Structure and Dynamics of Trapped Ions

Xiao Peng Xi, Xiangguo Shi, Joel H. Parks [1]

The Rowland Institute at Harvard, 100 Edwin H. Land Blvd., Cambridge, MA 02142

Our research group has developed new experimental methods designed to be performed on ions stored within radio frequency (RF) ion traps. The talk will emphasize the integration of trap technology within different experimental arrangements in order to perform unique scientific measurements. The talk will describe measurements of trapped ion electron diffraction (TIED) of metal cluster ions [1] and radiative lifetimes of trapped biomolecular ions [2]. Apparatus for these measurements are shown schematically in Figures 1 and 2.

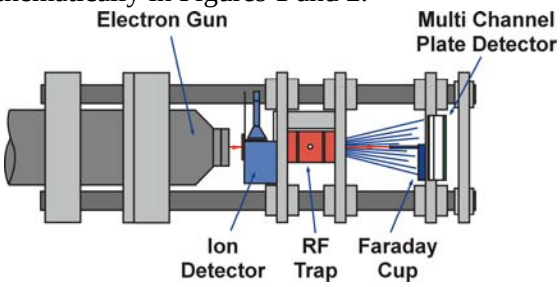

Figure 1. Diffraction Apparatus

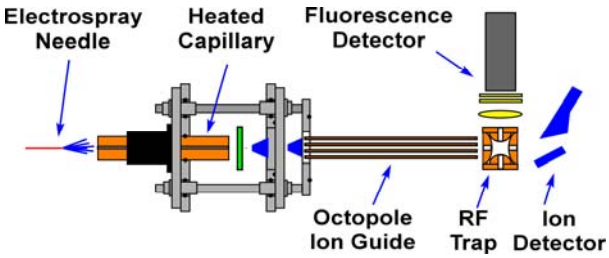

Figure 2. Fluorescence Apparatus

Ion traps have enabled a remarkable range of experiments to study the interaction of stored ions with both charged and neutral molecules, and with photons. The introduction of new ion sources, in particular metal cluster aggregation sources [3] and electrospray ionization sources [4] provided unique opportunities to produce ion beams composed of metal atom clusters and biomolecules respectively. The possibility to study the structures of these more complex species was of particular interest to investigate many-body properties and conformational dynamics on a size scale which is theoretically tractable. However the structures and dynamics of both clusters and biomolecules are strongly dependent on m/z; consequently, a method of isolating a single m/z species is essential for such studies. The ion trap mass spectrometer presented an excellent opportunity to isolate a specific m/z and store a sufficient number of thermally equilibrated, mass selected ions for a long enough time to accomplish physical measurements which otherwise could not be performed.

The talk will discuss two general areas of study which utilized an RF ion trap (i) to determine the evolution of metal cluster structures with size, and (ii) to probe local fluctuations of biomolecular conformations as a function of temperature. In each of these areas, tradeoffs in trap design were introduced which optimized high signal to noise (S/N) measurements of ion properties while maintaining acceptable mass spectrometry precision. This balance of ion trap capabilities with experimental data requirements was one of the most challenging issues in these research studies.

References

[1] Xiaopeng Xing, et al. Phys. Rev. B **74**, 165423 (2006).

[2] Xiangguo Shi, et al. J. Phys. Chem. B **112**, 12801 (2008).

[3] H. Haberland, et al., J. Vac. Sci. Technol A **10**, 3266 (1992).

[4] J. B. Fenn, et al. Science **246**, 64 (1989).

1 E-mail: parks@rowland.harvard.edu