J. Phys. B: At. Mol. Opt. Phys. **32** (1999) 1783–1794. Printed in the UK PII: S0953-4075(99)95673-0

Electron scattering by Ne, Ar and Kr at intermediate and high energies, 0.5–10 keV

G García†, M Roteta†, F Manero†, F Blanco‡ and A Williart§

† Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), Departamento de Fusión y Partículas Elementales, Avenida Complutense 22, 28040 Madrid, Spain

‡ Universidad Complutense de Madrid, Facultad de Física, Departamento de Física Atómica Molecular y Nuclear, Avenida Complutense sn, 28040 Madrid, Spain

§ Universidad Nacional de Educación a Distancia, Facultad de Ciencias, Departamento de Física de los Materiales, Senda del Rey sn, 28040 Madrid, Spain

Received 20 June 1998

Abstract. Semi-empirical total cross sections for electron scattering of noble gases (Ne, Ar and Kr) in the energy range 0.5–10 keV have been obtained by combining transmission-beam measurements for impact energies up to 6 keV with an asymptotic behaviour at higher energies according to the Born–Bethe approximation. The influence of the forward electron scattering on the experimental system has been evaluated by means of a Monte Carlo electron transport simulation. Theoretical values have also been obtained by applying the Born approximation in the case of inelastic processes and by means of an atomic scattering potential for the elastic part. The results of these calculations show an excellent agreement with the semi-empirical values in the above-mentioned energy range.

1. Introduction

Recently, an extensive paper devoted to obtaining analytical partitioning of total cross sections (σ_T) for electron scattering in noble gases was published [1]. As mentioned therein, cross section values for electron scattering over a wide energy range are required in many scientific and technological applications (astrophysics, plasmas for fusion, detector response simulations). Therefore analytical or empirical expressions reproducing data accurately are very useful in computational work related to these applications. It is obvious that these analytical fits must be based on accurate experimental or theoretical results. However, for energies above 1 keV, some important aspects have not been taken into consideration in the empirical fits of Brusa *et al* [1]. At these energies, the only experimental values obtained by a linear transmission-beam technique are those published by García *et al* [2]. However, these results were not considered in [1]. Their analysis at these energies was based on the experimental data of Zecca *et al* [3, 4], which were obtained using a Ramsauer-type device [5]. In recent studies on electron–molecule scattering [6–8] we found serious discrepancies between our results at higher energies and those obtained with the latter technique. Moreover, in a recent paper [9] we have shown that the electrons scattered in the forward direction are the main source of systematic errors at these energies, even in experiments with a reasonable angular resolution, and could be the cause of this discrepancy. These considerations have prompted the present work. In this work, the influence, in the case of our experimental set-up

0953-4075/99/081783+12$19.50

[2], of the forward scattering on total cross section measurements for electron–atom (Ne, Ar, Kr) collisions has been studied by means of a Monte Carlo electron transport simulation for impact energies of 1, 2 and 3 keV. The result of this calculation has been used to correct the experimental values where the contributions of this effect were appreciable. By combining the corrected experimental values with an asymptotic behaviour at higher energies according to the Born–Bethe theory [10–13], an analytical expression for σ_T has been obtained, which reproduces to a good approximation the experimental results in the energy range from 0.5 to 6 keV and could be used to extrapolate these values to higher energies.

The contribution of both elastic and inelastic processes to the total cross section has been calculated by means of different approximations. As may be deduced from previous works [2, 8], the inelastic cross sections are well described, at these energies, by the Born–Bethe theory. The elastic part has been calculated by using an atomic potential to integrate the scattering equation. The total cross sections obtained by adding these theoretical results are in good agreement with those given by the above-mentioned semi-empirical formula.

2. Procedure

2.1. Transmission beam measurements

Transmission beam experiments are based on the measurement of the attenuation of a linear electron beam through a gas cell containing the atoms or molecules to be studied. The recorded beam intensity (I) follows the law

$$I = I_0 \exp(-nL\sigma_a) \tag{1}$$

where I_0 is the intensity of the primary beam, L is the interaction region length, n is the atomic density and σ_a is the measured apparent cross section. Since in a real experiment the electron beam is not infinitely narrow and the solid angle subtended by the detector is not zero, this measured apparent total cross section tends to be lower than the true total cross section (σ_T),

$$\sigma_T = \sigma_a(1 + \Delta) \tag{2}$$

where the correction term Δ represents the relative contribution of the electrons scattered into the detection angle. The magnitude of this term depends on the scattering geometry of

