Molecular Dynamics Simulation of Coulomb Explosion Processes

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Irradiation of clusters with intense femtosecond laser pulses has been found to oftentimes produce highly charged ion fragments resulting from Coulomb explosion of the cluster under investigation. When a time-of-flight mass spectrometer is used for detection, double peaks can be observed for these multicharged species due to the different arrival times of backward and forward ejected ions. Kinetic energy release values can be calculated from these peaks splittings and also can be directly measured from cutoff potentials using a reflectron as an energy analyzer. The experimental values determined with both of these methods are surprisingly large, typically on the order of several hundred electronvolts. The purpose of the work reported herein is to model the temporal evolution of a cluster system after the ionization event, using MD simulations on a level of pure electrostatic interactions between the formed ion cores. The results give insight into how composition, size, structure, and charge distribution in the initially ionized cluster influence the kinetic energy distribution of the ejected ions.

Introduction

Study of the interaction of atoms, molecules, and clusters is made possible by the availability of strong optical fields produced in ultrafast laser pulses. Various investigations have revealed that sufficiently intense interactions can lead to multiple ionization events due to the ejection of large numbers of electrons from individual atoms, molecules, and clusters. The observation of multicharged ions through photoionization of atoms has been reported by many authors starting in the mid-1980s.[1−4] Studies[5−7] of N_2 irradiated with picosecond and subpicosecond laser pulses revealed the occurrence of multicharged atomic ion species. However, in all of these studies the atomic ions had comparatively low kinetic energies, typically in the range from a few to up to 20 eV. Kinetic energies of a similar magnitude also have been reported from experiments on the photoionization of individual HI molecules,[8] where charged fragments of iodine up to I^{5+} could be observed, and in studies of other diatomic molecules such as CO, O_2, and H_2[9−12] which showed the formation of multicharged species with comparable kinetic energy release values. Though the interactions of intense laser pulses with single atoms or molecules and solid targets[13,14] have been the subject of intense studies over the past decade, only recently have field matter interactions of femtosecond laser pulses with clusters become a subject of interest.

Several years ago we identified the role clustering has in effecting the facile formation of multiply charged cluster fragments and atomic ions in the case of molecular clusters subjected to modest laser fields of femtosecond duration. A study of the ionization of hydrogen iodide clusters as well as co-clusters of HI with argon with femtosecond laser pulses[15] revealed the surprising finding that multicharged iodine and argon ions as highly charged as I^{17+} and Ar^{8+} could be produced at relatively low laser fluences. Significantly, average kinetic energy releases of several hundred electronvolts were determined in the process of Coulomb explosion of these clusters, with maximum values extending into the several kiloelectronvolts energy range. Comparable values of kinetic energy carried by ionic fragments have been measured for a variety of small to medium size clusters, including noble-gas clusters seeded with trace amounts of hydrogen iodide,[16,17] acetone clusters,[18] and ammonia clusters.[19]

Rhodes et al.[20,21] found that highly charged atomic ions as well as the emission of X-rays can be observed upon irradiation of noble-gas clusters. As an extension to these earlier studies, more recently work by Ditmire[22,23] showed that the ejection of ions with maximum kinetic energies up to 1 MeV and charge states as high as +40 could be obtained with large noble-gas clusters consisting of up to 10 000 atoms heated with high-intensity laser pulses. The ion kinetic energies observed in their study is 3 orders of magnitude higher than observed in the Coulomb explosion processes of molecules and smaller clusters, leading them to conclude that there is a fundamental shift in the nature of field matter interaction, from a Coulomb explosion process operative in molecules and small clusters, toward the hydrodynamic explosion of a formed microplasma consisting of several thousand ions and electrons in the case of large size clusters.

Two ionization mechanisms have been proposed to account for the general observation of multicharged fragments formed during irradiation of molecules or clusters with intense optical fields. One is a mechanism formulated by Rhodes,[24,25] based on the coherent motions of the field ionization electrons (coherent electron motion model, CEMM). This model considers that the coherent electron motions enhance the number of ionization events because the electrons begin to behave as quasi-particles. Overall, in this model the formation of highly charged ions is considered as an electron impact ionization phenomenon. An alternative approach termed the ionization ignition model (IIM) proposed by Rose-Petruck and Barty,[26] considers that the highly ionized states arise due to the lowering of the ionization threshold by nearby ion cores created in the initial ionization events and is related to other considerations provided by Bandrauk et al.,[27]Seideman et al.,[28] and Jortner et al.[29] The

