Total Electron Scattering Cross Sections of He, Ne, Ar, Kr and Xe in the Energy Range 100 eV to 10 000 eV

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The total cross sections for electron scattering from He, Ne, Ar, Kr and Xe in the energy range from 100 eV to 10 000 eV have been calculated based on the optical-model potential. Our theoretical results are compared with the available experimental data. The consistency between them is also discussed. At higher energies (over 2000 eV for He, over 5000 eV for Ne, Ar, Kr and Xe), the total cross sections of electron scattering from these atoms are scarce, so our calculations will give a reference for further experimental and theoretical studies.

Key words: Electron Scattering; Total Cross Section; Optical-Model Potential.
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1. Introduction

The total electron scattering cross sections of He, Ne, Ar, Kr and Xe over a wide energy range are indispensable in many fields, such as plasma physics, astrophysics, atmospheric physics, semiconductor physics, and radiation physics [1 – 3]. A few groups have measured the total cross sections of electron scattering from these atoms above 1000 eV: for He, three experimental groups, Baek and Grosswendt [2], Ariyasinghe et al. [4], and Dalba et al. [5], for Ne, four experimental groups, Baek and Grosswendt [2], Ariyasinghe et al. [4], Garcia et al. [6], and Zecca et al. [7], for Ar, five groups, Ariyasinghe et al. [4], Garcia et al. [6], Zecca et al. [7], Baek and Grosswendt [2], and Noguerira et al. [8], for Kr, three groups, Ariyasinghe and Goains [1], Garcia et al. [6], and Zecca et al. [9], for Xe, three groups, Ariyasinghe and Goains [1], Garcia et al. [3], and Zecca et al. [9]. However, some discrepancies exist between the cross sections of the different experimental groups. For example, for He, the difference between the results of [4] and [5] is about 20% at 2000 eV. For Ar, the difference between those of [4] and [7] is about 10% at 3000 eV. For Kr, the difference between those of [1] and [9] is about 20% at 2500 eV. For Xe, the difference between those of [3] and [9] reaches 28% at 4000 eV. In the year of 2003, Salvat [10] and Stepanek [11] studied the electron elastic scattering by He, Ne, Ar, Kr and Xe with the optical-model potential. However, the total cross sections (elastic and inelastic) for electron scattering from these atoms have been seldom calculated in the energy range above 1000 eV.

With regard to these considerations, the total cross sections for electron scattering of He, Ne, Ar, Kr and Xe are calculated from 100 eV to 10 000 eV with the optical-model potential. These calculated cross sections are compared with the above experimental data.

2. Theoretical Model

In the present work, the optical-model potential method is employed to obtain the total cross sections for electron scattering from these atoms. In this method, the potential of an atom can be expressed as follows:

$$V_{\mathrm{opt}} = V_{\mathrm{s}}(r) + V_{\mathrm{e}}(r) + V_{\mathrm{p}}(r) + \mathrm{i}V_{\mathrm{a}}(r). \quad (1)$$

$V_{\mathrm{opt}}(r)$ is the complex optical potential. It incorporates all the important physical effects. The static potential $V_{\mathrm{s}}(r)$ for e-atom systems is calculated by using the atomic charge density, determined from the well-known Hartree-Fock atomic wave functions. Exchange potential $V_{\mathrm{e}}(r)$ and polarization potential $V_{\mathrm{p}}(r)$ are adopted by the form of Jiang, Sun, and Wan [12] and Zhang, Sun, and Liu [13], respectively. The imaginary part of the optical potential $V_{\mathrm{a}}(r)$ is the absorption potential, which represents the inelastic scattering. Here, we employ a semi-empirical absorption potential as discussed by Staszewska et al. [14], which is a function of atomic charge density, incident electron energy,

