

Chapter 6

Summary

The numerical simulation program PISA-QMS has been developed for analysis of ion trajectories in a three-dimensional RF electric field in QMS, which is classified into RF-QMF and ITMS. PISA-QMS provides simulations of ion motions during any process in mass spectroscopy, *i.e.* injecting ions, scanning to obtain a mass spectrum, and ejecting ions, which were not possible previously due to the excessive computational time. In PISA-QMS, the electric field is calculated by the modified BEM for RF-QMF and the multipole expansion method for ITMS. The ion trajectories in the electric field are calculated with the Shanks method. The effect of buffering gas and space charge can also be included as simple interaction models in PISA-QMS. All these numerical methods or models are adopted in PISA-QMS to reduce the computational time, while maintaining a very low numerical error of 0.01%.

The applications of our new program PISA-QMS to RF-QMF and ITMS have revealed several new aspects of the correlations between their performances and related factors as described below.

(1) PISA-QMS was applied to simulate ion trajectories at the entrance of RF-QMF. Through investigation of the dependence of the ion transmission efficiency on the focal position of ions at the entrance of RF-QMF, the optimum region of the focal position to enhance the transmission efficiency was found. In the case that ions are injected with higher energy of 100-200eV and decelerated at the entrance part, the transmission efficiency is determined by the actual stability region, which is shifted from the theoretical one. By applying PISA-QMS to the whole structure of RF-QMF, it is possible to clarify the mechanism of the ion transmission for improvement of

the transmission efficiencies.

(2) Through the PISA-QMS calculation of the trajectories of ions injected into ITMS, it has been proved for the first time that the addition of the second and third dominant oscillation modes to the fundamental oscillation one plays a crucial role in describing the motion of ions injected into ITMS. Furthermore, the optimum values of RF voltage and ion injection energy to improve the ion trapping efficiencies were clarified. Based on the optimum RF voltage, a new injection method to solve uneven sensitivity among different ion species was derived.

(3) Mass spectra have been simulated by calculating the ion motions during the conventional mass scanning at a constant speed in ITMS. Through the PISA-QMS simulations in several cases with various scan speeds, we clarified the relationship between the scan speed and the ITMS performance items such as mass resolution and mass accuracy. Based on this relationship, a new scanning method, in which the scan speed is varied according to the ion mass, was proposed. The new scanning method was proved to achieve high resolution without mass shift or scanning time expansion by simulations.

The above three results are significant in that they confirm PISA-QMS is a powerful tool for obtaining the optimal new design and operation of RF-QMF and ITMS. PISA-QMS should play a role improving the performance of RF-QMF and ITMS dramatically to that of other huge high performance mass spectrometers.