Fundamental Aspects of Ion Confinement in SLIM Devices

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Overview

- Structures for Lossless Ion Manipulation (SLIM) represent a novel class of ion optical devices based upon electrodes patterned on planar surfaces.
- Complex sequences of ion manipulations, ion mobility separation, MS/MS, etc., can be enabled by SLIM devices, and allowing e.g. analyses with greater speed and reduced sample size requirements.
- Ion dynamics in SLIM devices are analyzed using ion optics theory and computational modeling.

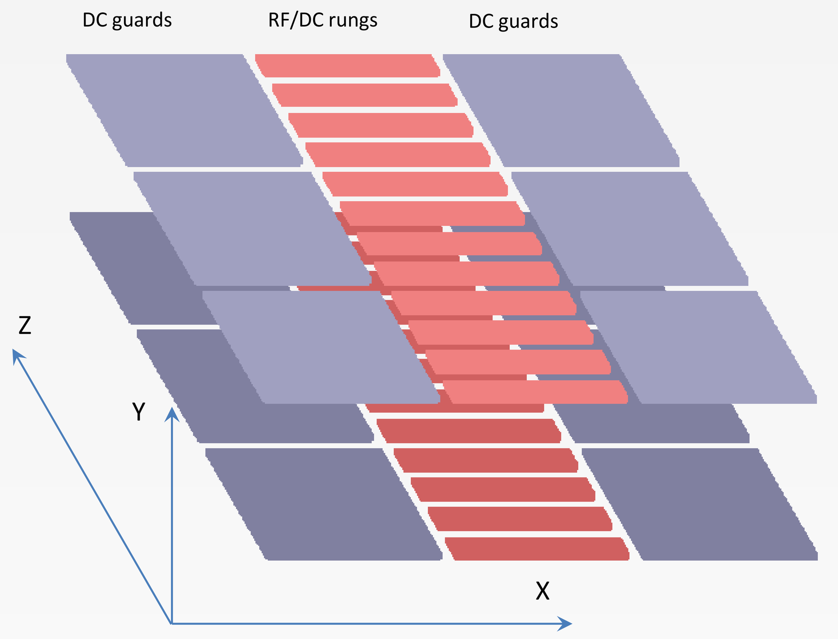

Fig. 1. A section of the Structure for Lossless Ion Manipulation, formed by two planar boards, each having DC guard electrodes and central RF/DC rung electrodes.

Introduction

Ion dynamics theory and modeling has facilitated mass spectrometry developments at our laboratory, ranging from new types of ion traps and guides to advanced FT ICR analyzer cells. The ion funnel design refinement depended crucially on modeling, and now such devices are common to many highly sensitive MS platforms.

We recently introduced Structures for Lossless Ion Manipulations (SLIM), a concept which builds upon similar capabilities for lossless ion transmission, and provides a potential basis for a wide range of ion manipulations, such as accumulation and storage, ion mobility separations, ion reactions and ion fragmentation. Here we present a theoretical treatment of the ion dynamics in SLIM devices.

Methods

The SLIM devices considered in this study are formed by two parallel surfaces, each having a sequence of radio frequency (RF) "rung" electrodes, bordered by DC "guard" electrodes. Ion motion is confined by the RF effective potential in the direction orthogonal to the boards, and limited by the guard DC potential in the transversal direction. The pressure was 4 torr (nitrogen), and we assumed an absence of gas dynamic contributions. The computer modeling was based on custom developed potential calculation approach [1], enabling precise potential calculations for complex 3D geometries.

