Role of Auger-type emission from diatomic molecular targets interacting with fast multicharged ions

Carmen A. Tachino, Mariel E. Galassi, and Roberto D. Rivarola
Instituto de Física Rosario (CONICET–UNR) and Facultad de Ciencias Exactas, Ingeniería y Agrimensura, Universidad Nacional de Rosario, Avenida Pellegrini 250, 2000 Rosario, Argentina
(Received 1 June 2009; published 24 July 2009)

Multiple electron emission in collisions between bare multiply charged ions and diatomic molecules is studied. The role played by Auger-type emission in cross sections for fixed number of ejected electrons is investigated. It is shown that this postcollisional reaction gives the main contribution to these cross sections at high enough impact velocities. This behavior is accentuated as the ionization degree increases.

DOI: 10.1103/PhysRevA.80.014701 PACS number(s): 34.50.Gb

I. INTRODUCTION

Multiple ionization processes produced by the impact of fast ions on diatomic molecules have been a matter of active research during the last decades (for reviews see, for example, Refs. [1,2]) since they are of great importance in areas such as astrophysics and biological physics. Two mechanisms are of our present interest: direct ionization and postcollisional electron emission. In the first one, the direct interaction of the projectile with the target electrons provokes the ejection to the continuum of one or more of them, leaving the residual target in a highly excited state with vacancies in inner shells. In the second mechanism, which is assumed to be produced once the projectile is far away, these vacancies created are filled by other target electrons. The energy generated in these transitions is employed to release photons or to produce autoionization of the remaining bound electrons through Auger-type emission [3–5]. This postcollisional reaction may correspond to intershell Auger and/or intrashell Coster-Kronig electron ionization, depending if the ejected electron is initially in a different or in the same shell than the one going to fill the vacancy. Thus, new vacancies are created and photons and/or autoionization of electrons are again produced. This process can be subsequently repeated so that additional Auger-type cascades can be observed.

For the case of atomic targets, previous experiments and theoretical calculations obtained using different models gave clear evidence that Auger-type ionization dominates multiple electron ionization at high enough collision energies as the q-ionization degree of the target increases [6–14]. In a recent work [15], hereafter referred as I, this physical behavior was also shown to appear in collisions of proton beams impacting on diatomic CO, N_2, and O_2 molecules. The scopes of the present work are to extend this study and to investigate the role played by Auger-type postcollisional emission in multiple ionization reactions for the case of higher charged projectiles colliding with these diatomic targets.

As in I, independent electron approximation and binomial distributions are employed to obtain the q-fold ionization cross sections. Also, in order to simulate the diatomic character of the target, this is described as composed of two atoms separated by a distance equivalent to the molecular equilibrium one. This simplified molecular picture was previously employed with success to study direct multiple electron emission from diatomic targets [16–18]. Single ionization probabilities are calculated using the three-body continuum distorted wave–eikonal initial state (CDW-EIS) model.

Atomic units will be used in the following except where otherwise stated.

II. THEORY

Let us consider the multiple ionization of a diatomic molecular target by an ion of nuclear charge Z_P at intermediate and high collision energies. The straight line version of the impact parameter approximation is employed and it is supposed that the internuclear molecular vector remains as frozen during the reaction. The last assumption is valid considering that the times associated with the vibration and the rotation of the molecule are much larger than the collision time at enough high impact velocities v. Details on the theoretical model are given in Ref. [15]. The relativistic character of the kinematics of the projectile at very high collision energies is taken into account in the present model. Following this work, the probability of emission of q_j electrons by direct interaction with the projectile and α_j Auger-type electrons, both from the j-molecular center $(j=1,2)$ composing the target, is given by

$$P_{q_j,\alpha_j}(b_j) = \sum_{q_{k_j}=0}^{N_{k_j}} \mathcal{P}(q_{1s_j}, q_{2s_j}, \ldots; \alpha_j) \sum_{k_j=1s,2s,2p,\ldots}^{q_{k_j}=q_j} \times \prod_{k_j=1s,2s,2p,\ldots} \binom{N_{k_j}}{q_{k_j}} p_{k_j}^{q_{k_j}}(b_j)[1-p_{k_j}(b_j)]^{N_{k_j}-q_{k_j}}, \quad (1)$$

where b_j is the impact parameter with respect to the j-molecular center, p_{k_j} is the single ionization probability per electron corresponding to the atomic orbital k_j, N_{k_j} and q_{k_j} are the total number of electrons and the number of electrons emitted from this orbital, respectively, and $\mathcal{P}(q_{1s_j}, q_{2s_j}, \ldots; \alpha_j)$ represents the probability of emission of α_j postcollisional electrons from the j center after emission

