Compression Ratio Ion Mobility Programming in Structures for Lossless Ion Manipulations

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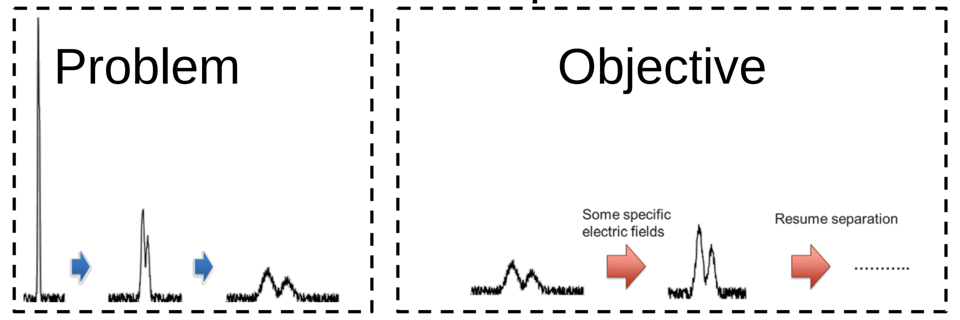
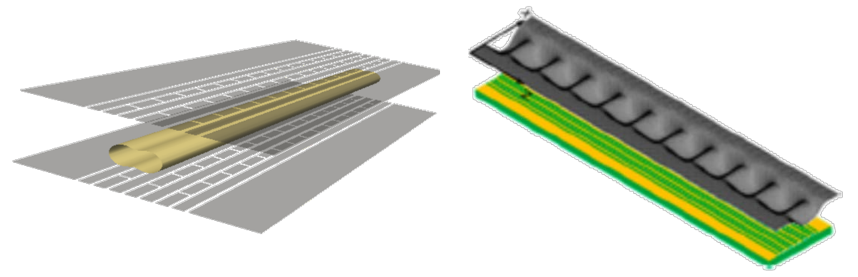
Overview

- IMS separates ions moving in an electric field over a given drift path.
- Structures for Lossless Ion Manipulations[1] (SLIM) allow very long drift paths, limited by diffusional peak broadening.
- We solve diffusional broadening to enable unlimited drift paths.



Introduction

- In SLIM, ions move within "traveling traps" created by rf and traveling wave (TW) potentials applied to electrodes patterned on surfaces.
- Serpentine ultra-long path with extended routing (SUPER) SLIM with multipass capability allows practically infinite IM drift length.[2]



- IMS peaks are defined by ions distributed in "N" TW traveling traps.[3]
- CRIMP uses this peak "quantization" to enable peak width reduction by integer ratios and enable high S/N with very long path lengths.