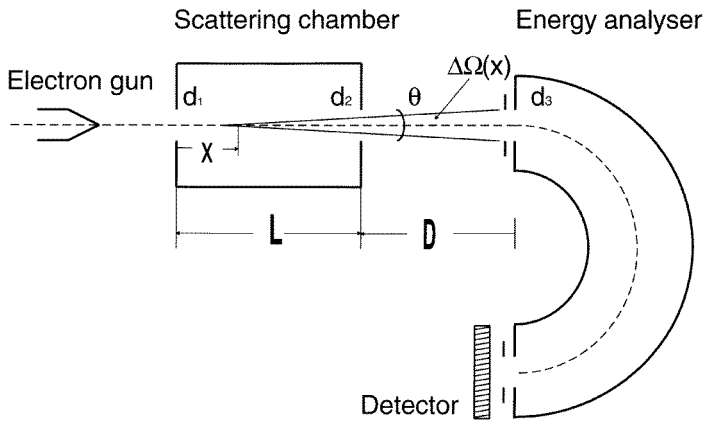

Figure 1. Sketch of the scattering geometry used in the experimental set-up of [2].

the experiment. The scattering geometry considered in the measurements of [2] is shown in figure 1. The geometrical characteristics are defined by the size of the apertures limiting the gas cell (d_1, d_2), which were of 2 mm in diameter in this case, the entrance aperture of the energy analyser (d_3), of 1 mm in diameter, the length of the collision chamber (L), which could be varied from 100 to 300 mm in this experiment and the distance between the end of the chamber and the entrance aperture of the analyser (D), which in this case was 50 mm.

The magnitude of the correction term due to the forward scattering can be evaluated by carrying out a Monte Carlo simulation of the electron transport through the experimental set-up used in [2].

2.2. Monte Carlo simulation

Calculations have been made for Ne, Ar and Kr at 1.0, 2.0 and 3.0 keV impact energies by using the elastic differential cross sections measured by Jansen *et al* [14] and Jansen and de Heer [15]. The corresponding total cross section data have been taken from [2]. Total elastic cross sections have been obtained by integrating an analytical fit to the differential cross section values given in [14, 15] by means of a nonlinear least-squares method. The inelastic part was evaluated by subtracting those values from the experimental total cross sections. As the energy resolution used in this experiment was sufficient to discriminate inelastic processes, the path of the colliding electrons was considered to terminate in the simulation when an inelastic collision takes place.

In accordance with the method used in [2], the simulation has been repeated for different target pressures ranging from 1 to 30 mtorr. Semi-logarithmic plots of the transmitted intensities (including and excluding elastically scattered electrons into the detection angle) were fitted by two straight lines. The relative difference between the simulated apparent and true cross sections $[(\sigma_T - \sigma_a)/\sigma_a]$ was deduced from the slope of these lines, and used to correct the measured σ_a.

2.3. Born–Bethe calculations

In accordance with [10–12], the total inelastic (σ_{inel}^{BB}) and the total elastic (σ_{el}^{BB}) cross sections for electron scattering by atoms, in a combined Born–Bethe approximation, can be written as

$$\frac{\sigma_{inel}^{BB}}{a_0^2} = 4\pi\left[M_{inel}^2\left(\frac{R}{E_0}\right)\ln\left(4c_{inel}\frac{E_0}{R}\right) + \cdots\right] \tag{3}$$

and

$$\frac{\sigma_{el}^{BB}}{a_0^2} = \pi\left[A_{el}\left(\frac{R}{E_0}\right) + B_{el}\left(\frac{R}{E_0}\right)^2 + C_{el}\left(\frac{R}{E_0}\right)^3 + \cdots\right] \tag{4}$$

respectively, where E_0/R is the incident energy in Rydberg units (1 Ryd = 13.605 eV) and a_0 is the Bohr radius. M_{inel}^2 and c_{inel} are defined in [12] as a function of the dipole-oscillator strength density per unit of excitation energy in the atom. Calculations of these parameters can be found in [12], for Ne and Ar, and in [13] for Kr. The parameters of the elastic part (A_{el}, B_{el} and C_{el}) are defined in [11] as

$$A_{el} = 8\int_0^\infty |Z - F(K)|^2 K^{-3}\,\mathrm{d}K \tag{5}$$

$$B_{el} = -Z^2 \tag{6}$$

$$C_{el} = 0 \tag{7}$$

where Z is the nuclear charge, K is the momentum transfer and $F(K)$ is the atomic form factor. Values of these parameters for Ne are given in [11]. The corresponding values for Ar and Kr can be calculated from the atomic form factors obtained by Salvat *et al* [16] by using an analytical screening function fitted to Dirac–Hartree–Fock–Slater self-consistent data.

By adding (3) and (4), the total cross section in the Born–Bethe approximation ($\sigma_{\mathrm{T}}^{\mathrm{BB}}$) can be written as

$$\frac{\sigma_{\mathrm{T}}^{\mathrm{BB}}}{a_0^2} = A_{\mathrm{tot}}\left(\frac{R}{E_0}\right) + B_{\mathrm{tot}}\left(\frac{R}{E_0}\right)\ln\left(\frac{E_0}{R}\right) + C_{\mathrm{tot}}\left(\frac{R}{E_0}\right)^2 + \cdots \tag{8}$$

where the constants A_{tot}, B_{tot} and C_{tot} can be deduced from the above-mentioned parameters.

