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Total ionization cross sections in particle and antiparticle collisions with rare gases

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Abstract

In this contribution we analyze the total ionization cross sections by impact of electrons, positrons, protons and antiprotons in Ne, Ar, Kr and Xe. We compare theoretical results using the continuum distorted wave eikonal initial state approximation with a detailed compilation of the available experimental data for the four projectiles in each target. The charge and mass effects, and the convergence at intermediate energies are discussed, which are important issues for antiparticle normalization. We remark the influence of the post-collisional Auger-like electron emission, which is decisive to describe the total ionization of Kr and Xe at impact velocities above 9 a.u.

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1. Introduction

Total ionization cross sections have been experimentally and theoretically studied for years. Reviews and compilations of data are available in the literature. For example, the electron impact compilations by Tawara and Kato (1987) [1] and by de Heer *et al* (1979) [2], and the review and suggested values for proton impact by Rudd *et al* (1985) [3]. The research on antiparticle impact processes has become a very active field in the last three decades. A recent *state of art* of antiproton impact ionization can be found in [4], and for developments and applications of the physics of positron impact in [5]. Well-known reviews on particle and antiparticle collisions are those by Schultz *et al* (1991) [6] and by Knudsen and Reading (1992) [7].

In this contribution we focused on the total ionization cross sections by $|Z| = 1$ projectiles, i.e. protons, antiprotons, electrons, and positrons, with a double purpose:

- to analyze the charge and mass effects, and convergence at high energies, important for antiparticle normalization,

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- to show the influence of post-collisional ionization in the total ionization at high impact energies.

The differences in the ionization cross sections by light (electrons and positrons) and heavy (protons and antiprotons) projectiles in the intermediate to low energy region is experimentally clear. The theoretical description of these collisions involves considering the projectile trajectories, finite momentum transferred and the energy thresholds. In the high energy region all these cross sections are expected to converge. However, this convergence and the minimum impact velocity for these cross sections to be equal is different for antiprotons, positrons or electrons. Usually the antiproton and positron data are normalized to electron data at high energies rather than to proton impact values. One of the objectives of this work is to present a broad view of the convergence of the different $|Z| = 1$ projectiles and possible alternatives for the antiparticle normalization, even at lower energies than 1 keV employed up to now [8, 9].

In the high energy region the post-collisional ionization is also important, which affects also the total ionization cross sections [10]. The post-collisional electron emission is a consequence of the ionization of the inner-shells that ends in multiple ionization due to rearrangement of the excited target (Auger-type processes). The manner of including the post collisional ionization within the total cross sections is by calculating the multiple ionization, both in direct collisions and in post collisional processes [11]. To analyze the particle-antiparticle behavior we consider the ionization of the heaviest rare gases (from Ne to Xe) by proton, antiproton, electron and positron impact. An extended compilation of the available data in comparison with the ab-initio CDW-EIS total cross sections [10, 11, 12, 13] is presented for the sixteen systems considered (four projectiles and four targets). The values studied here are pure ionization, not including charge transfer (for proton impact) or positronium formation.

In section 2 we summarize the theoretical calculations of total ionization cross sections from the multiple ionization values, and the inclusion of post collisional contributions. In section 3 we display and discuss the comparison of the total ionization values for the four projectiles. Finally some conclusions are presented in section 4

2. Theoretical considerations about the total ionization cross sections

The total ionization cross section, σ_{Total} , is calculated theoretically as

$$\sigma_{Total} = \sum_{nlm} \sigma_{nlm} \quad (1)$$

with σ_{nlm} being the contribution of the ionization of an electron initially in the nlm sub-shell. This value is also known as the inclusive single ionization cross section (ionization of at least one electron). Instead, the multiple ionization cross section $\sigma_{(q)}$ of exactly q electrons is known as exclusive cross section [14]. The gross cross and count cross sections are defined as different additions of the multiple ionization values as

