Optimization of a Dual In-Vacuum Ionization Source using Ion Optics Simulations

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INTRODUCTION

A high transmission ion optical system designed to incorporate a triple filament thermal ionization (TI) source and an electron ionization (EI) source coupled to an orthogonal Time-of-Flight mass analyzer is optimized using ion optics simulations. The TI source is in linear alignment with the ion optical axis of the ion beam sampled by the oTOF mass analyzer, while the EI source is mounted at right angles through a DC quadrupole lens used to deflect ions by 90 degrees. The ion optical system of the dual ionization source is designed and optimized to deliver space-velocity correlated ion beams, which are characterized by low turn-around time necessary for high resolution TOF mass spectrometry.

METHODS

Infrared optical pyrometry was performed on rhenium filaments and temperature gradients were monitored as a function of heating current. The non-contact infrared thermometer used for conducting the temperature measurements was a Minolta/Land instrument equipped with a a silicon photocell having a spectral response between 0.8 and 1.1 µm. Appropriate values for the emissivity of rhenium were used to adjust temperature readings. Experimentally determined temperature distributions are then used to modify the surface boundary of the potential array, thus allowing for an accurate simulation of the triple filament configuration. Optimization of the ion optical system was performed in SIMION™. Calculated potential arrays were further processed to incorporate the voltage gradient across the resistive filament and investigate the deflection ions experience during the early stages of their transport. Additional simulations were performed on the EI ion optical system.

RESULTS

Filament temperature distributions for the different heating currents are shown in Figure 1. Significant cooling of the filament is observed at the two supporting posts and the temperature difference relative to the center can be as high as 1000 K. At 5.0 A heating current the maximum temperature measured at the center is 2250 K. Figure 2 shows the voltage distribution across the filament calculated using pyrometric data and the following expression, $dV=-I\,(dl/A)\,\rho(T)$, where *dV* is the voltage drop that corresponds to a temperature drop across a filament length *dl*, *A* is the cross sectional area of the filament and $\rho(T)$ is rhenium resistivity dependence on temperature *T*.

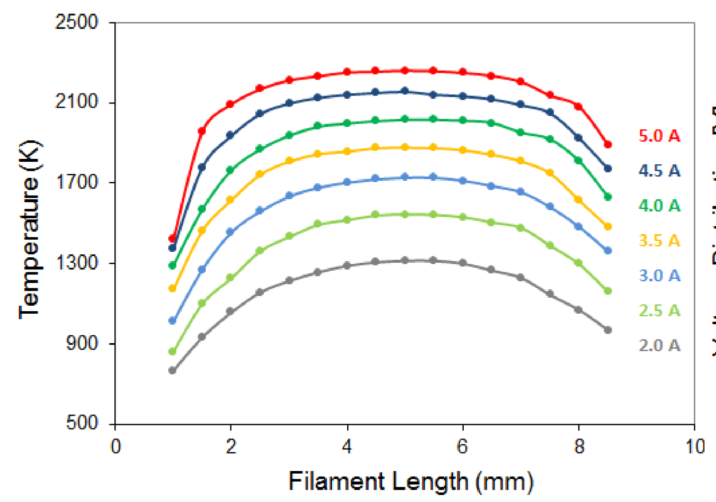

FIGURE 1. Filament temperature distributions as a function of current.

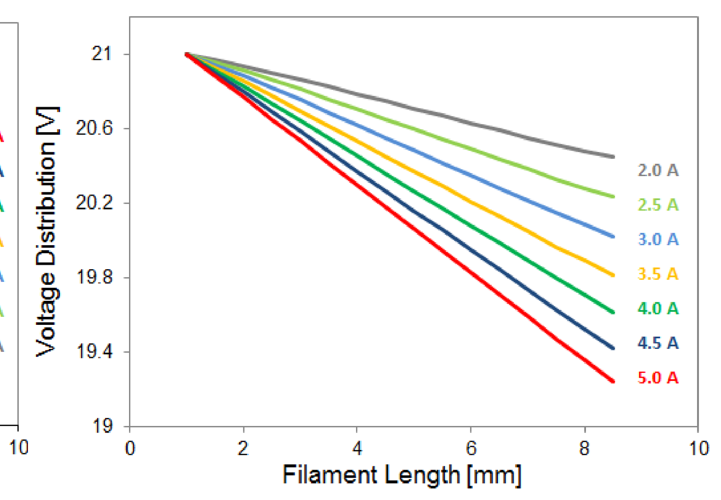

FIGURE 2. Corresponding voltage drop across the filament length.

