflate flanges.

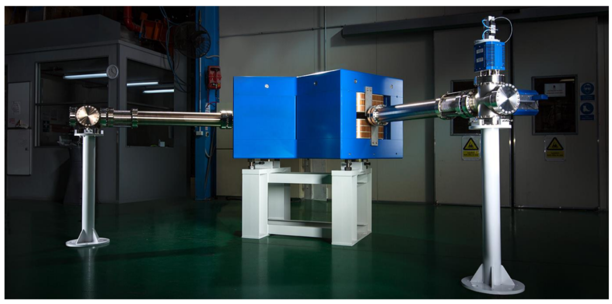

Figure 3: Final design of analyzing magnet system with resolution 1/1500.

BEAM ENVELOP SIMULATION

Particle Beam Optics Laboratory (PBO LabTM) software [5] was used to track the ions and simulate the beam envelope through the whole beam line including the analyzing magnet system. The PBO Lab enables the user to construct interactively and visually optical beam lines using a palette bar of accelerator element icons. A TRACE 3-D module is implemented to calculate beam envelopes and phase space ellipses.

Overview of the ion beam envelope tracked along the injector beam-line, as outputted by the PBO-Lab code. The red line is the vertical plane, and blue the horizontal. (For

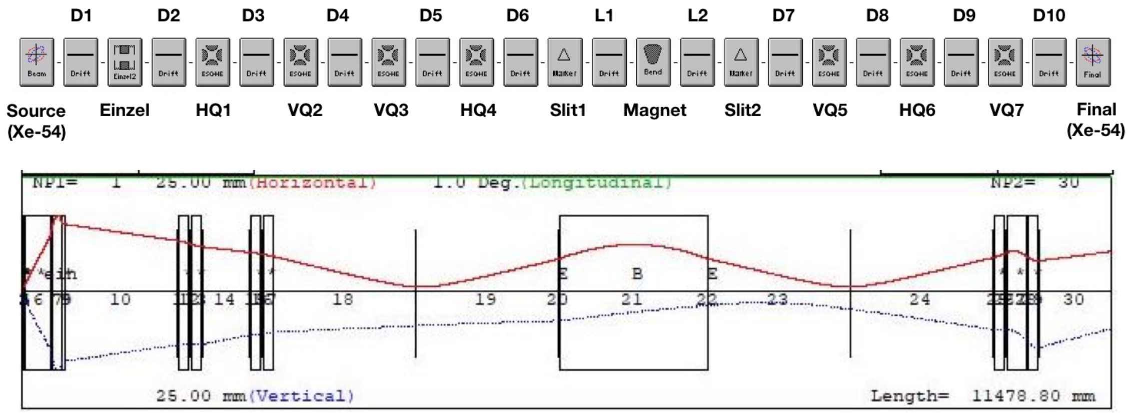

Figure 4: TRACE 3-D graph of the singly-charged Xe-54 ion beam envelope tracked along the injector beam-line

interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Injector line consists of an ECR ion source followed by an einzel lens system which features a symmetrical unipotential lens. The inner diameter of the cylinders is 40*mm*, the gap between the electrodes is 10*mm* and the total physical length of the einzel lens system is 430 *mm*. Next, two electric quadrupole doublets are placed to provide the required beam focusing and adaptation before the beam retches the entrance slit of the magnet. After the slit, a 1.5 *m* drift tube connects the line to the analyzing dipole entrance. Another 1.5 *m* drift tube connects the magnet to the exit slit.

A singly-charged Xe-54 ion is created in the ECR ion source with an effective ion temperature of about 1 eV. The beam size at the extraction point of the ion source is determined by the plasma chamber hole through which the beam is extracted. The final extraction energy from the ECR ion source is fixed at 50 keV, which corresponds to the analyzing magnet specifications. Next to the ion source, the einzel lens will preform the first focusing to form the beam as it travels to two electric quadrupole doublets. The transverse (x'-x, y'-y) phases spaces of the initial beams are restricted by the 50 keV beam input which is obtained from the ECR source extraction model. The transverse emittances of the 50 keV beam are 7.22 π-$mm - mrad$ which are the boundary value. The first step is to adjust manually the voltage of the einzel lens so that the beam is a reasonable size at the entrance to the first electrostatic quadrupole, and the value used is -23.0 kV. The second step is to use TRACE 3-D fitting model to adjust the fields of the electrostatic quadrupoles in order to fit the beam into the magnet entrance slit. The electrode voltage applied on for HQ1, VQ2, VQ3 and HQ4 are 4, 5, 106 and 164 V, respectivily, but one has to mention that this is not a unique solution. The overall length of the injector beam-line is 11478.80 *mm* and the ion beam envelope tracked along the line is shown in Fig. 4.

CONCLUSION AND OUTLOOK

A high resolution mass analyzing magnet system was designed and currently is being constructed to provide a singly-charged ion beam of energy up to 50 keV and mass up to 1500 *amu* with the mass resolution of $\Delta m/m = 1 : 1500$. The ion-optical calculations, the actual analyzing magnet system parameters and the simulation of the beam envelop which including the ECR ion source and the magnet are presented. The magnet is installed on its final position and the construction of the whole line will start as soon as other lab preparation services are completed.

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