$$\sigma_{gross} = \sum_q q \sigma_{(q)} \quad (2)$$

and

$$\sigma_{count} = \sum_q \sigma_{(q)}. \quad (3)$$

Physically, σ_{gross} is a measure of total electron production, while σ_{count} measures the production of positive ions. The *count/gross* difference is known and tabulated experimentally [2]. However, *total* ionization cross section has been used indistinctly for *gross* or *count* cross sections, producing misunderstandings. For example, in a recent review by Chiari *et al* (2014) [15] a discrepancy between the data by Marler *et al* (2005) [16] and by van Reeth *et al* (2002) [17] is mentioned, without noting that count cross sections were compared with gross cross sections. Similarly, the electron impact *count* cross sections by Sorokin *et al* (2000) [18] have been compared with the theoretical gross cross sections by Bartlett and Stelbovits (2002) [19], with the reasonable disagreement for Kr and Xe at high energies.

Sant'Anna *et al* (1998) [14] demonstrated that σ_{Total} given by Eq. (1) is exactly the same that σ_{gross} given by Eq. (2).

$$\sum_{nlm} \sigma_{nlm} = \sum_q q \sigma_{(q)}, \quad (4)$$

As explained in [10], the measurements of total electron flux, σ_{Total}^{exp} , include not only those electrons emitted in direct collisional process but also the post-collisional ones. So the experimental total ionization values can be theoretically calculated if the post-collisional ionization (PCI) is included. If we call $\sigma_{(q)}^{PCI}$ to the ionization cross section of exactly q electrons including direct ionization and PCI, then

$$\sigma_{Total}^{exp} = \sum_q q \sigma_{(q)}^{PCI}, \quad (5)$$

with

$$\sum_q q \sigma_{(q)}^{PCI} \geq \sum_q q \sigma_{(q)} = \sum_{nlm} \sigma_{nlm}. \quad (6)$$

The equality in Eq. (6) may be valid for low to intermediate impact energies, for which post-collisional ionization (PCI) is not important, or for targets with few electronic shells, because inner-shell ionization is decisive for PCI. As quantified in table 1 of [10] for proton and antiproton impact, the influence of PCI in the total cross sections is negligible in Ne and only 5% in Ar for high impact velocities (i.e. $v > 10$ a.u.). But for Kr and Xe, this difference exceeds 20% and 30% at similar high velocities [10].

