Fragmentation lifetimes and the internal energy of sputtered clusters

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Received 12 March 1998; received in revised form 28 August 1998

Abstract

We have compared the distribution of internal energies and fragmentation rate constants determined experimentally for sputtered Fe

cluster ions with theoretical Molecular Dynamics computer simulations. It is found that the experimental data and the simulation are complementary with respect to the fragmentation time scale involved. While the experiment is sensitive to fragmentation times of nanoseconds and above, the simulation can provide information about the time interval ranging from femtoseconds to about one nanosecond. From the experimental data, it is found that the distribution of fragmentation rates as a function of time after the emission of the clusters follows a power law rather than an exponential decay, thus indicating a broad distribution of fragmentation rate constants. From the simulation, we conclude that this dependence continues down into the sub-nanosecond time range with, however, increasing exponent as the times get shorter. Around fragmentation times at or below \(10^{-12}\) s, the rate distribution levels off due to a maximum possible rate constant of the order of the vibrational frequency of the cluster. The fragmentation rate constants are connected with the internal energy distribution of the sputtered clusters by means of statistical RRK theory. While the average internal energy determined by experiment and simulation agree quite well, significant differences are found in the width of the respective distributions, the origin of which is attributed to the different times scales explored by both techniques. © 1999 Elsevier Science B.V. All rights reserved.

1. Introduction

If a solid is bombarded with keV ions, a variety of particles are released into the gas phase. This process is called sputtering. It is well-known that the flux of sputtered material contains an abundant fraction of molecules or clusters. The formation of these species, which may contain up to several 100 atoms [1], represents an intriguing phenomenon in sputtering physics [2,3]. From a number of studies, it has been shown that Molecular Dynamics computer simulations are well suited to model the complex collisions and interaction processes which may lead to the ejection of polyatomic species in sputtering [4–10]. From such simulations, a picture has emerged in which the
formation of sputtered clusters is divided into two steps. First, nascent clusters are ejected from the surface due to correlated atomic collisions from the volume beneath the surface which is energized by the impinging primary ion. Due to the collisional nature of their formation, these clusters contain a relatively high amount of internal energy and are therefore mostly unstable with respect to dissociation. In a second step, nascent clusters will therefore undergo unimolecular fragmentation processes during their passage away from the surface, until at very large distances metastable or, ideally, only stable fragments remain. Generally, it is these final species which are readily accessible by experiment, since most experimental schemes detect the sputtered clusters at times of the order of microseconds after their formation at the surface. As a consequence, the information obtained from such data is always convoluted with the unimolecular decay processes which may significantly alter the measured cluster properties. In order to obtain information on the collisional processes governing the cluster formation mechanism in sputtering, it is on the other hand highly desirable to directly investigate the properties of sputtered nascent clusters. While this is relatively straightforward in computer simulations, it represents an extremely difficult experimental task due to the very short fragmentation times involved. Moreover, it is known that, at least for clean metals as investigated here, most of the sputtered atoms and clusters are neutral. To the best of our knowledge, no experimental approach exists to date which enables the determination of the internal energy of sputtered neutral clusters larger than dimers. Only recently, Dzhemilev and coworkers developed a method which utilizes the unimolecular decomposition of sputtered ionic clusters to determine their internal energy distribution shortly after their formation [11,12]. The time scale accessible by such an experiment is restricted to nanoseconds and above. However, by extrapolation to even shorter times, they tried to extract information about the internal energy distribution of nascent ionic clusters. It is the purpose of the present work to compare the results obtained with this method to those of corresponding Molecular Dynamics simulations. In particular, Fe$_n^+$ cluster ions sputtered from a metallic iron surface were chosen for the experiment, since the binding energies of these species are comparable to those obtained in the MD simulation using state-of-the-art many body interaction potentials. From the results, we will demonstrate that the combination of experimental data and MD simulation provides a very efficient tool to gain information about the fragmentation dynamics of sputtered clusters.

