Investigation of the on-axis atom number density in the supersonic gas jet under high gas backing pressure by simulation

Cite as: AIP Advances **5**, 107220 (2015); https://doi.org/10.1063/1.4934675
Submitted: 03 September 2015 . Accepted: 12 October 2015 . Published Online: 21 October 2015

Guanglong Chen, A. S. Boldarev, Xiaotao Geng, Yi Xu, Yunjiu Cao, Yiming Mi, Xiuli Zhang, Lili Wang, and Dong Eon Kim

AIP ADVANCES **5**, 107220 (2015)

Investigation of the on-axis atom number density in the supersonic gas jet under high gas backing pressure by simulation

Guanglong Chen,[1] A. S. Boldarev,[2] Xiaotao Geng,[3] Yi Xu,[1] Yunjiu Cao,[1] Yiming Mi,[1] Xiuli Zhang,[1] Lili Wang,[1] and Dong Eon Kim[3,4,a]
[1]*School of fundamental studies, Shanghai University of Engineering Science, Shanghai 201620, China*
[2]*Keldysh Institute of Applied Mathematics, Russian Academy of Science, Moscow 125047, Russia*
[3]*Department of Physics & Center for Attosecond Science and Technology(CASTECH), Pohang University of Science and Technology (POTECH), Pohang, Kyungbuk 376-73, Korea*
[4]*Max Planck Center for Attosecond Science, Pohang, Max Planck POSTECH / KOREA Res. Init. Kyungbuk 376-73, Korea*

(Received 3 September 2015; accepted 12 October 2015; published online 21 October 2015)

The supersonic gas jets from conical nozzles are simulated using 2D model. The on-axis atom number density in gas jet is investigated in detail by comparing the simulated densities with the idealized densities of straight streamline model in scaling laws. It is found that the density is generally lower than the idealized one and the deviation between them is mainly dependent on the opening angle of conical nozzle, the nozzle length and the gas backing pressure. The density deviation is then used to discuss the deviation of the equivalent diameter of a conical nozzle from the idealized d_{eq} in scaling laws. The investigation on the lateral expansion of gas jet indicates the lateral expansion could be responsible for the behavior of the density deviation. These results could be useful for the estimation of cluster size and the understanding of experimental results in laser-cluster interaction experiments. [http://dx.doi.org/10.1063/1.4934675]

I. INTRODUCTION

In the study of laser-cluster interaction, e.g., the deuterium-deuterium nuclear fusion,[1–3] plasma waveguide generation,[4] x-ray,[5] terahertz radiation,[6] the cluster size in a gas jet is an important parameter for the understanding of these experimental results. Usually, a clustered gas jet is produced by the adiabatic expansion of gas under a high backing pressure through a conical nozzle into vacuum and the average cluster size is estimated by Hagena scaling laws.[7,8] In the scaling laws, the average cluster size N_c depends on $(Kd_{\mathrm{eq}}{}^{0.85}P_0/T_0{}^{2.29})^{2.35}$, where K is a constant related to the property of a gas species,d_{eq} is the equivalent diameter of a conical nozzle and P_0, T_0 are an initial gas backing pressure in mbar and a gas temperature in Kelvin before expansion, respectively. Among these parameters, the determination of d_{eq} is important for the estimation of cluster size. In scaling laws, the definition of d_{eq} is based on an idealized straight streamline model in which the expansion angle of gas jet through a conical nozzle into vacuum is the same as the opening angle of the conical nozzle. From this idealized model, a conical nozzle corresponds to an idealized equivalent diameter d_{eq} of $0.74d/\tan\alpha$ for a rare gas, i.e., $d_{\mathrm{eq}} = 0.74d/\tan\alpha$, where d is the throat diameter and α the half opening angle of the conical nozzle. It is well known that the scaling law is based on the experimental data obtained at relatively low gas backing pressures, while in the usual laser-cluster interaction experiment, a high backing pressure is quite often employed to produce a gas jet with a high atom density. Thus one