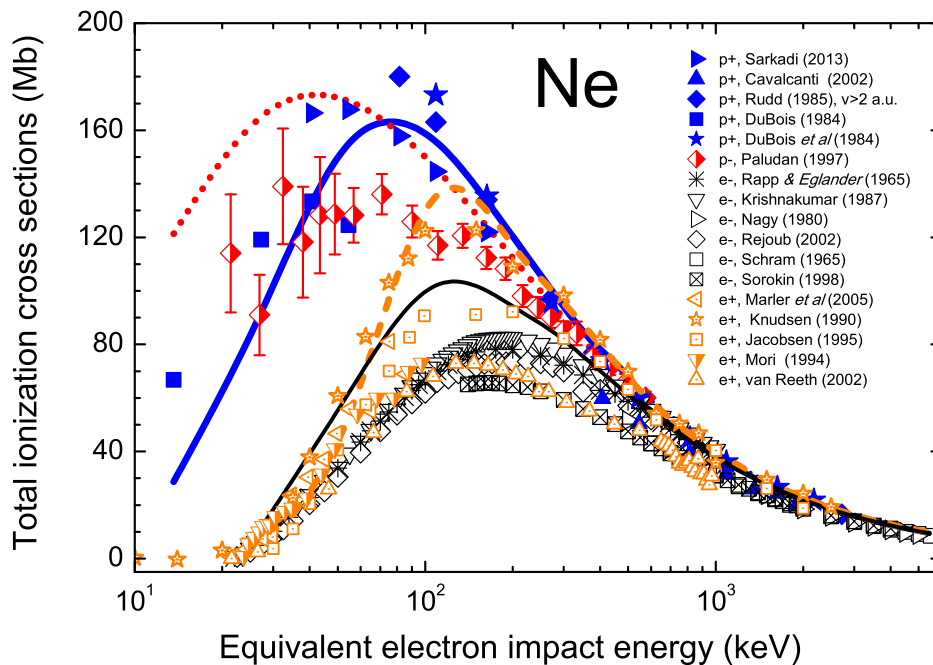


Fig. 1. Total ionization cross section of Ne by proton ($p+$), antiproton ($p-$), positron ($e+$) and electron ($e-$) impact. Different colors are employed for a visual improvement of the comparison: blue for protons, red for antiprotons, orange for positrons and black for electrons. Curves: CDW-EIS results by proton (thick solid-line), antiproton (dotted-line), positron (dashed-line) and electron impact (thin solid-line). Experimental data: **by proton-impact**, Sarkadi (2013) [42], Cavalcanti (2002) [22], Rudd (1985) [3], DuBois (1984) [39], DuBois *et al* (1984) [40]; **by antiproton-impact**, Paludan (1997) [44]; **by positron-impact**, Marler (2005) [16], Mori (1994) [48], van Reeth (2002) [17], Jacobsen (1995) [8], Knudsen (1990) [47]; **by electron-impact**, Schram (1965) [29], Rapp and Eglander-Golden (1965) [31], Nagy (1980) [32], Krishnakumar (1987) [33], Rejoub (2002) [35], Sorokin (1998) [38].

The underestimation at high impact energies of the total ionization cross sections by using Eq. (1) has been known for years. In 1977 McGuire [20] carried out a first approximation to the inclusion of PCI of inner-shells with a weighted addition of cross sections of different sub-shells. Despite being very extended in time, the experimental total

ionization cross sections of Kr and Xe, could not be theoretically described until recently, when multiple ionization and the post-collisional Auger contribution was included in the multiple ionization cross sections [10, 12].

The theoretical description of multiple ionization by energetic heavy ions corresponds to the last fifteen years for heavy ions [11, 21, 22, 23, 24], and only recently for light projectiles [12, 13]. These calculations work within the independent electron approximation, which is an advantage for dealing with multi-electronic targets (analytical expressions and computational codes), but also its limitation. This formalism that has been successful to describe the multiple ionization by protons [11, 25], antiprotons [10], electrons and positrons [12, 13], and proved to be better for Kr and Xe than for Ne or Ar [26]. The CDW-EIS total ionization cross sections included in section 3 take into account the PCI. They have been calculated in [10, 12, 13] by adding the multiple ionization cross sections as in Eq. (5).

