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Momentum Transfer Cross Section for e^-–Kr Scattering

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Abstract

The momentum transfer cross section for electrons in krypton has been derived over the energy range 0–4 eV from an analysis of drift velocity and D_T/μ data for hydrogen–krypton mixtures. At energies in the vicinity of the Ramsauer–Townsend minimum, the present work differs significantly from derivations based on analyses of drift velocity data alone. The overall uncertainty in the derived cross section reflects the experimental errors in the transport coefficients, the uncertainty in the cross sections used to represent the hydrogen component in the mixtures, and the uncertainty associated with the χ^2 minimisation. The present cross section is compared with recent theoretical calculations and other experimental derivations.

1. Introduction

The large number of derivations of the momentum transfer cross section for krypton, σ_m, from analyses of electron swarm transport data that exist in the literature, are in poor agreement (see for example Elford *et al.* 1992), reflecting uncertainties in the experimental data and the intrinsic non-uniqueness of cross sections derived from transport data. Despite accurate experimental data, recent derivations, such as that of Hunter *et al.* 1988 (based on an analysis of electron drift velocity data for pure krypton), suffer from significant uncertainty, arising from the relatively low sensitivity of the drift velocity to the momentum transfer cross section at energies in the vicinity of the Ramsauer–Townsend minimum. This manifests itself as poor uniqueness in the derived cross section. The problem of uniqueness in the derived cross section, discussed by Elford *et al.* (1992) and references therein, can be alleviated to some extent by using drift velocity data for krypton–hydrogen mixtures as the basis for deriving a cross section (England and Elford 1988; Mitroy 1990). The uncertainty in the derived cross section, due to the uniqueness problem, may be further reduced by basing the cross section on an analysis of two or more transport coefficients in such mixtures. In this paper we present a derivation of the momentum transfer cross section for electron scattering from krypton, using electron swarm transport data for hydrogen–krypton mixtures. In the present work, the sensitivity of the derived cross section to the experimental data has been enhanced by analysing three sets of data including: recent measurements of the ratio D_T/μ (Elford *et*

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al. 1992) (where D_T is the transverse diffusion coefficient and μ the electron mobility) for electrons in a 0·4673% hydrogen–99·5327% krypton mixture; and the drift velocity, W, for electrons in two hydrogen–krypton mixtures containing 0·4673% and 1·686% hydrogen respectively (England and Elford 1988). The use of hydrogen–krypton mixtures, rather than pure krypton, has a number of advantages (discussed in Elford *et al.* 1992), in spite of the introduction of uncertainties in the assumed set of scattering cross sections for hydrogen, which necessarily increase the uncertainty in the derived krypton σ_m.

The method of analysis is similar to that of Mitroy (1990), although several modifications have been made to the fitting procedure in addition to the inclusion of the recent D_T/μ data in the analysis. These modifications are discussed in Section 2, together with other details relevant to the analysis. The uncertainty associated with the cross section is discussed in Section 3.

In Section 4 we compare the present work with theoretical calculations and previous experimental determinations. The most recent *ab initio* calculations include an R-matrix optical potential calculation, in the range 1–20 eV (Baluja *et al.* 1991; Jain 1991) and the recent study by the 'York group' (Mimnagh *et al.* 1993), who have modified their non-relativistic polarised orbital calculation (McEachran and Stauffer 1990) to more accurately include the effects of polarisation. Finally we consider the Dirac–Fock calculation of Sienkiewicz and Baylis (1992).

2. Computational Details

The cross section $\sigma_m(\epsilon)$ for krypton was derived using a non-linear least squares fitting routine in which the following function was minimised:

$$\chi^2 = \sum_j \{[\Delta_j(W)]^2 + [\Delta_j(D_T/\mu)]^2\} . \tag{1}$$

In this function $\Delta_j(W)$ and $\Delta_j(D_T/\mu)$ are the relative differences between the calculated and experimental values of W and D_T/μ, respectively, for the jth E/N value. That is,

$$\Delta_j(W) = (1/w_j)[W^{\mathrm{calc}}(E/N)_j - W^{\mathrm{expt}}(E/N)_j]/W^{\mathrm{expt}}(E/N)_j ,$$

with a similar expression for D_T/μ. The w_j refer to relative weights assigned to each datum point (usually 1—see below). The calculated values of the transport coefficients are arrived at by an appropriate solution of the Boltzmann equation using a set of cross sections for krypton and hydrogen. The krypton $\sigma_m(\epsilon)$ was represented in parametric form and the parameters adjusted to minimise χ^2.

