Total electron scattering cross sections of Kr and Xe in the energy range 250–4500 eV

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Total electron scattering cross sections are reported for Kr and Xe for 250–4500 eV electrons by measurement of the electron-beam intensity attenuation through a gas cell. These cross sections are compared with the previous experimental measurements and the predictions by theoretical and semiempirical models. Discrepancies in experimental cross sections between different experimental groups are explained using the oscillator strengths and inelastic threshold of electron-energy-loss spectra. The correlation between the total electron scattering cross section and the atomic radius is discussed for Ne, Ar, Kr, and Xe atoms.

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I. INTRODUCTION

There is a renewed interest in the total electron scattering cross sections of noble gases at intermediate and high energies (300–5000 eV) [1–7] because accurate cross sections are essential in testing theoretical models to understand the electron-atom interaction process, and required as reference values in applications such as astrophysics, atmospheric physics, chemical physics, plasma physics, and semiconductor physics. A considerable number of experimental cross sections of light noble gases (He, Ne, and Ar) at these energies is reported in the literature and there is a reasonable agreement between these cross sections produced by different experimental groups with few exceptions. However, the cross sections of heavy noble gases (Kr and Xe) are not plenteous in the literature. At electron energies over 700 eV, only two experimental measurements each for Kr and Xe atoms are reported in the literature. Further, there are serious discrepancies between these reported cross sections, leaving greater uncertainty in the experimental cross sections of these two elements. First, Garcia, Arqueros, and Campos [8] have measured the electron scattering cross section of Kr in the energy range 700–6000 eV using the linear beam transmission technique with 6% experimental error. Then Zecca *et al.*. [7] have measured the Kr and Xe cross sections in the energy range 80–400 eV using a modified Ramsauer-type apparatus with 5% or lower experimental uncertainty. Recently, Garcia *et al.* [1] have measured the cross section of Xe using the linear beam transmission technique with an experimental uncertainty of 3% and found those to be 20%–25% higher than the cross sections reported in Ref. [7] at energies higher than 2000 eV. Also the Kr cross sections reported in Ref. [8] are about 35% higher than those reported in Ref. [7], again at higher electron energies.

A recent article by Zecca, Karwasz, and Brusa [4], where the discrepancies in experimental electron scattering cross sections of noble gases at intermediate and high electron energies are discussed, emphasizes the need for more accurate cross section measurements at these energies. Further, they pointed out that the discrepancies are dependent on the size of the target atom, negligible for Ne but of the order of 40% for Kr. As a response to some of the comments made in this article, Garcia *et al.*. [1] have measured the zero-degree energy-loss spectra of Ne, Ar, Kr, and Xe at 2500 eV energy and indicated that the discussed discrepancies in Ref. [4] result from the poor angular resolution of the modified Ramsauer-type apparatus. Recently, we have measured the intermediate- and high-energy scattering cross sections of He, Ne, and Ar atoms [9] using the linear beam transmission technique and made a comparison with the existing cross section. In this comparison it was found that the Ar cross sections measured using the linear beam transmission technique in different laboratories agree with each other within their experimental uncertainties but those measured using the modified Ramsauer-type apparatus are 10%–15% lower than those of the transmission beam technique at energies 2000 eV or higher. A parallel trend was observed in the He cross sections measured by these two techniques. At electron energies higher than 1500 eV, He cross sections measured using the Ramsauer technique are 10%–20% lower than those using the linear beam transmission technique. However, within the experimental uncertainties, the Ne cross sections measured at different laboratories agree with each other regardless of the experimental technique used.

In the present experiment, the total electron scattering cross sections of Kr and Xe are measured for 250–4500 eV electron energies using the linear beam transmission technique. These cross sections are compared with the existing experimental and theoretical cross sections and empirical models. Discrepancies in the cross sections determined using the linear beam transmission technique and modified Ramsauer techniques are discussed.