2. Experimental

The experimental procedure to determine the fragmentation rate of a sputtered cluster as a function of time after its ejection from the surface has been described in great detail elsewhere [12,13]. In short, a double focusing mass spectrometer consisting of a magnetic sector and an electrostatic prism is used to detect ionic clusters which are sputtered under ultrahigh vacuum conditions from clean metallic samples by 9 keV Xe$^+$ ions generated by a duoplasmatron ion gun. The secondary ions are accelerated from the sample surface by an extraction field of about $10^6$ V/m. The nominal kinetic drift energy of a singly charged particle leaving the surface with zero initial kinetic energy is then determined by the applied extraction voltage of $U_{ac} = 5000$ V. Keeping the pass energy of the electrostatic energy analyzer fixed at this value, the kinetic energy distribution of the sputtered particles can be measured by variation of the sample potential. Fig. 1 shows the resulting energy spectra for Fe$_n^+$ cluster ions sputtered from polycrystalline Fe surfaces. At kinetic energies higher than $eU_{ac}$, particles are detected which leave the surface with initial kinetic energies above zero, and the spectrum displayed for positive values of the ordinate therefore simply represents the kinetic energy distribution of sputtered (stable) particles. At kinetic energies lower than $eU_{ac}$, particles are detected which leave the surface with initial kinetic energies above zero, and the spectrum displayed for positive values of the ordinate therefore simply represents the kinetic energy distribution of sputtered (stable) particles. At kinetic energies lower than $eU_{ac}$, on the other hand, a long tail is detected which is more pronounced for larger clusters and practically absent for atoms. This tail towards “negative” kinetic energies is attributed to the occurrence of unimolecular fragmentation reactions of the type

$$X_n^+ \rightarrow X_{n-m}^+ + X_m$$  \hspace{1cm} (1)
during the acceleration of sputtered nascent $X^+$ ions. If fragmentation occurs at a distance $d$ from the surface, the kinetic energy of the fragment ion is lowered due to the mass loss, and the fragment ion will leave the acceleration region with a kinetic energy deficit of

$$E_d = eU(d) \frac{m}{n},$$  \hspace{1cm} (2)$$

where $U(d)$ denotes the electrostatic potential at distance $d$. If the initial kinetic energy of the cluster is negligible compared to $eU(d)$ and only one fragmentation channel corresponding to a particular value of $m$ is active, the distribution of $E_d$ will therefore unambiguously reflect the distribution of fragmentation time after sputter ejection or formation of the cluster by

$$\frac{dN}{dt}(t) = I(t)(E_d(t)) \frac{dE_d}{dt}$$  \hspace{1cm} (3)$$

with $E_d(d)$ given by Eq. (1) and the relation $d(t)$ determined by the equation of ion motion within the accelerating electric field. A detailed description of the conversion procedure as well as a thorough discussion of the underlying assumptions can be found in Refs. [11,12]. The temporal distribution of fragmentation rates which is calculated using Eq. (3) can then be connected with the internal energy of the sputtered cluster ions as discussed in Section 4.

For the conversion according to Eq. (3) to work, it is essential that only one fragmentation channel is open. For sputtered Fe$^+_n$ clusters, previous experiments – utilizing the fragmentation processes which occur within the first field free drift region of the mass spectrometer – show that this is the case with $m = 1$, i.e. the sputtered cluster ions preferably fragment by evaporation of a monomer.

3. Computer simulation

The molecular dynamics simulation as well as its extension towards the formation and fragmentation of clusters in sputtering has been described in great detail earlier [4,10]. In short, the classical equations of motion are solved numerically for all atoms of a crystallite which in the present case has a surface area of $40 \times 40 \text{Å}^2$, a thickness of 9 atomic layers and contains approximately 2300 metal atoms. The fcc-crystal was orientated such that the ion bombarded surface was an unreconstructed (1 1 1) plane. While the interaction between the impinging Ar$^+$ ion and the metal atoms was described by a conventional pair potential of the Molière type, a many-body potential designed by DePristo and coworkers [14,15] was used to describe the interaction between the target atoms. The functional form of this potential, which has been termed “Molecular Dynamics and Monte Carlo-Corrected Effective Medium” (MD/MC-CEM), as well as details about its construction can be found in Refs. [15,16]. For the present purpose, it is worth noting that this potential, which is fit to spectroscopic data of gas phase dimers as well as to the cohesion energy and elastic constants of the corresponding bulk material, is capable of

![Fig. 1. Measured energy spectra of Fe$^+_n$ cluster ions sputtered from a polycrystalline Fe surface under bombardment with 9-keV Xe$^+$ ions.](image)
providing a fairly accurate description of the bond energies of small metal clusters [10].