2.4. Atomic potential calculations

As shown previously [2], the inelastic processes in collisions of electrons with Ne, Ar and Kr can be described in terms of the Born approximation for energies above 500 eV. Therefore, in the energy range from 0.5 to 10 keV, total inelastic cross sections can be deduced from equation (3). However, this approximation overestimates the elastic cross sections even at 10 keV. For this reason elastic processes have been studied here by replacing the atom by an appropriate scattering potential (V_{sc}). As may be seen in [17], this potential can be described for elastic processes as

$$V_{\mathrm{sc}}(r) = V_{\mathrm{s}}(r) + V_{\mathrm{e}}(r) + V_{\mathrm{p}}(r) \tag{9}$$

where $V_{\mathrm{s}}(r)$ is the static potential for the electron–atom system, which has been calculated by using the atomic charge density deduced from Hartree–Fock atomic wavefunctions [18]. $V_{\mathrm{e}}(r)$ is the exchange potential which has been represented by the following semiclassical energy-dependent formula derived by Riley and Truhlar [19]:

$$V_{\mathrm{e}}(r) = \tfrac{1}{2}\left[\tfrac{1}{2}k^2 - V_{\mathrm{s}}(r)\right] - \tfrac{1}{2}\left[\left(\tfrac{1}{2}k^2 - V_{\mathrm{s}}(r)\right)^2 + 4\pi\rho(r)\right]^{1/2} \tag{10}$$

where k is the momentum of the incident electrons ($k^2 = E_0/R$ in these units) and $\rho(r)$ the above-mentioned atomic charge density. Finally, $V_{\mathrm{p}}(r)$ in equation (9) represents the target polarization potential, which has been described by the formula given by Zhan *et al* [20].

By means of this potential, differential ($\mathrm{d}\sigma_{\mathrm{el}}/\mathrm{d}\Omega$) and integral ($\sigma_{\mathrm{el}}$) elastic cross sections have been obtained in a partial-wave expansion, given by

$$\frac{\mathrm{d}\sigma_{\mathrm{el}}}{\mathrm{d}\Omega} = \frac{1}{4k^2}\left|\sum_{l=0}^{l_{\max}}(2l+1)\left(\mathrm{e}^{2\mathrm{i}\delta_l} - 1\right)P_l(\cos\theta)\right|^2 \tag{11}$$

$$\sigma_{\mathrm{el}} = \frac{4\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1)\sin^2\delta_l \tag{12}$$

respectively. $P_l(\cos\theta)$ is the Legendre polynomial and δ_l the lth partial-wave phase shift, which arises from the asymptotic behaviour of the $u_l(r)$ radial wavefunction defined by

$$\frac{\mathrm{d}^2u_l(r)}{\mathrm{d}r^2} + \left[k^2 - \frac{l(l+1)}{r^2} - 2V_{\mathrm{sc}}(r)\right]u_l(r) = 0. \tag{13}$$

In order to obtain the lth partial-wave phase shift, the variable-phase technique [21] has been used and the corresponding equation, in terms of the $j_l(t)$ and $n_l(t)$ Riccati–Bessel functions,

$$\frac{\mathrm{d}\delta_l(r)}{\mathrm{d}r} = -\frac{V_{\mathrm{sc}}(r)}{k}[j_l(kr)\cos\delta_l(r) - n_l(kr)\sin\delta_l(r)]^2 \tag{14}$$

has been integrated numerically by means of an adaptive-step-size fourth-order Runge–Kutta algorithm [22].

The l_{max} limit in (11) and (12) was taken to ensure a convergence of the calculations within 1%. The phase shifts corresponding to high l values (above $l = 60$) were generated by using the effective range given by Jiang *et al* [17].

3. Results and discussion

3.1. Semi-empirical total cross sections

The magnitudes of the correction to the total cross section due to the forward scattering contamination, deduced from the Monte Carlo calculation, for Ne, Ar and Kr at impact energies of 1.0, 2.0 and 3.0 keV are shown in table 1. As may be seen in this table, this effect increases with energy, but in all cases is less than 1% even at 3.0 keV. The experimental total cross sections of [2], corrected for forward scattering contamination at 1.0, 2.0 and 3.0 keV, are also shown in table 1. These results have been compared with those predicted by the Born–Bethe

Table 1. Total cross sections, in units of a_0^2, obtained by correcting the measurements of [2] with the Δ value deduced from the Monte Carlo simulation for Ne, Ar and Kr.