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latter model predicts that the rate of ionization is highly dependent upon the internuclear distance in a nonmonotonic fashion and assumes that ionization takes place by a nonvertical process with a sequential loss of electrons occurring over increasingly larger internuclear separation distances. Pump−probe experiments on acetone clusters[17,18] done in our laboratory indeed showed temporal oscillations in the production of multicharged carbon and oxygen atoms formed from Coulomb explosion of these clusters. This is in general accordance with the predictions by Bandrauk and supports the role of the ionization ignition model as the initializing mechanism in the Coulomb explosion process. However, evidence largely based on investigations of kinetic energies of the resulting multicharged fragments, which typically have been observed to be in a range of several tens to hundreds of electronvolts, have been reported which support each of the above mechanisms.

The temporal evolution of a Coulomb exploding cluster has been studied by Jortner et al.[30] using molecular dynamics simulations on xenon and mixed HI/Ar clusters of sizes up to 60 atoms. Their study proved valuable in evaluating the magnitudes of the expected kinetic energies of ions formed in the Coulomb explosion process and the dependence of this energy on cluster size and charge states. Specifically their findings show an increase of final average atomic velocity with increasing cluster size and at constant cluster size with increasing ion charge.

Herein we present the results of recent experiments on the ionization of clusters with femtosecond laser pulses and the results of MD simulations, which give insight into the magnitudes and distribution of kinetic energies that can arise from Coulomb explosion processes involving clusters of different size, ion charge, and structure. A major objective is to model the effect of the atomic/molecular arrangement on the distribution of kinetic energies that can arise.

Experimental Findings

Using high-intensity laser pulses with different wavelengths and intensities to ionize clusters in a molecular beam produced in a supersonic expansion, we have studied a variety of different cluster systems including xenon, krypton, argon, hydrogen iodide, ammonia, and acetone. As the theoretical models predict, in all cases we could not observe any multicharged species, unless clusters were present in the molecular beam. For the Coulomb explosion of ammonia clusters, recent work[31] in our laboratory employing covariance mapping showed for the first time direct evidence for the connection between clusters and the formation of highly charged species (N^{4+}, N^{3+}, and N^{2+}) produced during Coulomb explosion of molecular ammonia clusters irradiated with a femtosecond laser beam. Although the formation of clusters is necessary for the observation of multicharged fragments, these experiments found a correlation between multicharged fragments and small ammonia clusters and an anticovariance between multicharged ions and larger ammonia clusters, indicating only a weak dependence on cluster size as predicted by the ionization ignition model.[26]

To further reveal the role of clusters in Coulomb explosion processes at moderate laser fluences and the kinetic energy distribution of multicharged ions formed in these processes, recently we conducted a wide range of experiments on methyl iodide clusters. In the course of pump−probe experiments on methyl iodide clusters using higher laser fluence than in previous studies,[30] we also observed the formation of multicharged carbon and iodine ions. Pump−probe spectra of methyl iodide clusters and multiply charged fragments resulting from Coulomb explosion of these clusters show a strong anticorrelation between the formation of cluster ions and the formation of multicharged fragments, in agreement with other systems studied earlier in our laboratory, e.g., the acetone cluster system.[18] Figure 1 shows pump−probe traces for $CH_3ICH_3^+$, $(CH_3)_2^+$, and the multicharged fragments I^{2+}, C^{2+}, and C^{3+}. It is apparent that the singly charged cluster fragments exhibit a pronounced dip at delay times where the multicharged species appear in the TOF mass spectra. The observed correlation between the dip in the cluster response and the pump−probe response for the multicharged fragments indicates that the formation of multicharged fragments results from the Coulomb explosion of clusters. Related experiments in which the laser beam was scanned through the molecular beam, by changing the timing between opening the pulsed nozzle and firing of the laser, showed that the formation of highly charged carbon and iodine ions is strongly correlated with the onset of cluster formation in this packet.[33] It can be observed that when the laser is focused into a region of the neutral molecular beam containing predominantly monomer species, no multicharged species can be observed. By contrast, in regions of the molecular beam that contain significant amounts of clusters, formation of multicharged species can be observed. Preliminary results further indicate that the magnitude of kinetic energies of these multicharged ions is correlated with the size distribution of clusters in the neutral molecular beam.

