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Multiple Ionization Cross Sections of Ne and CO Induced by Very High-q Fast Projectiles ($q/v > 1$)

Man Zhou, Zhenye Wang, Sufen Li, Peng Xu, Haoxin Zhou

Rocket Force University of Engineering, Xi'an, China
Email: zhouman1984@qq.com

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Abstract

In this paper, we extend our previous work of classical over barrier ionization (COBI) model to study the multiple ionization cross section of Ne and CO molecule collided by very high-q fast projectiles(q/v > 1). The model gives similar results to the independent-electron-approximation calculation and is in good agreement with experimental data. The very small computational time required makes it a good candidate for studying the multiple ionization of complex molecules under high linear energy transfers.

Keywords

Multiple Ionization, High-q Projectiles, Strong Coupling Regime, Model Calculation

1. Introduction

Multiple ionization of multi-electron atoms and molecules impacted by high-q fast projectiles has been investigated widely. The underlying physics is of major importance not only for basic research in astrophysics, plasma physics, and chemical physics, but also for technological applications such as in material science [1] [2] [3] [4].

Numerous theoretical works for multiple ionization of atoms and molecules impacted by ions have been reported recently. The most widely used approach is the eikonal-classical trajectory Monto Carlo (CTMC) method [5], in which the ion trajectories are simulated and the initial momentum distribution of the target electron is assumed. Then, the whole system is evaluated numerically. This method provides a good description of multiple ionization. However, its application to more complex molecules is limited by its consuming. In a perturbative regime, the first-order semi-classical approximation (SCA) model [6] and statistical energy deposition (SED) model [7] [8] can give a reasonable description of

multiple ionization mechanism. However, when it comes to a strong coupling regime ($q/v > 1$), remarkable deviations from the first-order results have been found. Lately, a method using the independent-particle model (IPM) is suggested for estimating multiple ionization cross sections of heavy atoms colliding with highly charged ions [9], but some of the theoretical explanation is insufficient. In recent years, the calculation by using non-perturbative quantum mechanical approach shows good agreement with experimental results over a wide range of energy from 20 keV to several MeV in proton–water collision [10] [11]. However, a non-parameter model for the multiple ionization of atoms and molecules induced by very high-q and fast projectiles ($q/v > 1$) is extremely scarce.

In previous work, we used the classical over barrier ionization (COBI) model [12] [13] [14] [15] [16] to interpret the relative multiple ionization cross sections of Ar impacted by He^+ ions at energies from 10 to 800 keV/u, and by 34 MeV Cl^{q+}. Now, we extend our previous work of COBI model to the multi-electron systems, and calculate the multiple ionization of Ne and CO molecule collided by very high-q fast projectiles in a strong coupling regime.

The paper is organized as follows: the COBI model is presented in Section 2. Calculation results of the relative multiple ionization cross sections each as a function of projectile energy and projectile charge q for Ne are presented and compared with the experimental data in Section 3. Then, the scenarios of multiple ionization of CO molecules by very high-q fast projectiles are discussed. Finally some conclusions are drawn from the present study in Section 4. Atomic units are used throughout, unless otherwise specified.

2. Model

The present model used to calculate multiple ionization cross sections of complex targets is based on our previous work of COBI model and also on Bohr's over barrier (OB) model [17]. Based on Bohr's classical over barrier model (COBM), ionization is introduced in COBI to describe the double-ionization process in the strong coupling regime. According to COBM, the release distance is given as $R_r = \frac{Z+2\sqrt{qZ}}{I}$, where Z and q are charges of the projectile and the target core, and I is the electron's binding energy. The capture distance is $R_c = \frac{2q}{v^2}$, where v is the velocity of projectile. If release occurs within the capture distance R_c electrons will be captured; if release occurs outside the capture distance, electrons will not be ionized until they obtain enough kinetic energies to escape. When the projectile approaches the distance R_I, the Stark energy transferred to the kinetic energy of the released electron is larger than its ionization energy of quasi-molecular state, the ionization will occur. So, the ionization distance R_I satisfy the equation