[a]Author to whom correspondence should be addressed: kimd@postech.ac.kr

expects the cluster size deviation when the scaling law is used to estimate the cluster size under a high gas backing pressure. Up to now, there have existed many papers about the investigation of the gas jet and its cluster size,[9–19] and there have been papers reporting the cluster size deviation from the size expected by the scaling laws[20,21] and some works concerned about the understanding of the deviation.[22] In Ref. 22, the d_{eq} was investigated by experimentally measuring the dimension of a gas jet. It was found that the experimental dimension was larger than the idealized one. And thus it was concluded that the actual d_{eq} was smaller than the idealized d_{eq}. Actually, the deviation of dimension from the idealized dimension denotes the existence of the lateral expansion of a gas jet. As stated in Ref. 22, the definition of d_{eq} is directly based on the on-axis atom number density of a gas jet, rather than the dimension of gas jet. Considering the spatial distribution of atom density in a gas jet, the investigation of the on-axis atom density becomes more important than that of the dimension for the understanding of the deviation of d_{eq} and the effect of the lateral expansion on it. In this work, a large number of simulations about argon gas jet produced from the conical nozzle were made using the Boldarev's 2D model.[21] It aims to investigate the on-axis atom number density and try to show the behavior of on-axis atom number density under the effect of the lateral expansion of gas jet. The on-axis atom number density was investigated in detail by comparing the simulated atom density of a gas jet with that expected by the straight streamline model. The deviation of d_{eq} from the idealized one was then discussed. In this work, eighteen cases were considered in simulations: six nozzle lengths (L = 5, 10, 15, 20, 25 and 30 mm) and three half opening angles (α = 8.5°, 14° and 19.3°) for each nozzle length. For each nozzle, the on-axis atom number densities of gas jets at sixteen different heights above a nozzle exit were examined under five different gas backing pressures (P_0 = 10, 20, 30, 40 and 50 bars). It is demonstrated in simulation that due to the lateral expansion of gas jet, the formula $0.74d/\tan\alpha$ of the idealized d_{eq} for a rare gas could be valid only when the conical nozzle with a long nozzle length and a large opening angle is used under a low backing pressure.

II. THE DIMENSION OF GAS JET AND THE EQUIVALENT DIAMETER OF CONICAL NOZZLE

Figure 1 shows the schematic diagram for the idealized streamline of a gas jet into vacuum from a conical nozzle. From Fig. 1, the idealized dimension of gas flow $2l_T$ can be given by the expression $2l_T = 2(L + h)\tan\alpha + d$, where L is the length of the conical nozzle, h the height above the nozzle exit and d, α the throat diameter and the half opening angle of the conical nozzle, respectively. It is clear that the idealized dimension is related to the opening angle, the height and the nozzle length.

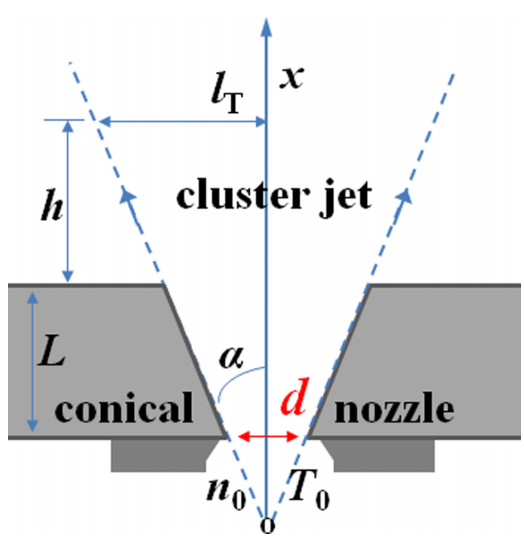


FIG. 1. The schematic diagrams for streamline of gas jet into vacuum from a conical nozzle based on the idealized straight streamline model.

Based on the idealized straight streamline model,[7,8] at a few diameters of conical nozzle throat downstream, the idealized on-axis atom number density n_T in the gas jet can be expressed as 0.15 $(x/d_{eq})^{-2}\,n_0$, where n_0 is the atom number density at the gas source. To compare the atom number density in the gas jet between the simulated results and the results from the straight streamline model, the on-axis atom number density ratio η is defined as n_T/n_c, where n_c is the on-axis atom number density in gas jet by simulation. And thus the simulated equivalent diameter $d_{eq}{}^c$ is the idealized d_{eq} ($=0.74d/\tan\alpha$) by $\eta^{-0.5}$, i.e., $d_{eq}{}^c = \eta^{-0.5}d_{eq}$.