	Ne		Ar		Kr	
Energy (keV)	Δ (%)	σ_T (a_0^2)	Δ (%)	σ_T (a_0^2)	Δ (%)	σ_T (a_0^2)
1.0	0.11	3.28	0.16	8.62	0.38	11.9
2.0	0.28	1.89	0.37	5.05	0.47	8.22
3.0	0.39	1.34	0.89	3.71	0.57	6.29

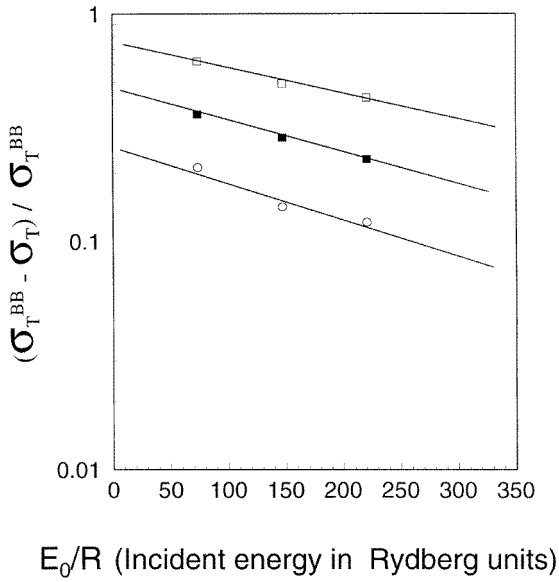

Figure 2. Relative difference between the experimental cross sections of [2] corrected by the Monte Carlo simulation (σ_T) and those predicted by the Born–Bethe approximation (σ_{BB}). ○, data for Ne; ■, data for Ar; □, data for Kr.

Table 2. Born–Bethe parameters, in atomic units, of equations (3), (4) and (8) for Ne, Ar and Kr.

Atom	A_{el}	B_{el}	C_{el}	M_{inel}	c_{inel}	A_{tot}	B_{tot}	C_{tot}
Ne	63.6	−100	0	1.393	0.4089	211.8	24.38	−314.2
Ar	231	−324	0	2.255	0.8114	800.9	63.90	−1018
Kr	592	−1296	0	2.709	0.6998	1954	92.22	−4071

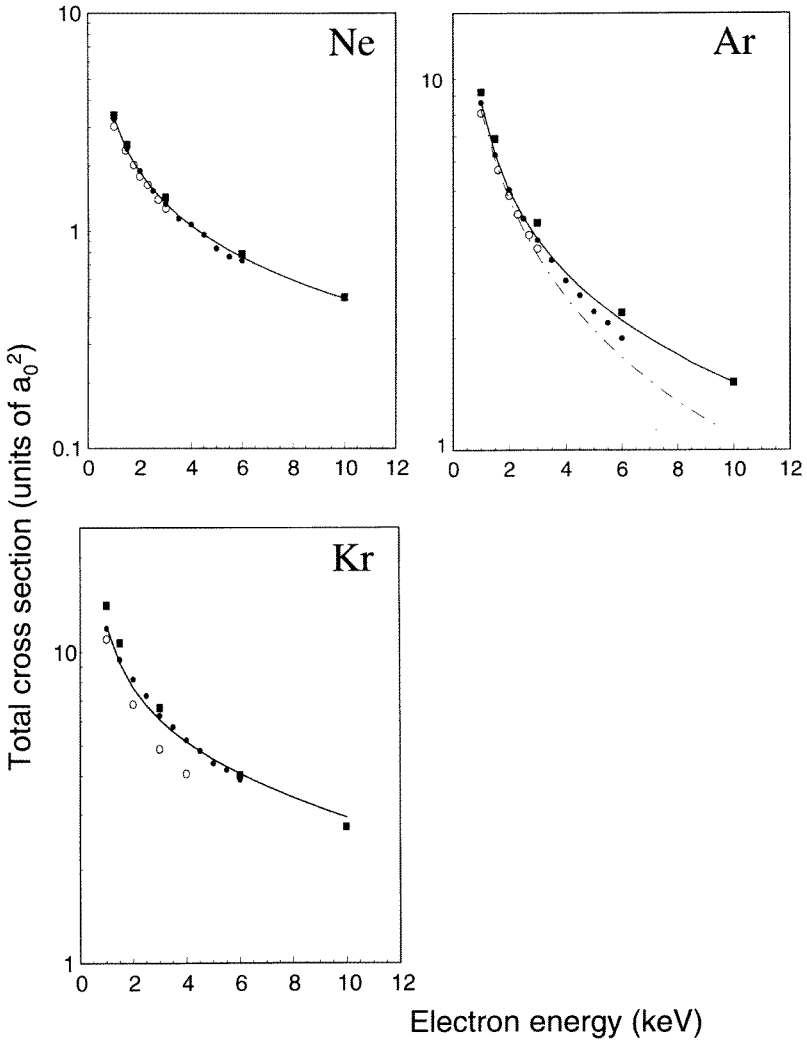

Figure 3. Total cross section (in units of a_0^2) for electron scattering by Ne, Ar, and Kr. ——, present semi-empirical values; — · —, empirical formula deduced in [1]; ●, experimental values of [2]; ○, measurements of [3, 4]; ■, theoretical values obtained by adding the Born–Bethe total inelastic cross section to our integral elastic cross section calculated by means of a scattering potential.

approximation for Ne, Ar and Kr. The parameters required to evaluate equations (3), (4) and (8) are shown in table 2. In all cases the values calculated with equation (8) are higher than the experimental ones. However, this discrepancy tends to be less as the energy increases. Hence

Table 3. Best fit of the parameters α and β (in Ryd) of equation (16).