$$\frac{q}{R_I} \geq I + \frac{q}{R_r} \tag{1}$$

The electrons released within the capture distance R_c will be captured; others released outside the capture distance will not be ionized until the ion enters the ionization distance of R_I. Then, one-electron release, capture and ionization probability for each impact parameter b are given as

$$P_r = \frac{2\sqrt{R_r^2 - b^2}}{vT} \tag{2}$$

$$P_c = \frac{2\sqrt{R_c^2 - b^2}}{vT} \tag{3}$$

$$P_I = P_r - P_c = \frac{2}{vT}\left(\sqrt{R_r^2 - b^2} - \sqrt{R_c^2 - b^2}\right) \tag{4}$$

where v is the collision velocity, and $T = 2\pi n^3/Z^2$ is the orbital period of the target electron, n is principal quantum number. Equations (2)-(4) are the obtained single electron ionization and capture probabilities P_I and P_c for a given atomic orbit.

It is important to note that, the projectile charge is very high in the present model, the ionization distance R_I is of one to two orders of magnitude larger than the molecular dimension. Thus, atoms of the molecule can be seen as being at the origin of the coordinate. To improve the calculation efficiency and maintain the accuracy, when apply P_I of atomic orbital to CO, we neglect the orientation effect of molecules. The existing literature [18] [19] also indicates that the orientation effect will not exceed a few percent even in the highly charged cases for the collisions in a strong coupling regime. For the same reason, in the strong coupling regime the ionization distance R_I is far larger than molecular size, the fine structure of molecular electron cloud will not play an important role. Therefore, our calculation of molecular orbitals is not rigorous solution but several atomic orbitals instead. In addition, the multi-electron probabilities are extracted from the one-electron probabilities by using the method of independent event model (IEVM) [20] [21], which have been proved more adequate than IPM for multi-electron targets.

In summary, in present work, atoms of the molecule are all located at the origin of coordinate, out shell electrons are staying at their orbitals with the ionization energy I_i and the period $T_i = \pi \cdot n/I_i$. The ionization energy I_i presented in **Table 1** is obtained by employing the quantum chemical Molpro program [22] [23] [24]. Then, with the statistical method of multinomial distribution, the relevant q-fold ionization probability can be obtained as

$$P_I^{q+} = \sum_{i,j,\cdots,n} P_{Ii} P_{Ij} \cdots P_{In} \prod_{s \neq i,\cdots,n} \left(1 - P_{Is} - P_{cs}\right) \tag{5}$$

Table 1. Calculated values of ionization energy (in eV) for CO molecule and molecular ions for different states of ionization.

	1	2	3	4	5	6	7	8
CO	14.05	27.47	40.27	55.12	68.27	86.34	105.41	131.15

The cross sections are obtained by integrating the probability $P_1^{q+}(b)$ over-all impact parameters as

$$\sigma^{q+} = \int_{-\infty}^{+\infty} P_1^{q+}(b) \cdot 2\pi b \mathrm{d}b \tag{6}$$

3. Results and Discussion

Figure 1 shows the ratios of multiple to single ionization of Ne impacted by 34 MeV Cl^{q+}, each as a function of projectile charge *q*. They are compared with the SCA calculation results [6] and the available experimental data (uncertainty is about 25%) [25]. It can be seen that both calculation results are in good agreement with the experimental data. On the whole, the results of SCA model are underestimated, and the COBI model is overestimated. Compared with the SCA, the results of COBI model are closer to the experimental data. For different values of projectile charge, the ratios $R_{q1} = \sigma_q/\sigma_1$ (q = 2, 3) are of the same order of magnitude. The ratios are found to increase slightly with projectile charge increasing.

In **Figure 2** we report on the calculated relative multiple ionization cross sections each as a function of projectile energy for the Cl^{12+} + Ne collisions. It also includes the SCA calculation results of Ref. [6] and the experimental data of Ref. [25]. The overall agreement is excellent. Double, triple ionization cross sections are about 40%, 20% of the single ionization cross section respectively. For different values of projectile energy, the ratios $R_{q1} = \sigma_q/\sigma_1$ (q = 2, 3) are also of the same order of magnitude. The ratios are found to decrease very slowly with projectile energy increasing.