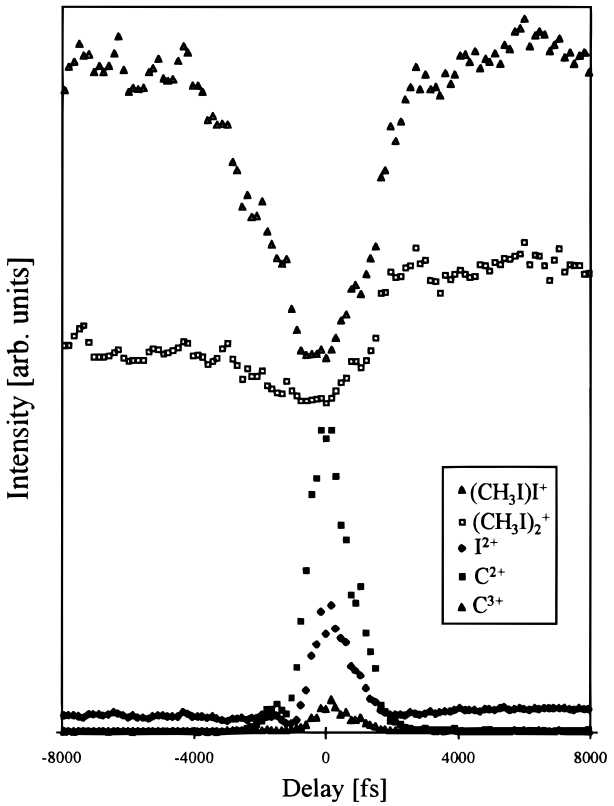

Figure 1. Pump probe traces for $(CH_3I)I^+$, $(CH_3I)_2^+$, and the multicharged fragments I^{2+}, C^{2+}, and C^{3+}. The ion $(CH_3I)I^+$ is a fragment of larger clusters and therefore an indicator of cluster formation. The asymmetry in the pump−probe trace of $(CH_3I)_2^+$ is due to the different wavelengths of laser pulses used as pump (λ = 266 nm) and probe (λ = 400 nm).

Simple electrostatic repulsion considerations immediately reveal that ion kinetic energies of several hundred electronvolts experimentally measured for highly charged argon and iodine ions resulting from Coulomb explosion of HI and mixed Ar/HI clusters, and up to more than 2000 eV for highly charged carbon

ions found with acetone clusters, cannot be accounted for by Coulomb repulsion forces inside individual molecules. Taken together, all experimental data available indicate that the kinetic energy released during the course of Coulomb explosion is a function of the size of the cluster irradiated by the laser pulse. Although this can be considered as a general understanding, theoretical work is necessary to estimate the magnitude of kinetic energies to be expected from the Coulomb explosion of small to medium size clusters.

The calculations presented in the next section were done with the intention of modeling the temporal evolution of an ionized cluster system using MD simulations on a level of pure electrostatic interactions between ions. No considerations have been included concerning the mechanism of the ionization event or the time frame within which ionization of the cluster is complete, and a totally vertical ionization process is assumed. Nevertheless, the results give insight into how composition, size, structure, and charge distribution in the ionized cluster influence the kinetic energy distribution of the ejected ions.

Numerical Approach and Results

Calculations are performed with a C program code which we wrote that can run either on a PC or a RISC 6000 workstation, depending on the size of the cluster system treated. The Coulomb explosion process of clusters is modeled on a hard sphere level using pure electrostatic interactions between the ions. This treatment seems appropriate because all experimental evidence points to the rapid loss of large numbers of electrons from the cluster prior to significant nuclear motion, so that this initial configuration can be chosen to study the effect of size and charge state on the acquired kinetic energy distribution.

The simulation is started from an initial configuration resembling the geometry of the neutral cluster by placing ions in their atomic positions. During the simulation the electrostatic force resulting from all charges in the cluster on each individual ion is calculated.

$$F_i = z_i e_0 \sum_j -\nabla f_j \quad \text{with} \quad F_j = \frac{z_j e_0}{4\pi e_0}\left(\frac{1}{r_{ij}}\right) \tag{1}$$

With the force acting on ion i being known, the equations of motion for this particle can be solved according to

$$\vec{F} = m\cdot\vec{a} \quad \text{and} \quad \vec{s} = \vec{v}t + {}^1/_2\vec{a}t^2 \tag{2}$$

where v is the velocity of the particle and t is the duration of a time step in the simulation.