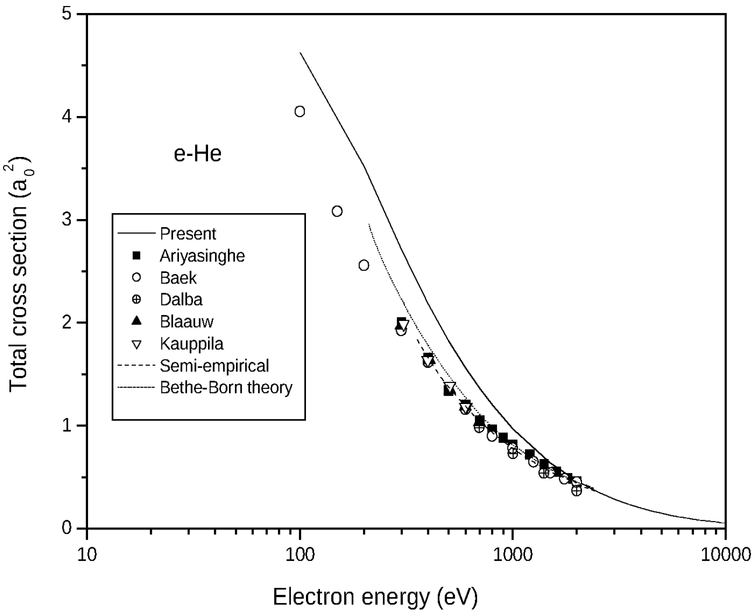

Fig. 1. Total cross sections for He. Solid line: present results. Experimental data: Baek and Grosswendt [2], Ariyasinghe et al. [4], Dalba et al. [5], Blaauw et al. [15], Kauppila et al. [16]. Semi-empirical data of Brusa et al. [17]. Bethe-Born theory [18, 19].

and the excitation threshold Δ of the target as following:

$$V_a(r) = -\rho(r)(T_L/2)^{1/2}(8\pi/5k^2k_f^3) \cdot h(k^2 - k_f^2 - 2\Delta)(A+B+C), \quad (2)$$

where

$$T_L = k^2 - V_s - V_e - V_p,$$

$$A = 5k_f^3/2\Delta,$$

$$k_f = [3\pi^2\rho(r)]^{\frac{1}{3}},$$

$$B = -k_f^3(5k^2 - 3k_f)/(k^2 - k_f^2)^2,$$

$$C = 2h(2k_f^3 + 2\Delta - k^2)(2k_f^2 + 2\Delta - k^2)^{5/2}/(k^2 - k_f^2)^2.$$

Here, k and k_f are the momentum of incident electron and the Fermi momentum, respectively. $\rho(r)$ is the atom charge density, $h(x)$ the Heaviside function.

The total cross sections σ_T of the atom are obtained by the method of partial waves:

$$\sigma_T = \frac{\pi}{k^2}\sum_{l=0}^{l_{max}}(2l+1)[|1-s_l|^2 + (1-|s_l|^2)]. \quad (3)$$

To obtain s_l we solve the following radial equation:

$$\left(\frac{d^2}{dr^2} + k^2 - 2V_{opt} - \frac{l(l+1)}{r^2}\right)u_l(r) = 0 \quad (4)$$

under the boundary condition

$$u_l(kr) \sim kr[j_l(kr) + i n_l(kr)] + s_l kr[j_l(kr) + i n_l(kr)], \quad (5)$$

where j_l and n_l are spherical Bessel and Neumann functions separately. The limit l_{max} is taken, which is enough to generate the higher partial-wave contributions until a convergence of less than 0.5% is achieved in the total cross section calculation.

3. Results and Discussion

With the optical-model potential, the total cross sections for electron scattering from He, Ne, Ar, Kr and Xe have been calculated in the energy range from 100 eV to 10 000 eV. The results are listed in Table 1. The present calculations along with the available experimental data are given in Figures 1 – 5.