The relative multiple ionization cross sections present a weak dependence on

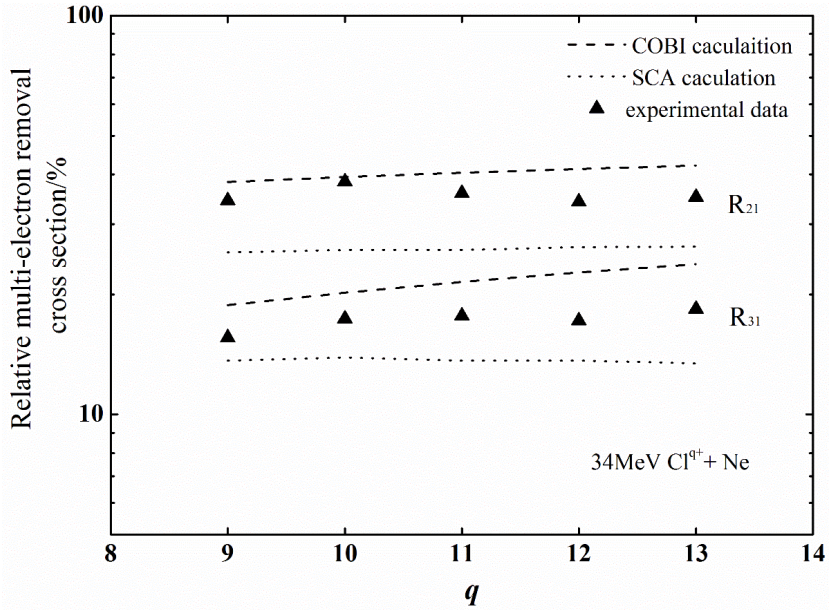

Figure 1. Relative multiple ionization cross sections each as a function of projectile charge for 34MeV Cl^{q+} + Ne. The lines represent the model results, and symbols denote the experimental data.

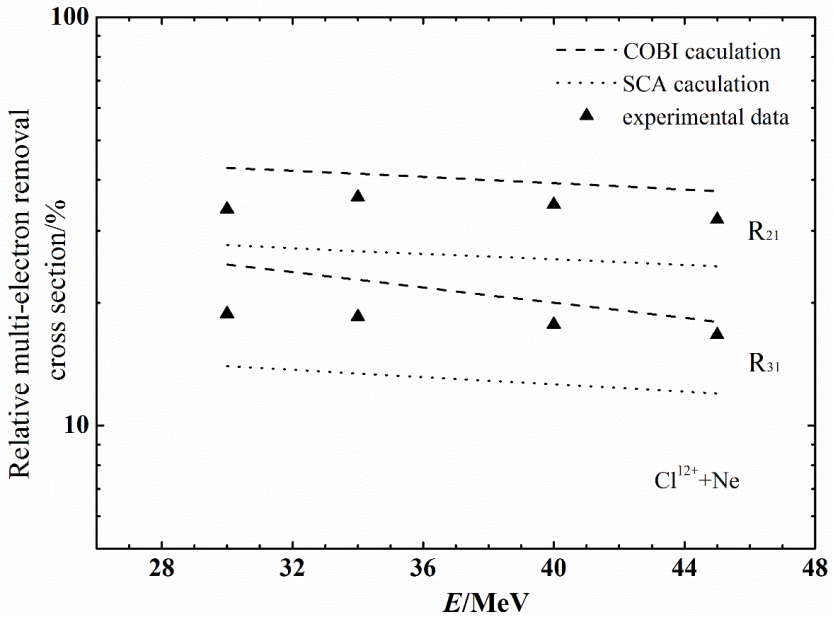

Figure 2. Relative multiple ionization cross sections each as a function of projectile energy for Cl^{12+} + Ne. The lines represent the model results, and symbols denote the experimental data.