The steps are repeated for all ions i to N (N = number of ions included), and each is moved accordingly. To avoid too large movements of an individual ion during this process, the time steps for the simulation are kept very small at 0.1 fs. Despite these small time steps, simulations involving up to 500 ions and a simulated time frame of up to 20 ps can be performed within a reasonable computational time.

To compare the kinetic energy values from the simulations with the experimental values, considerations have to be made concerning the angular distribution of the ions of high kinetic energy which are ejected. The kinetic energy values taken from the simulation are absolute values of kinetic energy, not considering the spatial direction in which an individual ion is ejected. If only one individual cluster is considered, the kinetic energy of ions ejected into a certain angle of space will depend highly on the orientation of this cluster. For an ensemble of a large number of clusters with random and equally probable orientations as can be expected in a molecular beam, the kinetic energy distribution of ions ejected into a certain angle of space in the laboratory reference frame will resemble the distribution of absolute values of kinetic energy in all directions.

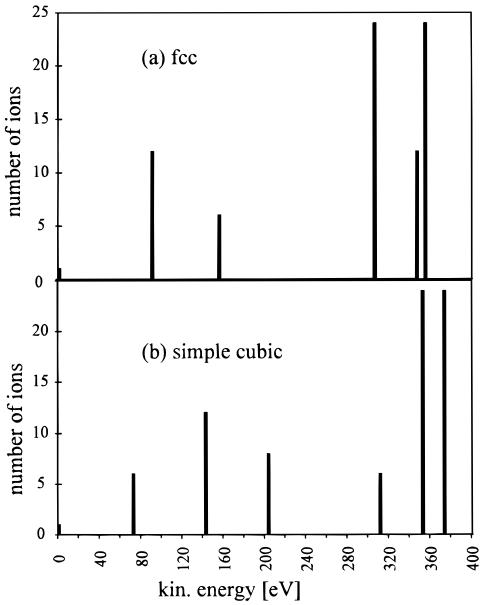

Figure 2. Simulated kinetic energy distributions for a face-centered-cubic Ar_{79} (a) and simple cubic Ar_{81} (b) cluster. All argon ions are set to a doubly charged state.

Experimental kinetic energy distributions are determined using time-of-flight mass spectrometry, a technique that determines kinetic energies from different flight times, i.e., velocities of the particles, and generally is only sensitive to velocity differences along the time-of-flight axis. Nevertheless, a direct comparison of calculated and experimentally determined kinetic energies is possible because particles having just a slight off-axis velocity component will not reach the detector of the time-of-flight instrument. For the apparatus used in our experiments, it can be calculated that all ions with more than 0.6 eV kinetic energy in either one of the off-axis velocity components do not strike the detector. Except for ions with very low kinetic energy below 0.6 eV, it follows that calculated kinetic energy distributions can be compared directly to those experimentally determined. This might also explain the center peaks observed in the split peaks of some multicharged fragment ions reported in earlier publications.[15]

Coulomb Explosion of Noble-Gas Clusters. Molecular dynamics simulations performed by Jortner et al.[30] for Xe cluster systems revealed the role the shell structure of the cluster has on the final kinetic energy distribution. To further investigate the effect of initial structures, we performed calculations for different symmetric and asymmetric arrangements. Simulations performed for noble-gas clusters involved Ar ions with charge +2 based on an initial cluster configuration of a face-centered-cubic arrangement with an interatomic distance of 3.8 Å, equivalent to the interatomic distances of argon atoms in solid argon. The structure is arranged around a central ion, and all 78 other ions enclosed in a sphere with radius 9 Å around this central ion are included. The kinetic energy distribution resulting from the Coulomb explosion of 79 argon atoms arranged in a fcc lattice is shown in Figure 2a. It shows maximum kinetic energies of up to 360 eV. For comparison, the kinetic energy to be expected from the Coulomb repulsion of two Ar^{2+} ions at the same internuclear distance of 3.8 Å is