of q_{k_j} electrons from each k_j orbital due to direct ionization. Then, the probability for q degree of ionization of the molecular target as a function of the impact parameter **b** (defined with respect to the middle point of the molecular equilibrium distance) can be obtained using the expression

$$P_q(\mathbf{b}) = \sum_{\substack{q_1,q_2,\alpha=0 \\ q_1+q_2+\alpha=q}}^{N_1,N_2,\alpha^{\max}} \sum_{\substack{\alpha_1,\alpha_2=0 \\ \alpha_1+\alpha_2=\alpha}}^{\alpha_1^{\max},\alpha_2^{\max}} P_{q_1,\alpha_1}(b_1) P_{q_2,\alpha_2}(b_2), \qquad (2)$$

with α as the total number of electrons postcollisionally emitted and N_j as the total number of electrons of the j-molecular center. The probability for q-degree direct electron ionization (excluding postcollisional emission) can be easily obtained by taking $\alpha_j=0$ [which is equivalent to consider $\mathcal{P}(q_{1s_j}, q_{2s_j}, \ldots; \alpha_j)=1$] in expression (1). In our model p_{k_j} is calculated into the CDW-EIS approximation and the probabilities of emission of α_j postcollisional electrons are calculated (as we proceeded in Ref. [15]) using the photoionization experimental data obtained for the case of only one electron remotion from the k_j subshell, while all the other ones remain bound to the target [19]. In this procedure we have assumed that the postcollisional ionization reaction is independent of the nature of the primary vacancy production.

Cross sections σ_q for q-ionization degree can be determined integrating the probability P_q on the impact parameter **b** and averaging the result over all molecular orientations.

III. RESULTS AND DISCUSSIONS

Cross sections σ_q are presented in Fig. 1 for impact of H^+, He^{2+}, and C^{6+} ions on CO targets as a function of the impact energy per atomic mass unit. Calculations with and without Auger-type contributions are discriminated, showing that like in the case of protons (previously considered in Ref. [15] and where a very good agreement with experimental data [20,21] was found) postcollisional emission dominates the multiple ionization reaction as q becomes larger. It is observed that this behavior is produced at higher impact energies (it means at higher collision velocities) as Z_P increases. It can be understood from the fact that at high velocities the direct single ionization probabilities p_{k_j} present a Z_P^2 dependence with the projectile nuclear charge. As a consequence, as we have numerically verified, the production of q_{k_j} electrons by direct ionization of the k_j orbital increases for larger Z_P while α_j postcollisional emission following the vacancy of the q_{k_j} electrons gives the same contribution for any value of the projectile charge, independently of the collision velocity. Thus, higher impact energies must be considered to observe the dominance of the Auger-type mechanism as Z_P increases. In Figs. 2 and 3, it is shown that a similar comportment also appears for impact of H^+, He^{2+}, and C^{6+} on N_2 and O_2 molecules.

In Fig. 4, σ_q ionization cross sections shown in Fig. 1 are presented as a function of the Bohr parameter Z_P/v. It is found that this parameter is appropriate to determine the region where postcollisional mechanisms begin to dominate

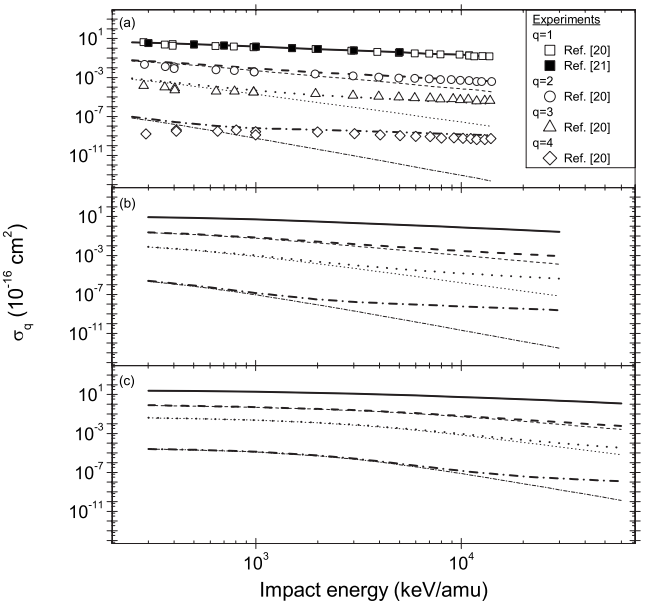

FIG. 1. Cross sections for q-ionization degree of CO molecules by (a) H^+, (b) He^{2+}, and (c) C^{6+} impact. The thin lines represent direct ionization contributions and the thick ones correspond to cross sections including postcollisional emission contributions; $q=1$ (—), $q=2(\times 10^{-1})$ (– – –), $q=3(\times 10^{-2})$ (···), and $q=4(\times 10^{-5})$ (–·–).