A schematic diagram of the dual ionization source is shown in Figures 3 (a) and (b) in the XZ and YZ planes respectively. Ions generated in the TI and EI sources are directed through a high vacuum lens to control initial conditions for the TOF experiment.

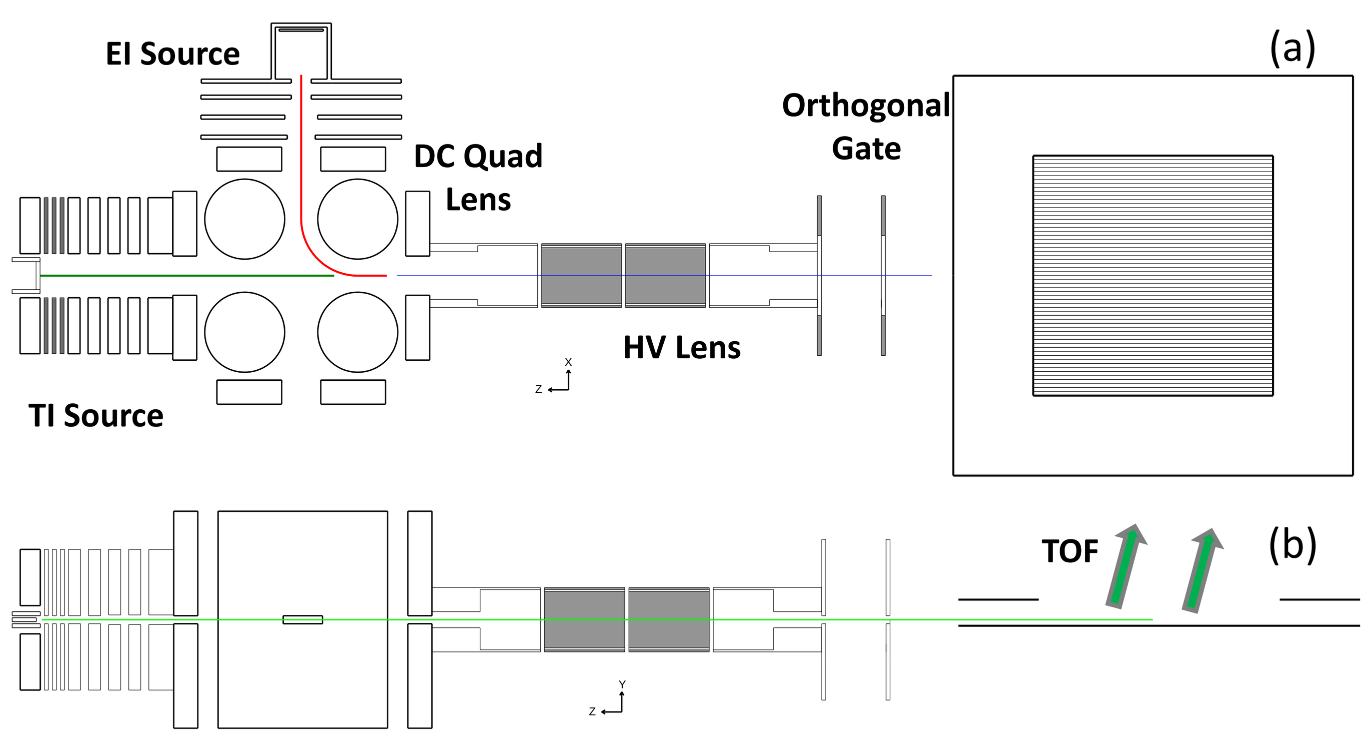

FIGURE 3. Schematic diagram of the dual ionization source in (a) XZ and (b) YZ planes comprising a TI source, a EI source, a DC quadrupole lens, a high-vacuum lens and the orthogonal acceleration gate for TOF mass analysis.

