IRSTI 29.27.47 https://doi.org/10.26577/phst2024v11i1a11

Analytical formula for multiple ionization cross sections of rare gas atoms by electron and positron impact

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(Received March 26, 2024; received in revised form April 30, 2024; accepted May 11, 2024)

The paper presents an analysis of data on the single and multiple ionization cross sections of rare gas atoms by electron impact and single ionization cross sections by positron impact. To approximate the cross section for single ionization of atoms of rare gases, as well as a large number of atoms of other elements, a semi-empirical formula with four parameters was proposed, which gives an accuracy of several percent in a wide energy range. Here we generalize our approach to the case of multiple ionization of an atom by electron impact and single ionization by positron impact. For the selected sets of experimental data, the recommended values of the approximation coefficients for a wide range of collision energies have been calculated and determined. The approximation formula reproduces the values of the ionization cross sections for rare gases in a wide range of energies with an accuracy of the order of error of the available experimental data and it has physically reasonable asymptotics.

Key words: multiple ionization cross sections, electron impact, positron impact, approximation of cross sections.
PACS number(s): 34.80.Bm, 34.80.Dp, 51.50.+v, 52.80.Dy.

1 Introduction

To analyze and simulate processes in low-temperature plasma, it is necessary to know the kinetic coefficients, in particular, the cross sections for ionization of atoms by electron impact. This work is a continuation of our works [1-4], in which experimental and theoretical data on electron-atomic collision cross sections are analyzed [5-11]. In 1912, Thomson, based on the consideration of the problem of the collision of two electrons, one of which is at rest, determined the following formula for the ionization cross section [5]:

$$\sigma_{ionization}(\varepsilon) = \frac{\pi e^4}{\varepsilon}\left(\frac{1}{I} - \frac{1}{\varepsilon}\right) \equiv 4\pi a_0^2 \frac{Ry^2(\varepsilon - I)}{I\varepsilon^2}, \quad (1)$$

where I – ionization energy, $\varepsilon > I$ – incident electron energy, a_0 – Bohr radius, Ry=13.6 eV. This formula gives a linear increase in the ionization cross section at a small excess of the collision energy over the ionization potential. The formula for approximating the initial part of the curve of dependence of the ionization cross section on the energy of the incident electron was first proposed by Compton and van Voorhis in 1925 [6]: $\sigma_{ionization}(\varepsilon) = C_i(\varepsilon - I), \quad I < \varepsilon < 2I$. Vanier in [11] took into account the interaction of the incident and bound electrons and obtained the following approximation of the initial section:

$$\sigma_{ionization}(\varepsilon) = C_i(\varepsilon - I)^{1.127}, \quad \varepsilon > I. \quad (2)$$

The first ionization potential I can serve as the natural scale of energy when an electron collides with an atom, so here and below it is convenient to pass to the dimensionless energy $x = \varepsilon / I$, $\Delta = x \quad x - 1, x > 1$. In the case of high energies ($\varepsilon > 300$ eV) dependence of the ionization cross section on the electron-impact energy can be described by the Born-Bethe type formula:

$$\sigma_{ionization}(\varepsilon) \propto \frac{\ln x}{x}. \quad (3)$$

Formulas of that type are widely used for fitting the excitation and ionization cross sections (see, e.g. [12]).

In our paper [4], we proposed a formula for the electron impact ionization cross section of an atom with four approximation coefficients α, β, γ, δ:

$$\sigma_{ionization}(\varepsilon) = \frac{\alpha \Delta x^{\delta}}{(1+\beta \Delta x)^{\gamma}}. \quad (4)$$

Here the constant α has the dimension of area, and the constants β, γ, δ are dimensionless quantities. To search for them, the problem of minimizing the root-mean-square relative deviation of cross sections from their experimental values was solved using the coordinate descent method. For $\alpha = 4\pi a_0^2 (Ry/I)^2, \beta = 1, \gamma = 2, \delta = 1$ formula (4) coincides with Thomson's formula (1). The maximum value of the cross section according to this formula is achieved when Δx = δ/(β(γ − δ)). Formula (4) allows one to take into account the deviation of the dependence of the cross section from linearity near the threshold, and at high energies it allows one to take into account the logarithmic correction of the Bethe-Born approximation. It turns out that a power-law decrease in the ionization cross section $\sigma_{ionization}(x) \propto 1/x^{\gamma-\delta}$ at high energies makes it possible to obtain quite satisfactory agreement with experimental and theoretical data for all inert gases. The errors of the approximation of experimental data by analytical dependence (4) for rare gases, alkali and vapors of other metals, as well as for H, Si, P, S lie in the range of 1-10% [4], which corresponds in order of magnitude to the error of the experiments themselves.