The momentum transfer and inelastic scattering cross sections for hydrogen of England *et al.* (1988) were used in the calculations. The same set of cross sections was also used by both England and Elford (1988) and Mitroy (1990) in their respective derivations of the krypton σ_m from drift velocity data in krypton and hydrogen–krypton mixtures. The maximum value of E/N considered in this study was 2·0 Td (1 Td $\equiv 10^{-21}$ V m^2), in order to limit the energy range of the present investigation to $0 \leq \epsilon \leq 4$ eV. The upper limit is set by the availability of

cross sections for hydrogen, which are assumed to be known sufficiently accurately over this energy range (Crompton and Morrison 1993; present issue p. 203).

It was found that the juxtaposition of the onset of the 0–1 vibrational transition in hydrogen, and the Ramsauer–Townsend minimum in krypton, at $\approx 0 \cdot 5$ eV demanded use of a 'multi-term' solution of the Boltzmann equation (Ness and Robson 1986) to correctly describe the diffusion of the electron swarm transverse to the applied electric field. In the present case, the relatively small amount of hydrogen used in the mixture ensured that the difference between the diffusion coefficients, as calculated by the multi-term and 'two-term' codes (as employed by Mitroy), was limited to a maximum of a few percent at the highest values of E/N. Note that a two-term solution of the Boltzmann equation is sufficient to accurately describe both the drift velocity of the swarm and the diffusion of the swarm parallel to the applied field.

However, the need for a relatively high speed algorithm for solving Boltzmann's equation militated in favour of the 'two-term' solution as used by Mitroy (1990), instead of the more computationally intensive multi-term code of Ness and Robson (1986). It was necessary to account for the differences in the values of D_T calculated by the two codes where appropriate. This was achieved by running the multi-term code once, over the relevant range of E/N, using a model cross section (the krypton σ_m of McEachran and Stauffer 1988 was used), in order to obtain a table of estimates of the difference between the values of D_T predicted by the two-term solution and those of the fully converged multi-term code. Once this was established, the transport coefficients calculated by the two-term code could be suitably modified for comparison with the experimental data. After a satisfactory fit was obtained using this method, the resultant cross section was fed into the multi-term code and a new table established. This procedure converged to the final cross section after only three such iterations.

The parametric representation of the krypton σ_m and the fitting procedure employed in the present work are adapted from Mitroy (1990). In Mitroy's work, the scattering phase shifts for krypton below ≈ 1 eV (and hence the σ_m in this region) were represented by a six-parameter modified effective range theory (MERT), while Mitroy assumed that the shape of σ_m above 1 eV was an average of the experimentally derived cross sections of Hunter *et al.* (1988) and England and Elford (1988). In the present work, the krypton σ_m was represented by a cubic polynomial $F_{\mathrm{P}}(\epsilon)$ in the energy range ≈ 1–4 eV. In the modified algorithm, the energy, ϵ_j, at which the representation of the fitted cross section given by MERT, $F_{\mathrm{M}}(\epsilon)$, joins that given by the cubic polynomial, is also a free parameter. The coefficients of this polynomial were fitted, subject to the constraints:

$$F_{\mathrm{M}}(\epsilon_j) = F_{\mathrm{P}}(\epsilon_j), \qquad \left.\frac{\partial F_{\mathrm{M}}(\epsilon)}{\partial \epsilon}\right|_{\epsilon=\epsilon_j} = \left.\frac{\partial F_{\mathrm{P}}(\epsilon)}{\partial \epsilon}\right|_{\epsilon=\epsilon_j}. \tag{2}$$

which ensured that the transition between the two representations was smooth. The parameters in the MERT formalism describing the low energy σ_m are as defined by Mitroy (1990).

It should be noted that the two lowest-order coefficients of the cubic polynomial were determined by the constraints (2) and were not free parameters in the fit. A value of $16 \cdot 744$ a.u. (Dalgarno and Kingston 1960) was used initially for the

dipole polarisability α_d of krypton and an initial value of 8·0 a.u. represented the effective quadrupole polarisability α_q (Mitroy 1990; Buckman and Mitroy 1989). After an initial fit to the experimental data, both the dipole and quadrupole polarisabilities were allowed to vary. In all, eight parameters, including α_d and α_q, were fitted in addition to the two free parameters describing the cubic polynomial and one parameter defining the maximum energy of the MERT representation.