II. EXPERIMENTAL PROCEDURE AND ERRORS

The present experimental arrangement to determine the total electron scattering cross sections by a linear transmission technique for Kr and Xe has been discussed in detail in previous papers [10–12]. Briefly, a 250–4500 eV energy electron beam obtained from an electron gun was passed through a 24.5-cm-long gas cell with 1.0-mm-diam entrance and exit apertures. Electrons emerging from the gas cell passed through a double-focusing electrostatic energy analyzer (ESA) whose entrance was 4.5 cm away from the exit of the gas cell. The ESA was operated in the constant 50 eV energy transmission mode with 1.0-mm-diam entrance and exit apertures. At these settings, the ESA resolution is 0.75 eV (full width at half maximum) or better and the accuracy of the energy scale is 0.1 eV or better. Electrons transmitted through the ESA were collected on a Faraday cup and the intensity, typically about 10^{-10}–10^{-12} A, was measured by an electrometer. The Faraday cup, ESA, gas cell, and electron gun were shielded from the Earth's magnetic field and other stray magnetic fields and maintained in a vacuum in the low 10^{-7} Torr region. When the gas was present in the gas cell, the pressure in the regions where the Faraday cup, ESA, and electron gun were located was 1×10^{-5} Torr or better.

As discussed in previous papers [10–12], the cross sections were determined by measuring the electron beam attenuation through the gas cell. According to the Lambert-Beer law, the attenuation of an electron beam passing through a length L of a target gas at pressure P can be expressed by the relation

$$I = I_0 e^{-\sigma n P L} \quad (1)$$

where I is the attenuated electron beam current, I_0 is the primary electron beam current, n is the number density of the gas, and σ is the electron scattering cross section. Therefore, the variation of $\ln(I/I_0)$ with P is a linear function whose slope is a measure of the scattering cross section.

The beam currents I and I_0 were determined by measuring the currents generated at the Faraday cup attachment to the ESA with and without the gas present in the gas cell. First, I_0 was measured just prior to gas being admitted into the gas cell from a needle valve. The current I was measured subsequently when the pressure in the gas cell had reached an appropriate level. The pressure in the cell was measured by a capacitance manometer. Times between the measurements of I and I_0 were kept short, typically, 4–6 s, in order to minimize errors due to current drifts and fluctuations. Further, upon closing the gas needle valve, it was made sure that the current returns to its original value of I_0 after the gas cell was pumped down to zero pressure in the capacitance manometer. Both Kr and Xe gases were commercially purchased research-grade gases with the minimum purity 99.9% or better. Gas purities were monitored throughout the experiment with an on-site residual gas analyzer, attached to the vacuum chamber where the ESA was housed, to ensure that there was no atmospheric contaminant leak into the gas cell during the gas transfer. During this process the purity of gases was confirmed with 0.3%–0.4% uncertainty.

The errors in the cross sections reported in this experiment are the same as those discussed in the previous papers [10–12]. Briefly, the errors arise from essentially five sources: (i) gas-electron interaction length determination (2% or less), (ii) pressure measurement (2% or less), (iii) contribution from the zero-degree elastic scattering (1% or less), (iv) current measurement including the possible current fluctuations during the experiment (2% or less), and (v) statistical errors in determination of the slope (1% or less). These random errors combined quadratically to assign a random error of 4% or less for the cross sections reported here.

TABLE I. The total electron scattering cross sections of Kr and Xe in units of 10^{-20} m^2 determined in the present experiment.

Energy (eV)	Kr	Xe
250	7.31±0.29	9.34±0.35
300	6.68±0.25	8.61±0.34
400	5.70±0.23	7.72±0.31
500	5.01±0.21	6.91±0.28
600	4.60±0.18	6.39±0.26
700	4.09±0.16	5.80±0.23
800	3.81±0.15	5.38±0.21
900	3.58±0.14	5.06±0.20
1000	3.33±0.13	4.69±0.19
1200	2.94±0.12	4.26±0.17
1400	2.65±0.11	3.92±0.16
1600	2.44±0.10	3.62±0.14
1800	2.29±0.09	3.37±0.13
2000	2.17±0.09	3.17±0.13
2500	1.93±0.08	2.78±0.11
3000	1.72±0.07	2.52±0.10
3500	1.56±0.06	2.25±0.09
4000	1.40±0.06	2.05±0.08
4500	1.32±0.05	1.91±0.07

III. RESULTS

Given in Table I are the measured total electron scattering cross sections of Kr and Xe in the energy range 250–4500 eV in the present experiment. These cross sections are mean values of six to ten individual measurements. Each individual measurement was obtained by measuring the attenuated electron beam current for eight to ten different gas pressures, plotting ln (I/I_0) against the pressure graph and determining the slope of it.