In principle, there are hundreds of experimental and theoretical works on the determination of ionization cross sections. But at the same time, errors are often not given, because, generally speaking, they cannot be determined without knowing the exact answer. By increasing the number of measurements, the statistical error can be reduced, but in the case of an experiment, a systematic error remains. Therefore, the experimental data themselves from various sources may differ tenfold, while errors in the range of 3-7% are often indicated. In addition, the ionization of an atom as a multielectronic system, based on theoretical consideration, usually involves the use of simplifying assumptions, which makes it difficult to determine the accuracy of the result.

2 Approximation of the single ionization cross sections by 1 term formula

The largest amount of experimental and theoretical data is available for cross sections of single ionization of atoms. The observed variation in the experimental data for cross sections is due to the fact that the cross section is not a directly measurable quantity, but is calculated as a result of processing other measured parameters. To analyze and approximate them, we took data from [13,14], where recommended cross-section values were obtained for single ionization of rare gas atoms by analyzing experiments and theories.

The work [15] presents the results of measurements of the ionization cross sections of helium, neon, argon, krypton, and xenon upon electron impact for energies in the range from the first ionization threshold to 1000 eV. In addition to single ionization cross sections, this work obtained data on multiple ionization cross sections. Briefly, during cross-section measurement, the vacuum chamber is filled with the target gas and the electron gun generates pulses. These pulses pass through the gas between the two plates, and the electrons produced by ionization are going at a collector. The data from [15], which claim higher accuracy, confirm the correctness of the single ionization cross sections recommended in [13, 14].

The results of the approximation of experimental data [13,14] according to formula (4) for inert gases are given in [4]. In this work, for comparison, we added the results of approximation of experimental data on single ionization [15]. The root-mean-square relative error of approximation in both cases lies in the range from one to five percent, i.e. within experimental errors. As an example, Fig. 1 for Xe shows the experimental data from [14] and [15], as well as their approximations according to formula (4). The data [14] on the right tail is significantly higher than in [15]. Table 1 shows the values of the parameters for approximating the ionization cross sections of rare gas atoms as well as the values of the root-mean-square relative error, the maximum ionization cross section $\sigma(\varepsilon_m)$ and the energy ε_m, at which it is achieved.

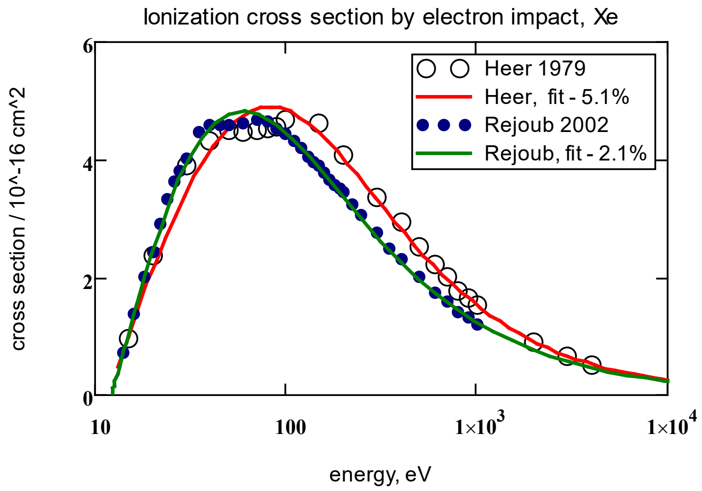

Figure 1 – Single ionization cross sections of Xe atoms by electron impact.

Table 1 – Parameter values for approximating the ionization cross sections of rare gas atoms by electron impact.