III. RESULTS AND DISCUSSIONS

In this work, the simulations were done for the argon gas flow using the 2D hydrodynamic model described in detail in Ref. 21. The capability of this model for the gas density has been demonstrated.[19,21,23] In this work, the gas jets of eighteen conical nozzles with the same throat diameter d of 0.5 mm under five gas backing pressures were simulated for the on-axis atom number density. As examples, the results about density at the gas backing pressure of 50 bars are shown in Fig. 2. The colored solid symbols are used for the simulation results about n_c and the black symbols for the idealized densities n_T. Note that the densities for the nozzles with the same opening angle are plotted using the same color. For examples, the red symbols in Fig. 2 denote the densities for six nozzles with $\alpha = 8.5^o$ at h = 1.8, 2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4, 3.6, 3.8, 4.0, 4.2, 4.4, 4.6, 4.8 mm, respectively. The six nozzles correspond to the nozzle lengths L = 5, 10, 15, 20, 25 and 30 mm from left to right, respectively. That is to say, the first group of red symbols represent the densities at every height for nozzle of L = 5 mm (the corresponding $L + h$ is from 6.8 mm to 9.8 mm), and the second group of red symbols represent the densities at every height for a nozzle of L = 10 mm (the corresponding $L + h$ is from 11.8 mm to 14.8 mm), and so on. From Fig. 2, in general, we note the following points: (1) the bigger the opening angle or the height is, the lower the atom density in gas jet is for a given nozzle length. Moreover, it is also noted that the atom density decreases with the increase of the nozzle length L for a given opening angle. These results can be easily understood based on the geometrical structure of conical nozzles. For a conical nozzle, the radius of nozzle exit will become larger when the opening angle and the nozzle length increase. The dimension of a gas jet should then increase, which leads to the decrease of density. It is in agreement with the result from the idealized straight streamline model. (2) However, as expected, the on-axis atom number density n_c is generally lower than the idealized one n_T, i.e., there exists the deviation between them. If the density ratio η is used to denote the density deviation, η is generally bigger than one. Based on the definition of atom density ratio η and the formula ($d_{eq}{}^c = \eta^{-0.5}d_{eq}$), one expects the deviation of the equivalent diameter from the

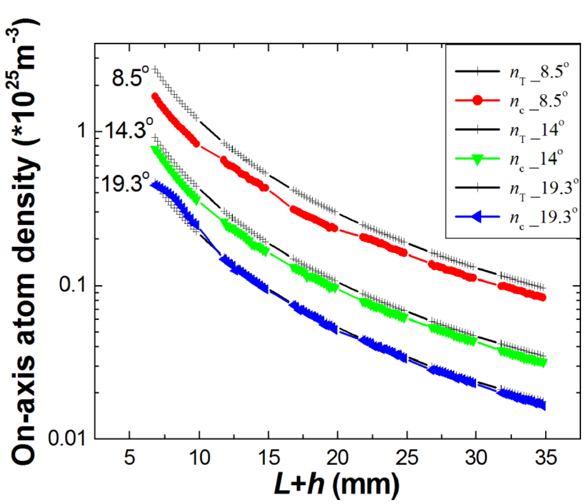


FIG. 2. Comparison of the on-axis atom number density in gas jet at different heights above nozzle for conical nozzles with three opening angles and six nozzle lengths under a gas backing pressure of 50 bars. (The colored and the black symbols denote the densities in simulation n_c and those predicted by the straight streamline model n_T, respectively).