The data used in the fit were: the drift velocity data of England and Elford (1988) for the two mixtures of 0·467 and 1·686% hydrogen in krypton at 293 K over the E/N ranges $0{\cdot}08 < E/N < 2{\cdot}0$ Td and $0{\cdot}1 < E/N < 2{\cdot}0$ Td respectively; and the D_T/μ data of Elford *et al.* (1992), for a 0·467% hydrogen–krypton mixture at 295 K, over the E/N range $0{\cdot}025 < E/N < 1{\cdot}4$ Td. The data sets were smoothed before fitting in order to minimise small-scale fluctuations in the χ^2 space. The resultant cross section was compared to the original data, using the multi-term code as described above. An investigation into the influence of the relative weighting [w_j in equation (1)] of the three data sets on the 'fit' indicated that the relative weights given to the data could be varied by at least a factor of 2 without significantly altering the final fit. In all, 38 drift velocity and 24 D_T/μ datum points were included in the fit. The energy dependence of the final cross section is given in Table 1 (see also Fig. 1 later) together with the calculated

Table 1. Present momentum transfer cross section for krypton

The MERT parameters (as defined by Mitroy 1990) describing the cross section in the region $0 \leq \epsilon \leq 0{\cdot}995$ eV are $\alpha_d = 16{\cdot}74, \alpha_q = 8{\cdot}0, A = -3{\cdot}3528, D = 170{\cdot}33, F = -212{\cdot}593, A_1 = 13{\cdot}322$, $H = 15{\cdot}362$ and $A_2 = 4{\cdot}2$. In the region $0{\cdot}995 \leq \epsilon \leq 4$ eV the cross section has the form $0{\cdot}1151\epsilon^3 - 0{\cdot}3039\epsilon^2 + 2{\cdot}4207\epsilon - 1{\cdot}5322$

Energy (eV)	Cross section (10^{-16} cm^2)	Error (%)	Energy (eV)	Cross section (10^{-16} cm^2)	Error (%)
0·000	39·6	98–104	0·700	0·196	90–108
0·010	25·8	97–103	0·800	0·329	94–108
0·020	20·9	96–102	0·900	0·497	95–107
0·030	17·6	95–102	1·000	0·700	95–106
0·040	15·1	95–101	1·100	0·916	95–104
0·050	13·1	95–101	1·200	1·13	95–104
0·100	7·09	94–101	1·300	1·35	95–104
0·150	4·12	95–101	1·400	1·58	96–103
0·200	2·45	96–101	1·500	1·80	96–104
0·250	1·45	97–103	1·600	2·03	96–104
0·300	0·850	98–105	1·700	2·27	96–104
0·350	0·485	97–108	1·800	2·51	96–104
0·400	0·271	96–112	1·900	2·76	96–105
0·450	0·155	94–115	2·000	3·01	96–105
0·500	0·102	88–117	2·100	3·28	96–105
0·510	0·0966	87–116	2·200	3·55	96–105
0·520	0·0931	86–116	2·300	3·83	96–106
0·530	0·0910	85–115	2·400	4·12	96–106
0·540	0·0902	84–114	2·500	4·42	96–106
0·550	0·0906	84–113	2·750	5·22	95–106
0·560	0·0921	84–111	3·000	6·10	95–106
0·570	0·0946	84–110	3·250	7·07	93–105
0·580	0·0982	85–109	3·500	8·15	91–105
0·590	0·103	85–108	3·770	9·44	89–104
0·600	0·108	86–108	4·000	10·6	87–104

maximum and minimum uncertainties, given as a percentage of the best-fit cross section. The parameters associated with the best-fit cross section are also given in Table 1.