Atom, I, eV	α, Å²	β	γ	δ	Δ, %	ε_m, *eV*	$\sigma(\varepsilon_m)$ Å²	Reference
2, He 24.59	0.406	0.330	2.01	1.11	1.0%	116	0.35	A, Heer, [13]
	0.372	0.312	2.03	1.13	1.6%	124	0.34	B, Rejoub, [15]
10, Ne 21.57	0.451	0.23	2.22	1.33	1.3%	162	0.71	A, Heer, [14]
	0.343	0.182	2.33	1.33	4.2%	179	0.67	B, Rejoub, [15]
18, Ar 15.76	3.19	0.326	1.92	1.08	2.5%	78	2.87	A, Heer, [14]
	4.26	0.541	1.93	1.26	3.6%	71	2.66	B, Rejoub, [15]
36, Kr 14.0	3.77	0.302	1.86	1.07	2.7%	77	3.82	A, Heer, [14]
	7.08	0.641	2.19	1.52	4.3%	64	3.61	B, Rejoub, [15]
54, Xe 12.13	3.66	0.178	1.66	0.836	5.1%	81	4.90	B, Heer, [14]
	5.64	0.365	1.79	1.05	2.1%	59	4.83	A, Rejoub, [15]

The analysis of the data presented in Table 1 allows us to estimate experimental errors and improve the accuracy of determining cross sections. It can be noted that there is a correlation between the approximation error of the experimental data [13-15] by the analytical dependence (4) and the proximity of the parameter β to the value of 0.33. Therefore, for He, Ne, Ar, Kr we recommend data from [13,14], and for Xe from [15]. In the last column of Table 1, the letter A – marks the most accurate approximation, and B – marks the less accurate one. Note that in the recommended approximations, the values of the coefficient δ are in the range from 1.05 to 1.33, i.e. the Vanier correction (2) with the value δ = 1.127 allows us to more correctly describe the initial part of the dependence of the ionization cross section on the collision energy.

Formula (4) approximates well the behavior of the dependence of ionization cross sections on energy for most elements (see [4]). But for some elements, as shown in Fig. 1 for Xe, this dependence has a two-humped nature due to the knocking out of electrons from the inner shells. In these cases, a fairly good accuracy is achieved by approximating experimental data with two-term formula

$$\sigma_{ionization}(\varepsilon) = \frac{\alpha_1 \Delta x_1^{\delta_1}}{(1+\beta_1 \Delta x_1)^{\gamma_1}} + \frac{\alpha_2 \Delta x_2^{\delta_2}}{(1+\beta_2 \Delta x_2)^{\gamma_2}},$$

where $x_1 = \varepsilon / I_1$, $\Delta x_1 = x_1 - 1$, $x_1 > 1$, $x_2 = \varepsilon / E_2$, $\Delta x_2 = x_2 - 1$, $x_2 > 1$, E_2 – potential from the inner shell. We used this two-term formula in [4] to approximate the single-ionization cross sections of

Xe, Cs, Cu, and U atoms, which made it possible to reduce the approximation error for these elements by one and a half times and qualitatively reproduce the two-humped nature of the dependence of the cross section on the collision energy.

3 Approximation of the multiple ionization cross sections of atoms by one term formula

With a sufficiently high energy of the incident electron, it can knock out several electrons at once:

$$e + A \rightarrow e + A^{n+} + ne, \quad n \geq 1$$

Analysis of the experimental data [16] on multiple ionization (MI) cross sections σ_N showed that the majority of the cross sections has a similar shape and the electron-impact energy dependence can be described by the Born-Bethe type formula (3) [17]. Namely, for cases with n>=3, based on formula (3), a semi-empirical formula for the dependence of the cross sections MI of atoms by electron-impact is obtained [18]:

$$\sigma_n(x) = \frac{\alpha_{n,N} Ry^2 (x-1)\ln x}{I_n^2 x^2}. \quad (5)$$

where dimensionless energy $x = \varepsilon / I_n$, $\Delta x = x - 1$, $x > 1$. The threshold energy $I_n = \sum_{i=0}^{n-1} I_{i,i+1}$, corresponds to the minimal ionization energy I_n, required to remove n outmost electrons, $I_{i,i+1}$ – is the one-electron ionization energy from the charge i to $i+1$. The coefficient $\alpha_{n,N}$ should depend only on two parameters: the number of ejected electrons n and the total number of the target electrons N, and a power-law approximation was found for it. Formula (5) does not allow correctly taking into account the asymptotes for $n=1, 2$, and for $n>2$ in many cases the error is very large. Semi-empirical formulas for the cross sections for the double ionization of light positive ions by electron impact were obtained in [19].

