Reflectron Time-of-Flight Mass Spectrometer with Improved Convergence of an Ion Beam*

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Introduction

Time-of-flight mass spectrometry (TOF-MS) is widely employed for mass analysis of various ion species as it enables us to **measure their mass spectra in a wide mass range instantaneously**.

As it is often supposed that analyte **ions are generated in a small volume** in the ion-extraction region, its performance is not optimized for ions spread over a large volume.

It should be noted for reflectron TOF-MS that **an ion reflector itself causes diverging ion trajectories**. In a conventional RTOF-MS, the electric field created in an ion reflector has a cylindrical symmetry where the symmetry axis is tilted to guide the ion beam to an ion detector. As faster ions penetrate deeper in the ion reflector than slower ones, the ions arrive at different positions on the ion detector. Therefore, ions spread over a large volume in the first extraction field could reach even out of the detector, as illustrated in Figure 1, due to their significantly dispersed kinetic energies.

Trajectory simulation of a conventional RTOF-MS

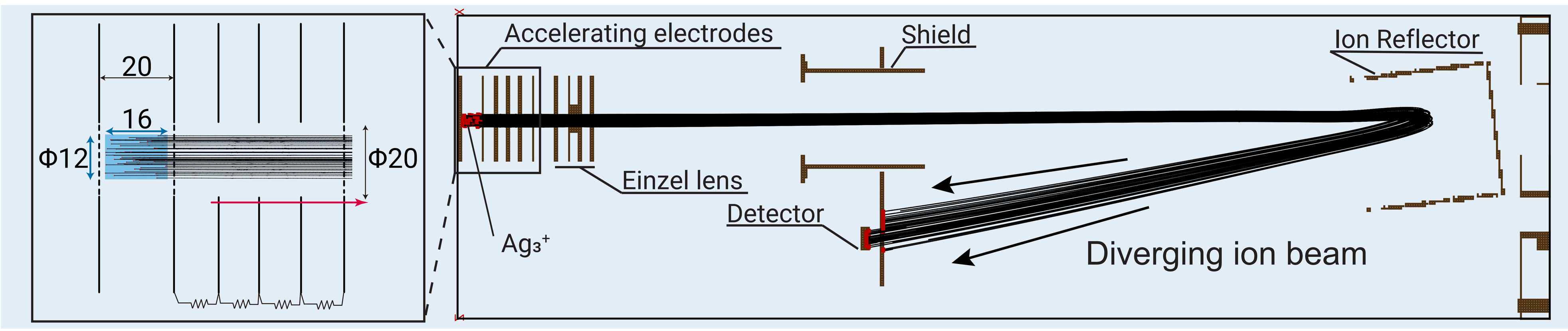

Fig. 1 Ion trajectory simulation of **a conventional RTOF-MS**. When the volume of the ions in the acceleration region is large, the **detection efficiency** is degraded as well as **mass resolution**.

In this work, we develop a new RTOF-MS that improves convergence of ion beams to overcome the problem mentioned above.

