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RESEARCH PAPER

Research of Unidirectional Ion Ejection in Printed-Circuit-Board Ion Trap

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Abstract: Printed-circuit-board ion trap (PCBIT) is a novel ion trap mass analyzer, which is capable of optimizing its internal electric field distributions to improve the analytical performance by adjusting the radio frequency (RF) voltage-divided ratio. This work introduced odd electric field components into the trapping volume to achieve unidirectional ion ejection by applying asymmetric RF voltages to x electrode pairs of PCBIT. In this case, the center of ion vibration was displaced away from the geometrical center of PCBIT and ions were ejected predominantly through one of x electrode pairs. The relationship between asymmetric voltage-divided ratio ΔV and internal electric field distributions was investigated by simulation software SIMION and AXSIM. In addition, the ion trajectories and simulated mass spectrum peaks were calculated. The results showed that, for ions with m/z 609 Th, a mass resolution of over 2500 and an ion unidirectional ejection efficiency of over 90% were achieved in PCBIT with ΔV = 20% at an appropriate frequency of AC. Using this method, the ion detection efficiency of PCBIT was significantly improved while maintaining a high mass resolution, which made the PCBIT more suitable for developing miniaturized mass spectrometer.

Key Words: Printed-circuit-board ion trap; Simulation; Unidirectional ion ejection; Odd-order electric field

1 Introduction

Due to its advantages such as structure simplicity, small size, high sensitivity, low vacuum requirement[1] and capability of MSn[2,3], ion trap mass spectrometer had been commercialized and used in many fields[4,5] since it was invented. It is well known that a linear ion trap (LIT) has higher trapping efficiency and greater ion capacity than a traditional three-dimension (3-D) ion trap[6]. Therefore, LIT has higher sensitivity and dynamic range than that of 3-D ion trap. In the last decade, novel LITs with simplified geometry[7,8] were developed and attached great importance. The simplified LIT has advantages such as ease of manufacture and assembly, high machining precision and relatively low cost, which makes it the first choice of miniaturized mass spectrometer.

Ouyang *et al*[7,9] built a rectilinear ion trap (RIT) which was mainly composed of two pairs of rectangular electrodes with planar-shaped surface instead of hyperbolic-shaped electrodes as that used in a conventional LIT. The rectangular electrodes introduced a large amount of nonlinear electric fields, which degraded its analytical performance. Sudakov *et al*[10,11] introduced another type of LIT with planar-shaped surface, the triangular electrodes LIT (TeLIT). The TeLIT was composed of two pairs of triangular electrodes instead of the rectangular electrodes as that used in RIT. The TeLIT reduced nonlinear electric field components and improved analytical performance, because its geometry was more approximate to hyperbolic shape than RIT's. Li *et al*[12] developed a LIT featuring half round rod electrodes (HreLIT) with two pairs of half-round-shaped electrodes. The nonlinear electric field components were further reduced and the analytical

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performance was further improved.

Jiang *et al*[13] built a printed circuit board ion trap (PCBIT) with low cost material-PCB. In a PCBIT, each PCB electrode was fabricated to specially designed patterns with several separate electric strips (one central strip, two side strips and two corner strips). Its internal electric field distributions were capable of being optimized by adjusting the RF voltage-divided ratio, and 67% was finally selected as the RF voltage-divided ratio according to the optimized experiment results. In this case, the performance of PCBIT was much superior to that of RIT. He *et al*[14] changed the method of applying AC voltages on PCBIT and removed the two corner strips to further optimize the performance of PCBIT. The simulation results indicated that the mass resolution increased by a fact of 25% and 16% respectively.

For existing LITs (only for radial ejection LITs), ions were ejected from both sides along the x axis, which means that the ion detection efficiency would not be higher than 50% if only one ion detector was used, as it usually does[7,11–13]. To solve this problem, two ion detectors was used in commercialized LIT mass spectrometer. However, this configuration requires relatively large vacuum chamber, and apparently higher cost, which is undesirable for developing miniaturized mass spectrometers.