Results

Effective Potential

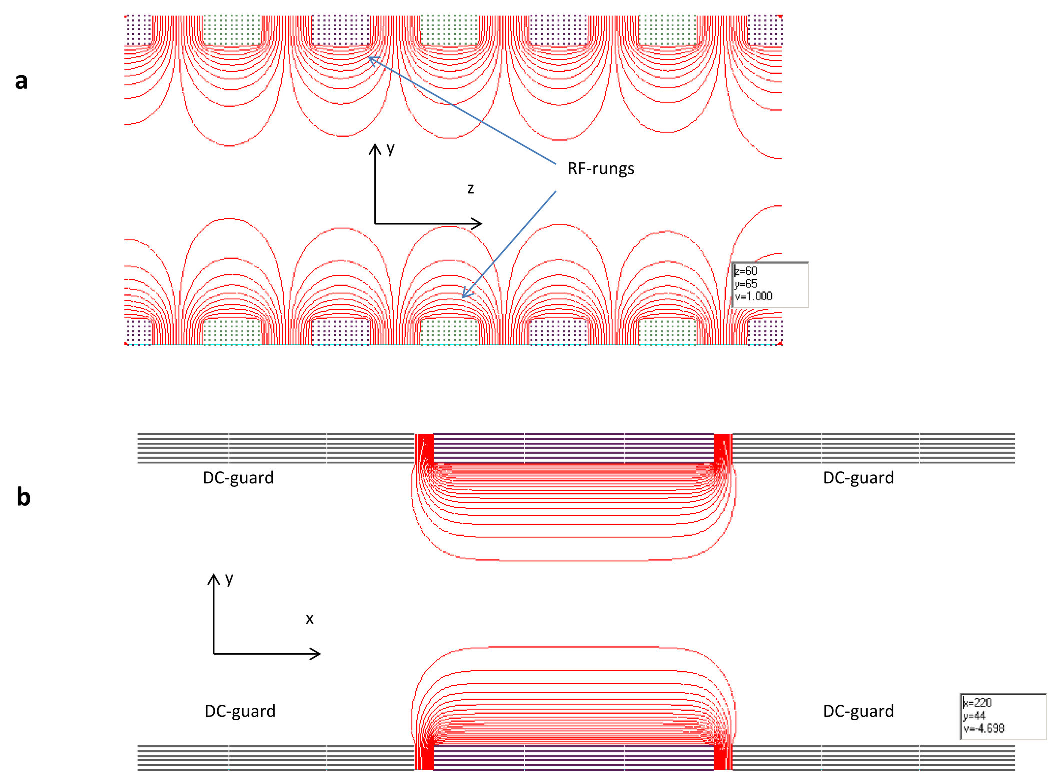

Fig. 2. Equipotential contours representing distribution of the RF field.
(a) cross section along YZ plane of symmetry.
(b) transverse cross section, XY plane.

The RF field distribution between the two SLIM surfaces shows intense electric fields in areas close to rungs; at the plane of symmetry in the center the field intensity is reduced, forming a nearly field-free region. The transverse cross section, Figure 2b, shows a uniform X-distribution in the center region. Such a distribution produces effective potential wells near the RF rung electrodes, and a nearly flat potential at mid-plane. The guard DC offset constrains the ion motion in the X dimension and focuses ions in the central region.

Optimal Dimensions

Two example geometries are considered in Fig. 3, showing the DC potential as a function of X for a guard DC offset of 10 V. A wider gap between the surfaces (5.7 mm) leads to an increased penetration of the DC potential to the center, ~2.5 V at the minimum. In the case of a narrow gap (2.7 mm,) the central DC potential is reduced to ~0.45 V. The smaller penetration for the narrower gap results in weaker ion focusing in the transversal directions, i.e., a wider area around the center that can be occupied by ions.

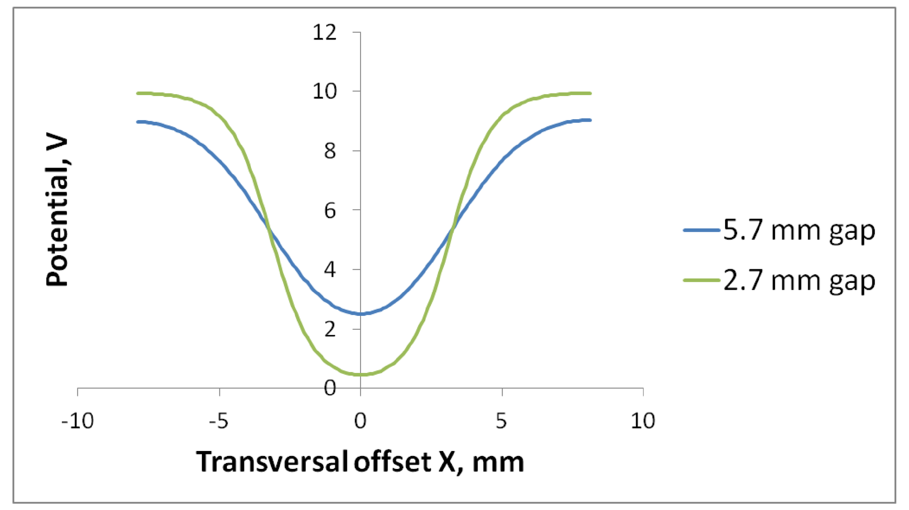

Fig. 3. SLIM width and gap dimensions optimization. DC potential profiles for rungs 5.3 mm wide, comparison for 2.7 mm and 5.7 mm spacing between the two surfaces. The wider gap (5.7 mm) provides tighter focusing in the transverse dimension.