There is a large amount of experimental data for multiple ionization of rare gas atoms (see references in [20, 21]). We took more recent experimental data for multiple ionization of rare gas atoms from [15], which are in good agreement with the data from [20]. Table 2 shows the results of approximation of the cross section for multiple ionization of rare gas atoms by electron impact using formula (4). Figures 2-4 for Ne, Ar and Xe show experimental data from [14] and [15], as well as their approximations using formula (4).

Table 2 – Parameter values for approximating the multiple ionization cross sections of rare gas atoms by electron impact.

Atom	n, I_n, eV	α, Å^2	β	γ	δ	Δ, %	ε_m, eV	$\sigma(\varepsilon_m)$, Å^2
2, He	2, 79.01	0.005	0.643	3.59	2.25	3.7%	285	0.0013
10, Ne	2, 62.53	0.137	0.648	4.60	3.15	3.2%	272	0.0306
	3, 126.0	0.011	0.572	5.32	3.0	4.5%	411	0.0015
18, Ar	2, 43.39	12.48	1.89	4.07	3.04	6.2%	111	0.1803
	3, 84.30	0.014	0.45	2.44	1.43	32%	350	0.0089
	4, 144.1	0.005	0.63	8.76	6.96	19%	1028	0.0015
36, Kr	2, 38.36	121	2.68	4.68	3.8	3.0%	100	0.297
	3, 75.31	0.047	0.379	2.31	1.41	7.9%	387	0.039
	4, 127.8	0.078	0.94	4.75	3.84	2.5%	702	0.0097
56, Xe	2, 33.10	33.2	2.35	3.64	3.0	6.6%	99.0	0.471
	3, 64.15	127	2.35	5.69	4.78	14%	208	0.175
	4, 106.4	28.3	2.06	6.12	5.15	22%	380	0.0471
	5, 160.5	31.5	2.59	6.26	5.0	9.5%	406	0.0116
	6, 227.16	35.6	2.91	7.30	6.0	13%	587	0.0019

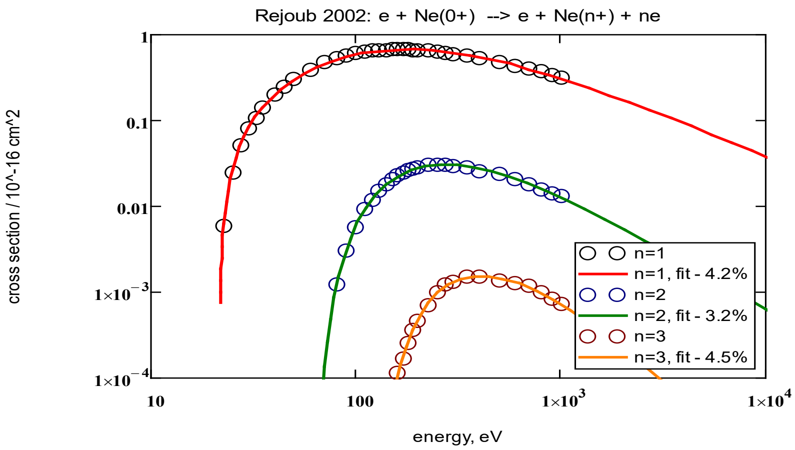

Figure 2 – Single, double and triple cross sections for ionization of Ne atoms by electron impact.

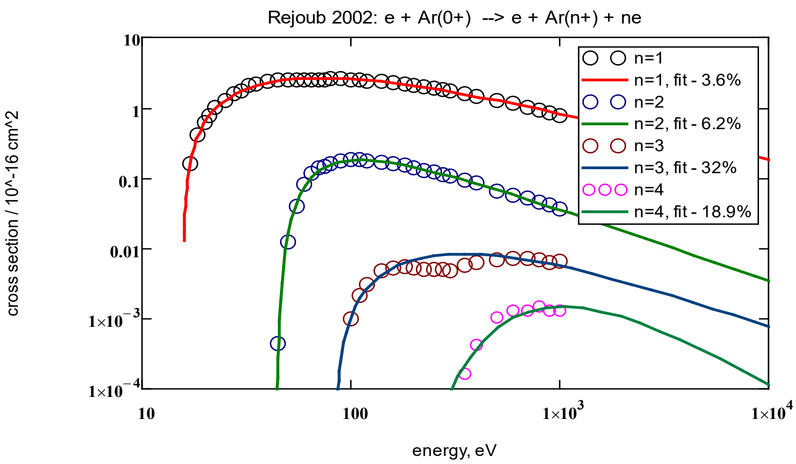

Figure 3 – Single, double, triple and four-fold cross sections for ionization of Ar atoms by electron impact.