Methods

CRIMP Concept: Re-binning of an IMS peak

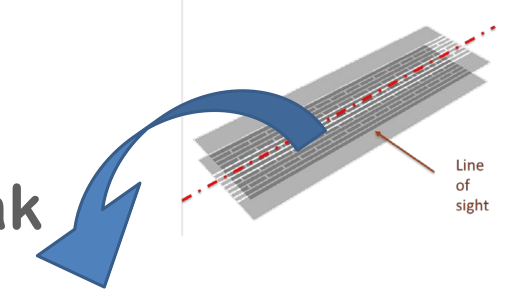
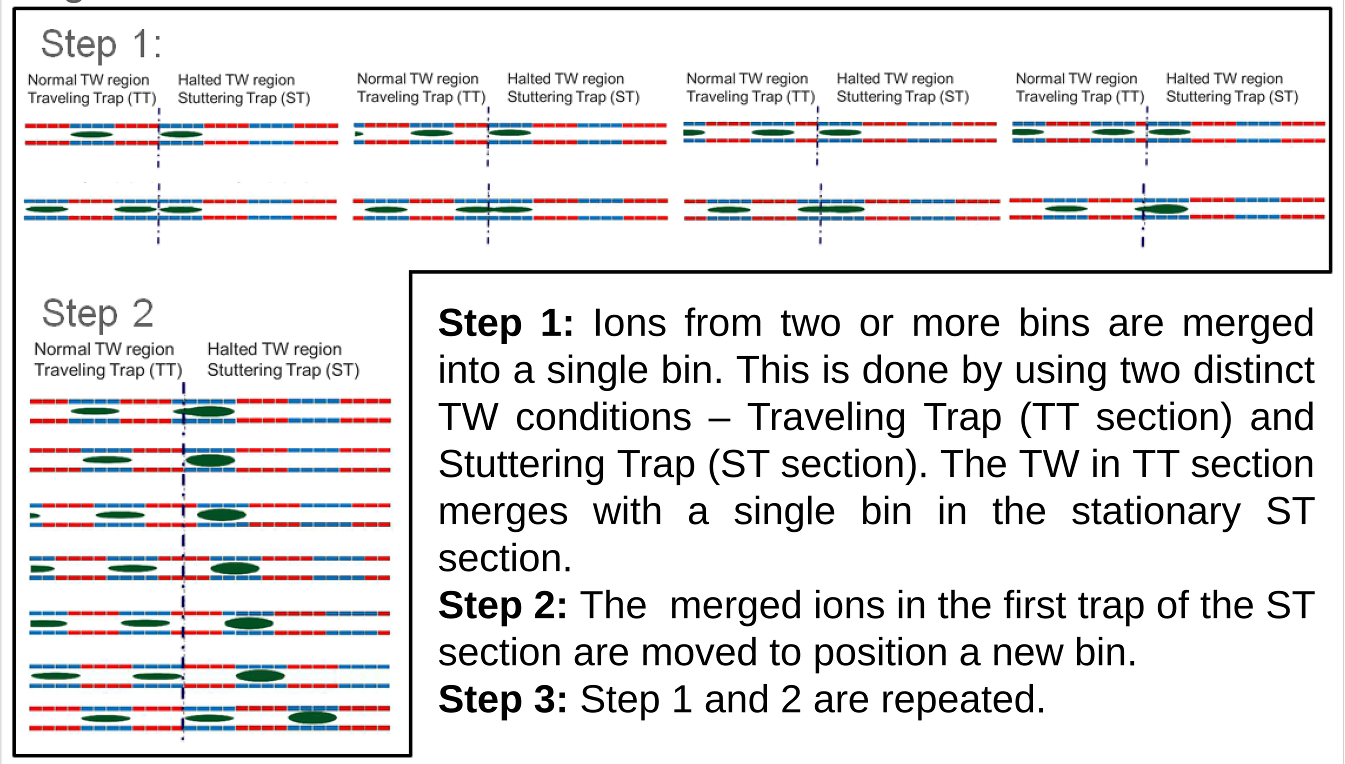


Figure 1



Step 1: Ions from two or more bins are merged into a single bin. This is done by using two distinct TW conditions – Traveling Trap (TT section) and Stuttering Trap (ST section). The TW in TT section merges with a single bin in the stationary ST section.
Step 2: The merged ions in the first trap of the ST section are moved to position a new bin.
Step 3: Step 1 and 2 are repeated.

Figure 2

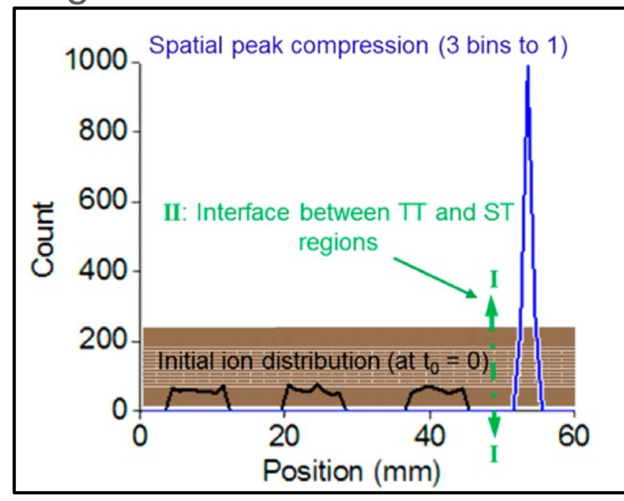


Figure 2. Simulation shows the merging of 3 "bins" from the TT section to a single "bin" in the ST section. The black traces represent initial ion distribution (in three TT). The blue trace represents the final ion distribution in a single ST after spatial compression using CRIMP.