3. Results and discussion

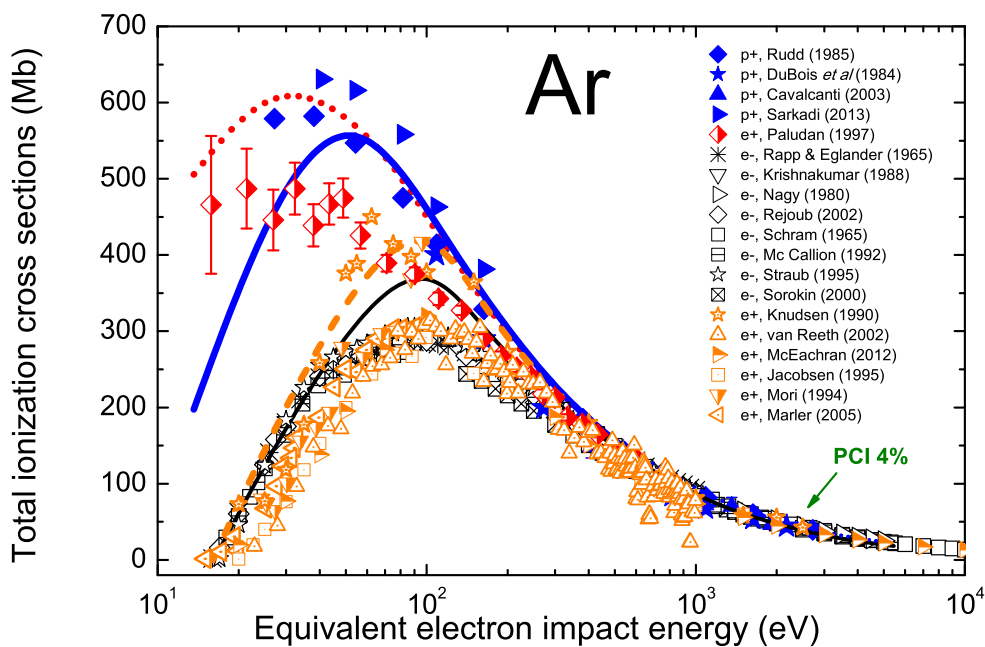


Fig. 2. Total ionization cross section of Ar by proton, antiproton, positron and electron impact. Colors and curves as in figure 1. Experimental data: **for electron-impact**, Schram (1965) [29], Rapp and Eglander-Golden (1965) [31], Nagy (1980) [32], Krishnakumar (1987) [33], Rejoub (2002) [35], Straub (1995) [37], McCallion (1992) [36], Syage (1992), Sorokin (2000) [18] (count cross sections); **for proton-impact**, DuBois *et al.* (1984) [40], Rudd (1985) [3], Cavalcanti (2003) [23], Sarkadi (2013) [42]; **by antiproton-impact**, Paludan (1997) [44]; **by positron-impact**, by Marler (2005) [16], by Mori (1994) [48], by McEachran (2012) [54], van Reeth (2002) [17], Jacobsen (1995) [8], Knudsen (1990) [47].

The experimental data compiled here is very extended, covering to our knowledge, all the values available in the literature: for electron impact the values by Schram and collaborators [27, 28, 29, 30], and by Rapp and Eglander-Golden (1965) [31], to the present measurements [18, 32, 33, 34, 35, 36, 37, 38]; for proton impact the data by DuBois, Manson and Rudd [3, 39, 40, 41] up to now [22, 23, 42]; for antiparticles the experimental work corresponds only to the last 30 years, the measurements for antiproton impact ionization by Knudsen group at CERN [43, 44, 45], and for positron impact in [8, 9, 16, 46, 47, 48, 49, 50, 51, 52, 53, 54].

In figures 1 to 4 we display this compilation of experimental data together with the CDW-EIS results for the total ionization cross sections including PCI for protons, antiprotons, electron and positron impact in the four rare gases in