Atom	α	β (in Ryd)
Ne	0.290	300
Ar	0.475	425
Kr	0.750	475

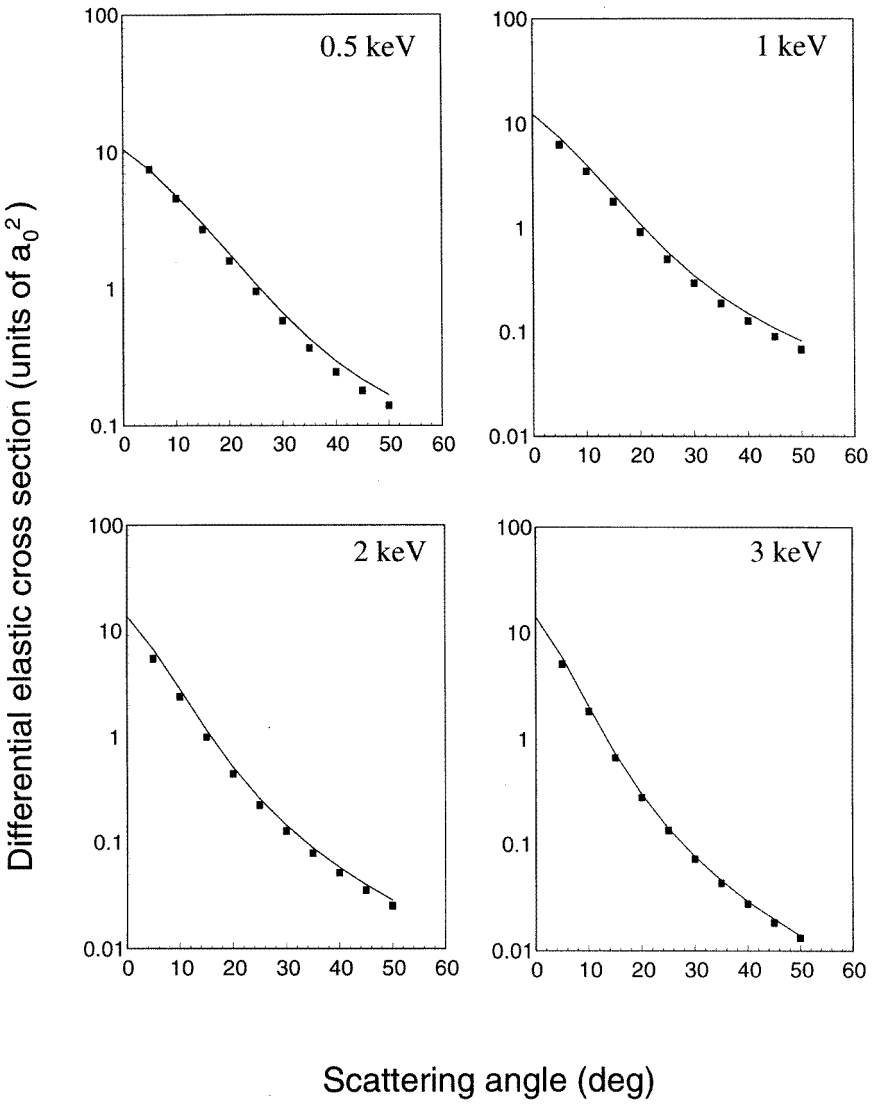

Figure 4. Differential elastic cross sections for electron scattering by Ne: ——, present calculations; ■, experimental values of Jansen *et al* [14].

we have studied their relative difference as a function of energy. Figure 2 is a semi-logarithmic plot of $\left(\sigma_{\mathrm{T}}^{\mathrm{BB}} - \sigma_{\mathrm{T}}\right)\big/\sigma_{\mathrm{T}}^{\mathrm{BB}}$ versus E_0/R. For each atom, the plotted points can be fitted by the