IV. DISCUSSION

The cross sections reported in the literature by other experimental groups are compared to those measured in the present experiment by normalizing the cross sections of others to the present cross sections and scaling those as a function of energy. Since the objective of this normalization is merely to compare the cross sections produced by others to the present cross sections, the present cross section at a given energy is used as the standard cross section at that energy and the cross sections of others are divided by that value to obtain the normalized cross sections. The interpolated present cross sections are used for the energies of those cross sections that are not measured in the present work. These normalized cross sections are displayed in Figs. 1 and 2, respectively, for Kr and Xe where the normalized cross section value 1.0 refers to the cross sections of this work.

As can be seen from Fig. 1, within the experimental uncertainties, the Kr cross sections produced in the present experiment are in good agreement with those of Garcia, Arqueros, and Campose [8] for the entire energy range. Also the

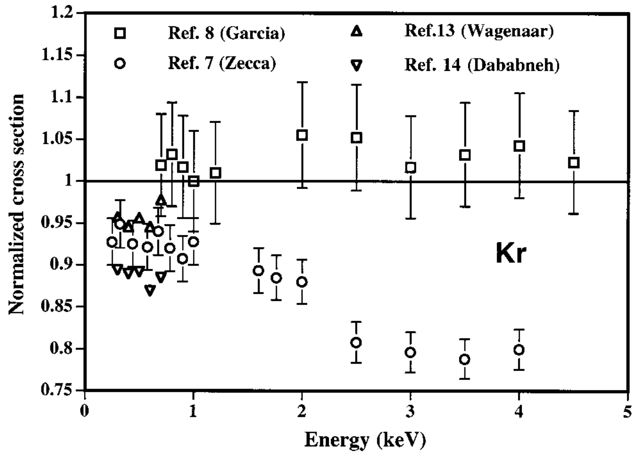

FIG. 1. Comparison of the Kr cross sections produced by other experimental groups with those in the present experiment by normalizing the cross sections of others to the present measurements. In the figure, the normalized cross section value 1.0 refers to the present measurements. Interpolated present cross sections have been used to normalize the cross sections at energies where the cross sections were not measured in the present experiment.

cross sections reported in Ref. [13] are in fair agreement with the present measurements in the energy range of their study. However, the cross sections reported by Zecca *et al.* [7] are lower than the present measurements for the entire energy range and the deviation between the two experiments increases with increasing energy up to 2500 eV and reaches the highest deviation of about 20% at energies 2500 eV and higher. At 1000 eV and lower energies the deviation of the measurements in Ref. [7] is not significant but the results do not agree within the experimental uncertainties of two experiments. Also the cross sections reported in Ref. [14] are 10%–14% lower than the present measurements at the energies in their study.

It is apparent from Fig. 2, where the relative Xe cross sections are scaled, the overall agreement and disagreement between the cross sections among the five experimental groups are parallel to those of the Kr cross sections. The

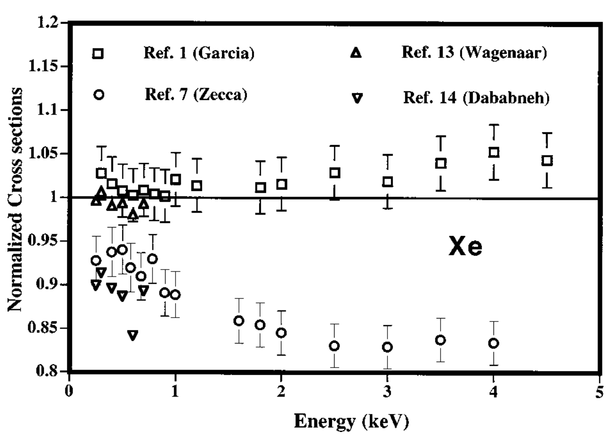

FIG. 2. Comparison similar to Fig. 1 for Xe. Again, some interpolated present cross section values have been used to normalize the cross sections at energies where the cross sections were not measured in the present work.

cross sections reported in Ref. [1] (Garcia *et al.*) and Ref. [13] are in good agreement with the present measurements while those of Ref. [7] (Zecca *et al.*.) and Ref. [14] are lower than the present cross sections. The deviation between the cross sections reported in Ref. [7] and those of the present experiment begins to appear below 1000 eV energy, increases with increasing energy up to 2500 eV, and reaches the maximum deviation of about 18% at energies 2500 eV and higher.