the cross sections σ_q. The separation between curves corresponding to include or not Auger-type contributions is produced in the region $Z_P/v \lesssim 0.3$, with a small shift to larger values of the Bohr parameter as the ionization degree increases. This behavior observed for CO targets is found in a similar way for N_2 and O_2 molecules.

IV. CONCLUSIONS

Postcollisional electron emission in multiple ionization of diatomic targets by impact of multiple charged ions was ana-

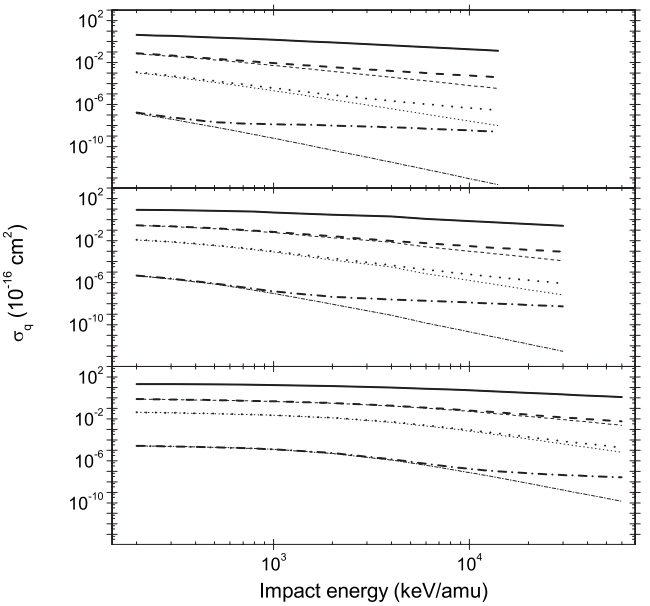

FIG. 2. Same as Fig. 1 but for N_2 molecules.

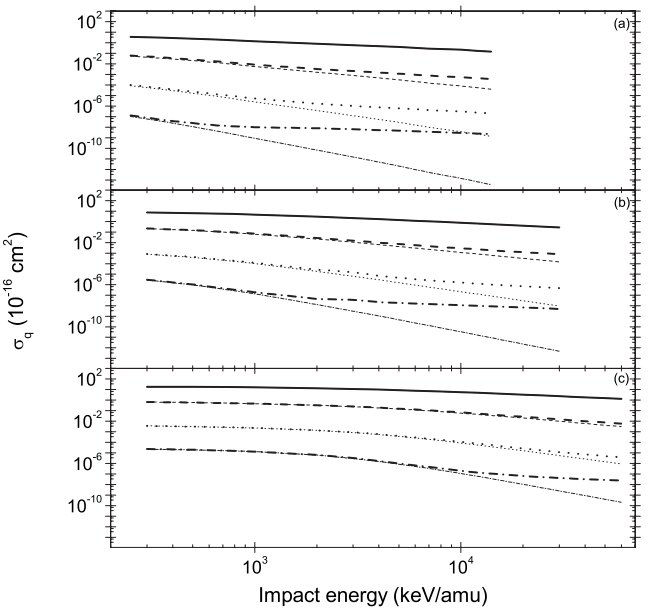

FIG. 3. Same as Fig. 1 but for O_2 molecules.

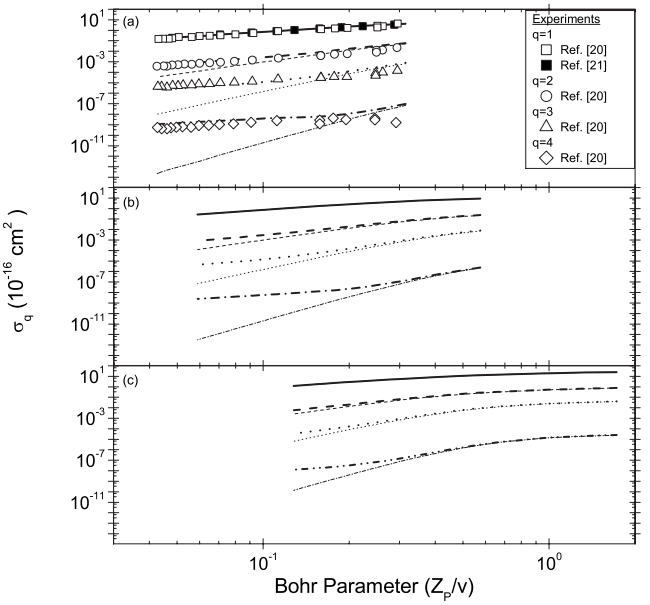

FIG. 4. Same as Fig. 1 but as a function of the Bohr parameter Z_P/v.