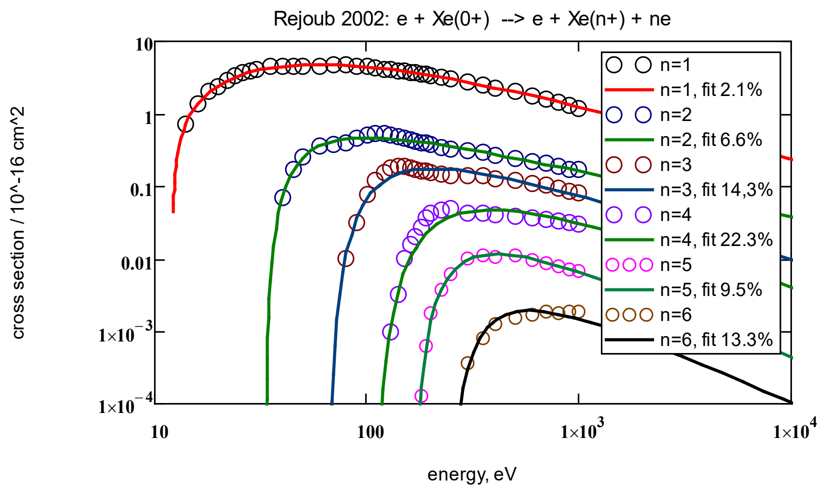

Figure 4 – Single, double, triple, 4-, 5- and 6--fold cross sections for ionization of Xe atoms by electron impact.

For triple and 4-fold ionization of Ar atoms and two-, three-, 4-, 5- and 6-fold ionization of Xe atoms, the cross-section curve has a two-humped character due to the ionization of electrons from the inner shells. To take this effect into account more accurately, it is necessary to use two-term approximation, as we did in [4] for Xe, Cs, Cu, and U.

4 Approximation of the single ionization cross sections of rare atoms by positron impact

The papers [22, 23] present the cross sections for ionization by a positron impact for atoms of rare gases. For these data, we calculated the approximation coefficients according to formula (4). The results are shown in Table 3.

Table 3 – Parameter values for approximating the multiple ionization cross sections of rare gas atoms by positron impact.

Atom	n, I_n	α, $Å^2$	β	γ	δ	Δ, %	ε_m, eV	$\sigma(\varepsilon_m)$, $Å^2$	Reference
2, He	1, 24.59	1.06	0.501	3.55	2.33	3.4%	118	0.54	Ratnavelu, [23]
10, Ne	1, 21.57	0.644 0.487	0.337 0.196	2.84 2.40	1.93 1.32	4.4% 3.1%	157 156	0.885 0.803	Kara, [22] Ratnavelu, [23]
18, Ar	1, 15.76	1.88	0.198	2.67	1.42	3.0%	106	2.96	Ratnavelu, [23]
36, Kr	1, 14.0	2.77 3.47	0.284 0.316	2.33 2.87	1.42 1.80	8.8% 7.2%	91 89	3.48 4.15	Kara, [22] Ratnavelu, [23]
56, Xe	1, 12.13	4.59 5.40	0.207 0.277	1.99 2.55	1.03 1.47	8.3% 5.6%	75 72	5.86 6.27	Kara, [22] Ratnavelu, [23]

Figure 5 shows cross sections of single ionization of helium atoms by electron-impact for experimental data from [13, 15] and positron impact for experimental data from [23].

Figure 6 shows cross sections of single ionization of krypton atoms by electron impact for experimental data from [14, 15] and positron impact for experimental data from [22, 23]. This figure clearly shows the more complex nature of the dependence of the ionization cross section by positron impacts compared to electron impacts. The reason apparently lies in an additional ionization channel with the formation of positronium in a positron-atom collision. In addition, measurements of positron-atomic collisions have a large error.