The triple filament configuration is employed in TI mass spectrometry to enhance ionization efficiency for species with ionization potentials greater than the work function of the polycrystalline substrate. The central filament is maintained at a lower temperature to control evaporation rate while side filaments operate at high temperature to promote ionization. Temperature gradients and related fringe fields near the filament have a strong influence on ion transmission. Ion optical solutions are found for the cases were the voltage gradient of the two high temperature filaments is in the same as well as in opposite directions, and results are shown in Figures 4 (a) and (b) respectively.

A collimated low voltage ion beam is produced by forming consecutive lenses across the electrode stack and generating multiple focal points in the transverse direction. Stray ion trajectories are associated with fringe fields near the filament and the effect can minimized by increasing the intensity of the surrounding electric field. However, the magnitude of the acceleration is limited by the defocusing action imparted to the ions during deceleration further downstream. Figure 5 shows the axial profiles for the two solutions discussed with reference to Figures 4 (a) and (b).

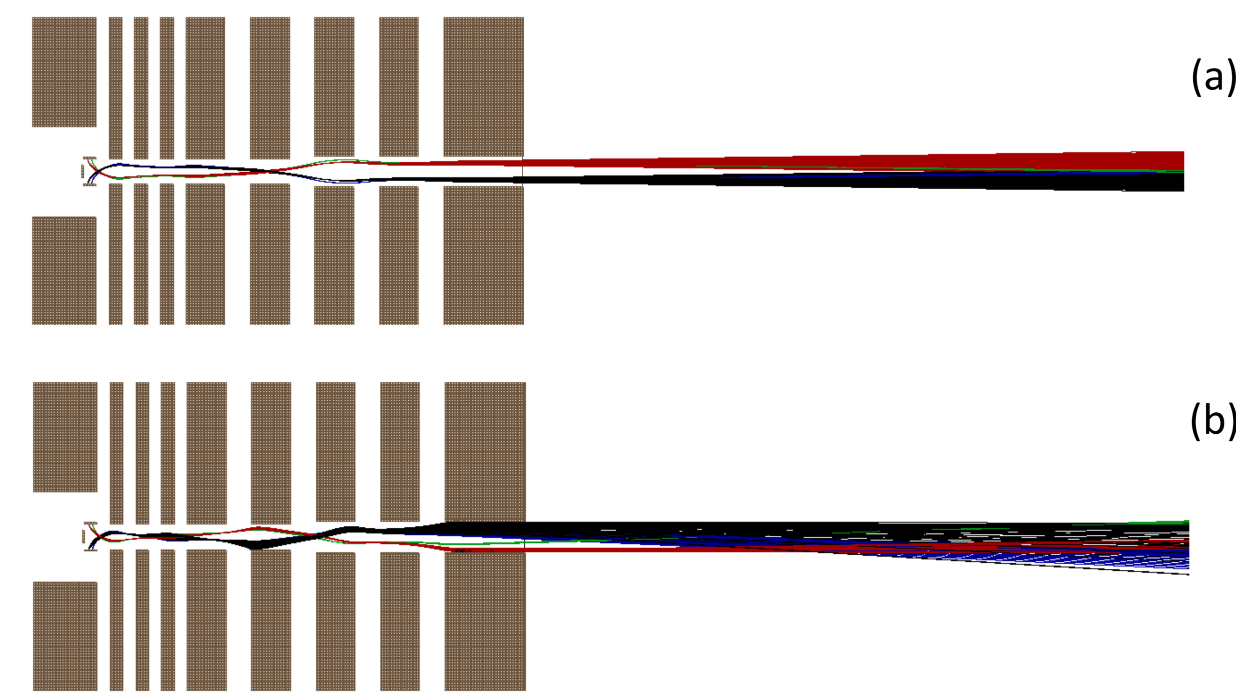

FIGURE 4. Ion trajectories for the triple filament TI source configuration with (a) parallel-direction and (b) counter-direction side filament heating currents .

