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Characterization of the impact of the ejection slit on miniature rectilinear ion trap analysis

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ABSTRACT

The rectilinear ion trap (RIT) has always been one of the ideal candidates for mass analyzer miniaturization because of its simple configuration. In this work, the effect of the ejection-slit dimensions on the ion ejection efficiency of a miniature rectilinear ion trap (mRIT) with full-scale dimensions of 5 mm × 4 mm × 25 mm was investigated by using SIMION8.1 simulation. Six mRITs with the same dimensions as those simulated and with different slit widths, whose X electrodes were fabricated by the stainless steel chemical etching process, were tested and characterized on a homemade mass spectrometer platform. It is shown that the ejection slit dimensions have a significant impact on both the signal intensity and mass resolution. For an mRIT with these full-scale dimensions, the optimized slit dimensions are 0.6 mm × 18 mm. The optimized mRIT demonstrated capabilities including a mass/charge range of over 1000 Th, unit mass resolution at m/z 332, and a passable tandem mass spectrometry capability, which are better than the non-optimized RIT with the same dimensions.

1. Introduction

As a universal chemical analysis method with high specificity and sensitivity, mass spectrometry has been widely applied in the fields of food safety [1,2], environmental monitoring [3,4], space exploration [5], and public safety [6,7]. The demand for in situ analysis continuously increases the need for portable mass spectrometers [8,9]. As early as 1989, Kaiser and Cooks have conducted studies on the miniature mass spectrometer [10]. Several researches on the portable mass spectrometer have been reported over the past two decades [11–14]. In addition, the development of MEMS technology has provided a favourable method for the further miniaturization of mass spectrometers. Several relevant MEMS components [15–18] and complete MEMS mass spectrometers have also been investigated and reported [19,20]. However, it is generally recognized that the miniaturization of components is achieved at the cost of reducing the system performance. To maintain good analytical performance during the course of mass spectrometer miniaturization, the problems concerning the great reduction of ion storage capacity and ejection efficiency have to be taken into primary consideration, because the reduced dimensions and intensified space charge effect will directly reduce the system's detection sensitivity and resolution [21].

In 2004, Ouyang developed a novel mass analyzer – the rectilinear ion trap (RIT) – using plate electrodes instead of the hyperboloid electrodes in traditional ion traps [22]. With a powerful ion storage capacity and simple structure, which reduces the processing difficulty and cost, the RIT has become a good choice for mass analyzer miniaturization [23–25]. For rectilinear ion traps, previous studies have optimized the X and Y electrodes' dimension scale [26–28], operation mode [22,29], working air pressure [30], and electrode surface roughness [31]. However, with the further miniaturization of RIT mass analyzers, the relative area ratio between the slit and the plate has to be increased due to the limitations of manufacturing technology, so its impact on the analytical performance will become more obvious and important. Several researchers have reported the approximate expressions for nonlinear electric fields in the ion traps with apertures on the electrodes [32–34], indicating theoretically the influence of the aperture size on the multipole coefficients of radio-frequency (RF) ion traps, which is also applied to the ejection slit of the mRIT. However, the multipole field theory cannot predict the analytical performance directly.

In this study, the relation between the ejection slit dimensions and ion ejection efficiency was characterized quantificationally by computer simulation, and the experimental verification showed that the ion slit dimensions had a significant influence on both

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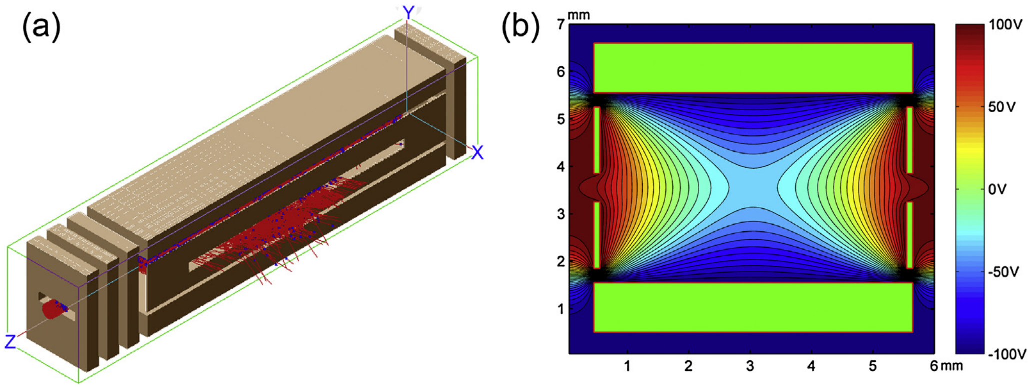

Fig. 1. (a) Simulation model by SIMION 8.1, the distances between two electrode pairs are 5 mm (X), 4 mm (Y), 27.5 mm (Z), the size of the ion optic lens is 1 mm (electrode) and 1.25 mm (space), the injection aperture size is 0.5 mm × 3 mm, the thickness of the electrode X is 0.2 mm, and the ejection slit dimensions are 0.6 mm × 18 mm; (b) trapping field of the mRIT calculated by MATLAB.

the signal intensity and mass resolution. The simulation and experiment results demonstrated the same optimal dimensions. Furthermore, several experimental studies on the mass analysis range, resolution, and tandem mass spectrometry capability of the optimized ion trap were conducted to verify its performance.