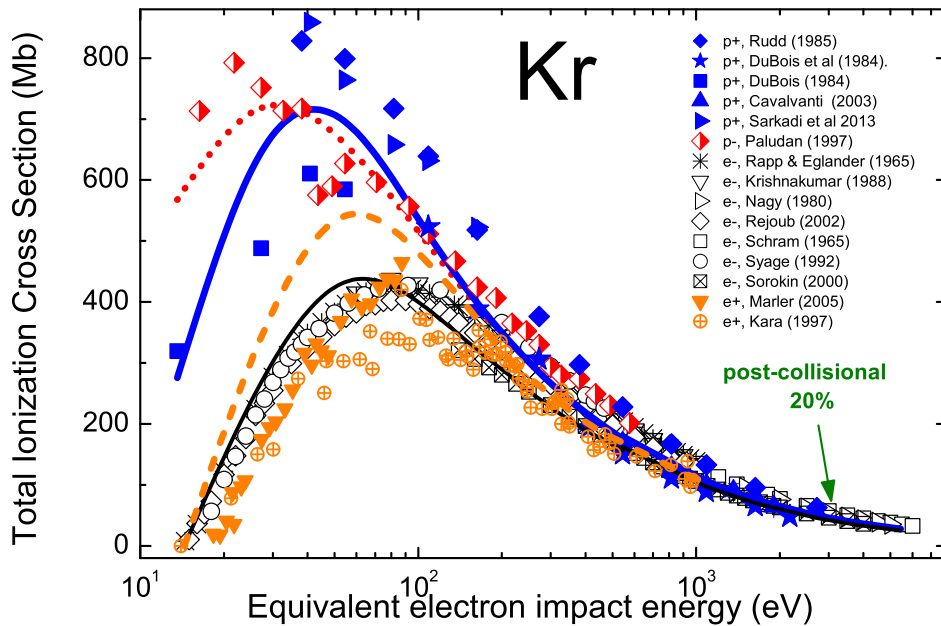


Fig. 3. Total ionization cross section of Kr by electron and proton-impact. Colors and curves as in figure 1. Experimental data: **by electron-impact**, Schram (1965) [29], Rapp and Eglander-Golden (1965)[31], Nagy 1980) [32], Krishnakumar (1988) [33], Rejoub (2002) [35], Syage (1992) [34], Sorokin (2000) [18] (count cross sections); **by proton-impact**, DuBois (1984) [39], DuBois *et al* (1984) [40], Rudd (1985) [3], Cavalcanti [23], Sarkadi (2013) [42]; **by antiproton-impact**, Paludan (1997) [44]; **by positron-impact**, by Marler (2005) [16], Kara (1997) [9].

[10, 12, 13]. The comparison is performed on equal velocity, and the figures are plotted as function of the equivalent electron impact energy. The change to proton impact is forthright.

The experimental values shown in these figures have been measured directly as total ionization cross sections, σ_{Total}^{exp} , [3, 16, 29, 31, 48]; or they have been obtained from the experimental multiple ionization cross sections as $\sigma_{Total}^{exp} = \sum q \sigma_{(q)}^{exp}$, [8, 9, 17, 22, 23, 32, 33, 34, 35, 36, 39, 40, 44, 47]. The electron impact data by Sorokin and collaborators [18, 38] is also included despite being count cross sections because these values are usually used in normalization of data.

In general the CDW-EIS description of proton and antiproton values is correct within the experimental uncertainties. For light particles the description improves for Kr and Xe, while for Ne and Ar overestimates around the maximum. One explanation for this is that the CDW-EIS employs the independent electron approximation, being better for Kr or Xe (much more electrons involved) than for Ne or even for Ar [26]. It is worth noting that the curves displayed in these figures include PCI. This is indicated explicitly in figures 2, 3 and 4 with an inset showing the amount of PCI contribution.

Some general behaviors may be drawn from the comparison made in these four figures:

- Antiproton values are close to proton ones, and positron to electron around the maximum of the cross sections. This shows clearly the mass effect: smaller cross sections for electron and positron impact as compared to the equally charged heavy projectiles. As expected, equal mass affects the ionization more than equal charge in the low and intermediate energy region.
- Theoretically, the CDW-EIS predicts the positron impact ionization cross sections to be above the electron impact for all the targets. It may be said that positrons are more effective than electrons in the ionization. This is difficult to be tested experimentally. There are positron measurements above the electron data ([8, 47, 48])