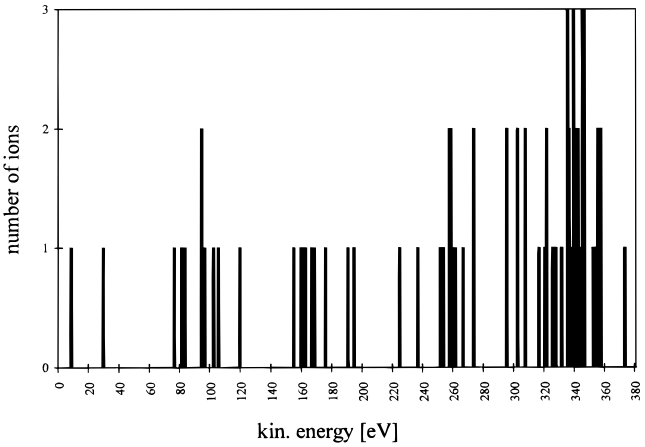

Figure 3. Simulated kinetic energy distribution of a nonsymmetric Ar_{79} cluster showing a broader distribution of kinetic energies due to the lower symmetry of the cluster.

only 7.46 eV. The discrete energy distribution of ions is a result of the high symmetry of the initial configuration. Ions having a similar location within the cluster will gain similar kinetic energy during the Coulomb explosion process, and ions placed on the surface of the initial arrangement gain the highest kinetic energy, while those in the center of the cluster gain only very little. The ion exactly in the center experiences a completely symmetric electric field and thus gains no kinetic energy at all during the course of Coulomb explosion. For comparison, and to reveal the effect of initial structure, Figure 2b shows the kinetic energy distribution calculated for the Coulomb explosion of a argon cluster with 81 ions starting from a simple cubic arrangement. The distances between the ions are chosen to be 3.4 Å, leading to a similar charge per volume in the cluster as used for the above structure of a fcc arrangement. Similar to the fcc structure, the initial configuration includes all ions enclosed in a sphere with radius 9 Å around a central ion. Because of the simple cubic arrangement, this spherical cluster contains two ions more than the equivalent fcc structure. Due to the lower symmetry of this initial structure, the kinetic energy distribution for this cluster differs from the one calculated for the fcc structure. Again, ions that acquire high values of kinetic energy are ones initially positioned in the outer shells of the cluster.

The high symmetry of the initial cluster arrangement can be disturbed by either a nonsymmetrical initial arrangement or random assignment of different charges to the ions. Figure 3 shows a simulation starting with 79 Ar^{2+} ions in a asymmetric fcc arrangement. As can be seen, the discrete kinetic energy changes to a broader distribution of kinetic energies due to the lower symmetry of the initial cluster. Figure 4 shows the initial asymmetric cluster structure. Final kinetic energies gained by the ions in the Coulomb explosion process are indicated by different gray scales. The lighter the color, the more kinetic energy this ion gains during the Coulomb explosion. The dark colored ions located in the center of the cluster are those gaining the least kinetic energy. These simulations show that different initial cluster structures lead to different kinetic energy distributions of the ions resulting from Coulomb explosion. The findings suggest that a rigorous evaluation of kinetic energy distributions could be indicative of the cluster's initial symmetry.

The discrete distribution of kinetic energies shown in Figure 2a also broadens when ions of unlike charge state are assumed to be present in the cluster. Figure 5 shows the result of a simulation of 77 Ar atoms in the same fcc arrangement as used for the simulations shown in Figure 2a, but now a random

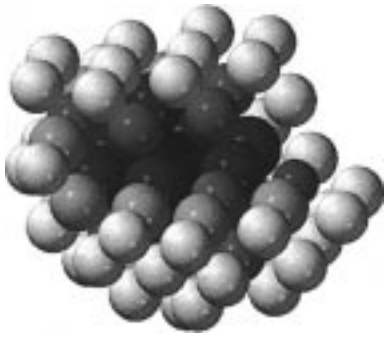

Figure 4. Final kinetic energy values of the ions gain in the Coulomb explosion process are indicated by different gray scales. The lighter the color, the more kinetic energy this ion gains during the Coulomb explosion. The dark colored ions located in the center of the cluster are those gaining the least kinetic energy.

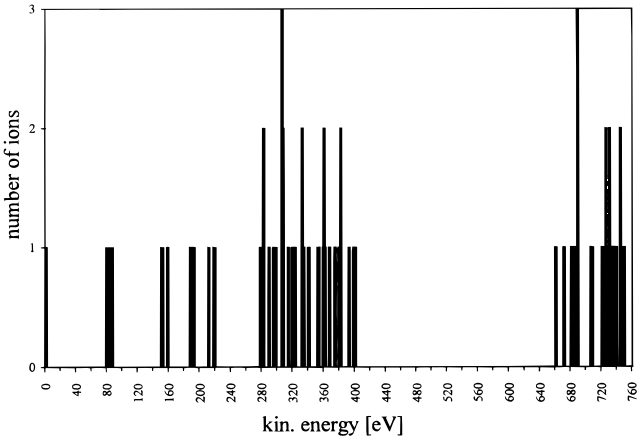

Figure 5. Simulated kinetic energy distribution from Coulomb explosion of a Ar_{79} cluster with doubly as well as triply charged Ar ions randomly distributed in the cluster.