Since the interest of this article is the cross sections at intermediate and high electron energies, the remaining discussion of comparison of experimental cross sections will be focused only on the cross sections reported by Garcia *et al.*. [1], Garcia, Arqueros, and Campose [8], Zecca *et al.* [7], and the present experiment. In a previous article [9] where the cross sections of Ar and Ne, measured in three laboratories, are compared, it was revealed that the Ne cross sections agree with each other for the entire energy range (300–3000 eV) while the Ar cross sections produced in Zecca *et al.*'s. [7] laboratory are lower than those produced in Garcia *et al.*'s [8] laboratory and the present laboratory at energies higher than about 2000 eV. The present cross sections as well as Garcia *et al.*'s cross sections are measured using the linear beam transmission technique while those of Zecca *et al.* [7] are measured using the modified Rainsauer technique. When combining the observation in Ref. [9] with the observation in Figs. 1 and 2, it is clear that the discrepancies of cross sections between the two experimental techniques depend on target size and energy; Ne cross sections produced by the two techniques agree with each other for the entire energy range 300–3000 eV, Ar cross sections produced by the two techniques deviate from each other at energies higher than about 2000 eV, and Kr and Xe cross sections produced by the two techniques deviate at energies higher than about 1000 eV. As stated in Sec. I of this article, Garcia *et al.* [1] have claimed that the discrepancies in the cross sections result from the poor angular resolution of the Ramsauer-type technique. Following are further supportive facts for Garcia *et al.*'s claim.

Unlike the electrostatic energy analyzers used in the linear beam transmission technique which has constant energy resolution of 0.75 eV (or better), the energy resolution of the Ramsauer technique is stated to be approximately 1% of the primary energy of the incident electron beam. Due to the decreasing energy resolution of the Ramsauer technique with increasing energy, errors in the cross sections determined by this device would be expected at energies above the point where its energy resolution reaches the energy thresholds for inelastic scattering in the forward direction. At energies above this point, the Ramsauer technique has decreasing ability to distinguish inelastically scattered electrons in the forward direction from unscattered electrons, causing the cross section to be underestimated. A qualitative understanding of this underestimation can be obtained for noble gas atoms by considering the oscillator strength distributions of these target atoms.

The oscillator strength distributions, determined from the fast electron-energy-loss spectra, give the relative probability of inelastically scattering of high-energy electrons in the forward direction as a function of energy loss [15]. The energies at which these oscillator strengths occur are indicative of the transition or ionization energies of the target atom. The lowest-energy-loss oscillator strength therefore defines the inelastic threshold of the target atom, which is the minimum energy loss possible for inelastic electron scattering in the forward direction. According to the fast electron-energy-loss spectra of Chan *et al.* [16,17] the inelastic threshold energy for Xe is about 8.5 eV and the maximum oscillator strength occurs at about 11.5 eV while the inelastic threshold of Ne is about 17 eV and the maximum oscillator strength occurs at 32 eV. Furthermore, according to the oscillator strengths reported in Refs. [16,17], the relative probability for high-energy electrons to be scattered in the forward direction for Xe is nearly ten or more times greater than that of Ne. If a primary energy of 1000 eV of the electron beam is used on Xe with the Ramsauer-type apparatus, its energy resolution of 10 eV is not adequate to resolve the primary beam and the inelastically scattered electrons in the forward direction at energies between approximately 991.5 eV (1000−8.5 eV) and 989.5 eV (1000−11.5 eV) or at a few eV lower than 989.5 eV. On the other hand, 10 eV resolution is adequate to resolve 1000 eV energy primary electrons on Ne from inelastically scattered forward electrons because the highest-energy inelastically scattered electrons appear at about 938 eV (1000−17 eV) or lower energy, with the maximum number appearing at 968 eV (1000−32 eV). Further, these inelastically scattered electrons are not insignificant in the case of Ne because the number of such electrons is only 1/10 or a lower fraction of those in Xe. Considering the peak oscillator strength of Ne, it is obvious that even for 3000 eV energy primary electrons, where the resolution is 30 eV, the contribution from the inelastically scattered electrons in the forward direction is insignificant. This is the primary reason behind the agreement of the Ne cross sections produced in the two experimental methods for the energy range 300−3000 eV. For Xe, the cross sections begin to deviate from each other around 800 eV (or even lower), the deviation increases to about 2500−3000 eV, and continues constant at higher energies because the number of inelastically scattered electrons is negligible at about 20 eV below the inelastic threshold of Xe [17].