idealized d_{eq}. Thus the simulation results reveal that the actual equivalent diameter of a conical nozzle $d_{eq}{}^{c}$ is smaller than the idealized d_{eq}, i.e., the equivalent diameter is overestimated in idealized straight streamline model. For example, for the nozzle (L = 5 mm, α = 8.5°), η is about 1.5 at h = 2.4 mm. And then $d_{eq}{}^{c}$ is about 0.8 times lower than the idealized d_{eq}. (3) From Fig. 2, it is found the density deviation decreases when the nozzle length or the opening angle increases. That is to say it shows a clear dependence on the nozzle length and the opening angle. For example, the deviations are about 7.2×10^{24} m^{-3} and 2.4×10^{23} m^{-3} for the nozzle (L = 5 mm, α = 8.5°) and the nozzle (L = 25 mm, α = 8.5°) at h = 2.4 mm, respectively, while it becomes 1.0×10^{22} m^{-3} for the nozzle (L=25 mm, α = 19.3°). These results are similar with those discussed for the conical nozzle with L = 5 mm in Ref. 22. It is noted that the deviation shows a weak dependence on the height. That is to say, the deviation generally decreases with the increase of the height, but the density ratio η hardly changes with the height for a given nozzle, which is different from that discussed for the conical nozzle with L = 5 mm in Ref. 22, as discussed below.

It is necessary to note the dependence of the on-axis atom number density on the gas backing pressure. We calculated the atom densities at a height of 2.4 mm for eighteen nozzles under the backing pressures of 10, 20, 30, 40 and 50 bars, respectively. From the results, it is found that the deviation of n_c from n_T shows a dependence on the backing pressure. As examples, n_c and n_T for the nozzles (L = 5 mm, α = 8.5° and L = 25 mm, α = 8.5°) are shown in Fig. 3(a) and Fig. 3(b), respectively.

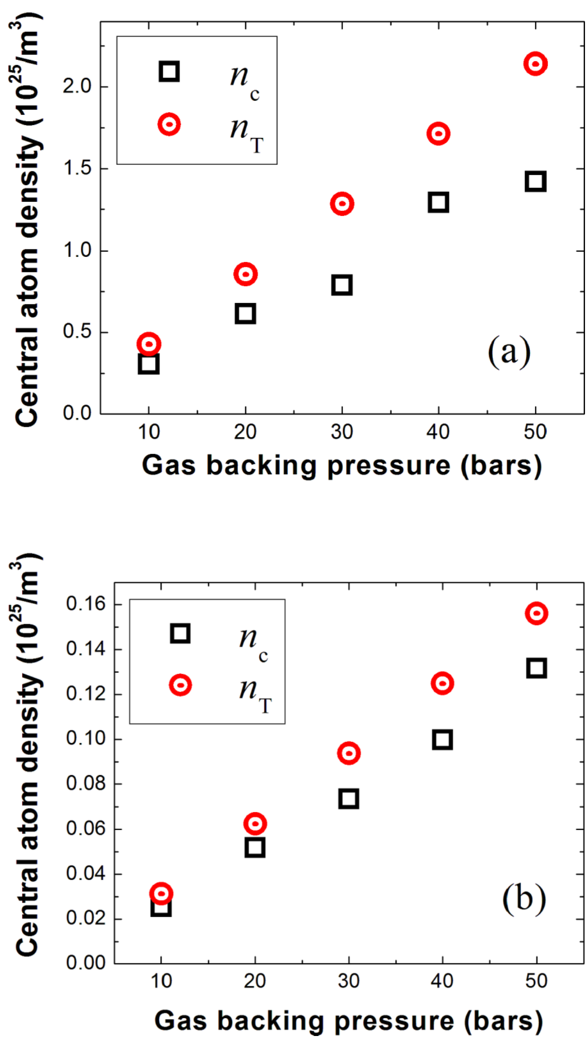


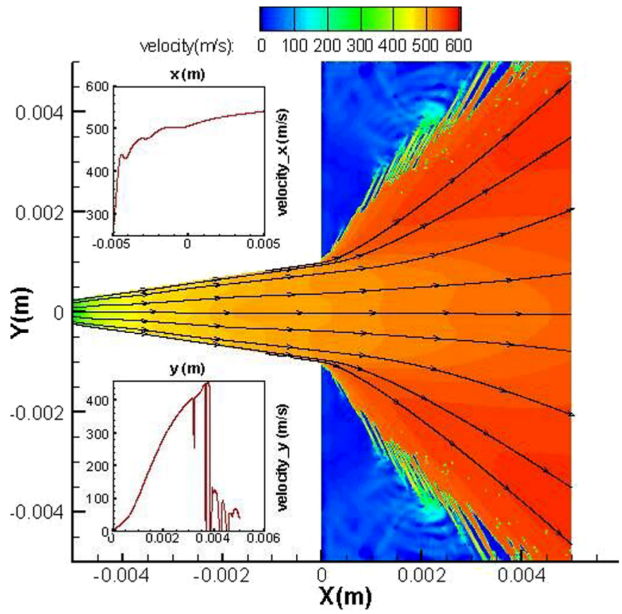
FIG. 3. Comparison of on-axis atom number density between the simulation results and the idealized ones in the straight stream model at h = 2.4 mm under different gas backing pressures. (a) L = 5 mm, α = 8.5° and (b) L = 25 mm, α = 8.5°.