Experimental Setup:

Figure 3

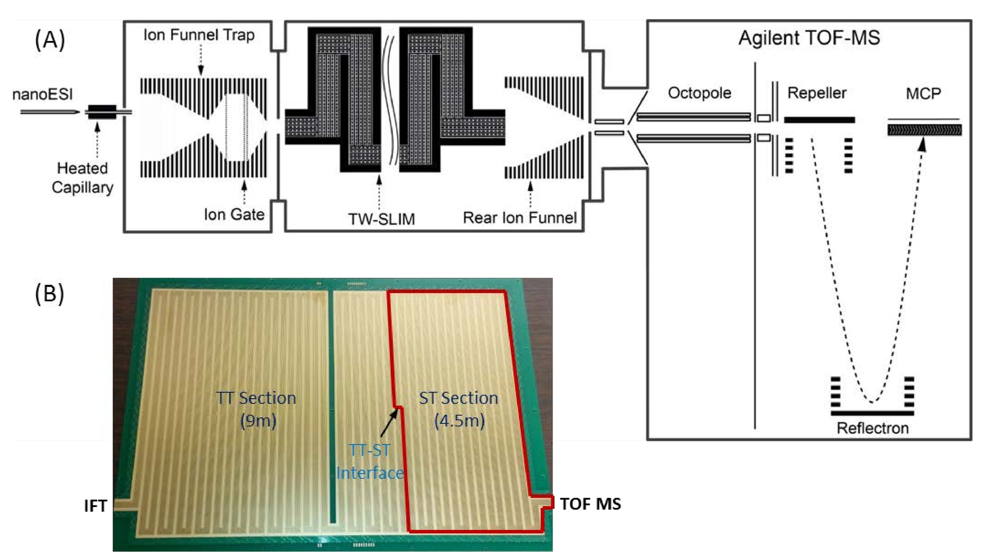


Figure 3. (A) Schematic of experimental setup. (B) One SLIM surface with 9 m of TT section and 4.5 m of ST section.

Results

Temporal Peak Compression (an example):

Figure 4

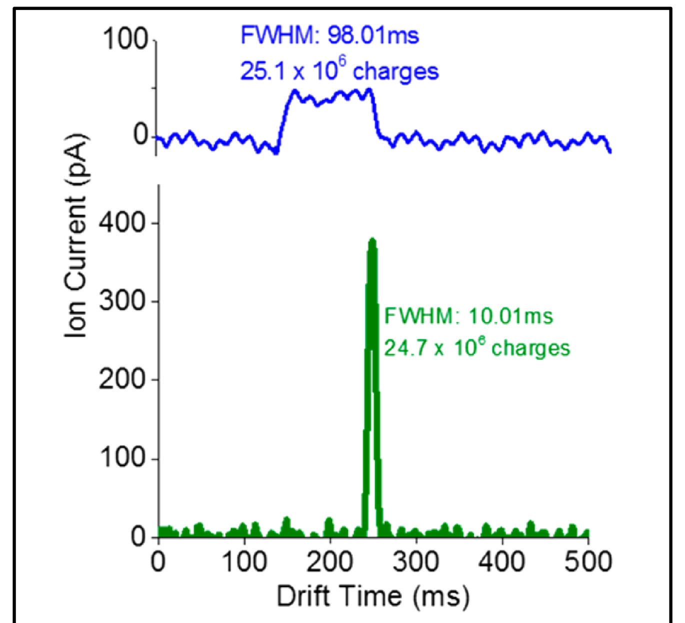
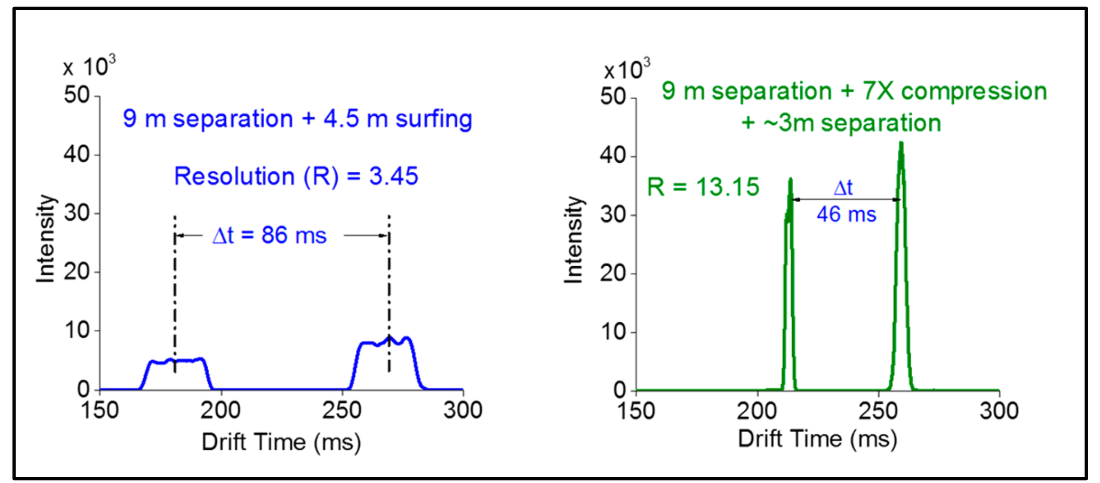