As discussed in Ref. [9], the He cross section produced by the Ramsauer technique is significantly lower than that produced by the beam transmission technique at 2000 eV. Comparison at 1500 eV is somewhat questionable because of the uncertainty in the experimental errors of the cross sections produced in Ramsauer technique. When the He cross section at 2000 eV is measured using the Ramsauer technique, the highest-energy inelastically scattered forward electrons are within the limits of the instrumental resolution. As can be seen from Chan, Cooper, and Brion's work [15] the inelastic threshold of He is 21 eV below the primary energy and the maximum oscillator strength due to ionization occurs within about 2−2.5 eV after the inelastic threshold. Considering the magnitude of the oscillator strength along with the 1% instrumental resolution at 2000 eV, the maximum oscillator strength for He is estimated to be about 22 eV below the primary electron energy. Although the magnitude of the maximum oscillator strength is of the same order as that of Ne, the electron scattering cross section of He at 2000 eV is 25% of that of Ne. Therefore, contributions from the inelastically forward scattered electrons are significant and these electrons are within the reach of the instrumental resolution in the Ramsauer technique for He at 2000 eV.

The discrepancies of the cross sections of Ar and Kr determined by the two experimental techniques can also be explained by the use of inelastic thresholds, oscillator strengths, and the energies of the oscillator strengths given in Refs. [16,17]. When the resolution of the Ramsauer technique reaches the limits of minimum energy loss, the apparatus does not distinguish the inelastically scattered electrons arising from the inelastic threshold, and the total cross section determined by this technique will begin to deviate. As the primary electron beam energy is increased further, the resolution of the Ramsauer technique decreases, and more and more inelastically scattered electrons in the forward direction will become unresolved in the measurements of the unscattered electron intensities, causing the cross-section measurements by this technique to become more and more underestimated. On the other hcand, the instrumental resolution in the beam transmission technique is less than 1 eV, independent of primary electron energy, and far beyond the reach of the inelastic threshold energies of noble gases.

For fast-moving charged particles, the Bethe theory gives an asymptotic formula for the total inelastic cross sections [18,19] while the Born approximation gives the total elastic cross sections [20]. The combined Bethe-Born theory of Inokuti [18] expresses the total cross sections ($\sigma_{\rm BB}$) in terms of the following formula:

$$\frac{E}{R}\frac{\sigma_{\rm BB}}{\pi a_0^2} = \left[A + B\left(\frac{R}{E}\right) + C\left(\frac{R}{E}\right)^2 + \cdots + 4M^2 \ln\left(4C_t\frac{E}{R}\right)\right], \tag{2}$$

where a_0 is the Bohr radius, E is the incident electron energy, R is the Rydberg constant, and the parameters A, B, C, M, and C_t are constants depending on the physical properties of the target atom. For He, Ne, and Ar, these parameters are given in Refs. [2,19,20]. In the past, it has been proven [8,21] that the Bethe-Born formalism overpredicts the total cross sections even at energies as high as 4000 eV. Recently, Garcia *et al.* [1] have proposed an empirical formula to predict the cross sections of noble gases by fitting the experimental cross sections of Ne, Ar, Kr, and Xe given in Refs. [1,8]. This model expresses the cross section (σ) as

$$\sigma = A(\alpha_P)E^{-B(Z)} \tag{3}$$

where

$$A(\alpha_P) = 0.57\alpha_P + 2.08, \tag{4}$$

and

$$B(Z) = 0.89 - 0.006\,32Z. \tag{5}$$

Here, $A(\alpha_P)$ and $B(Z)$ are fitting parameters based on the atomic polarizability (α_P) and atomic number (Z). Another semiempirical formula to predict the total cross sections of noble gases was developed by Brusa, Karwaz, and Zecca [5] and by Zecca *et al.* [4]. This formula is developed by fitting the experimental cross section with a minimization based on