projectiles energy E and charge q. We can give a reasonable interpretation to the behavior. For the very high-q projectiles, the release and ionization distance both reach the same asymptotic form of

$$R_{\mathrm{I}} = \frac{1}{I}\frac{2q\sqrt{Z}}{2\sqrt{Z}+\sqrt{q}} \xrightarrow{q>>Z} \frac{2\sqrt{qZ}}{I} = R_{\mathrm{r}}$$

indicating that

$$P_{\mathrm{I}} = P_{\mathrm{r}} \approx \frac{2R_{\mathrm{r}}}{vT} \propto \sqrt{\frac{q}{E}}$$

Therefore the ionization probability is determined by the single release probability. Since the single release probability is proportional to $(q/E)^{0.5}$, which is insensitive to q and E, and with the complementary role of P_{I} and $1 - P_{\mathrm{I}}$ in the multinomial distribution, the very weak q and E dependence of multiple ionization probabilities is expected.

We show in **Figure 3** our results of relative multiple ionization cross sections of Ne impacted by 2.4 MeV/u Ar^{14+} ion. It is observed that the COBI model calculation gives similar results to the independent-electron-approximation calculation [26] and is in good agreement with the experimental data. We can find that highly charged recoiled ions are copiously produced when they are impacted by fast highly charged Ar^{14+} ions. From single to 6-fold ionizations, the cross sections only drop off from 8.55×10^{-15} cm^2 to 1.3×10^{-16} cm^2. Even for 6-fold ionization, cross sections are still on the order of 1% of single ionization cross section. Totally, the multi-charged fractions contribute more than half of the recoiled ions.

The calculated results of CO molecules impacted respectively by 2.4 MeV/u Ar^{14+} ions are compared with the experimental data in **Figure 4**. As can be observed, between the two molecular descriptions COBI model gives the better agreement between experiments and theory. From **Table 2**, we find that highly charged recoiled ions are copiously produced, multi-electron removal is about 30% of the ionizing events. Note that the slopes of the curves do not increase

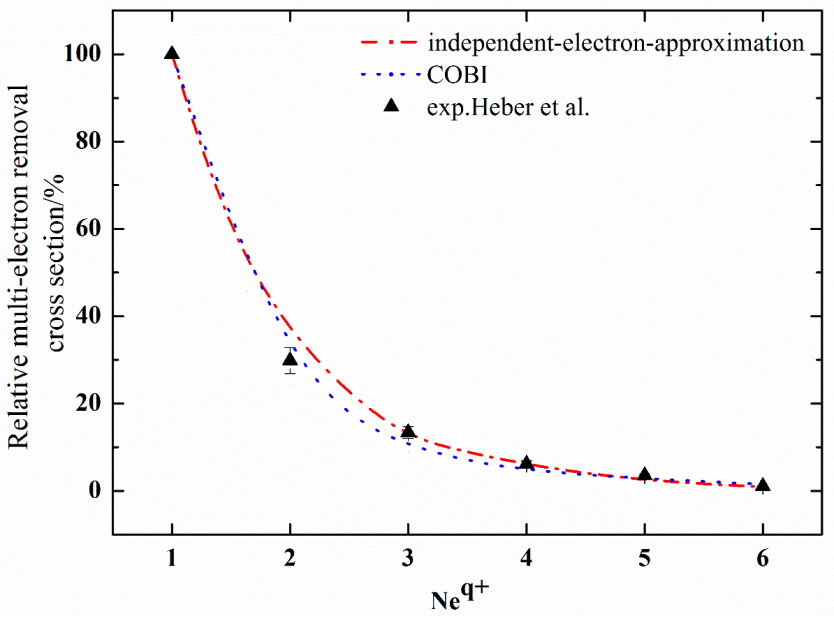

Figure 3. Relative multiple ionization cross sections of Ne for 2.4 MeV/u Ar^{14+} ion impact. The dot line and dash dot line represent the COBI model results and independent-electron-approximation calculations respectively, symbols denote the experimental data.

