A combined mass gate–energy discriminator

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A mass gate allows transmitting a selected mass in a time-of-flight mass spectrometer and to block other masses. The conventional stopping-potential mass gate does not discriminate against spontaneous fragments, which are generated in the drift tube. We present a simple improved version of a mass gate, which discriminates against fragments by using the fact that their kinetic energy is lower than that of the parent ion. © *1997 American Institute of Physics.* [S0034-6748(97)03512-0]

Starting from the early days of cluster science, cluster fragmentation (photoinduced[1] and spontaneous[2,3]) has attracted substantial scientific attention. While photoinduced fragmentation is an intentional action, spontaneous metastable decomposition is usually undesirable. Measurements of fragmentation yields can probe cluster binding energies.[3] More often, however, they pose a serious obstacle in cluster research, in masking the real size dependence of the measured phenomena. In this note, we introduce a simple method of cluster mass selection, which discriminates against spontaneous fragmentation prior to the measurement.

The widely used Wiley–McLaren (WM) time-of-flight (TOF) mass spectrometer (MS)[4] is based on the concept that all masses to be separated are accelerated to a given kinetic energy with some energy spread. Each mass is characterized by its own velocity, and different masses are separated according to their different velocities. When spontaneous fragmentation occurs during drift flight time, both the parent and the fragment ions share practically the same velocity (if one ignores the small recoil energy gained in the fragmentation process). Each mass peak with a given flight time, which seems to be comprised of one mass only, may contain the parent ion as well as its fragment daughters. Spontaneous fragmentation in the drift tube cannot be observed by a WM TOF MS. In a well-tuned reflectron MS,[5] spontaneous fragmentation can be detected,[3] if it occurs prior to the reflection, since the flight time in the reflector depends on the kinetic energy of the particles.

Having a mass spectrum, one often uses a mass gate (MG) to isolate a cluster of a given size from the cluster distribution. Most mass gates are based on the principle of deflecting[6] or stopping[7] the undesirable ions. The deflecting MG applies an electric field, which deflects the ions from their trajectory, while the stopping MS maintains a repelling electrical bias, which prevents the ions from coming through. At the proper timing, the voltage drops to zero and lets the desired charged species pass through the gate with no obstruction. The MG would select both daughter and parent ions in the case of spontaneous fragmentation, since they share the same velocity. However, while sharing the same velocity, their kinetic energies are different due to their different masses. We take advantage of this fact in our MG design. As in the conventional stopping design, our MG operates under a constant repelling dc voltage, slightly higher ($1.01E_k$) than the ion energy, to block the ions. At the right timing, a positive pulse is added to reduce the voltage to the extent that will let *only* the parent ion (which possesses a higher kinetic energy than its daughters) to pass through the gate. According to this principle, the effective potential during the pulse should be lower than the kinetic energy of the parent, and higher than this value times the biggest-daughter/parent mass ratio.

We have used a tandem TOF-reflectron MS in order to test our energy selecting version of the stopping MG. Figure 1(a) shows the reflectron MS picture of I^-Xe_8 with its four biggest daughters, after being selected by a conventional stopping MG. Figure 1(b) also shows the reflectron MS picture of I^-Xe_8, however, without its fragments, due to the new MG configuration. Note, that our MG can be used to discriminate against fragments just prior to the experiment, as it can be placed very close to interaction zone of the mass-selected cluster.

Another feature of this MG is its spatial focusing properties: it operates as an electrostatic lens that partially fo-