From Fig. 3, it is found that (1) the dependences of the density on gas backing pressure for the simulation results and the idealized results are similar, which are nearly proportional to gas backing pressure. (2) There exists the deviation of the density from the idealized one for a given gas pressure (n_T is higher than n_c), and the deviation between them generally increases when the gas backing pressure changes from 10 bars to 50 bars. (3) By comparing Fig. 3(a) with Fig. 3(b), the density deviation indicates a smaller variation for the nozzle with a long length when the gas backing pressure increases. For an example, when the gas backing pressure increases from 10 to 50 bars, the density deviation changes from 1.2×10^{24} m^{-3} to 7.2×10^{24} m^{-3} for the nozzle length of 5 mm (i.e., it increases by 6 times), while it only changes from 5.7×10^{22} m^{-3} to 2.5×10^{23} m^{-3} for a nozzle length of 25 mm (i.e., it increases by about 4.4 times). Hence the deviation is related to the backing pressure and the nozzle length.

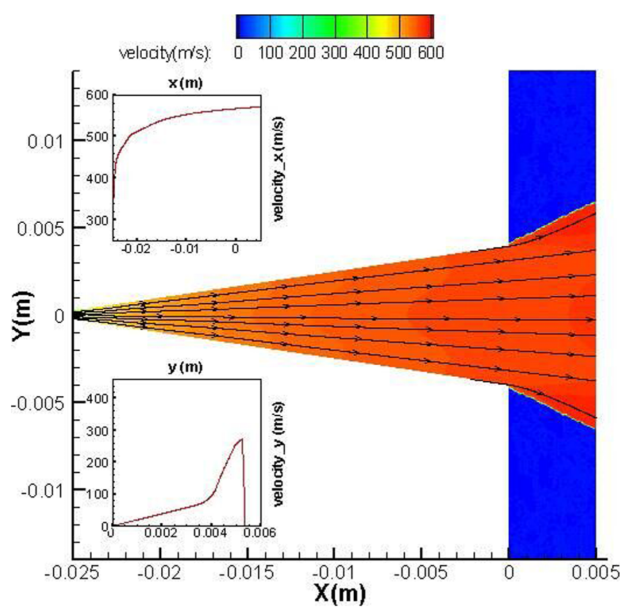
From discussion above, it is concluded that there does exist the deviation between the n_c and n_T, and the deviation is mainly related to the conical nozzle length, the opening angle, the gas backing pressure. The deviation behaves like this: it increases when the gas backing increases or the nozzle length, the half opening angle decreases. The on-axis atom density in gas jet is close to that predicted by the idealized model only for the nozzle with a longer length and a big opening angle under a low gas backing pressure. Because it leads to the increase of the dimension of a gas jet, the lateral expansion of a gas jet could result in the decrease of the on-axis density. The relation between the behavior of the density deviation and the lateral expansion of gas jet will be discussed below. It is necessary to note that if the deviation of the simulated dimension of a gas jet from the idealized dimension is investigated, as shown in Ref. 22, the dimension deviation shows a similar behavior. However, both the dimension deviation and the ratio of the dimension to the idealized dimension show the stronger dependences on the height above the nozzle, the opening angle, the nozzle length and the gas backing pressure. This could result from the fact that the dimension is easier than the on-axis density to be affected by the lateral expansion of gas jet.