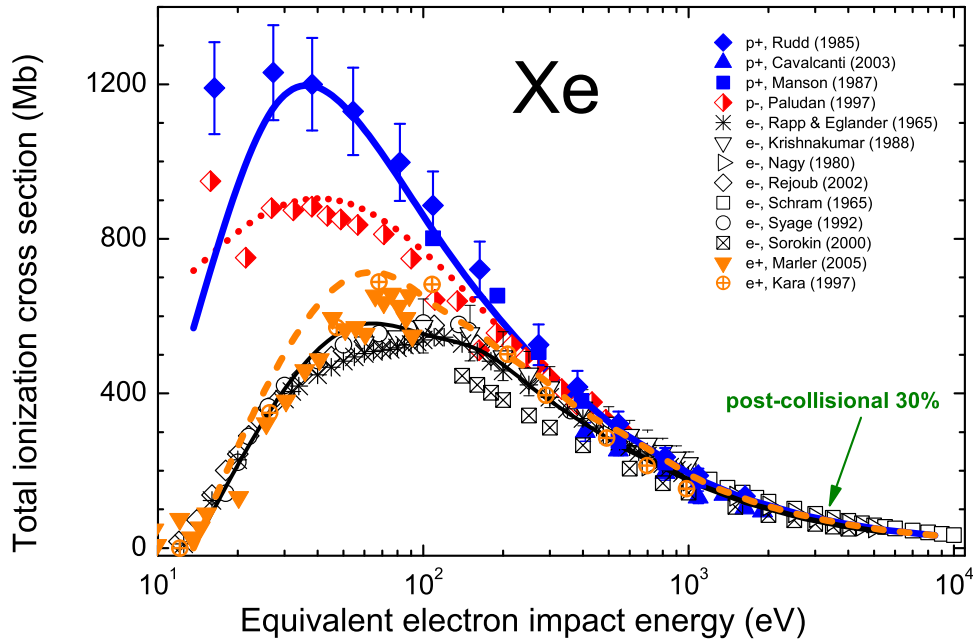


Fig. 4. Total ionization cross section of Xe by electron and proton-impact. Colors and curves as in figure 1. Experimental data: for electron-impact, Schram (1965) [29], Rapp and Eglander-Golden (1965) [31], Nagy (1980) [32], Krishnakumar (1988) [33], Rejoub (2002) [35], Syage (1992) [34], Sorokin (2000) [18] (count cross sections); for proton-impact, Cavalcanti (2003) [23], Rudd (1985) [3], Manson (1987) [41]; by antiproton-impact, Paludan (1997) [44]; by positron-impact, by Marler (2005) [16], Kara (19917) [9].

for Ne and Ar, [9, 16] for Xe), but there are also measurements similar to the electron-impact ones. The normalization of the positron measurements to electron impact data plays an decisive role in this even though it is performed at 1 keV.

- Around and below the maximum of the cross sections, the CDW-EIS results ordered from highest to lowest are: antiproton > proton > positron > electron for Ne and Ar; antiproton \simeq proton > positron > electron for Kr; proton > antiproton > positron > electron for Xe. This inversion in the antiproton/proton relative values for heavy targets is found theoretically and also experimentally! This issue represents an interesting challenge for future research.
- At high energies, the four $|Z| = 1$ projectiles are quite similar for impact energies above 1 keV electron impact (1.8 MeV proton impact). But antiproton values converge to proton ones for much lower energies, depending on the target.
- The electron impact data converge to the proton values around 600 keV for Ne and Ar, and 1 keV for Kr and Xe, while positron impact cross sections converge to the equal velocity proton impact ones at even lower energies than electron: equal charge seems to be more decisive than equal mass at sufficiently high energies.
- In the high energy region, the experiments are nicely described for the sixteen systems considered here. In the case of Kr and Xe this is due to the calculation using the multiple ionization values taking into account PCI.

4. Conclusions

In this contribution we present a detailed comparison of the total ionization cross sections of Ne, Ar, Kr and Xe by ± 1 charged particles, including a compilation of the experimental data available for the 16 different systems, and

the theoretical CDW-EIS results. The mass effect (protons/positrons, electrons/antiprotons) and the charge effect (proton/antiproton, electron/positron) are clear experimentally, and correctly described by the theory. The CDW-EIS total cross sections are obtained from the multiple ionization ones including the post-collisional Auger type contributions to the final ionization. This proved to be very important for the heaviest target considered here. This comparison also shows details on the convergence of the cross section for the different projectiles that cast doubts on the normalization of data in certain cases, and may be useful for the future work.

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