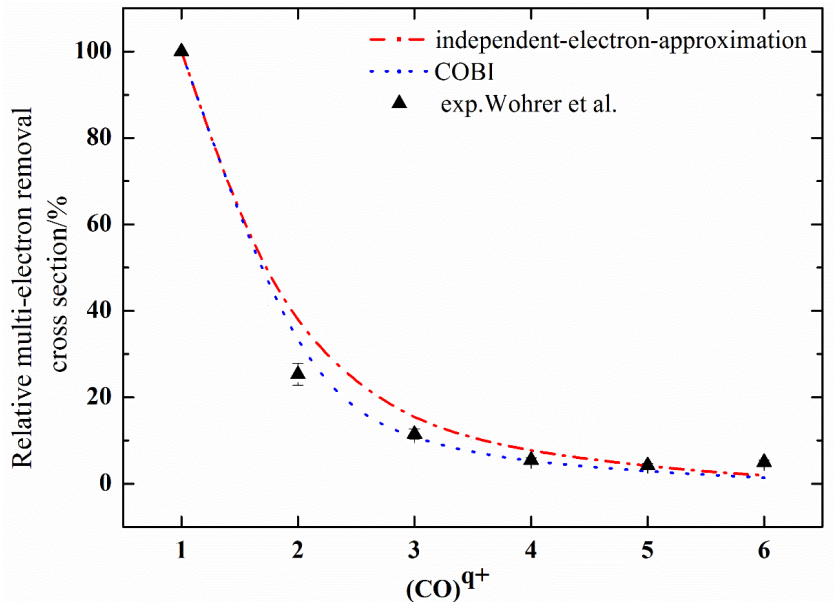

Figure 4. Relative multiple ionization cross sections of CO for 2.4 MeV/u Ar^{14+} ion impact. The dot line and dash dot line represent the COBI model results and independent-electron-approximation calculations respectively, symbols denote the experimental data.

Table 2. Absolute cross sections (in 10^{-15} cm^2) for multiple ionization of Ne and CO by 2.4 MeV/u Ar^{14+} ion impact.

	σ_1	σ_2	σ_3	σ_4	σ_5	σ_6
Ne	8.55	2.06	0.77	0.39	0.24	0.13
CO	14.4	3.27	1.34	0.72	0.40	0.20

rapidly with the increase of the recoiled ion charge states. The COBI model is on the assumption that single electron release probability is an important parameter in determining the multiple ionization cross sections induced by very high-q and fast projectiles. According to Equations (1)-(4), the single electron release probability is proportional to $(q/E)^{0.5}$. This is quite different from the data and the calculation results in the perturbation regime, where the slope increases quickly with ionization degree increasing. Moreover, one can see that the data of Ar^{14+} + Ne and Ar^{14+} + CO collisions do not exhibit a significant difference. The fractions of double and triple ionization cross section are some 20% and 10% respectively; for the 6th fold ionization, the relative cross section is about 1%. Moreover, the data of 2.4 MeV/u Ar^{14+} +CO and 6.7 MeV/u Xe^{44+} +CO collisions [14] are very similar. The results show that the multiple ionization of atoms and simple molecules is related to the number and ionization energy of outer electron, and has nothing to do with the type of projectiles in a strong coupling regime ($q/v > 1$).

4. Conclusions

In this paper, our previous work of COBI model is extended to the descriptions of the multiple ionization cross section of Ne and CO induced by very high-q fast projectiles ($q/v > 1$). By using the IEVM and the multinomial distribution, the COBI model results are in excellent agreement with available experimental data of atoms and molecules. The measurement and model both show that the relative multiple ionization cross sections present a rather weak dependence on q and E, which is quite different from the data and the calculation results in the perturbation regime. The COBI model assumes that multiple ionization is directly proportional to the single electron release probability P_r is proportional to $(q/E)^{0.5}$, which is insensitive to q and E, with the complementary effect of P_r and $1 - P_r$ in multinomial distribution, the relative multiple ionization cross sections will show weak dependence on q and E.

From a series of studies, we think that multiple ionizations of atoms and molecules impacted by very high-q fast projectiles ($q/v > 1$) probably can be seen as sequential release processes occurring at large distances rather than violent binary encounters between projectile and target electrons.

In addition, the simplicity of the COBI model in obtaining the multiple ionization fractions of complex molecules induced by very high-q fast projectiles ($q/v > 1$), providing a convenient way to study the high linear energy transfer (LET) irradiation of biological matter when a rapid computation is required as

happens in radiobiology.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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