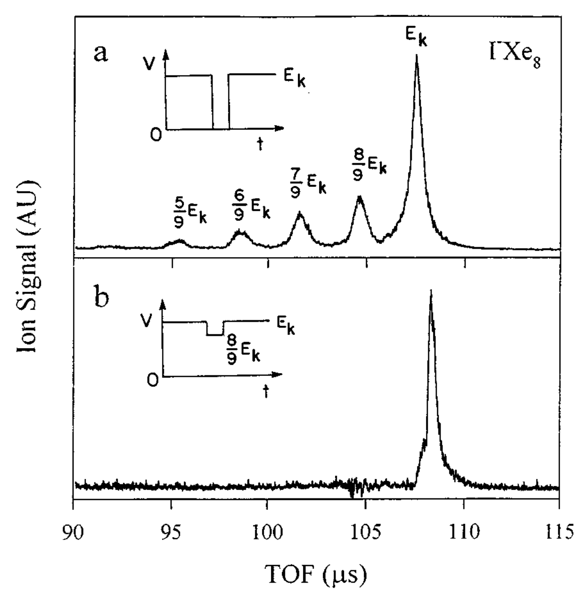

FIG. 1. A reflectron MS spectrum of the I^-Xe_8 (a) together with its daughters, after being selected by a conventional stopping MG, and (b) with no daughter peaks, after being selected by the MG-energy discriminator.

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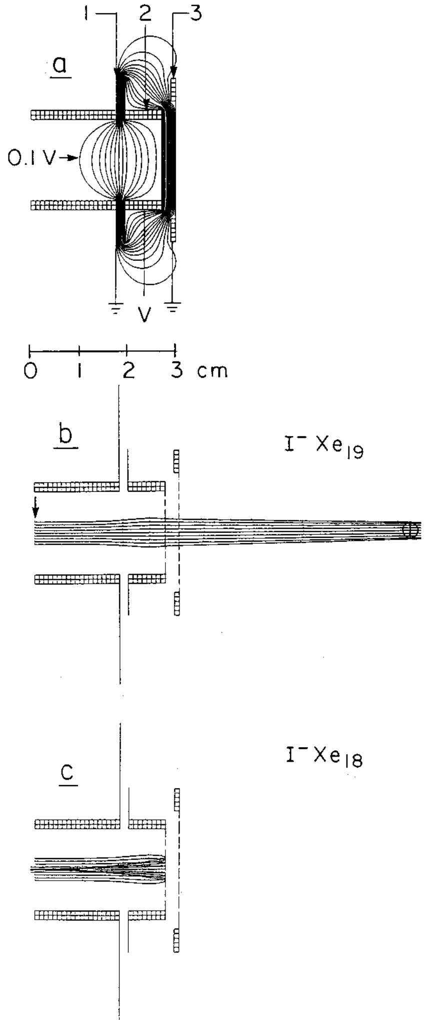

FIG. 2. The design and the simulation of the MG (the voltage regime on each electrode is described in detail in the text): (a) The MG consists of two electrodes at ground potential 1 and 3 (grid) and of a grid-stopping-electrode 2. The electric-field contours of the MG imply its focusing properties. (b) The I^-Xe_{19} parent ion is selected with a pulse, which starts at the arrow and lasts 3.4 μs, and is focused into the ionization zone (marked by a cross). (c) Its biggest daughter, I^-Xe_{18}, is fully blocked, under the same voltage regime.

cuses the ions into the ionization zone to allow a better overlap with an ionizing laser beam.

In Fig. 2, we display the structure of the MG and demonstrate in simulations[8] its characteristics. The potential contours of Fig. 2(a) suggest the focusing lens properties. We have chosen the I^-Xe_{19} cluster, a typical cluster in our in photodetachment experiments,[9] as the parent ion in our simulation. We attribute to it a kinetic energy of 1520 eV. The voltage on the gate is pulsed to 1450 V. This voltage exceeds by a few volts 1520 V times the mass ratio between the parent I^-Xe_{19} and its biggest daughter, I^-Xe_{18}. Note that the parent can easily pass the gate [Fig. 2(b)] and focus to some extent at the ionization zone (marked with a cross), while the daughter is back reflected [Fig. 2(c)].

Note that the selection resolution of the MG depends on the primary energy spread of the ions at the acceleration zone of the TOF MS. As the energy spread reduces, this mass gating technique would be more accurate. High-energy daughters would not slip through the gate together with low-energy parent ions, allowing us to differentiate a heavy parent from its relatively mass-close daughters.

In conclusion, we have presented a relatively simple device that both assures the exclusive selection of a certain charged particle, and increases the signal density by focusing that charged particle at the ionization zone.

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