Design

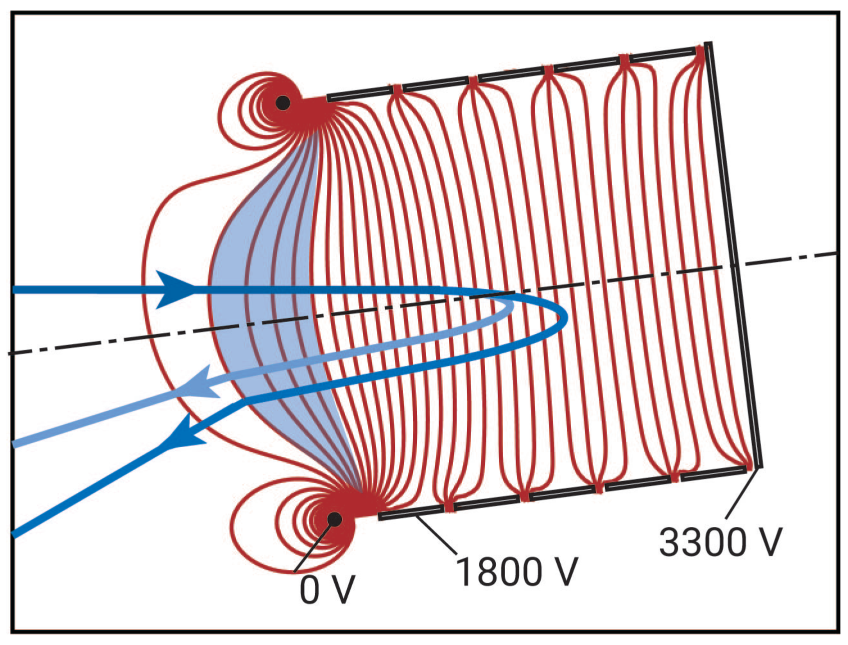

Fig. 2 Mechanism of ion-beam divergence in a conventional RTOF-MS. **The electric-field gradient in front of the reflectron causes the ion beam to be dispersed** by kinetic energy difference when the ion-beam path deviates from the cylindrical symmetry axis of the reflectron.

If the ion beam passes along the axis of the cylindrical symmetry, the electric-field gradient causes convergence of the ion beam upon exiting the reflectron.

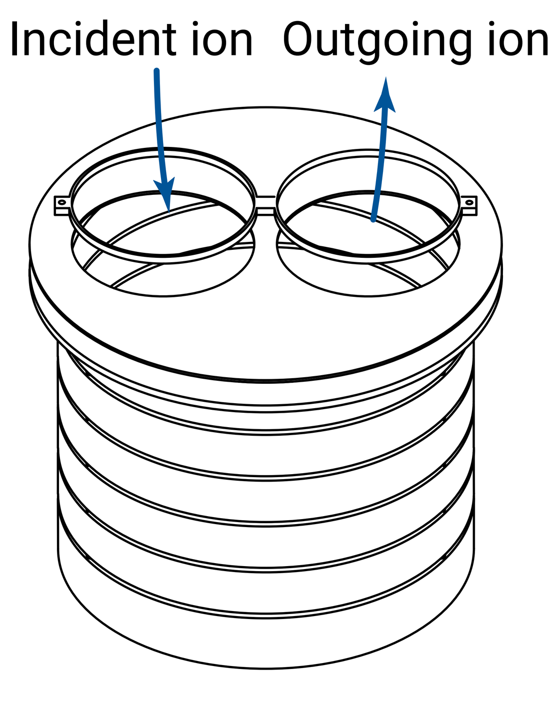

Fig. 3 Design of a new ion reflector.

We designed a new ion reflector equipped with two ion lenses both for incoming and for outgoing ions, as shown in Fig. 3. **The ion trajectory through the center of the lenses leads to convergence of the ion beam.**