In Figure 1, our results for He are compared with the measurements of [2], [4], [5], Blaauw et al. [15], Kauppila et al. [16], the semi-empirical data of Brusa et al. [17] and the calculated data of the Bethe-Born theory [18, 19]. From Figure 1, we can see that our results are higher than the measurements, the semi-empirical data, and the results of the Bethe-Born theory below 2000 eV. Fortunately, the difference decreases quickly as the incident energy of electron increases. Above 2500 eV, there are no experimental and theoretical results for He. So, further experiments and theoretical

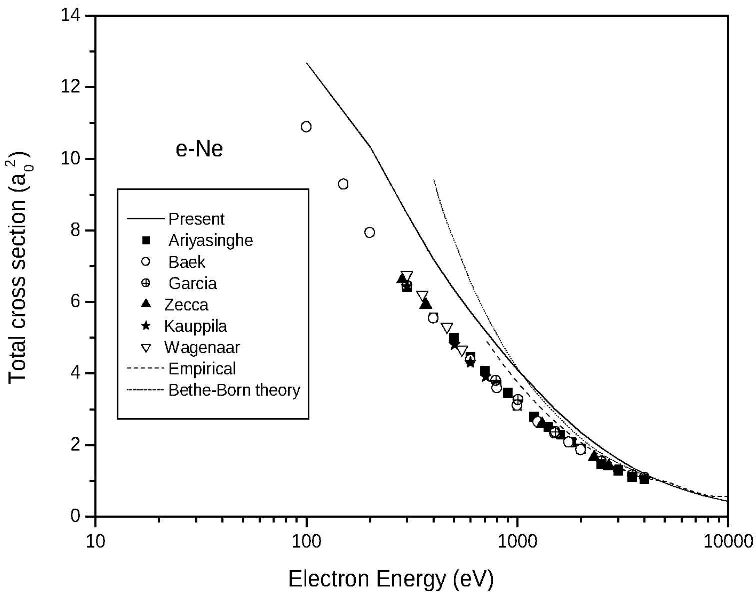

Fig. 2. Total cross sections for Ne. Solid line: present results. Experimental data: Baek and Grosswendt[2], Ariyasinghe et al. [4], Garcia et al. [6], Zecca et al. [7], Kauppila et al. [16], Wagenaar and De-Heer [20]. Empirical data of Garcia et al. [3]. Bethe-Born theory [18, 19].

Table 1. The calculated total cross sections for electron scattering from He, Ne, Ar, Kr and Xe from 100 eV to 10 000 eV in atomic units (a_0^2).

Energy (eV)	He	Ne	Ar	Kr	Xe
100	4.62	12.68	28.66	35.58	53.16
200	3.51	10.33	21.12	26.73	43.34
300	2.71	8.46	17.36	21.74	37.20
400	2.18	7.18	14.73	18.32	32.99
500	1.82	6.35	12.77	15.82	30.02
600	1.56	5.72	11.24	13.91	27.36
700	1.36	5.21	10.02	12.42	24.91
800	1.20	4.78	9.02	11.22	22.73
900	1.08	4.42	8.20	10.24	20.76
1000	0.97	4.10	7.51	9.43	19.00
1500	0.64	3.00	5.29	6.84	12.89
2000	0.46	2.35	4.08	5.45	9.62
2500	0.36	1.91	3.34	4.58	7.69
3000	0.29	1.60	2.83	3.98	6.41
3500	0.24	1.37	2.46	3.53	5.49
4000	0.20	1.19	2.18	3.19	4.81
4500	0.17	1.05	1.96	2.90	4.27
5000	0.15	0.93	1.78	2.67	3.85
5500	0.13	0.84	1.63	2.47	3.50
6000	0.12	0.76	1.51	2.29	3.20
6500	0.10	0.70	1.40	2.14	2.96
7000	0.093	0.64	1.31	2.01	2.75
7500	0.085	0.59	1.23	1.89	2.56
8000	0.077	0.55	1.15	1.78	2.40
8500	0.071	0.51	1.09	1.69	2.26
9000	0.065	0.48	1.03	1.60	2.14
9500	0.060	0.45	0.98	1.52	2.02
10000	0.055	0.42	0.93	1.45	1.92

calculations are required in the region from 2500 eV to 10 000 eV.