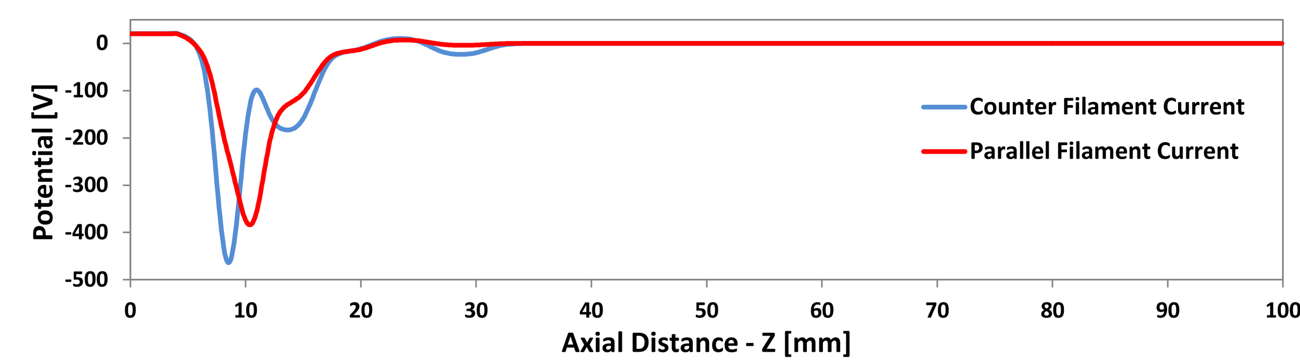

FIGURE 5. Axial voltage distributions for ion optical solutions shown in Figure 4.

Results obtained with the EI source are also presented. The EI ion optical model incorporates a series of consecutive electrodes to focus ions emitted from the source at the entrance of the DC quadrupole lens. The latter is designed for 90 degree deflection in order to align the ion beam relative to the ion optical axis sampled by the oTOF mass analyzer. The ion optical design can be used to sample ions either from the TI source or the EI source independently by switching the voltages applied to the DC quadrupole lens. A 3D model of the EI source, the DC quadrupole lens and ion trajectories are shown in Figures 6 (a) and (b) respectively.

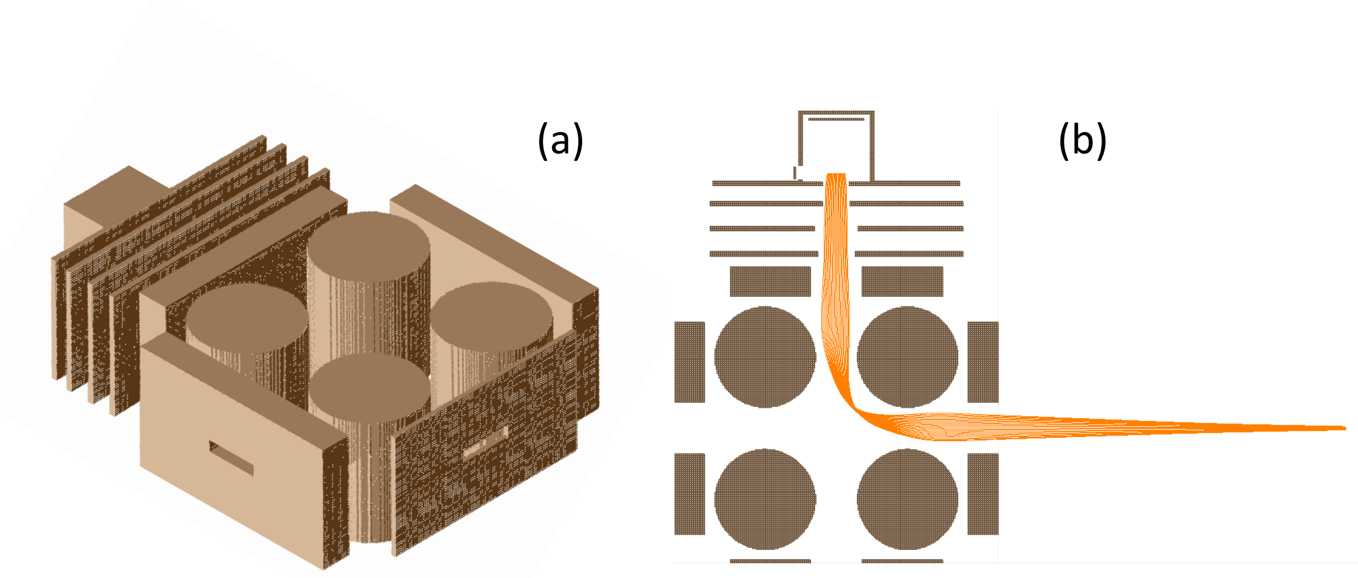

FIGURE 6. 3D model (a) and ion trajectories (b) for the EI source coupled to the DC quadrupole lens.