Trajectory simulation of a new RTOF-MS

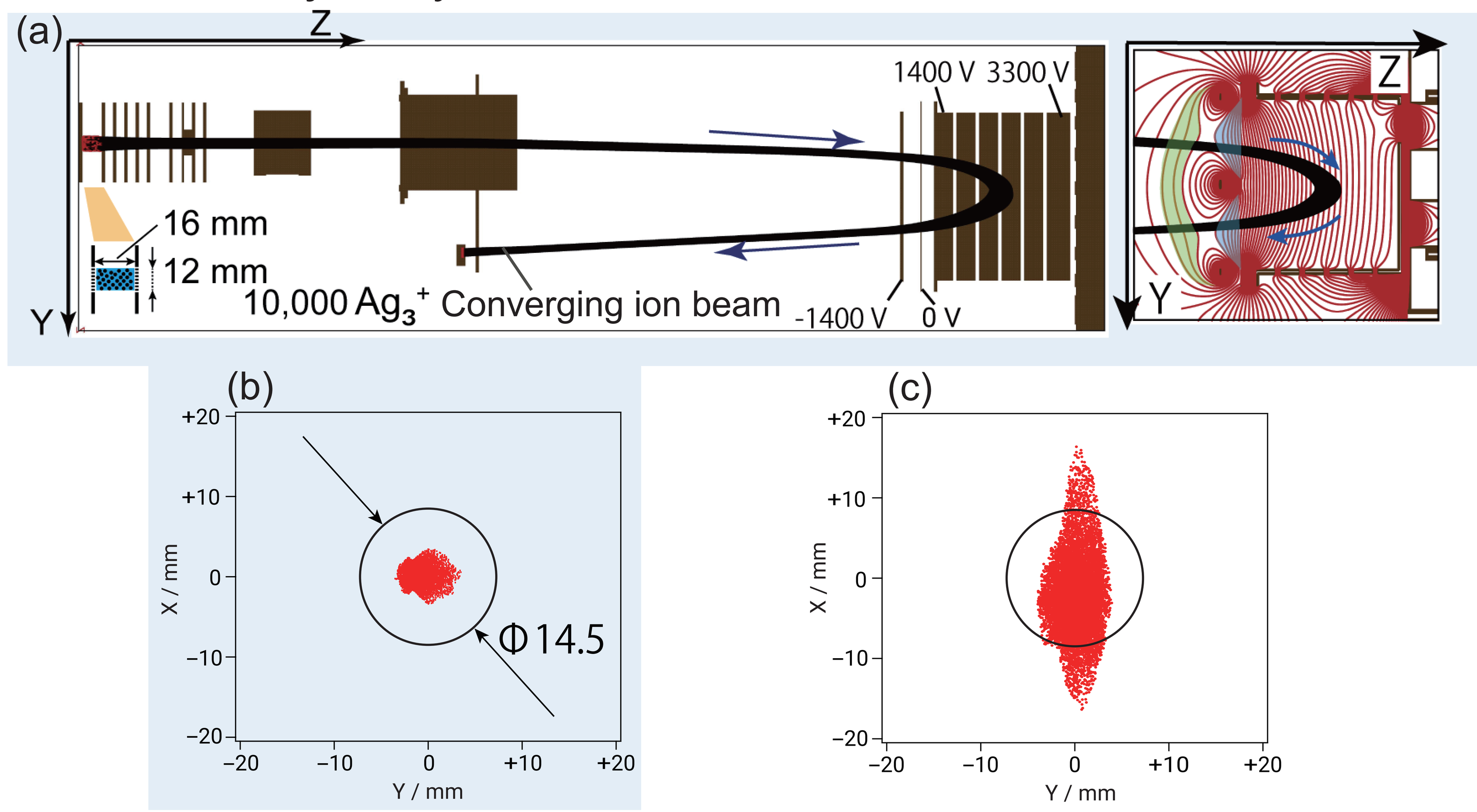

Fig. 4 (a) An ion trajectory simulation of RTOF-MS using a new ion reflector. **All the ions reach the ion detector** without diverging after reflection. The sectional view of the equipotential surfaces displays that the ion beam converges by the electric field gradient in front of the reflectron because it passes through the center of the lenses. (b,c) 2D profiles of ions on the MCP detector for dfferent reflectors. (b) **Original design of an ion reflector mounting a lens with 65 mm apertures.** All the ions successfully converge on the detector with an effective diameter of 14.5 mm. (c) Without eyeglasses-frame lens, ions are significantly diverged in the X direction. Both the two apertures and eyeglasses-frame electrode are thus essential to guide all the ions to the detector.