The ion density distribution is defined by combined action of the DC field from the guard electrodes and the effective RF focusing generated by the rungs. The profiles for $V_{eff} + V_{DC}$ as a function of the vertical coordinate (Y) can have a local maximum in the center (Y = 0). A pronounced local maximum is seen in the case of wider gap, 5.7 mm, in Fig. 4, blue; the "hump" is reduced for 4.2 mm gap (red), and completely removed in the case of narrow gap, 2.7 mm (green).

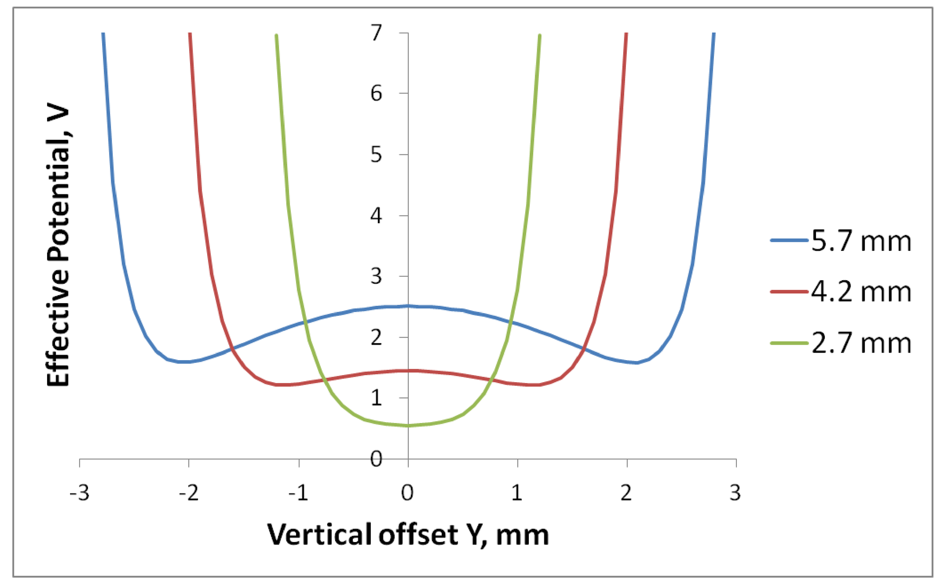

Fig. 4. SLIM effective potential in the vertical (Y) dimension, at the mid plane X = 0, for different inter-board spacings. RF 0.8 MHz, 100 V_{pp}, m/z 1000.