The identification and classification of sputtered clusters was done in the same way as described in detail in Ref. [4]. Briefly, the trajectory integration of the collision cascade initiated by the impinging primary particle was continued until the total energy of all atoms within the model crystal (i.e. those which are not detected to be sputtered) had fallen below zero, or a maximum integration time limit of 1000 fs was reached. Upon termination, the list of ejected atoms obtained for a given primary ion impact was examined for agglomerates of two or more atoms, the total (i.e. the sum of potential and relative kinetic) energy $E_{\text{tot}}$ of which was detected to be negative. These species, which we call “nascent clusters” consisting of $n$ atoms, were then subjected to a stability check by evaluating their total internal energy according to

$$E_{\text{int}} = E_{\text{tot}} + E_a(n)$$

and comparing it to the dissociation energy $E_d$, i.e. the lowest energy threshold

$$E_{\text{th}}^m = E_a(n - m) + E_a(m) - E_a(n)$$

for unimolecular decomposition reactions described by Eq. (1). The cluster atomization energies $E_a$ as given by the MD/MC-CEM potential were determined by means of an additional MD simulation involving repetitive melting and freezing of the cluster, for details of this procedure the reader is referred to [10].

As described in Sections 2 and 4, the experimental data on internal energies was accumulated for $\text{Fe}^+_n$ cluster ions sputtered from a polycrystalline Fe surface. Ideally, it would of course be desirable to perform MD calculations for ion bombardment of the same material. Unfortunately, solid Fe has bcc crystal structure, which is not predicted to be the most stable structure by spherically symmetric potentials like the MD/MC-CEM potential. In the present work we have therefore used a potential which was fit to the properties of solid silver and the Ag$_2$ dimer, respectively. The reason for choosing this particular potential is that we have worked with it before and know that it predicts reasonable yields and kinetic energy distributions of sputtered particles, and in particular allows a fairly accurate description of the yield distribution of sputtered silver clusters. Nevertheless, we regard the simulation results as representative for a generic metal (Me), the clusters of which (Me$_n$) are characterized by the bond energies and dissociation thresholds displayed in Table 1. It is of note that these energies are quite comparable to those of $\text{Fe}^+_n$ cluster ions (see also Table 1). We are therefore confident that at least the general trends predicted by the simulations are valid for Fe as well.

### 4. Results and discussion

Fig. 2 shows the internal energy of sputtered $\text{Fe}^+_n$ cluster ions which was determined from the data displayed in Fig. 1. The data reduction procedure employed to extract this information has been described in detail in Refs. [11–13], its application to the results on sputtered $\text{Fe}^+_n$ clusters has been published elsewhere [17]. However, the general line will be repeated here, since it is im-

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<tr>
<td>$E_a(\text{Me}_n)$</td>
<td>1.10</td>
<td>1.30</td>
<td>1.45</td>
<td>1.61</td>
<td>1.66</td>
<td>1.71</td>
<td>1.76</td>
<td>1.80</td>
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<tr>
<td>$E_a(\text{Fe}^+_n)$</td>
<td>1.47</td>
<td>1.63</td>
<td>1.81</td>
<td>2.02</td>
<td>2.17</td>
<td>2.20</td>
<td>2.26</td>
<td>2.31</td>
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<tr>
<td>$E_d(\text{Me}_n)$</td>
<td>1.65</td>
<td>1.91</td>
<td>2.03</td>
<td>2.31</td>
<td>2.06</td>
<td>2.09</td>
<td>2.11</td>
<td>2.21</td>
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<tr>
<td>$E_d(\text{Fe}^+_n)$</td>
<td>1.67</td>
<td>2.11</td>
<td>2.53</td>
<td>3.06</td>
<td>3.11</td>
<td>2.40</td>
<td>2.70</td>
<td>2.74</td>
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*For comparison, experimental data of $\text{Fe}^+_n$ cluster ions are included which were taken from the literature [19]. Values are given in eV.*
important for the further discussion. First, the temporal distribution of fragmentation rates calculated according to Eq. (3) is approximated by a function