Manufacture

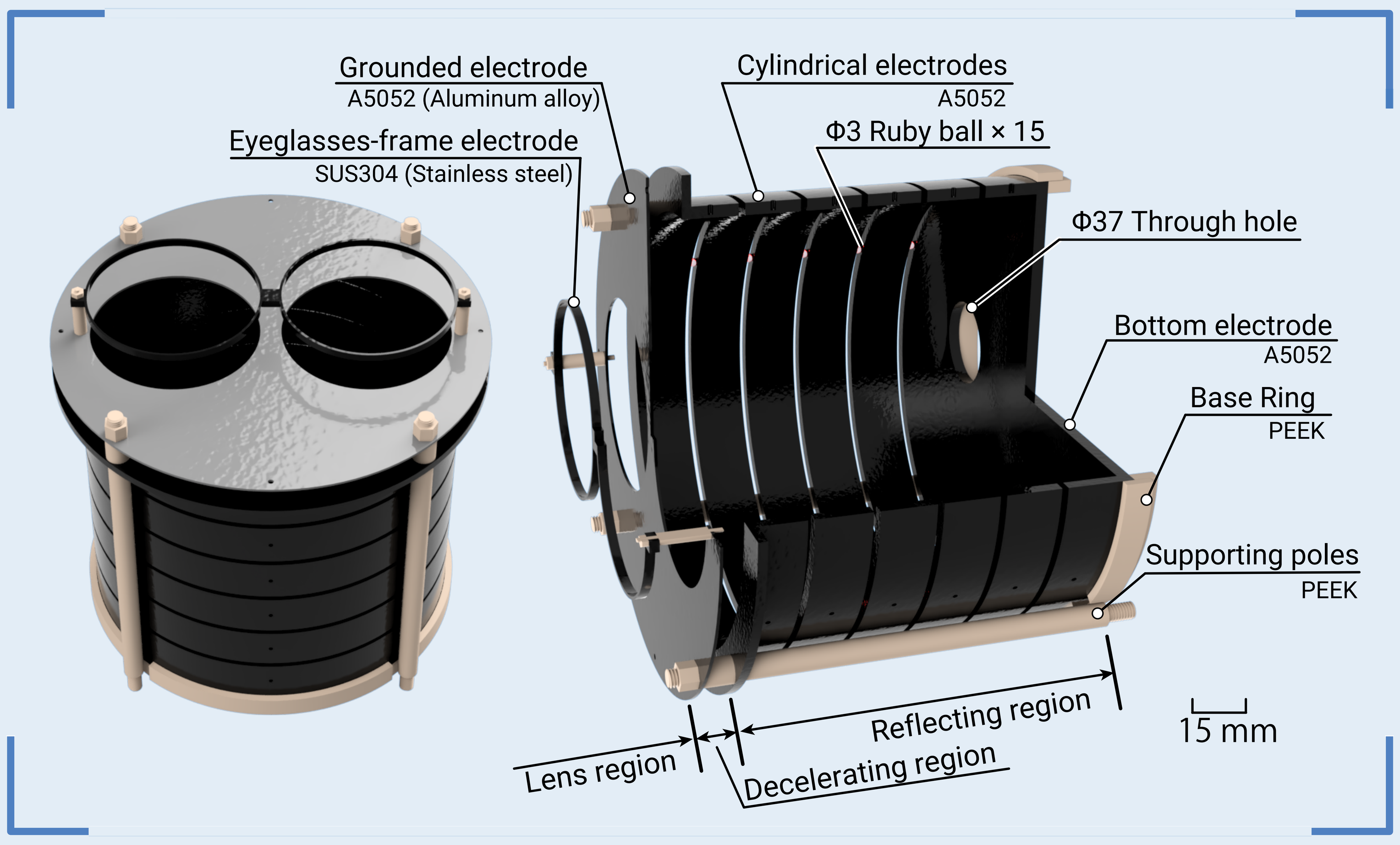

Fig. 5 Rendered views of the new ion reflector which was fabricated based on the results of simulation.

Main features of the new ion reflector

- An eyeglasses-frame electrode (extracting electrode) and a grounded electrode with two apertures (Φ65 mm) play important roles **in ion beam convergence**.
- **The electrodes are made of aluminum**, except for the eyeglasses-frame electrode, to reduce the total weight less than 800 g.
- The reflector electrodes are wired by a series of 10 MΩ resisters. Ruby balls (Φ3 mm) are used for insulators.
- The Φ37 through hole on the bottom electrode serves as a window for irradiation of laser or soft X-ray.