distribution of doubly and triply charged argon ions is considered. It is obvious that the average kinetic energy of ions ejected is higher than observed in the case where only doubly charged ions have been considered. This is in accordance with general expectations due to the higher Coulomb repulsion between triply charged ions and the higher total charge of the cluster. Furthermore, the distribution of kinetic energies changes from a discrete distribution to a broader distribution but still shows a significant difference in kinetic energy between ions placed in the inner shells of the cluster and those ions in the outer shell. The latter distribution probably more closely resembles the experiment, as it cannot be assumed that the ionization event is generating ions with only one specific charge state throughout the whole cluster.

Besides information about the final values of kinetic energies carried by the ions, the simulation provides the possibility to monitor the time evolution of the Coulomb exploding cluster, either by monitoring the positions of ions or by monitoring the kinetic energy ions have gained after a certain time. Figure 6 is a plot of the kinetic energy of each ion versus time evaluated from the simulation of the 79 argon ion cluster with charge states +2 starting from a fcc lattice configuration. As already shown in Figure 2, a separation into five distinct groups of ions with kinetic energies greater zero can be observed, stemming from different shells of the cluster. More interesting is the short time period during which the process of Coulomb explosion occurs. As can be seen, the ions gain kinetic energy very rapidly within the first 200 fs after starting the simulation and reach their maximum value after about 400 fs, a time scale comparable

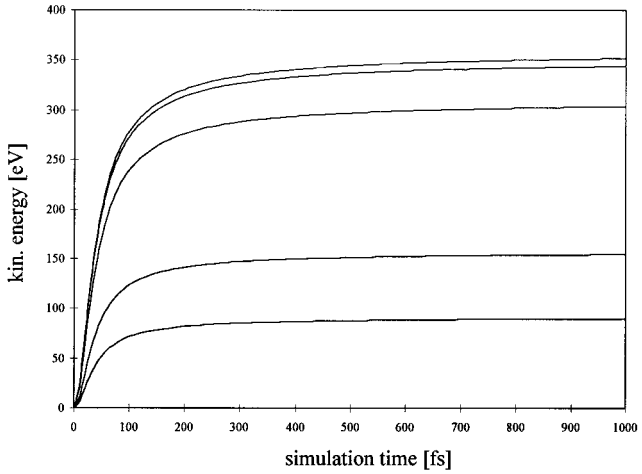

Figure 6. Time evolution of the kinetic energies for individual ions during Coulomb explosion of the symmetric Ar_{79} cluster during the first 1000 fs of simulation.

to the times calculated by Jortner et al.[30] for Xe clusters. During this time the ions are separated far enough that they do not gain any further energy from repulsion between each other.

Experimental studies provide values of ion kinetic energies resulting from the Coulomb explosion of a collection of clusters having a size distribution, which in most cases is not well-known due to the difficulty of measuring the size distribution of clusters in the neutral molecular beam. Numerical studies on the other hand open the possibility to calculate kinetic energies of ions ejected in the Coulomb explosion of clusters with a predefined size and charge state. To investigate the change of kinetic energy release with cluster size, a series of simulations have been performed on argon clusters of varying size. The argon ions are arranged in a face-centered-cubic structure as described for the aforementioned simulations with charge state of +2 located at an interionic distance of 3.8 Å to completely fill the volume of a sphere encircled by a radius r. Cluster systems covering a range of sizes between $r = 4$ Å, which is equivalent to 13 argon ions, and up to $r = 16$ Å, equivalent to 429 argon ions, were studied. The smallest cluster studied consisting of only 13 Ar ions resulted in average kinetic energy values of only 70.8 eV. Increasing cluster size leads to an increasing value of the average kinetic energy carried by ejected ions, a result already reported by Jortner et al.[30] The largest cluster system studied in the simulation contains 429 Ar ions and shows kinetic energy values of 905 eV averaged over all ejected ions. Values for the maximum kinetic energies found in these simulations vary accordingly from 76.7 eV for the cluster consisting of 13 Ar ions up to 1304 eV for the largest cluster studied.

