SIMULATION OF A QUADRUPOLE MASS FILTER EMPLOYING A DIGITAL WAVEFORM AND DISCONTINUOUS ION INTRODUCTION TO OBTAIN HIGH RESOLUTION AND TRANSMISSION

INTRODUCTION

Generally quadrupole mass filters exhibit an inverse relationship between resolution and transmission. Typical commercial quadrupoles (100% efficiency, 800mm, 900mm outer length) lose transmission to more than 90% at 10,000 resolution. This is because their maximum acceptance is limited by the number of RF cycles. At higher resolutions that have stable trajectories undergo lower acceptance relative to their initial positions, hence lower fillable stable regions. For a given stable acceptance region, there is a single phase value (x) where we see high acceptance in both r1 and r12 stable regions. In order to obtain the quadrupole on this phase we would have high acceptance with respect to the entire period of the ion motion. This is practically impossible however as the phase limit value is very large, the ion acceptance is on a very small and steep gradient, and needing to cross the fringing fields of the entrance of the quadrupole.

For the EC1 to r12 systems we plot the iAPC for resolutions of 10,000 and 50,000. These are shown in Figure 1. There is a range of initial phase values where the acceptance is high in the r1 and r12 stable regions. In particular, the acceptance is high in the r1 and R~60k for the r12 region. This allows us to estimate the theoretical resolution limits for the EC system.

The key to obtaining high resolution and transmission is to use larger phase space acceptance (i.e. within the high acceptance region) and then start application of the acceptor. Initially the acceptance is fully within the quadrupole (i.e. distant from any fringing fields), hence the acceptance is accessible using the correct timed application of the waveform.

According to the Mathieu stability equation, the value of m is a function of initial RF phase. Hence it is effectively a measure of the positional offset of the top of the rods relative to the mid point of the rod.

The iAPC plotted in Figure 3 consider only acceptance related to initial position. Initial phase acceptance is not improved by the EC waveform, hence we need to control the initial velocity spread of the ions. Due to the high positional tolerance of the EC system and the conservation of energy, these ions will experience a sufficient number of 1MHz digital waveform cycles to reach a stable acceptance position. However, previous analysis have shown the positional spread of the ions beam leading to a resolution in the velocity spread. From previous studies of the positional spread of the beam up to a standard resolution of 10,000 forms a velocity spread equivalent to a thermal temperature of ~2K.

The AtoC plots in Figure 2 consider any acceptance related to initial position. Initial phase acceptance is not improved by the EC waveform, hence we need to control the initial velocity spread of the ions. Due to the high positional tolerance of the EC system and the conservation of energy, these ions will experience a sufficient number of 1MHz digital waveform cycles to reach a stable acceptance position. However, previous analysis have shown the positional spread of the ions beam leading to a resolution in the velocity spread. From previous studies of the positional spread of the beam up to a standard resolution of 10,000 forms a velocity spread equivalent to a thermal temperature of ~2K.

In our present work we demonstrate that 1MHz different digital waveforms can be employed in the transfer optics to improve the positional spread and allow a greater number of RF cycles to be used. This results in an increased positional spread.

RESULTS

Figure 3 shows the results for the EC waveform. Both stability diagrams are plotted with the initial ion velocity spread and the initial phase spread. The principal advantage of the EC waveform is the increased stability, allowing 100% transmission even at a resolution limit of ~30k.

The 1MHz digital waveform: In order to obtain a reasonable resolution (10,000) we need a number of RF cycles to reach the acceptance region. A 1MHz digital waveform allows more than 100 RF cycles before the ions leave the acceptance region. Figure 4 shows the results for the digital system.

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Figure 5 shows the results for the EC system.

Figure 6 shows the results for the EC waveform. Both stability diagrams are plotted with the initial ion velocity spread and the initial phase spread. The principal advantage of the EC waveform is the increased stability, allowing 100% transmission even at a resolution limit of ~30k.

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METHODS

We have implemented the realistic approach to solving the Mathieu equations using a matrix method approach. This method was used to generate realistic stability plots of the EC waveform. For the digital waveform we can assess that the ions experience an equivalent number of cycles to a given resolution in the transfer optics. This approach allows for a realistic estimate of the positional spread of the ions beam leading to a resolution in the velocity spread.

The iAPC method is used to generate realistic stability plots of the EC waveform. A grid scale of fringes was used to be sufficient to reproduce the realistic matrix method results.

To obtain the vector diagram of the stability region, the phase space acceptance is in the normal harmonic system on a standard resolution value (x=0). For a position value, 100MHz thermal energy for mass m4 is tuned in and used to simulate the real system. The mass acceptance is then simulated with a range of RF voltages and mass acceptance values. The grid scale of fringes was used to be sufficient to reproduce the realistic matrix method results.

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REFERENCES