Experiments

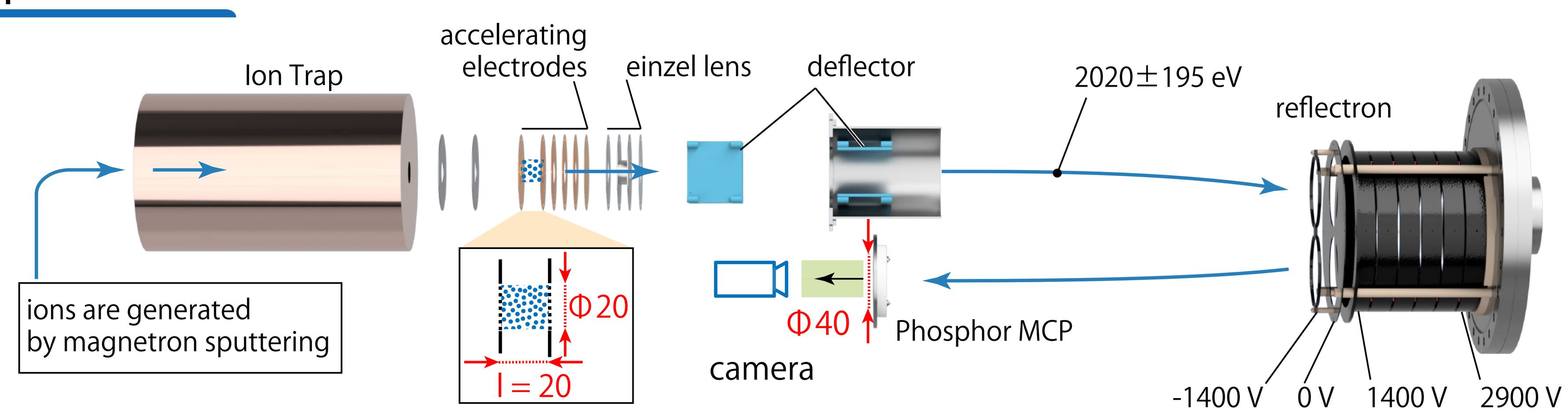

Fig. 6 Experimental setup.