To understand the behavior of the on-axis density, the lateral expanding velocity at $h = 2.4$ mm is investigated. As examples, Fig. 4(a) and 4(b) show the 2D flow velocity spatial distributions for the nozzles with $L = 5$ mm and $\alpha = 8.5^{\circ}$, and with $L = 25$ mm and $\alpha = 8.5^{\circ}$ under a gas pressure of 50 bars, respectively. The insert in the upper side shows the x-component of the velocity at the center of gas jet (i.e., the longitudinal velocity) along the jet direction (i.e., the x axis), while the insert in the lower side shows the y-component velocity at $h = 2.4$ mm (i.e., the lateral velocity along y axis). Clearly both x-velocity and y-velocity must be considered when the effect of lateral expansion is investigated. From Fig. 4, it is found that (1) the x-velocity generally increases as x and its increase gradually becomes slow. And thus the x-velocity at the exit of the 25 mm-nozzle (567 ms^{-1}) is a little higher than 507 ms^{-1} of 5 mm-nozzle. (2) The lateral velocity at $h = 2.4$ mm for the 25 mm-nozzle (its maximum velocity is about 270 ms^{-1}) is much lower than that for 5 mm-nozzle (its maximum velocity is about 460 ms^{-1}). It implies that the lateral expansion is obvious in the case of 5 mm-nozzle, i.e., the lateral expansion could make the obvious effect on the on-axis density for the short nozzle. Hence a bigger density deviation is expected for the nozzle with a short length. It is in agreement with the result above that the short nozzle corresponds to a big density deviation.

Similarly, the lateral expansion is investigated for the nozzles with different opening angles but a same nozzle length. The simulation results indicate the increase of the x-velocity at center of jet as the opening angle increases, while the lateral velocity nearly keeps the same. Thus the lateral expansion will be weak for a big opening angle. In this case for the nozzle with a big opening angle, the density deviation could be small. Meanwhile, for a given nozzle ($L = 5$ mm, $\alpha = 8.5^{\circ}$), the lateral expansions at $h = 2.4$ mm are compared under the gas backing pressures of 10 bars and 50 bars. As expected, it is found that the lateral velocity under 10 bars is lower than that under 50 bars, while the longitudinal velocity is nearly same. Thus the lateral expansion is weaker under a low gas backing pressure, which suggests a dependence of density deviation on gas backing pressure. The behavior of the lateral expansion is in agreement with the behavior of density deviation discussed above. It is reasonable to conclude that the lateral expansion of gas jet could be responsible for the density deviation and result in the dependence of the density deviation on the nozzle length, the opening angle and the gas backing pressure. Thus the effect of the lateral expansion on the on-axis atom density has to be considered in the study on the supersonic gas jet. It is noted that the nozzle surface could make effects on the gas



(a)



(b)

FIG. 4. The 2D velocity spatial distribution of (a) the nozzle with $L = 5$ mm and $\alpha = 8.5^o$, (b) the nozzle with $L = 25$ mm and $\alpha = 8.5^o$ under a gas pressure of 50 bars, respectively.

flow velocity near the nozzle wall and produce the boundary layer between the flowing gas and the stationary nozzle surface. And the boundary layer could have effects on the lateral expansion of gas flow. However, as stated in Ref. 9, the boundary layer thickness under high gas pressure is less than tens of micrometers. Hence its effects on the lateral expansion can be neglected under a gas backing pressure of several tens of bars. The reduction of the lateral expansion under a given condition will be helpful for the increase of the on-axis atom density, which could be useful for the production of large-size clusters.

IV. CONCLUSIONS

In conclusions, we investigated the on-axis atom number density and the lateral expansion in the supersonic gas jet for further understanding the deviation of the equivalent diameter of a conical nozzle. The on-axis atom number density is generally lower than the idealized one and the density deviation increases when the gas backing increases or the nozzle length, the half opening angle decreases. This behavior of the density deviation results from the behavior of the lateral expansion of a gas jet. Because the definition of d_{eq} is directly based on the on-axis atom number density of a gas jet, the density deviation implies the deviation of d_{eq}. The actual $d_{eq}{}^{c}$ is close to the idealized d_{eq} only where the conical nozzle with a long nozzle length and a large opening angle is used under a low gas backing pressure. The determination of d_{eq} is important for the estimation of cluster size in scaling laws, and thus the results could be helpful to estimate the cluster size in a gas jet from a conical nozzle in the case that there is still no proper method to directly measure the absolute cluster size experimentally up to now.

