Numerical Study of Ion Behaviors in Radiofrequency Quadrupole Mass Spectrometers

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Abstract

In recent years, mass spectrometers have become an indispensable instrument for identifying substances from their mass data in a wide variety of scientific research fields. Quadrupole mass spectrometers (QMS), which are categorized into radiofrequency quadrupole mass filters (RF-QMF) and quadrupole ion trap mass spectrometers (ITMS), have widespread use due to their versatility, compact size and comparatively low costs. However, the performance of RF-QMF and ITMS is, at present, inferior to that of other mass spectrometers. Performance items such as mass resolution, mass accuracy and sensitivity, which need to be improved, are related to many parameters, *e.g.* three-dimensional electrode structure, voltages applied to the electrodes, pressure of neutral buffer gas, mass analysis scanning method, *etc.*

To clarify the influences of such parameters on the performance, we have developed a new simulation program PISA-QMS to trace ion motions numerically during any process in mass spectroscopy, *e.g.* injecting ions, scanning to obtain a mass spectrum and ejecting ions, by calculating the three-dimensional electric field formed within actual shaped electrodes. The features of PISA-QMS are as follows.

(1) For the electric field calculation, the boundary element method (BEM) is modified so that the interpolative functions are definable for each element. Since all boundary values are solved by inputting DC unit values of ± 1 for the potential values on the electrode elements, ion motions are computed by calculating the electric field by multiplying the absolute RF voltage values by the fractional potential. This modified BEM ensures the electric field within the actual shaped electrodes is calculated with a very low numerical error (about 0.01%) without expansion of computational memory and time. Moreover, for ITMS, the electric field formed by the actual shaped electrodes can be expanded in multipole terms to investigate the influence of the

multipole fields which are closely related to the ITMS performance.

(2) Ion trajectories are calculated using the Shanks method with fairly high accuracy for the least number of electric field calculation times. The Shanks method is adopted in PISA-QMS, as the integration method for the equation of ion motion in the RF-QMF.

(3) The presence of buffer gas and space charge is unique to the ITMS. As an ion - buffer gas interaction, a viscous model is adopted in which damping force on the ion is proportional to its velocity while the ions are moving among the rarefied gas atoms in the state of thermal equilibrium. For a space charge model, the Coulomb force is generated by a virtual sphere at the center of the ITMS, in which charges are distributed uniformly.

We have applied PISA-QMS to RF-QMF and ITMS. Several new aspects of the correlations between their performance and the related factors were investigated. According to the results, some advanced methods were proposed as shown briefly in the following.

(1) Ion trajectories at the entrance part of RF-QMF are simulated. The influence of the ion beam focusing position around the entrance on the ion transmission efficiency is investigated. From this, the optimum region of the focal position to enhance the transmission efficiency is found. In the case that ions are injected with higher energy of 100-200eV and decelerated at the entrance part, the mechanism how the transmission efficiency is determined is clarified.

(2) Ion trapping efficiencies are evaluated by calculating the trajectories of the ions injected into ITMS. The influence of injection timing on the RF phase, amplitude of the RF voltage and ion injection energies are clarified. A new advanced injection method, in which the RF voltage is scanned during the injection period, is proposed and its effectiveness is investigated.

(3) Mass spectra obtained by ITMS are simulated by calculating ion motions during the mass analysis scan. The relationships between the performance and the mass scanning method

conditions such as scan speed or resonance voltage are investigated. A new advanced scanning method, in which the scan speed is changed nonlinearly with time, is proposed and its feasibility is examined.

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