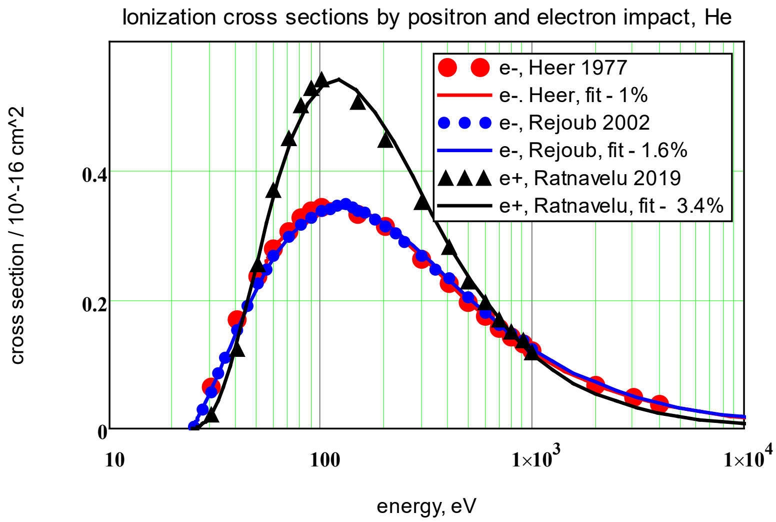

Figure 5 – Single-ionization cross sections of He by positron (e+) and electron (e-) impact.

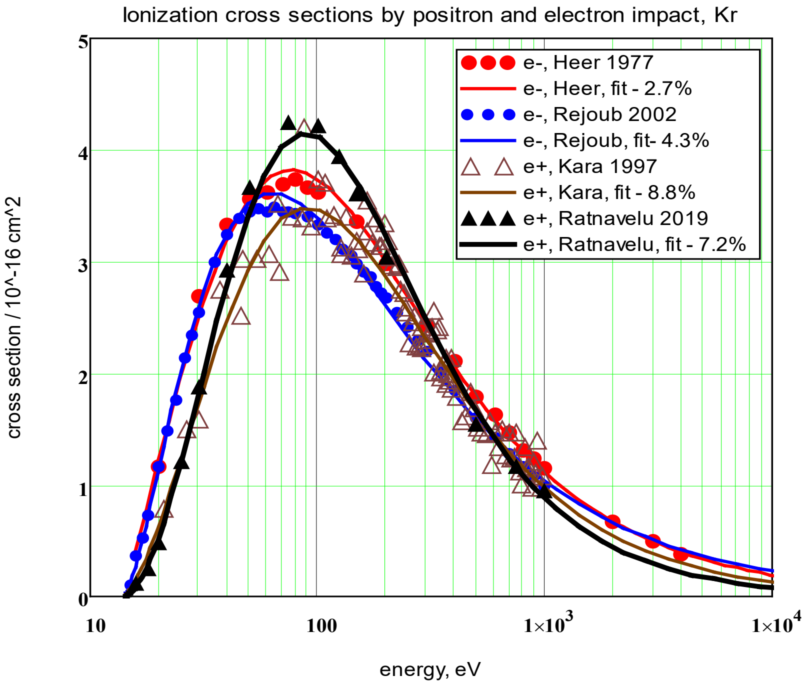

Figure 6 – Single-ionization cross sections of Kr by positron (e+) and electron (e-) impact.

5 Conclusions

Using the available and most reliable data on the ionization cross sections of atoms of inert gases, the cases of single and multiple ionization of atoms by electron impact and single ionization of atoms by positron impact are considered. For approximating the cross sections, a semi-empirical formula with four parameters is proposed. Smooth and asymptotically reasonable approximating dependencies make it possible to avoid errors in the numerical differentiation of experimental data, which in the mathematical sense is incorrect (that is, arbitrarily small errors in the data give an arbitrarily large error in the derivative). Therefore, the use of analytical formulas with physically reasonable asymptotes to find cross-section values by interpolation or extrapolation seems more preferable than the use of tabular experimental data.

The cross section of single ionization of atoms of rare gases by electron impact is approximated with an error of 1-3%. Since the error of the experimental data is an order of magnitude larger, the analysis of the fitting coefficients makes it possible to determine which data should be recommended for use.

Multiple ionization of atoms by electron impact is a more complex process in which the ionization of electrons from inner shells often plays an important role. But even in this case, it is possible to obtain an approximation error in the range of 3–30%. In order of magnitude, this error practically coincides with the error of the experimental data.

The cross section of single ionization of rare gas atoms by positron impact is approximated with an error of 3-9%. Since the ionization of an atom by a positron impact can be accompanied by the formation of positronium, this leads to a greater error in the experimental data.

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