Ion Mobility Spectrometer Based on SLIM

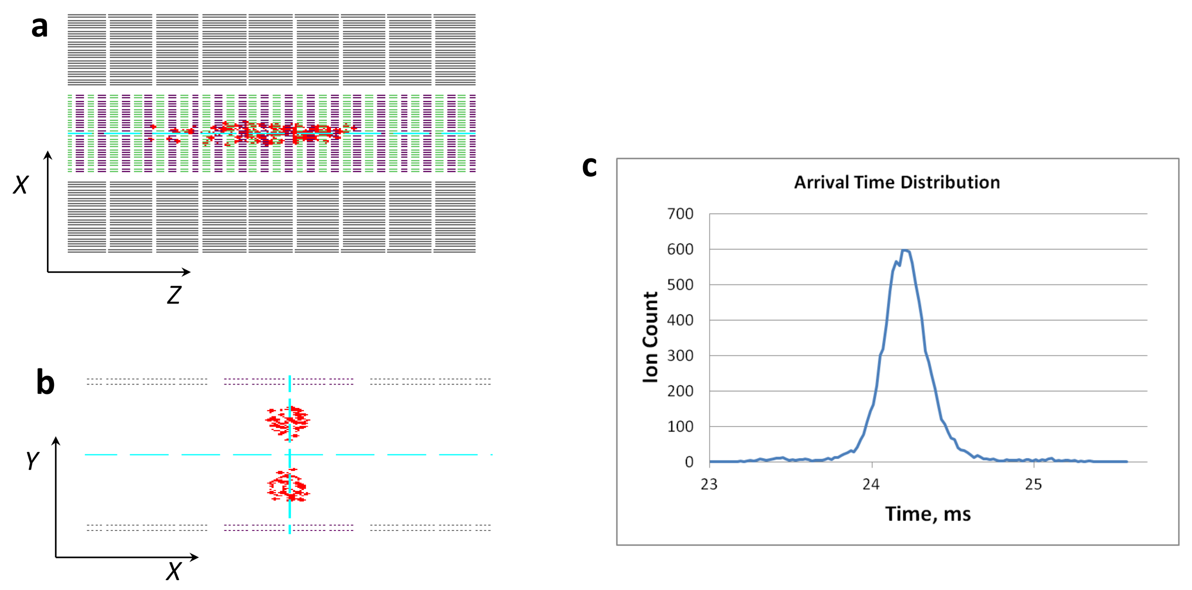

Fig. 5. Modeling results for a straight section SLIM component configured as an ion mobility spectrometer: (a) ion density in the *XZ* planar projection; (b) vertical *XY* cross section Ion density distribution; (c) arrival time distribution.

A computer model has been implemented to analyze the ion density distribution. Ions form into two elongated packets, each occupying a local Y-potential well. The ion density distribution along Z-axis takes the form of a Gaussian having the exponential width defined by diffusion. The vertical split is orthogonal to the ion drift, and does not affect the Gaussian arrival time distribution.

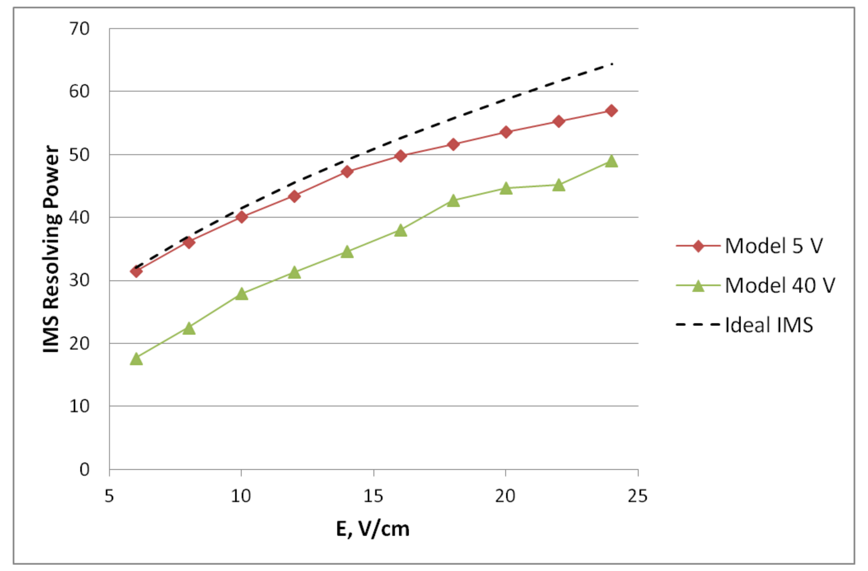

Fig. 6. Ion mobility resolving power as a function of electric field intensity: (diamonds) model, guard offset 5V, (triangles) model, guard offset 40 V, and (dashed) theoretical for an ideal IMS drift tube.

IMS resolving power modeling results. For the lower offset, 5 V, modeling results approach the theoretical IMS resolving power for low Z-electric fields, and trend lower for higher fields. With the guard offset increased to 40 V, the resolving power profile is lower than the theoretical across the range of electric fields, signifying an increased effect due to field irregularity.

Conclusions

- Ion confinement in SLIM is accomplished by a combination of the effective potential generated by the RF rung electrodes, and DC potential offset from the guard electrodes.
- RF rung electrode lengths shorter than the distance between surfaces creates a significant penetration of the guard DC potential into the central volume, a pre-condition for ion packet splitting into two volumes.
- Alternatively, geometries with smaller inter-surface gaps produce non-split ion packets, typically extending more in the transverse direction.
- Ion motion modeling supports lossless ion transmission.
- SLIM linear drift region components enable high quality ion mobility separations.
- Overall, the SLIM ion dynamics modeling studies are consistent with initial experimental observations, and support the potential robustness and versatility of these novel devices.

Acknowledgements

Portions of this research were supported by the NIH National Institute of General Medical Sciences (8 P41 GM103493-10), the U.S. Department of Energy (DOE) Office of Biological and Environmental Research (OBER) Pan-omics program at Pacific Northwest National Laboratory (PNNL) and performed in the Environmental Molecular Sciences Laboratory, a DOE OBER national scientific user facility on the PNNL campus. PNNL is a multiprogram national laboratory operated by Battelle for the DOE.AC05-76RL01830.

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