ACKNOWLEDGMENT

This research has been supported in part by Natural Science Foundation of China (Grant No. 51275283, 51503121, 11504228), by Global Research Laboratory Program [Grant No 2011-00131], by Leading Foreign Research Institute Recruitment Program [Grant No 2010-00471] and by Max Planck POSTECH/KOREA Research Initiative Program [Grant No 2011-0031558] through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(MEST) .

[1] T. Ditmire, J. Zweiback, V. P. Yanovsky, T. E. Cowan, G. Hays, and K. B. Wharton, Nature **398**, 489 (1999).
[2] Amol R. Holkundkar, Gaurav Mishra, and N. K. Gupta, Phys. Plasmas **21**, 013101 (2014).
[3] W. Bang, Phys. Rev. E **92**, 013102 (2015).
[4] T. Ditmire, R. A. Smith, and M. H. R. Hutchinson, Opt. Lett. **23**, 322 (1998).
[5] C. S. Liu, V. K. Tripathi, and Manoj Kumar, Phys. Plasmas **21**, 103101 (2014).
[6] Fazel Jahangiri, Masaki Hashida, Shigeki Tokita, Takeshi Nagashima, Masanori Hangyo, and Shuji Sakabe, Appl. Phys. Lett. **102**, 191106 (2013).
[7] O. F. Hagena and W. Obert, J. Chem. Phys. **56**, 1793 (1972).
[8] O. F. Hagena, Surf. Sci. **106**, 101 (1981).
[9] U. Even, Advances in Chemistry **2014**, 636042 (2014).
[10] K. Luria, W. Christen, and U. Even, J. Phys. Chem. A **115**, 7362 (2011).
[11] M. Hillenkamp, S. Keinan, and U. Even, J. Chem. Phys. **118**, 8699 (2003).
[12] Daniela Rupp, Marcus Adolph, Leonie Flückiger, Tais Gorkhover, Jan Philippe Müller, Maria Müller, Mario Sauppe, David Wolter, Sebastian Schorb, Rolf Treusch, Christoph Bostedt, and Thomas Möller, J. Chem. Phys. **141**, 044306 (2014).
[13] D. G. Jang, Y. S. You, H. M. Milchberg, H. Suk, and K. Y. Kim, Appl. Phys. Lett. **105**, 021906 (2014).
[14] A. M. Bush, A. J. Bell, J. G. Frey, and J-M. Mestdagh, J. Phys. Chem. A **102**, 6457 (1998).
[15] A. Ramos, J. M. Fernández, G. Tejeda, and S. Montero, Phys. Rev. A **72**, 053204 (2005).
[16] R. A. Smith, T. Ditmire, and J. W. G. Tisch, Rev. Sci. Instrum. **69**, 3798 (1998).
[17] F. M. DeArmond, J. Suelzer, and M. F. Masters, J. Appl. Phys. **103**, 093509 (2008).
[18] X. Gao, X. Wang, B. Shim, A. V. Arefiev, R. Korzekwa, and M. C. Downer, Appl. Phys. Lett. **100**, 064101 (2012).
[19] S. Jinno, Y. Fukuda, 1 H. Sakaki, A. Yogo, 1 M. Kanasaki, K. Kondo, A. Ya. Faenov, I. Yu. Skobelev, T. A. Pikuz, A. S. Boldarev, and V. A. Gasilov, Appl. Phys. Lett. **102**, 164103 (2013).
[20] H. Y. Lu, G. Q. Ni, R. X. Li, and Z. Z. Xu, J. Chem. Phys. **132**, 124303 (2010).
[21] F. Dorchies, F. Blasco, T. Caillaud, J. Stevefelt, C. Stenz, A. S. Boldarev, and V. A. Gasilov, Phys. Rev. A **68**, 023201 (2003).
[22] Guanglong Chen, Xiaotao Geng, Hongxia Xu, Yiming Mi, Xiuli Zhang, Lili Wang, and Dong Eon Kim, AIP Advances **3**, 032133 (2013).
[23] S. Jinno, Y. Fukuda, H. Sakaki, A. Yogo, M. Kanasaki, K. Kondo, A.Ya. Faenov, I.Yu. Skobelev, T.A. Pikuz, A.S. Boldarev, and V.A. Gasilov, Opt. Express **21**, 20656 (2013).