3. Uncertainty in the Derived σ_m

The estimation of the total uncertainty in the derived cross section is necessarily subjective, at least in part. In the present case a diverse combination of factors contribute to the total uncertainty. In addition to the so-called 'non-uniqueness' in the derived cross section, which we have mentioned previously and attempted to minimise in this work (that is the uncertainty in the fitted parameters), we must include the effects of the uncertainties in the experimental measurements on the derived krypton cross section, together with the impact of the uncertainties in the cross sections used to represent the hydrogen in the admixture in the Boltzmann equation (themselves the subject of considerable controversy—see for example Brunger *et al.* 1990, 1991). The transport data used in the present work are characterised by low statistical scatter (for example 0·2% in W values) and relatively larger systematic errors. The effect of the systematic errors in the data on the derived cross section was estimated in the following way.

The original transport data used to obtain the best estimate cross section σ_m were increased by the quoted systematic errors (Elford *et al.* 1992; England and Elford 1988) and a new cross section found by the procedure described in Section 2. The original transport coefficient data were then decreased by the quoted systematic errors and another cross section derived. The difference in these two cross sections represents the range of uncertainty in σ_m due to systematic errors in the data.

The uncertainty in the krypton σ_m due to the uncertainty in the momentum transfer cross section for hydrogen (quoted by Crompton *et al.* 1968 as 5%) was estimated in a similar manner, except that the hydrogen momentum transfer cross section was altered uniformly by ±5% and the krypton σ_m fitted to the best estimate experimental data using the modified hydrogen σ_m.

The impact of the uncertainty in the hydrogen inelastic cross sections on the derived krypton σ_m is more difficult to estimate. In the mixtures considered, the function of the cross sections of England *et al.* (1988), representing the accessible inelastic processes in hydrogen, is primarily as a sink for the energy gained by the electrons in the swarm from the electric field. To first order then, we need only consider the uncertainty in the inelastic cross sections as a whole, rather than the uncertainties associated with individual inelastic processes (see Crompton and Morrison 1993).

Using the neon momentum transfer cross section of Robertson (1972) and the momentum transfer cross section for hydrogen, given by England *et al.*, the magnitudes of all inelastic processes accessible in hydrogen were both incremented and decremented to points where satisfactory agreement no longer existed between the values of the drift velocity predicted by the Boltzmann code and those measured by England *et al.* This defined a maximum and a minimum for the magnitude of the entire accessible inelastic processes in H_2. Thus we determined that the uncertainty in the magnitude of the inelastic processes in hydrogen, in the range 0–4 eV, was 2–3% of the total, given by the sum of the inelastic processes considered in England *et al.* (1988). Then, using appropriately scaled

inelastic cross sections, the uncertainty in the krypton σ_m due to the uncertainty in the inelastic cross sections for hydrogen was estimated in the same manner as for the hydrogen σ_m above.

The contribution from each source of uncertainty in the derived σ_m was combined appropriately, together with cross sections corresponding to the uncertainties in the fitted parameters of Section 2. This total uncertainty appears in Fig. 1 as a 'band' associated with the present σ_m and is shown in Table 1 at representative energies. Note that this process yields an uncertainty which is not necessarily symmetric about the best-fit cross section as a function of energy.

O'Malley (1992) has suggested that the experimental data might be influenced by electron scattering from multiple krypton centres at the elevated pressures used in the experiments. This possibility was not treated in either of the experimental papers by England and Elford (1988) or Elford *et al.* (1992). The contribution to the total uncertainty in the present derived σ_m due to the possible influence of 'multiple scattering' on D_T/μ and W was investigated in the following fashion.

Since the theory of O'Malley (1992) applies only to the case of elastic scattering, the procedure adopted was to first calculate both W and D_T/μ as a function of N for pure krypton, using the present σ_m for krypton and O'Malley's theory, and plot them against D_T/μ for the mixture (as a rough guide to the mean energy of the swarm $\langle\epsilon\rangle$). The corrections to the transport coefficients for hydrogen–krypton mixtures at particular E/N and N values were then assumed to be those for pure krypton at the D_T/μ value corresponding to the E/N value used for the mixture. The assumption is that the presence of hydrogen in a hydrogen–krypton mixture only reduces the D_T/μ value at a given E/N and N without changing the correction itself. We consider this a 'worst case' estimate.