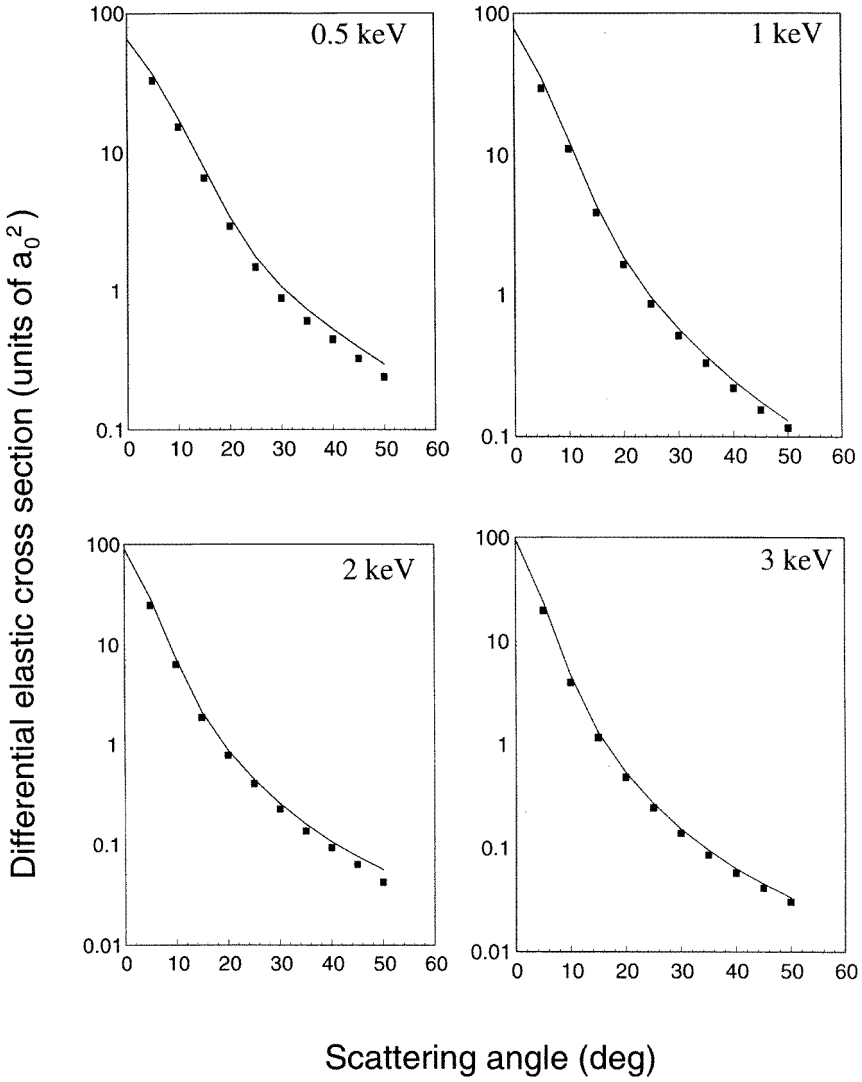

Figure 5. Differential elastic cross sections for electron scattering by Ar: ——, present calculations; ■, experimental values of Jansen *et al* [14].

following exponential function:

$$\frac{\sigma_{\mathrm{T}}^{\mathrm{BB}} - \sigma_{\mathrm{T}}}{\sigma_{\mathrm{T}}^{\mathrm{BB}}} = \alpha \exp\left(-\frac{1}{\beta}\frac{E_0}{R}\right). \tag{15}$$

Values of α and β for Ne, Ar and Kr are shown in table 3. Thus semi-empirical total cross sections for these atoms can be obtained from

$$\sigma_{\mathrm{T}} = \left[1 - \alpha \exp\left(-\frac{1}{\beta}\frac{E_0}{R}\right)\right]\sigma_{\mathrm{T}}^{\mathrm{BB}} \tag{16}$$

where $\sigma_{\mathrm{T}}^{\mathrm{BB}}$ is given by equation (8), and α and β in table 3.

In order to estimate the accuracy of the semi-empirical σ_{T} values, partial error contributions in (16) must be taken into account. In accordance with [2], the experimental errors have been