Ion detection efficiency could be greatly increased by unidirectional ion ejection even if only one detector was used. Wang *et al*[15] verified that odd-order fields could lead to unidirectional ion ejection using mathematical modeling approach. Splendore *et al*[16] employed an asymmetric trapping field on a traditional 3-D ion trap by adding an alternating voltage out of phase to the end-cap electrodes at the same frequency as the ring electrode. The experiment results indicated that unidirectional ion ejection occurred and the absolute ion abundance was doubled. Remes *et al*[17] created some models of hyperbolic LIT with asymmetric geometry and studied their performance using numerical simulation approach. The simulation results indicated that a high mass resolution that was comparable to an ideal quadrupole trap and a certain extent capacity of unidirectional ion ejection were achieved in these asymmetric traps.

In the present study, odd electric field components were introduced into the trapping volume to achieve unidirectional ion ejection by applying asymmetric RF voltages to x electrode pairs of PCBIT. In this case, the center of ion vibration was displaced away from the geometrical center of PCBIT and ions were ejected predominantly through one of x electrode pairs, which improved ion detection efficiency.

2 Experimental

2.1 Geometry of PCBIT

The geometry of PCBIT that had been optimized by He *et al*[14] was adopted in this study, and the cross-section of this geometry was shown in Fig.1A. In comparison with the prototype of PCBIT built by Jiang *et al*[13], the two corner strips were removed and the lengths of the other strips were adjusted in each PCB electrode. The geometrical parameters were shown as follows: the central strips C = 3 mm, the two side strips S = 2.8 mm, "field radius" $r = x_0 = y_0 = 5$ mm, the width of slits d = 0.8 mm, and the insulate gap l = 0.2 mm.

2.2 Field and ion trajectory simulations

The configuration of applying RF and AC voltages on PCBIT were shown in Fig.1A[14]. A RF voltage with opposite phase was applied to x electrodes and y electrodes with different RF voltage-divided ratio, and an AC voltage out of phase was only applied to the central strips of x electrodes. Figure 1B showed equipotential lines diagram with asymmetric voltage-divided ratio $\Delta V = \gamma - \alpha = \alpha - \beta = 15\%$, here $\alpha = 67\%$. The trapping field center was displaced towards the negative x electrode where the RF voltage-divided ratio was smaller than the other.

In any electric field, it is essential that the Laplace condition is satisfied and, consequently, the potential in PCBIT can be expressed in Cartesian coordinates as follows:

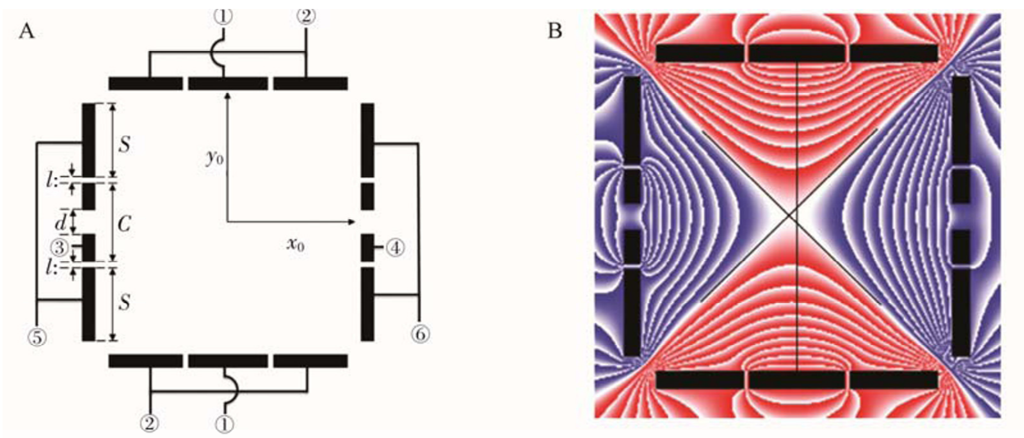

Fig.1 Printed-circuit-board ion trap: (A) mode of voltages applied to printed-circuit-board ion trap; (B) equipotential lines with asymmetric voltage-divided ratio ΔV of 15% (1. +RF; 2. +Arf; 3. –RF, –AC; 4. –RF, +AC; 5. –βRF; 6. –γRF)