Figure 7 shows the values for average and maximum kinetic energies found in these simulations versus the number of ions included in the cluster. The dashed line is the potential energy calculated from electrostatic repulsion of ions in the initial cluster arrangement. During the course of Coulomb explosion, the potential energy initially inherent in the cluster is completely transferred into kinetic energy of the ejected ions when they reach infinite separation. Therefore, the average kinetic energy of ejected ions is equal to the initial potential energy in the ion cluster divided by the number of ions. That the average kinetic energy of ions matches this value is a consistency check and shows that the MD simulation is performed correctly.

Extrapolation of this dashed line would indicate that the Coulomb explosion of an infinite size cluster (bulk material) would ultimately lead to infinite values of kinetic energies for

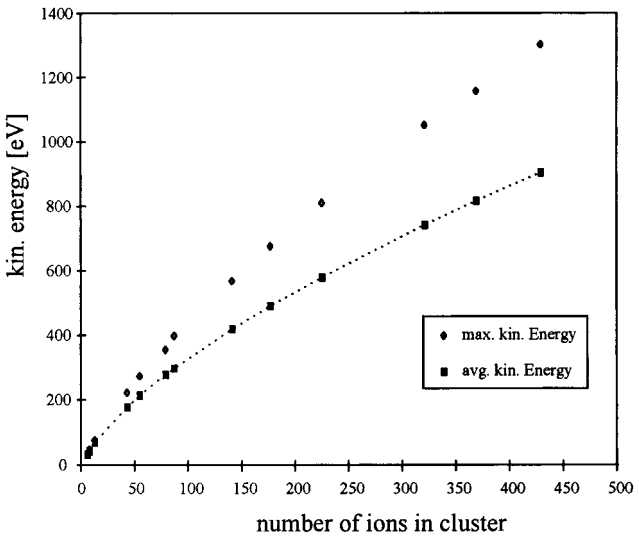

Figure 7. Maximum (▲) and average (■) values of kinetic energy found in simulations of the Coulomb explosion of spherical argon clusters with charge state +2 versus the cluster size. The dashed line indicates the average potential energy per ion in the initial configuration.

the ejected ions. These considerations clearly show that there are limits for the use of a simple electrostatic model to describe a Coulomb explosion process. The model used here assumes that when the Coulomb explosion is initiated, all free electrons resulting from ionization of atoms have a mean free path large enough that they can stream directly out of the cluster. Then, after all electrons have left the cluster, the remaining ion cores undergo a Coulomb explosion due to their electrostatic repulsion. For larger clusters this assumption is no longer valid, and it is estimated that for clusters with diameters of more than 50 Å electrons will undergo multiple collisions inside the cluster, keeping them from leaving the cluster. Ultimately, a dense expanding microplasma will be formed. A detailed treatment of the formation and expansion of plasmas formed in the interaction of intense laser pulses with large atomic clusters has been given by Ditmire et al.[34,35] and used to explain the observation of very high kinetic energy ions through irradiation of noble-gas clusters. However, the simulation of a 437 Xe^{18+} ions containing cluster with our simple electrostatic model resulted in an average kinetic energy of ejected ions of 85 keV and a maximum kinetic energy of 123 keV, without the necessity to invoke a plasma model to simulate the expansion of this cluster.

Coulomb Explosion of Acetone Clusters. Prompted by experiments in our laboratory on the Coulomb explosion of acetone clusters,[17,18] which under conditions of high laser fluence showed kinetic energy release values of 200 eV for O^{2+} and C^{2+}, 1500 eV for C^{3+}, and up to 2600 eV for C^{4+},[36] we also performed simulations on acetone cluster systems.

As input parameters for these simulations, the molecular structure of the neutral was used. To initiate the Coulomb explosion process, the atoms were assigned a charge +1 for hydrogen, +6 for oxygen, and +4 for carbon. These are the highest charge states observed experimentally. Simulation of an acetone monomer with the appropriate charges revealed kinetic energy values of not more than 482 eV for the oxygen ion. The oxygen ion gains this high kinetic energy due to its high charge state of +6, its close proximity to the central carbon ion also with a high charge of +4, and its direct ejection away from the remainder of the molecule without any further interaction. Kinetic energies found for the other ejected ions are significantly lower with values of 279 eV for the carbon