Figure 4. (Top) Injected ion packet. (Bottom) Compressed ion packet

- Ions injected into the TT region from the ion funnel trap (IFT) are transported through the SLIM in the "surfing" mode. The ions remain in their respective TTs.
- Blue trace in Figure 4 shows a 100 ms injected ion plume after traveling through the 13 m SLIM device.
- Compression Ratio is defined as CR = $\frac{\text{number of TT bins occupied before compression}}{\text{number of ST bins occupied after compression}}$
- Effects of compression on peak (with an initial temporal width T, TW speed *s*, width of a single bin x_w):
  number of bins spanned by peak after compression: $N_{\text{compressed}} = \left\lfloor \frac{1}{\text{CR}} \left\lfloor \frac{s}{x_w} T \right\rfloor \right\rfloor$
  temporal width after compression: $T_{\text{compressed}} = \frac{x_w}{s} \left\lfloor \frac{1}{\text{CR}} \left\lfloor \frac{s}{x_w} T \right\rfloor \right\rfloor$
- Once peak re-binning is achieved as shown in Figure 1 and 2, the stuttering wave in ST region is reverted to a normal TW to "lock-in" the spatial compression in temporal domain as well.
- CR = 10 used at the TT/ST interface to reduce the injected peak width from 100 ms to 10 ms

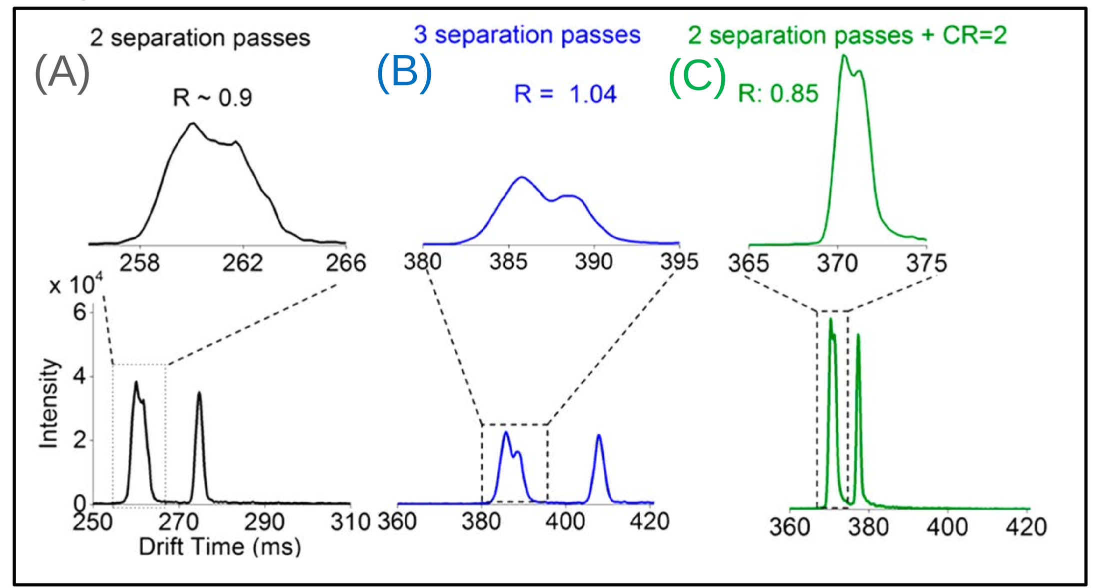
CRIMP with IM separations:

Figure 5



- Figure 5. (Blue traces): Two species of Agilent Tune Mix (m/z 622, K_o 1.17cm^2/Vs and m/z 922, K_o 0.97 cm^2/Vs) are injected as a 25 ms packet using IFT and separated in the first TT section (9 m). The ST region operated purely in "surfing" mode to lock the 9 m separation that was recorded.
- Figure 5 (Green traces): After 9 m separation, at the TT/ST interface the separation is subjected to CR = 7. After the separated packet is compressed, the stuttering wave in ST is replaced with another normal TW to perform an additional ~3 m separation

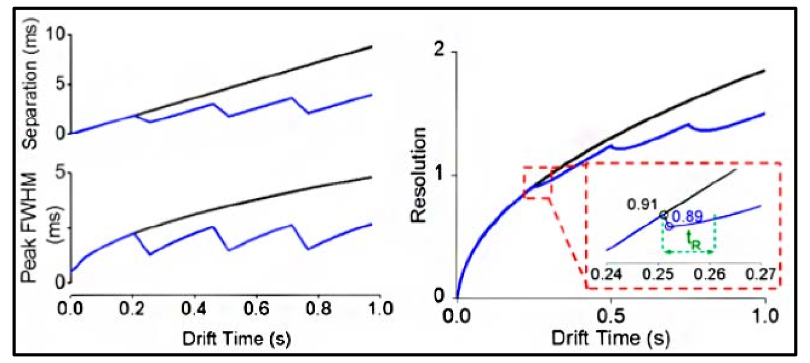
Figure 6



- Multi-pass capability of SLIM SUPER IM used to separate structurally similar isomers of human milk oligosaccharides.
- Figure 6A (Black traces): Lacto N-Hexose (LNH) and Lacto N-neohexaose (LNnH) after 2 passes through SLIM device (i.e. 26 m separation).
- Figure 6B (Blue traces): LNH and LNnH after 3 passes (39 m separation)
- Figure 6C (Green traces): LNH and LNnH after 26 m separation, followed by a CR = 2 and ions delivered to detector in the surfing mode.
- After CRIMP (as in 6C) the gain in the peak height can be used make practical more passes of separation.
- Any minor loss of resolution (0.9 to 0.85) due to CRIMP is quickly recovered

Results

Peak Resolution with CRIMP (Theory):



$$\Delta T_{\text{compressed}} = \frac{x_w}{s} \left\lfloor \frac{1}{\text{CR}} \left\lfloor \frac{s}{x_w} \Delta T \right\rfloor \right\rfloor$$

$$\langle t_{\text{fwhm}} \rangle_{\text{compressed}} = \frac{x_w}{s} \left\lceil \frac{1}{\text{CR}} \left\lceil \frac{s}{x_w} \langle t_{\text{fwhm}} \rangle \right\rceil \right\rceil$$

$$R_{\text{compressed}} \geq \frac{\left\lfloor \frac{1}{\text{CR}} \left\lfloor \frac{s}{x_w} \Delta T \right\rfloor \right\rfloor}{\left\lceil \frac{1}{\text{CR}} \left\lceil \frac{s}{x_w} \langle t_{\text{fwhm}} \rangle \right\rceil \right\rceil}$$

Conclusions

- TW-SLIM allow ions to be trapped within traveling traps, resulting in peak "quantization".
- IM peak "quantization" enables peak compression with integer compression ratios (CR).
- Any loss in IM resolution due to CRIMP can be recovered quickly by additional separation passes.
- CRIMP with SLIM SUPER TWIMS enables practically unlimited drift paths, overcoming diffusion.

Acknowledgements

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References

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2. Deng et al, 2016. "Ultra-High Resolution Ion Mobility Separations Utilizing Traveling Waves in a 13-m Serpentine Path Length Structures for Lossless Ion Manipulations Module." Analytical Chemistry 88(18), Analytical Chemistry
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Career Opportunities: For potential openings in Integrative Omics Group at PNNL please visit http://omics.pnl.gov/careers

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