\[ N(t) = b(t + c)^{-a} \]  

with parameters \( a \) and \( c \) being determined by a non-linear least squares fitting procedure and displayed in Table 2. The normalization factor \( b \) will be ignored in the following. With the assumption that \( N(t) \) represents a superposition of exponential decay functions

\[ N(t) = \int_0^\infty k \varphi(k) \exp(-kt) \, dk, \]  

this function can be converted into the distribution \( \varphi(k) \) of fragmentation rate constants \( k \)

\[ \varphi(k) \propto k^{a-2} \exp(-ck), \]  

which is then converted into the distribution of internal energies by

\[ \Psi(E_{int}) = \varphi(E_{int}) \frac{dk}{dE_{int}} \]  

using the quantum mechanical version of conventional Rice–Ramsperger–Kassel (RRK) [18] theory

\[ k = k_0 \frac{i!(i-j+s-1)!}{(i-j)!(i+s-1)!} \]  

to connect the fragmentation rate with the internal energy \( E_{int} = i\hbar k_0 \) and the dissociation threshold \( E_d = j\hbar k_0 \). In Eq. (10), \( k_0 \) represents a typical vibration frequency of the cluster, the value of which we arbitrarily set to \( 10^{13} \, \text{s}^{-1} \). The necessary values of the dissociation energies \( E_d \) of the cluster ions were taken from measurements of the kinetic energy release upon fragmentation as described in much detail in Ref. [12].

The internal energy spectra displayed in Fig. 2 can now be compared to the results of MD simulations. Fig. 3 shows the calculated internal energy

![Normalized internal energy distributions](image)

**Fig. 2.** Normalized internal energy distributions of sputtered \( \text{Fe}_{\text{n}}^{+} \) clusters. The data were evaluated from the data displayed in Fig. 1 using the procedures described in the text.

**Table 2**

Parameters \( a \) and \( c \) corresponding to the fragmentation rate constant distribution of sputtered \( \text{Fe}_{\text{n}}^{+} \) and \( \text{Me}_{\text{n}}^{+} \) clusters