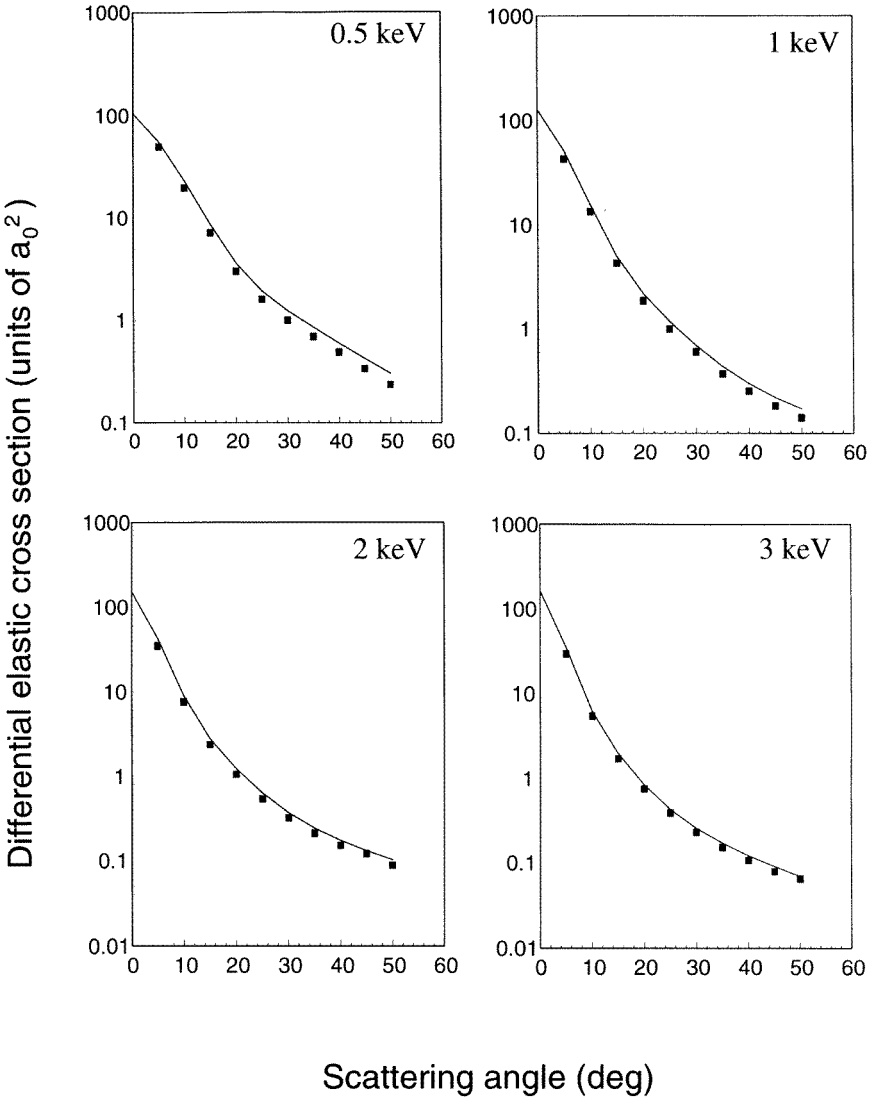

Figure 6. Differential elastic cross sections for electron scattering by Kr: ——, present calculations; ■, experimental values of Jansen and de Heer [15].

taken as ±6%. Concerning the σ_{BB} values, the spread of data for Ne, Ar and Kr obtained from wavefunctions of different accuracy [11–13, 16] is within 7%. Thus we have considered this value as a good indication of the precision of the calculations, with independence of the validity of the Born–Bethe approximation. By combining these uncertainties we have estimated an error limit of about 9% for the values given by (16) from 0.5 to 10 keV.

In figure 3 the semi-empirical total cross sections given by (16) are shown for Ne, Ar and Kr, respectively, together with previous experimental results [2–4] in the energy range from 1.0 to 10 keV. Data derived from the empirical formula proposed by Brusa *et al* [1] for Ar are also included for comparison. Similar data for Ne and Kr were not possible to obtain from equation (1) in [1] so either the value of the parameters needed or the equation must be wrong

in the paper by Brusa *et al* [1]. As may be seen in figure 3, there is a good agreement for Ne between the semi-empirical values given by (16) and previous experimental data. However, in the case of Ar, the empirical data of [1] based on the experiment of Zecca *et al* [3] deviate from the present ones when the energy increases, reaching discrepancies of about 40% at 10 keV. This discrepancy is even higher for Kr, where the result of Zecca *et al* [4] at 4 keV is about 30% lower than the present experimental and semi-empirical values. A similar situation was found in our measurements on electron–molecule scattering and has been discussed elsewhere [6–9]

Table 4. Integral cross section of electrons elastically scattered by Ne (in units of a_0^2).

Energy	Static potential (V_s)			V_{sc} (equation (9))
(keV)	[23]	[24]	This work	This work
1.0	1.74	1.76	1.73	1.93
1.5		1.32	1.30	1.43
2.0	1.05		1.04	
3.0			0.747	0.814
4.0	0.593		0.583	
6.0			0.406	0.439
8.0	0.321		0.312	
10.0			0.253	0.272

Table 5. Integral cross section of electrons elastically scattered by Ar (in units of a_0^2).

Energy	Static potential (V_s)			V_{sc} (equation (9))
(keV)	[23]	[24]	This work	This work
1.0	4.86	4.86	4.78	5.35
1.5		3.79	3.72	4.13
2.0	3.12		3.08	
3.0			2.32	2.55
4.0	1.91		1.88	
6.0			1.37	1.49
8.0	1.11		1.08	
10.0			0.895	0.969

Table 6. Integral cross section of electrons elastically scattered by Kr (in units of a_0^2).

Energy	Static potential (V_s)			V_{sc} (equation (9))
(keV)	[23]	[24]	This work	This work
1.0	6.68	7.42	6.58	7.41
1.5		6.03	5.31	5.91
2.0	4.61		4.53	
3.0			3.59	3.93
4.0	3.07		3.02	
6.0			2.34	2.53
8.0	1.97		1.93	
10.0			1.65	1.78