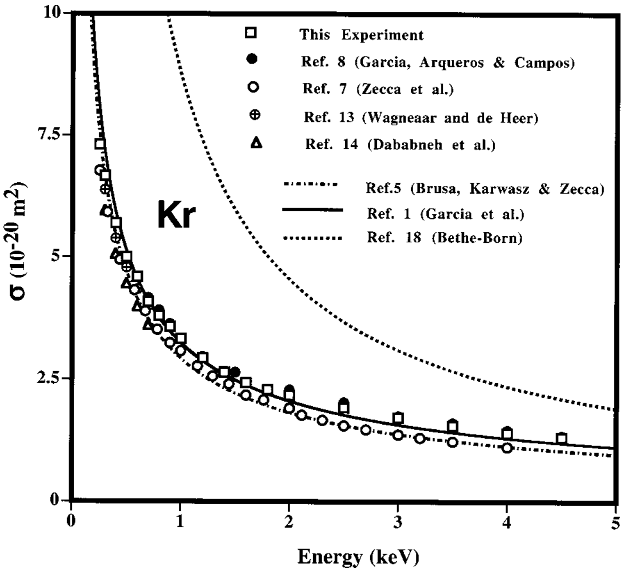

FIG. 3. Comparison of the experimental Kr cross sections with the predictions by Bethe-Born theory [18], the semiempirical formula of Brusa, Karwasz, and Zecca [5], and the empirical formula of Garcia *et al.* [1].

the simplex method and predicts a $1/E$ (E is the energy) dependence for the total cross sections as does the Born approximation. According to this formalism, the total cross section (σ) is expressed as a four-parameter formula as follows:

$$\sigma = \frac{1}{A(B+E)} + \frac{1}{C(D+E)} + \frac{2}{E}\sqrt{\frac{BD}{AC}}\frac{1}{|B-D|}\left|\ln\frac{E/D+1}{E/B+1}\right|, \tag{6}$$

where E is the incident energy, and A, B, C, and D are adjustable parameters fitted to the experimental cross sections.

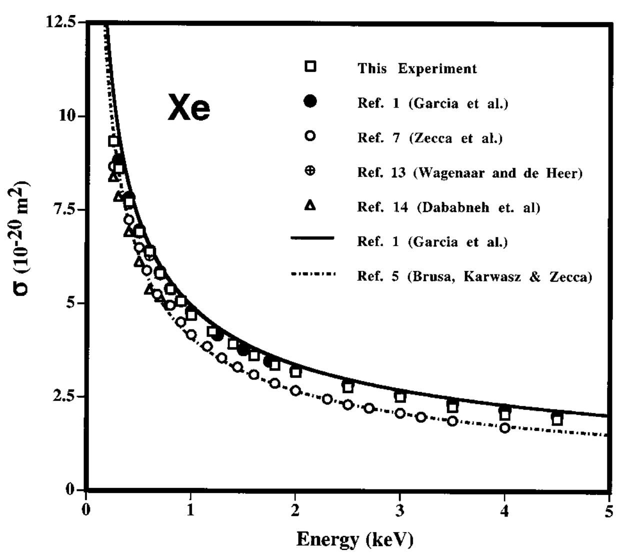

FIG. 4. Comparison of the experimental cross sections with the predictions by the semiempirical formula [5] and the empirical formula [1].