Figure 2 shows the variations of the total cross sections for electron-Ne scattering at energies from 100 eV to 10 000 eV. In the overlapping energy range, the experimental and our theoretical curve resemble well each other, while our results are systematically higher than the experimental data [2, 4, 6, 7, 16, 20]. Fortunately, the differences decrease as the incident energy increases. For example, the difference between the present results and the experimental data of [4] is about 31.6% at 300 eV, but descends to 14% at 4000 eV. Above 4000 eV, there are no experimental data, so our calculations are compared with the empirical data [3] and the results of Bethe-Born theory [18, 19]. Obviously, there is a very good agreement between them in the energy range from 4000 eV to 10 000 eV.

Total cross sections for Ar are plotted in Figure 3 and compared with the measurements of [2], [4], [6], [7], and [8]. The present results are in excellent agreement with all these experiments below 2500 eV. Above 2500 eV, the experiments of [4] and [6] are obviously higher than the present results. From 4000 eV to 10 000 eV, the empirical data [3] and the results of Bethe-Born theory [18, 19] are systematically higher than our results. Unfortunately, there are no experimental data in this energy range to be compared with our results.

In Figure 4, we present the total cross sections of Kr along with the experimental results of [1], [6], [9], Wagenaar and De-Heer [21], and Dababneh et

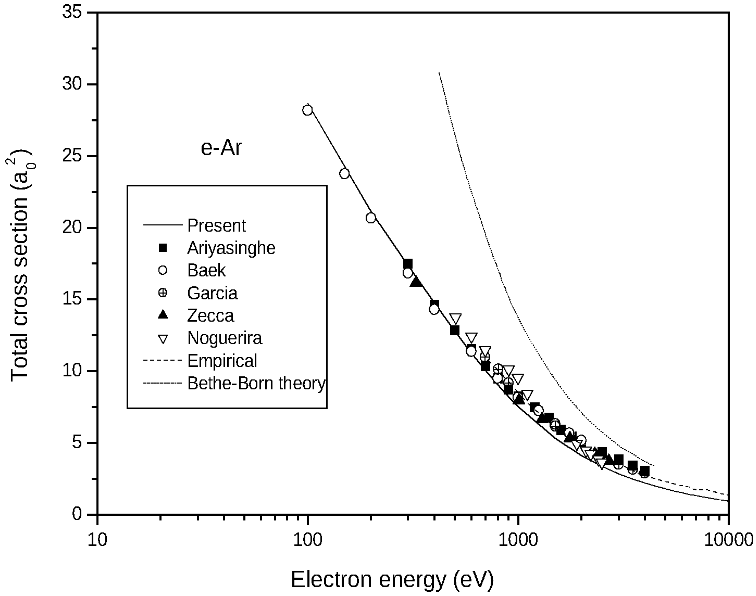

Fig. 3. Total cross sections for Ar. Solid line: present results. Experimental data: Baek and Grosswendt [2], Ariyasinghe et al. [4], Garcia et al. [6], Zecca et al. [7], Noguerira et al. [8]. Empirical data of Garcia et al. [3]. Bethe-Born theory [18, 19].

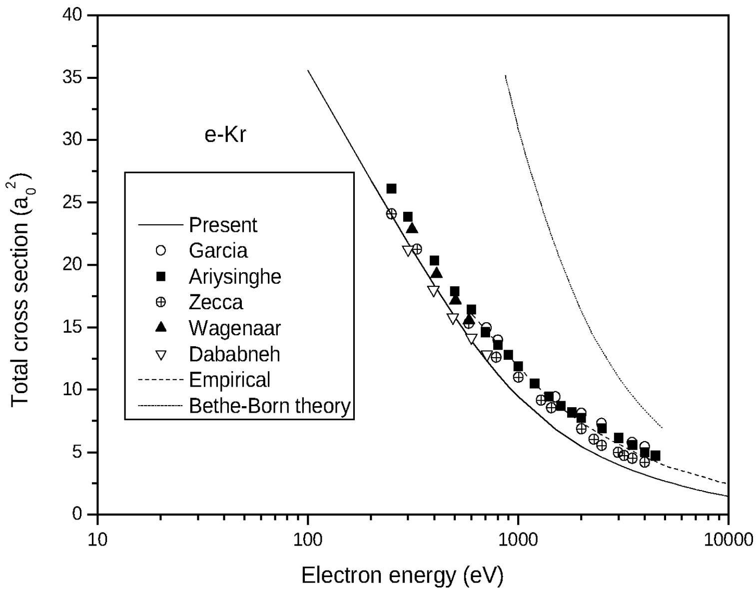

Fig. 4. Total cross sections for Kr. Solid line: present results. Experimental data: Ariysinghe and Goains [1], Garcia et al. [6], Zecca et al. [9], Wagenaar and De-Heer [21], Dababneh et al. [22]. Empirical data of Garcia et al. [3]. Bethe-Born theory [18].