3.2. Theoretical elastic and inelastic cross sections

The differential elastic cross sections, obtained by the method described above (equation (11)), for electron scattering by Ne, Ar and Kr are shown in figures 4–6, respectively, at impact energies of 0.5, 1.0, 2.0 and 3.0 keV. The experimental results of Jansen *et al* [14] and Jansen and de Heer [15] are also included for comparison. As may be seen in these figures, our calculations are in good agreement with the experimental values. The corresponding integral elastic cross sections for Ne, Ar and Kr, given by (12), are shown in tables 4–6, respectively, for energies ranging from 1 to 10 keV. Previous calculations of elastic scattering cross sections for noble gases were made by Riley *et al* [23] and by Fink and Yates [24] considering a static potential with relativistic corrections. We have checked our computational method by integrating equation (13) only with the static term (V_s) of the potential (9). As may be seen in tables 4–6, data obtained in this way reproduce the results of [24], also confirming that relativistic corrections for Ne, Ar and Kr are not relevant in the energy range from 0.5 to 10 keV. The contribution of the exchange term in (9) tends to be significant when the energy decreases, introducing a correction of the integral cross sections of between 3% and 7% at 400 eV. The effect of the polarization term (V_p) was found to be appreciable for the whole energy range, leading to corrections to the integral elastic cross sections of the order of 10%.

Finally, theoretical total cross sections have been obtained by adding the integral elastic cross section values of tables 4–6 to the inelastic ones given by the Born–Bethe theory (3). Data obtained in this way are in good agreement with our semi-empirical results over the whole energy range considered (see figure 3).

4. Conclusions

The semi-empirical method proposed here gives reliable total cross sections (within 9%) for electron scattering by atoms in the energy range from 0.5 to 10 keV. By using theoretical approximations we have obtained a partition into elastic and inelastic processes in accordance with the present semi-empirical results. In the energy range considered, inelastic collisions can be described in terms of the Born–Bethe theory. However, a scattering potential calculation is required to obtain the elastic part in agreement with previous experimental values [14, 15]. The consistency of our previous total cross section measurements [2] and the calculated values has also been demonstrated. However, the previous measurements of Zecca *et al* [3, 4] for Ar and Kr, using a Ramsauer-type apparatus, deviate from the present theoretical and semi-empirical results when the energy increases, reaching discrepancies, in the case of Kr, of about 40% at 4 keV. For these atoms, the energy dependence given by the present semi-empirical formula for the total cross section is in agreement with that predicted by the Born–Bethe theory at high energy, while the E^{-1} dependence deduced by Brusa *et al* [1] from the experimental data of Zecca *et al* [3, 4] diverges from this theoretical prediction when the energy increases. These considerations seem to indicate that experimental data obtained by using a Ramsauer-type apparatus at high electron energies (above 1 keV) must be revised.

Acknowledgments

This work was performed with partial financial support from the Spanish DGES (project no PB96-0136).

References

[1] Brusa R S, Karwasz G P and Zecca A 1996 *Z. Phys.* D **38** 279
[2] García G, Arqueros F and Campos J 1986 *J. Phys. B: At. Mol. Phys.* **19** 3777
[3] Zecca A, Oss S, Karwasz G, Grisenti R and Brusa R S 1987 *J. Phys. B: At. Mol. Phys.* **20** 5157
[4] Zecca A, Karwasz G, Brusa R S and Grisenti R 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 2737
[5] Dalba G, Fornasini P, Grisenti R, Lazzizzera R, Ranieri J and Zecca A 1981 *Rev. Sci. Instrum.* **52** 979
[6] García G and Manero F 1996 *Phys. Rev.* A **53** 250
[7] García G and Manero F 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 4017
[8] García G and Manero F 1998 *Phys. Rev.* A **57** 1069
[9] García G, Roteta M and Manero F 1997 *Chem. Phys. Lett.* **264** 589
[10] Inokuti M 1971 *Rev. Mod. Phys.* **43** 297
[11] Inokuti M and McDowell M R C 1974 *J. Phys. B: At. Mol. Phys.* **7** 2382
[12] Inokuti M, Saxon R P and Dehmer J L 1975 *Int. J. Radiat. Phys. Chem.* **7** 109
[13] Inokuti M, Dehmer J L, Baer T and Hanson J D 1981 *Phys. Rev.* A **23** 95
[14] Jansen R H J, de Heer F J, Luiken H J, van Wingerden B and Blaaw H J 1976 *J. Phys. B: At. Mol. Phys.* **9** 185
[15] Jansen R J and de Heer F J 1976 *J. Phys. B: At. Mol. Phys.* **9** 213
[16] Salvat F, Martínez J D, Mayol R and Parellada J 1987 *Phys. Rev.* A **36** 467
[17] Jiang Y, Sun J and Wan L 1995 *Phys. Rev.* A **52** 398
[18] Cowan R D 1981 *The Theory of Atomic Structure and Spectra* (London: University of California Press)
[19] Riley M E and Truhlar 1975 *J. Chem. Phys.* **63** 2182
[20] Zhang X Z, Sun J F and Liu Y F 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 1893
[21] Calogero F 1967 *Variable Phase Approach to Potential Scattering* (New York: Academic)
[22] Willian H P 1994 *Numerical Recipes in Fortran* (Cambridge: Cambridge University Press)
[23] Riley M E, McCallum C J and Biggs F 1975 *At. Data Nucl. Data Tables* **15** 443
[24] Fink M and Yates A C 1970 *At. Data* **1** 385