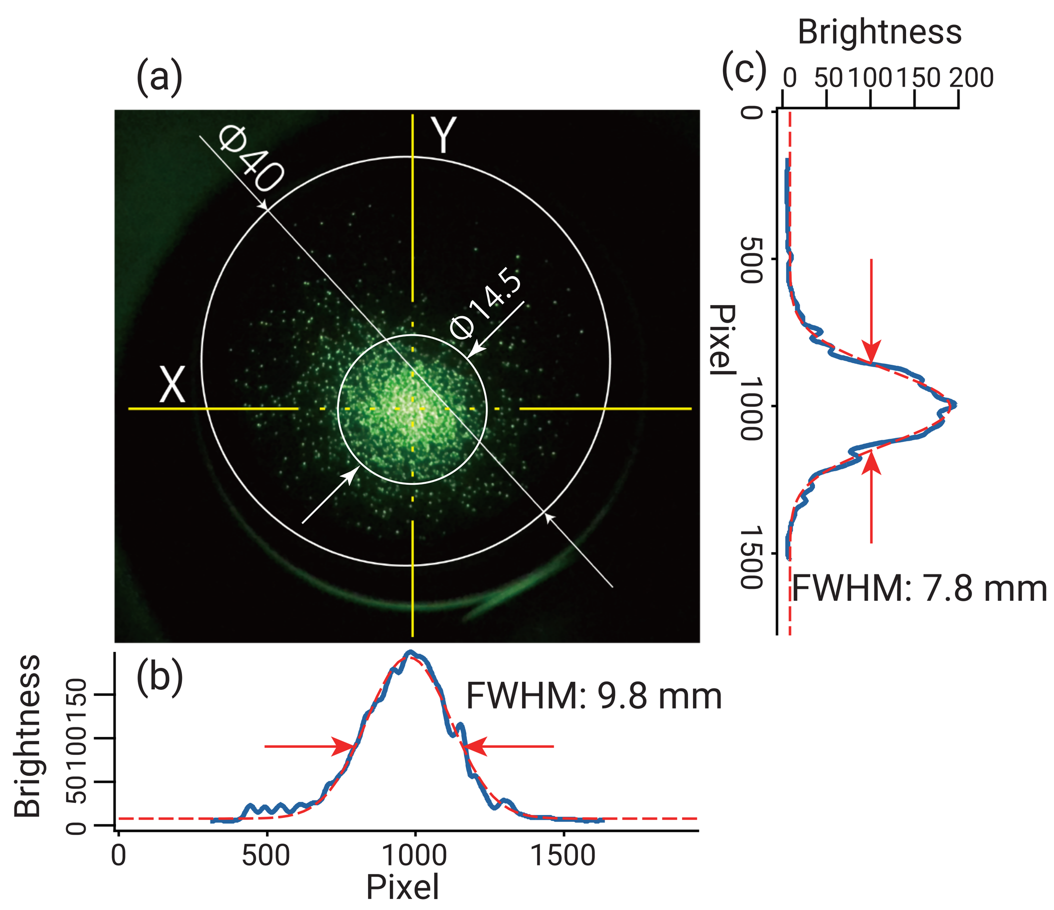

Fig. 7 (a) An image of Ag_3^+ spatial distribution measured using a MCP coupled with a phosphor screen (effective diameter = Φ40 mm) and a CMOS camera. (b)&(c) Intensity profiles along the X and Y axes, respectively. **The ions are successfully converged within the diameter of the fast-response MCP(ϕ14.5).**

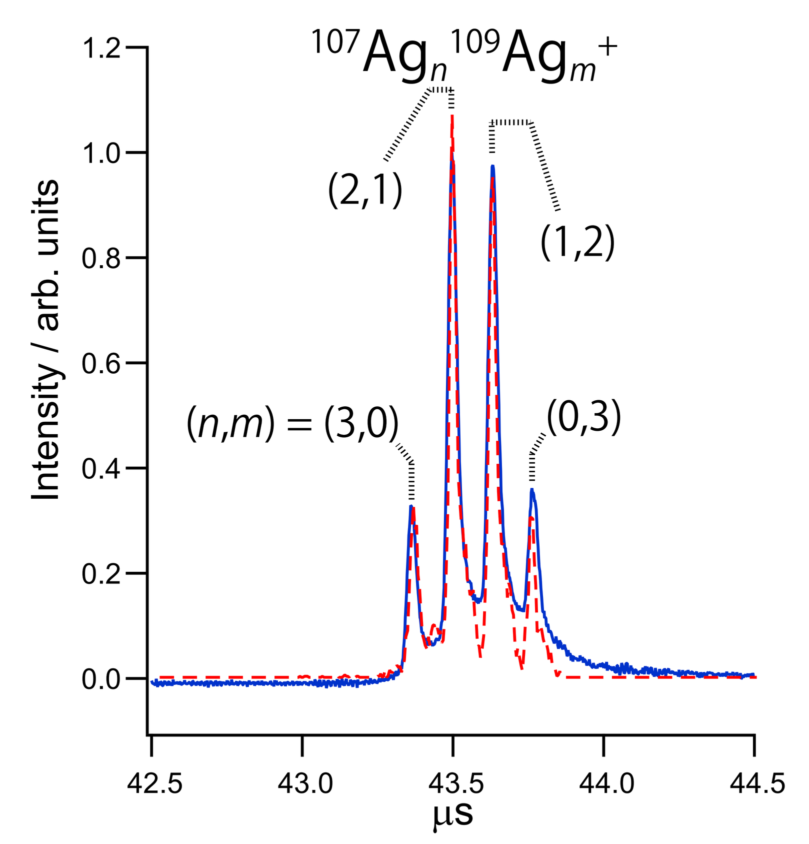

Fig. 8 The measured (blue solid line) and simulated (red dotted line) TOF spectra of Ag_3^+. The peaks are sufficiently sharp to observe Ag_3^+ isotopologues separately. **The mass resolving power is estimated to be $M/\Delta M$ ≒ 600**. The good agreement between the observed and simulated TOF spectra indicates that the new RTOF-MS works as designed.

Summary

- Based on extensive ion trajectory simulations, we have designed **a new RTOF-MS that exhibits improved convergence of an ion beam.**
- We experimentally confirmed the improved performance, where **the ion beam diameter at the detector was measured to be 9 mm in FWHM** for ions initially distributed in the volume of Φ20 mm diameter ×20 mm long in the accelerating region.
- Our new RTOF-MS has a **mass resolving power of $M/\Delta M$ ≒ 600 at M = 323**, which enables efficient measurements of TOF mass spectra for various ion species that spread over a large volume in the accelerating region.

Acknowledgements

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Reference

T.Handa et al., Int. J. Mass. Spectrom. 451, 116311 (2020).