2. Methodology and simulation

2.1. Theoretical basis of rectilinear ion trap

The rectilinear ion trap, which consists of a pair of rectangular Y electrodes, a pair of rectangular X electrodes with ejection slits, and two endplate Z electrodes with injection apertures, is a simplified structure of a hyperbolic linear ion trap [22]. In this paper, the RIT was operated in the mass-selective instability scan mode under the excitation of a double-phase RF power supply. The ions can be scanned out of the RIT through the slits in the X electrodes. As shown in Eq. (1), scanning the RF voltage amplitude loaded on the X and Y electrodes of the RIT can change the value of the Mathieu parameter q, which affects the ion stability [35], and when q exceeds 0.908, the ions will be ejected from the ion trap and be detected by a multiplier detector [36,37].

$$q = \frac{8zv}{m(x_0^2 + y_0^2)\Omega^2} \quad (1)$$

where v is the amplitude of the RF voltages applied on the X and Y electrodes, Ω is the frequency of the RF signals, m/z is the mass-to-charge ratio of ions, and x_0 and y_0, the quadrupole field radii of the RIT, are the half-distances between the X-electrodes pair and the Y-electrodes pair, respectively. In order to increase the ejection efficiency, an auxiliary alternate current (ac) at the approximate frequency of ion motion is applied on the X electrodes during the RF scanning [22]. Thus, the target ions will be scanned out before q reaches 0.908.

2.2. Simulation and optimization of ejection slit dimensions

First, a miniature rectilinear ion trap (mRIT) with field radii of 2.5 mm (x_0) and 2 mm (y_0) and a length of 25 mm was designed and simulated by SIMION 8.1, a software package primarily used to calculate the electric fields and trajectories of charged particles in electromagnetic fields (Scientific Instrument Services). As illustrated in Fig. 1a, three ion optic lens for focusing the ions, two pairs of X and Y electrodes for forming the quadrupole field, and a terminal Z electrode composed the simulation model. Fig. 1b gives the quadrupole electrical field distribution inside the ion trap.

Then, to guarantee that the ion traps with different slit dimensions can be operated under identical simulation conditions, m/z was set as 174 (arginine), the frequency of the RF signal was set as 1 MHz, the auxiliary ac frequency was 375 kHz, with an amplitude of 5 V. And 100 target ions were injected as a group synchronously, where the initial ions position was set as a circular distribution with the radius of 0.5 mm in front of the central position of the first ion optic lens, while the initial kinetic energy was 1 eV and towards the z direction. On the basis of Eq. (1), the parameter q of the Mathieu equation was scanned from 0.6 to 1.0, the terminal Z electrode was set to 32 V during the simulation, and the number of the ions ejected through the slits was recorded by the software to represent the ejection efficiency. The ejection efficiency in the simulation is used for comparison with the signal intensity in the experiments; because the signal intensity is related to the number of ejected ions, the ejection efficiency can predict the signal intensity to some degree.

The slit optimization process was divided into the length optimization and width optimization.

(1) *Length optimization*: The length of the slit was increased from 9 to 24 mm while the width was set as 500 μm. For each length, ten simulations were implemented accordingly, and the simulation results for the effect of the slit length on the ejection efficiency are shown in Fig. 2.

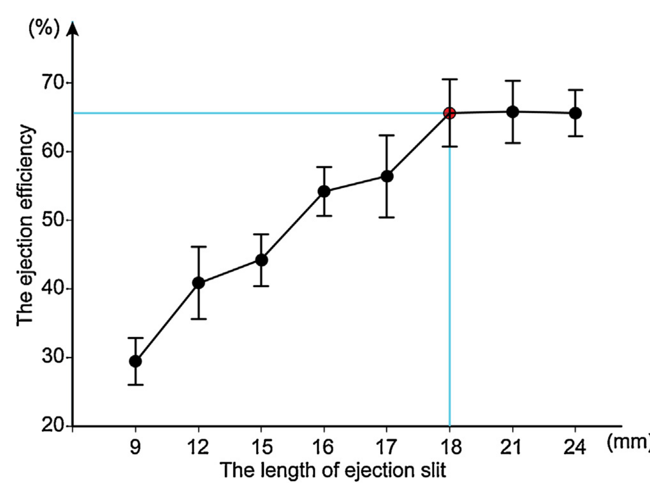

Fig. 2. The effect of the length of the ejection slit on the percentage of ions successfully ejected by the mRIT (the width was 500 μm) with the terminal Z electrodes set to 32 V. Bars represent the standard deviation of analysis for ten replicates.