An additional lens is employed to focus ions into the orthogonal gate of the oTOF mass analyzer and control the extent of space-velocity correlation. An estimation of the turn-around time and the mass resolving power of the TOF system can be made by monitoring phase space distributions at the exit of the HV lens.

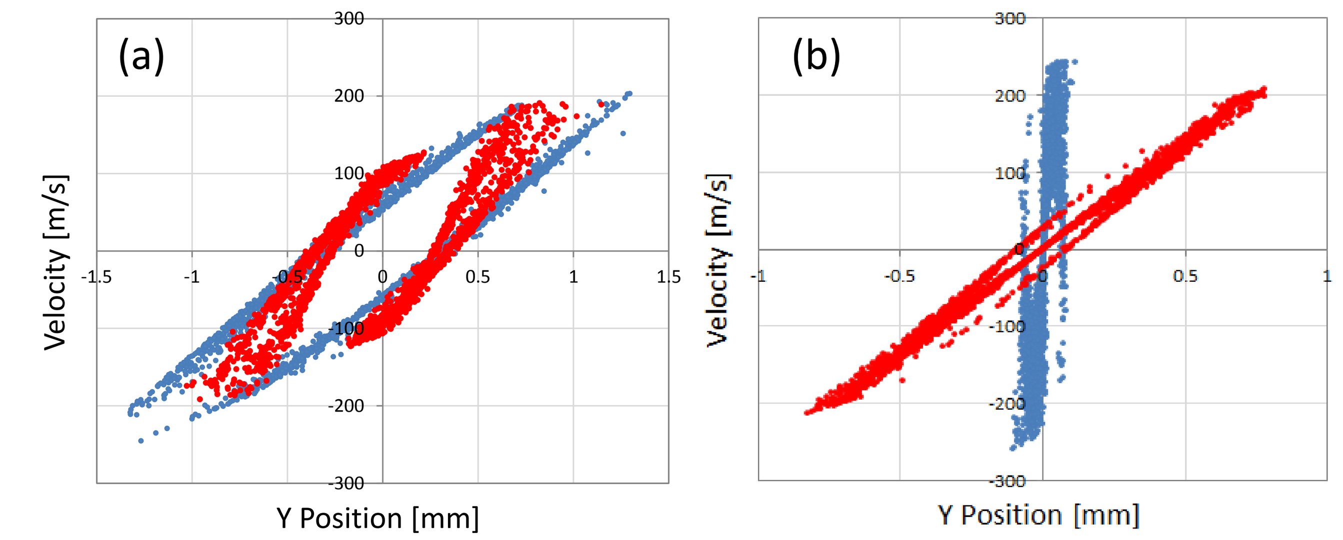

FIGURE 7. Phase space distributions (Y, Vy) for m/z=100 obtained with the (a) TI source and the (b) EI source.

For the triple filament TI source configuration and 50 V/mm acceleration field applied for the TOF experiment, turn around time is reduced from 4.5 ns to 3.3 ns by stretching phase space in Y and reducing maximum velocity from 110 m/s to 80 m/s respectively. The correlated phase space distribution produced by the EI source has a pronounced effect on the turn around time where time spread is reduced from 10 ns to less than 2 ns.

CONCLUSIONS

The design of a dual ionization source coupled to an orthogonal TOF mass analyzer is presented using ion optical simulations. The effect of the voltage gradient on the filament employed for ionization is critical and unless accounted for in the ion optical model can lead to significantly attenuated ion transmission. The EI source optics are coupled through a DC quad lens to the oTOF system. Ion optics are designed to produce correlated phase space distributions and reduce the effect of turn around time on the final time spread of the ions.