lyzed, showing that like in the case of protons they dominate the corresponding cross sections in comparison with direct ionization contributions at high enough collision velocities as the ionization degree increases. Moreover, it is shown that this behavior appears at larger collision velocities as the projectile nuclear charge increases. It is also observed that the Bohr parameter Z_P/v is adequate to estimate the physical conditions under which Auger-type emission mechanisms start to give the main contribution to the mentioned cross sections.

ACKNOWLEDGMENTS

This work was partially supported by the Agencia Nacional de Promoción Científica y Tecnológica (Project No. PICT 1912) and by the Consejo Nacional de Investigaciones Científicas (Grant No. PIP 5335), both institutions from the República Argentina. M.E.G. also acknowledges financial support through Project No. PICT 32070 of the Agencia Nacional de Promoción Científica y Tecnológica. C.A.T. expresses her thanks to the Fundación Josefina Prats from Rosario (Argentina) for financial support.

[1] N. Stolterfoht, R. D. DuBois, and R. D. Rivarola, *Electron Emission in Heavy Ion-Atom Collisions* (Springer, New York, 1997).
[2] R. D. Rivarola and P. D. Fainstein, Nucl. Instrum. Methods Phys. Res. B **205**, 448 (2003).
[3] P. Auger, Compt. Rend. **177**, 169 (1923).
[4] P. Auger, Compt. Rend. **180**, 65 (1925).
[5] P. Auger, J. Phys. Radium **6**, 205 (1925).
[6] R. D. DuBois and S. T. Manson, Phys. Rev. A **35**, 2007 (1987).
[7] O. Heber, G. Sampoll, B. B. Bandong, R. J. Maurer, E. Moler, R. L. Watson, I. Ben-Itzhak, J. L. Shinpaugh, J. M. Sanders, L. Hefner, and P. Richard, Phys. Rev. A **39**, 4898 (1989).
[8] T. Kirchner, H. J. Lüdde, and R. M. Dreizler, Phys. Rev. A **61**, 012705 (1999).
[9] T. Kirchner, M. Horbatsch, and H. J. Lüdde, Phys. Rev. A **66**, 052719 (2002).
[10] T. Spranger and T. Kirchner, J. Phys. B **37**, 4159 (2004).
[11] E. Cavalcanti, G. Sigaud, E. Montenegro, M. SantAnna, and H. Schmidt-Böcking, J. Phys. B **35**, 3937 (2002).
[12] E. Cavalcanti, G. Sigaud, E. Montenegro, and H. Schmidt-Böcking, J. Phys. B **36**, 3087 (2003).
[13] C. Archubi, C. Montanari, and J. Miraglia, J. Phys. B **40**, 943 (2007).
[14] M. E. Galassi, R. D. Rivarola, and P. D. Fainstein, Phys. Rev. A **75**, 052708 (2007).
[15] C. A. Tachino, M. E. Galassi, and R. D. Rivarola, Phys. Rev. A **77**, 032714 (2008).
[16] K. Wohrer and R. L. Watson, Phys. Rev. A **48**, 4784 (1993).
[17] C. Caraby, A. Cassimi, L. Adoui, and J. P. Grandin, Phys. Rev. A **55**, 2450 (1997).
[18] L. Adoui, C. Caraby, A. Cassimi, D. Lelièvre, J. Grandin, and A. Dubois, J. Phys. B **32**, 631 (1999).
[19] T. Carlson, W. Hunt, and O. Krause, Phys. Rev. **151**, 41 (1966).
[20] E. Wells, V. Krishnamurthi, K. D. Carnes, N. G. Johnson, H. D. Baxter, D. Moore, K. M. Bloom, B. M. Barnes, H. Tawara, and I. Ben-Itzhak, Phys. Rev. A **72**, 022726 (2005).
[21] M. Rudd, Y. Kim, D. Madison, and J. Gallagher, Rev. Mod. Phys. **57**, 965 (1985).