al. [22]. The present results show good agreement with the experimental results below 1000 eV, while the results of the Bethe-Born theory [18] deviate far away from our results. Above 1000 eV, the measurements of [1], [6], [9], and the empirical data of [3] are much higher than the present results. At the same time, we must notice that large difference exists between the experimental results of [1] and [9] over 2000 eV.

Figure 5 shows the total cross sections of the present calculations for Xe together with the measurements obtained by [1], [3], [9], [21], [22], Nickel et al. [23] and Szmytkowski et al. [24] in the energy range from 100 eV to 10 000 eV. From Figure 5, we can see that the present results are in good accordance with all experimental data from 1000 eV to 2000 eV. Above 2000 eV, the experimental data of [9] are slightly higher than our results, while the experimental data of [3] are

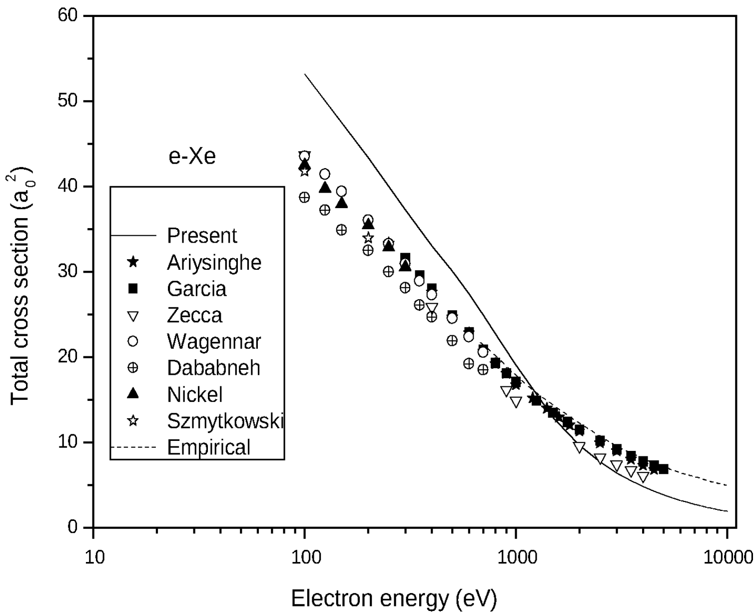

Fig. 5. Total cross sections of Xe. Solid line: present results. Experimental data: Ariysinghe and Goains [1], Garcia et al. [3], Zecca et al. [9], Wagennar and De-Heer [21], Dababneh et al. [22], Nickel et al. [23], Szmytkowski et al. [24]. Empirical data of Garcia et al. [3].

much higher than our results. In the energy range from 1500 eV to 10 000 eV, the empirical data of [3] are also much higher than the present results. Therefore, more precise measurements and theoretical results for Xe are needed to elucidate our calculations from 2000 eV to 10 000 eV.

4. Conclusions

In this paper, the total cross sections for electron scattering from He, Ne, Ar, Kr and Xe are calculated in the range from 100 eV to 10 000 eV. The calculated cross sections for He are higher than the available experimental cross sections below 2000 eV. For Ne, our cross sections are systematically higher than the experimental cross sections below 4000 eV, but the difference decreases with increasing energy. In the energy range from 4000 eV to 10 000 eV, our calculations give very good accordance with the empirical data. To our knowledge, no experimental total cross sections for electron scattering from Ar, Kr and Xe between 5000 eV and 10 000 eV seem to exist in the literature. We hope that more detailed experiments in this energy range can be presented in future.

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