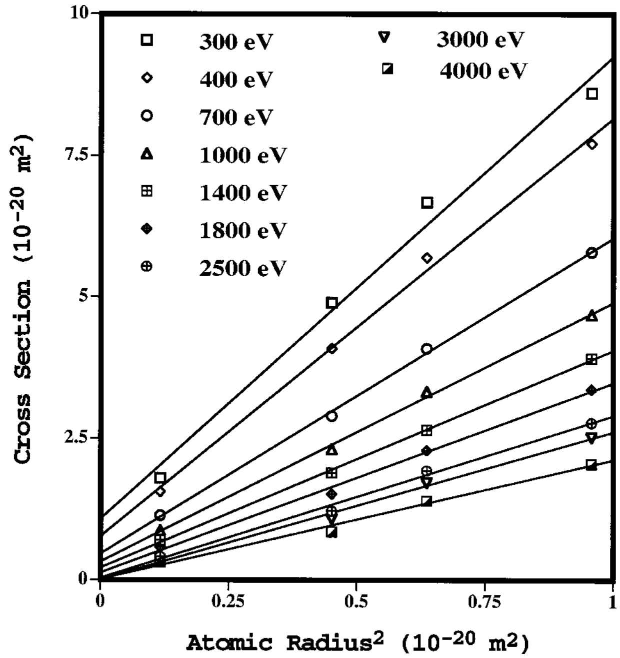

FIG. 5. Variation of the electron scattering cross section with the square of the atomic radius for Ne, Ar, Kr, and Xe at selected energies between 300 and 4500 eV. Atomic radii are taken from Ref. [23].

In order to compare the present experimental cross sections with predictions of these theoretical and empirical expressions, the present cross sections are scaled as a function of energy and displayed in Figs. 3 and 4, respectively, for Kr and Xe. In the same figures the experimental cross sections produced in other laboratories as well as the predictions by the above expressions are given for comparison. Since the Bethe-Born parameters are not available in the literature for Xe, the experimental Xe cross sections are compared only with the two empirical models given in Eqs. (3) and (6).It can be seen from Fig. 3 that the Bethe-Born theory overpredicts the cross sections by 100% or more for the entire energy range of this study for Kr. In Ref. [9] where the cross sections of He, Ne, and Ar are compared to the Bethe-Born theory it was revealed that the theory well predicts the He cross sections but overpredicts the Ne and Ar cross sections with greater overprediction for the Ar cross section. According to this pattern of the deviation of Bethe-Born theoretical predictions from the experimental cross sections, it is obvious that the Bethe-Born theoretical predictions of Xe cross sections would be 200% or more greater than the experimental cross sections.

As displayed in Fig. 3 for Kr and Fig. 4 for Xe, the empirical formula given in Eq. (3) agrees well with the cross sections produced by the transmission beam technique while the semiempirical formula given in Eq. (6) agrees with those produced by the Ramsauer technique. In Ref. [9], where the experimental cross sections of Ar and Ne are compared with these two expressions, nearly the same feature was seen with the exception of Ne cross sections below 2000 eV At these energies the experimental cross sections of Ne indicate a better agreement with the semiempirical formula given in

Eq. (6). Overall better representation of the experimental cross sections may be obtained by a combination of the concepts governing the two expressions and the accurate experimental cross sections.

Both experimentalists and theorists have discussed the correlation between the atomic parameters and the electron scattering cross sections [1,2,5,19,22]. The number of target electrons and the atomic polarizability are the most commonly employed parameters in the development of empirical and semiempirical formulas to predict the cross sections. However, the classical picture of the scattering cross sections is related to the atomic radius. In order to examine this feature the present cross sections and the cross sections reported in Ref. [9] are scaled as a function of the square of the atomic radius for Ne, Ar, Kr, and Xe at each primary electron energy and displayed in Fig. 5. This figure clearly indicates a linear relationship between the measured cross sections and the square of the atomic radius for the four atomic targets. However. the He cross section falls below the values of this linear relationship. Currently, the correlation between the cross section and the atomic radius is under further investigation.

V. CONCLUSION

The total electron scattering cross sections of Kr and Xe for 250–4500 eV have been measured by employing the linear beam transmission technique with the experimental uncertainties 4% or less. The present experimental cross sections are in good agreement with those produced by Garcia *et al.* [1] and Garcia, Arqueros, and Campos [8] but greater than those produced by Zecca *et al.* [7]. The discrepancies in these cross sections may have resulted from the poor angular resolution of the apparatus used in Ref. [7]. The empirical formula of Garcia *et al.* [1] agrees closely with the experimental cross sections but the semiempirical formula proposed by Brusa, Karwasz, and Zecca [6] underpredicts the cross sections. There exists a linear relationship between the experimental cross sections and the square of the atomic radius of Ne, Ar, Kr, and Xe atoms.

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