<table>
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<tr>
<th>( n )</th>
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<tr>
<td>(a) ( \text{Fe}_{\text{n}}^{+} ) (experiment)</td>
<td>( a )</td>
<td>2.2</td>
<td>1.9</td>
<td>1.7</td>
<td>1.6</td>
<td>1.6</td>
<td>1.6</td>
<td>1.7</td>
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<tr>
<td>( c(10^{-8} \text{s}) )</td>
<td>1.16</td>
<td>1.57</td>
<td>1.58</td>
<td>1.93</td>
<td>2.34</td>
<td>1.90</td>
<td>3.12</td>
<td>3.97</td>
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<tr>
<td>(b) ( \text{Me}_{\text{n}}^{+} ) (simulation)</td>
<td>( a )</td>
<td>2.9</td>
<td>4.0</td>
<td>4.4</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>( c(10^{-12} \text{s}) )</td>
<td>1.1</td>
<td>5.2</td>
<td>7.6</td>
<td>–</td>
<td>–</td>
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* \( \text{Fe}_{\text{n}}^{+} \) data were obtained by fitting Eq. (6) to the experimental data. The \( \text{Me}_{\text{n}}^{+} \) data were evaluated by fitting Eq. (8) to the simulated rate constant distributions displayed in Fig. 6.*
distributions of sputtered nascent Me₃, Me₄ and Me₅ clusters. Note that since no electronic degrees of freedom are included in the simulation, the simulated data refer to sputtered clusters irrespective of their charge state. In contrast, the experimental data presented above are restricted to sputtered ionic clusters, since the experimental approach used to determine the internal energy distributions depicted in Fig. 2 does not work for sputtered neutral clusters. In principle, the properties of sputtered neutral and ionic species may of course differ due to the additional ionization processes involved in the production of secondary ions. However, we feel that the formation as well as the internal (vibrational) excitation of sputtered nascent clusters are largely determined by the collisional processes initiated by the impinging primary ion and are therefore largely decoupled from the electronic processes leading to the ionization of the sputtered species. In other words, we assume that the ionization probability of a sputtered nascent cluster is largely independent of its vibrational excitation. At present, the validity of this assumption can only be judged by the comparison of experimental and MD simulation data as shown in Figs. 2 and 3. From the data presented in Fig. 2, it is seen that the internal energy distributions of Fe₄⁺, Fe₅⁺, Fe₆⁺, and Fe₇⁺ are centered at peak energies which are of the same order of magnitude as those observed in Fig. 3. As seen from Fig. 4, this means that both the magnitude and the cluster size dependence of the average internal energy of sputtered Fe₇⁺ cluster ions agrees quite well with that determined from the simulation. However, the shape (i.e. predominantly the width) of the experimental distributions differs significantly from that of the simulated ones. In order to illuminate the possible cause of this finding, we examine the data evaluation procedure described above in a little more detail. The central equation regarding the conversion of experimentally determined fragmentation rates and the distribution of fragmentation rate constants is Eq. (7). The implicit assumption behind this equation is that the rate constant distribution ϕ(k) and,
hence, the internal energy distribution of the clusters does not change with time. This means, that any modification of the rate constant distribution induced by fast decay processes occurring on sub-nanosecond time scales and the resulting evaporative cooling of the clusters are disregarded. From the MD simulation, on the other hand, we know that many fragmentation steps occur on time scales of picoseconds and below [4,10]. Therefore, the fragmenting clusters observed in the experiment may have undergone many sequential decay processes, before the final fragmentation step is detected in the experimentally accessible time range. In order to further discuss this problem, Fig. 5 shows the fragmentation rate constant calculated by Eq. (10) as a function of the reduced internal energy $\hat{e} = E_{\text{int}}/E_d$. At a postemission time of $t = 1$ ns, clusters with life time $\tau < t$ will already have decomposed. The values of $\hat{e}$ which correspond to a lifetime of $\tau = 10^{-9}$ s are listed in Table 3. It is important to note that these values impose an upper limit to the experimentally determined internal energy distribution, since only clusters with $\hat{e} < 1$ are stable with respect to fragmentation and will not decompose at all. These two restrictions explain the extremely narrow internal energy distribution which is determined for Fe$^+_3$. In fact, if we evaluate the upper half width limit, i.e. the energy at which the distributions in Fig. 2 have fallen to half of their maximum value, we find a one-to-one correspondence with the upper limits imposed by the experimental time range (see Table 3). In other words, the experimental distributions displayed in Fig. 2 represent the internal energy distributions of sputtered cluster ions at a time of approximately 1 ns after their emission/formation at the surface.

In contrast, the simulated data in Fig. 3 describe the properties of nascent clusters at times of approximately one picosecond after the impact of the primary ion. A detailed analysis shows that many of the subsequent fragmentation steps undergone by these clusters occur on a picosecond time scale and, most importantly, involve fission reactions (Eq. (1) with $m > 1$) as well as monomer evaporation [4]. As a consequence, it seems virtually impossible to obtain the properties of nascent clusters by extrapolation of experimental $N(t)$ data. In order to illustrate this, we convert the simulated internal energy distributions of Fig. 3 into fragmentation rate constant distributions by means of Eq. (10). The results are displayed in Fig. 6. It is seen that the distributions peak at rate

![Fig. 5. Fragmentation rate constant vs. relative internal energy $\hat{e} = E_{\text{int}}/E_d$ of small clusters as predicted by statistical RRK theory (Eq. (10)).](image)

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<tr>
<td>$\varepsilon$ ($10^9$ s$^{-1}$)</td>
<td>1.01</td>
<td>1.19</td>
<td>1.46</td>
<td>1.76</td>
<td>2.07</td>
<td>2.29</td>
<td>2.71</td>
<td>3.03</td>
</tr>
<tr>
<td>$\varepsilon_{\text{high}}$</td>
<td>1.01</td>
<td>1.19</td>
<td>1.51</td>
<td>2.69</td>
<td>2.67</td>
<td>2.81</td>
<td>3.02</td>
<td>3.11</td>
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The values of $\varepsilon_{\text{high}}$ correspond to the points at which the distributions of Fig. 2 have fallen to their half maximum value.