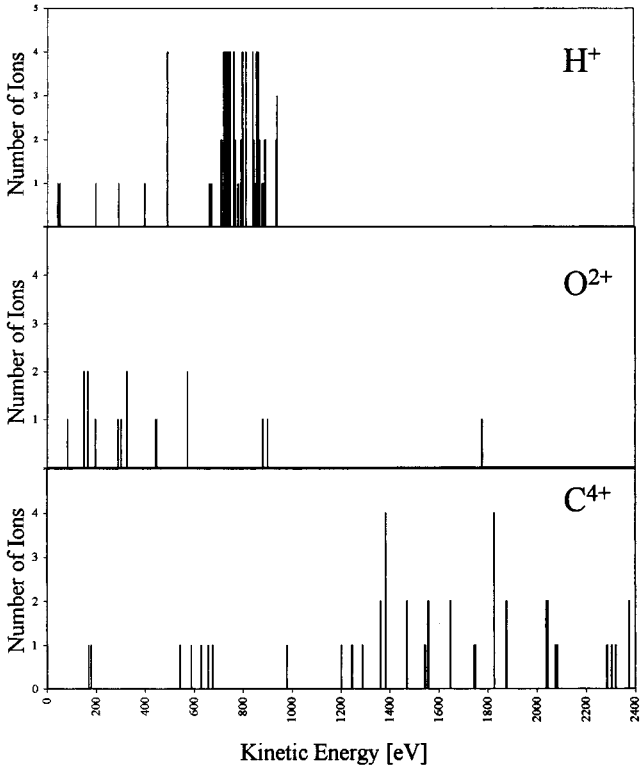

Figure 8. Simulated kinetic energy distribution resulting from the Coulomb explosion of a acetone 19-mer with the charge states H^+, O^{2+}, and C^{4+}. Distributions for hydrogen (top), oxygen (center), and carbon (bottom) ions are separated.

ions in the methyl groups and only 1 eV for the carbonyl carbon. Kinetic energies for the ejected hydrogen ions have been calculated to be 136 and 154 eV, respectively. Compared to the experimental values, it is obvious that the kinetic energies released from Coulomb explosion of a monomeric acetone molecule, even if the high charge states could be accessed, cannot account for the high values of kinetic energy release found experimentally.

Significantly higher values of kinetic energy are found for simulations of acetone clusters. Simulations of the Coulomb explosion of an acetone 19-mer were performed by arranging 19 acetone monomer subunits in a cubic structure occupying the center, faces, and edges of a cube to form a cluster. The eight corner positions are left out. Again the initial acetone monomers with high charges are assumed to have the same geometry as the uncharged acetone molecule for the purpose of this simulation. Kinetic energy release values for this cluster system are higher by an order of magnitude compared to the monomer. Maximum values are around 4400 eV found for oxygen ions, and the average kinetic energy in this system is 1384.5 eV.

To more closely model the experiment, in a further simulation we used the charge states observed with the highest abundance instead of the maximum charge states observed. In this simulation the same structure of the acetone 19-mer as described before was used, but now oxygen ions were assigned to be O^{2+}, carbon C^{4+}, and hydrogen H^+. Kinetic energies found for these three ion species are shown in Figure 8. The simulation predicts that hydrogen ions have a relatively narrow kinetic energy distribution around 800 eV. Doubly charged oxygen ions are calculated to have kinetic energies in the range 200−600 eV (experimental value 200 eV), and C^{4+} are predicted to gain kinetic energies between 1400 and 2400 eV (experimental value 2600 eV) and agree well with experimentally determined values.

Conclusions

The results from simulations on the Coulomb explosion of individual molecules and cluster systems show that the high values of kinetic energies found for ions ejected during the course of Coulomb explosions cannot be explained by Coulomb interactions between highly charged ion cores within single molecules. However, if these molecules are part of a larger cluster, Coulomb explosion of this highly charged cluster can easily lead to the high values of kinetic energy found experimentally solely from the Coulomb repulsion between highly charged ion cores. For small to medium size clusters in which it can be assumed that Coulomb explosion is mainly the result of direct Coulomb interactions between like charged ions, the model used in this simulation appears to be a simple and valuable method to explain the kinetic energies found experimentally. A more rigorous and detailed analysis of kinetic energy distributions from Coulomb explosions of clusters in connection with an electrostatic repulsion model using different cluster geometries as input might even prove valuable in the very tedious attempt to determine the structure of clustered particles.

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