<table>
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<td>Relative internal energy $\varepsilon = E_{\text{int}}/E_d$ which corresponds to a fragmentation rate constant of $10^9$ s$^{-1}$ (first row) and upper half width value $\varepsilon_{\text{high}}$ of measured Fe$^+_n$ cluster ion internal energy distribution (second row) vs. cluster size $n$</td>
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</table>

constants of the order $10^{12}$ s$^{-1}$. We would like to point out that fragmentation processes proceeding this fast correspond to dissociation within only a small number of vibrational periods, and, hence, complete energy redistribution between vibrational modes cannot a priori be assumed or even expected. Then, the statistical description of fragmentation rate constants given by RRK theory and hence the applicability of Eq. (10) becomes questionable. Nevertheless, we approximate the data depicted in Fig. 6 by the functional dependence of Eq. (8), treating $a$ and $c$ as fitting parameters. The resulting least square fitting curves are included in Fig. 6, the corresponding parameters $a$ and $c$ are displayed in Table 2. It is seen that the resulting values of $a$ are considerably larger than those obtained from the experimental data, while, as expected from the above discussion, the time constant $c$ is found to be of the order of $10^{-12}$ s, i.e. several orders of magnitude lower than the values extracted from the fits in Fig. 2. Note that the parameter $a$ corresponds to the power law exponent of $N(t)$, which apparently increases with decreasing fragmentation time. Interestingly, the fitting curves displayed in Fig. 6 (corresponding to the parameters depicted in Table 2) do not describe the simulated data in the entire range of $k$. While the agreement is fairly good for $k \approx 10^{11} \cdots 10^{12}$ s$^{-1}$, in particular for Me$_5$, the fragmentation rates are underestimated at lifetimes of $10^{-11} \cdots 10^{-10}$ s. Indeed, if one restricts the fitting procedure to include only data points up to $k \leq 10^{11}$ s$^{-1}$, a significantly lower value of $a = 2.8$ is obtained, thus indicating that the slope of the double logarithmic plot of $N(t)$ depends on $t$. Hence, we conclude that the simple extrapolation of the experimental $N(t)$ data by means of Eq. (6) is presumably inadequate. Instead, the fragmentation rate curve is expected to bend upwards in the time region between $10^{-9}$ s and $10^{-11}$ s, until at about $10^{-12}$ s a plateau is reached, which corresponds to a maximum achievable fragmentation rate constant comparable to the vibrational frequency of the cluster.

5. Conclusion

The combination of experimental data and Molecular Dynamics simulations provides a very efficient tool to investigate the fragmentation dynamics of nascent clusters formed during sputtering. Due to the measurement procedure involved, the experimental data is sensitive to fragmentation times of nanoseconds and above. At the present time, it seems virtually impossible to extend the method to time scales below this range. In order to gain information about fragmentation processes occurring on shorter time scales, one must therefore rely on an extrapolation of the measured data into that time region. The simulation, on the other hand, is restricted to time scales ranging from femtoseconds up to several hundred picoseconds. For larger simulation times, the MD scheme becomes impractical due to the accumulation of numerical errors. As a consequence, experiment and simulation yield complementary information,
the combination of which leads to a more complete picture regarding the temporal evolution of the fragmentation of sputtered clusters. In particular, the simulation can provide information about the quality of the extrapolation employed to interpret the experimental data. To this end, the simulated data clearly demonstrate that the parameter $c$ introduced above should be of the order of $10^{-12}$ s. Also, at fragmentation times between $10^{-12}$ and $10^{-9}$ s, the data suggest that the time dependence of the fragmentation rate may significantly deviate from the simple power law dependence assumed in Eq. (6).

Acknowledgements

The authors are very much indebted to the State Committee of Science and Technology of the Republic of Uzbekistan and the German Secretary of Education, Science and Technology (BMBF) for supporting this work in the frame of the scientific and technological cooperation between Germany and Uzbekistan. Moreover, thanks are due to the European Community for funding this work within the INTAS program (project no. INTAS-96-0470). We would also like to express our gratitude to B.J. Garrison for helpful cooperation regarding the Molecular Dynamics simulations.

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