The largest multiple scattering correction calculated for the W data of England *et al.* (1988) at any of the experimental conditions used in their measurements was approximately 0·2%, i.e. of the order of the scatter in the data. In the case of the D_T/μ data used in the present derivation, the corrections to the best-estimate values were found to be less than 0·2% for all $E/N > 0{\cdot}7$ Td. The corrections increased as E/N decreased, being 1·5% at 0·025 Td, the lowest E/N value used. In view of the fact that the cross section is constrained by MERT at these low energies and that only a few of the large number of datum points used in the fitting are possibly affected by multiple scattering, we believe that no additional uncertainty is introduced into the derived σ_m from this source.

There is, however, some evidence for the presence of multiple scattering effects in Fig. 3, where the differences between calculated and experimental D_T/μ values are presented as a function of E/N. It can be seen that the points at the lowest three E/N values appear to be somewhat lower than the general trend, the differences increasing as E/N decreases. This is consistent with multiple scattering as described by O'Malley. The small trend in this case, however, is well inside the stated uncertainty and it is therefore difficult to draw firm conclusions.

4. Discussion

Because of the very large number of momentum transfer cross sections for krypton in the literature, we have arbitrarily limited comparisons to those published since 1988. The cross sections shown in Figs 1*a* and 1*b* have all been derived from transport coefficient data, while those compared with the present

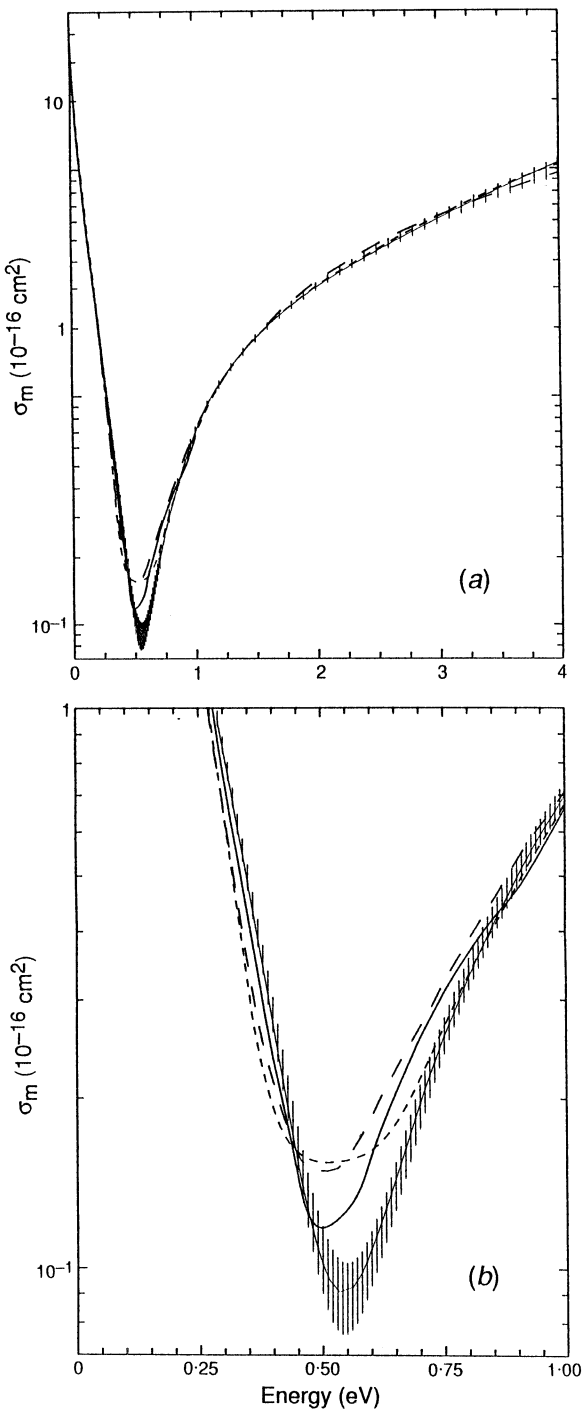

Fig. 1*a*. Present momentum transfer cross section for krypton 0–4 eV. The present σ_m (with uncertainty band) is compared with the experimentally derived cross sections of Mitroy (solid curve), England and Elford (—), and Hunter *et al.* (– –). Note that Mitroy is only plotted to 1·0 eV, whereafter it is a scaled average of Hunter *et al.* and England and Elford.

Fig. 1*b*. Detail of the momentum transfer cross section for krypton 0–1 eV. The legend is the same as for Fig. 1*a*.

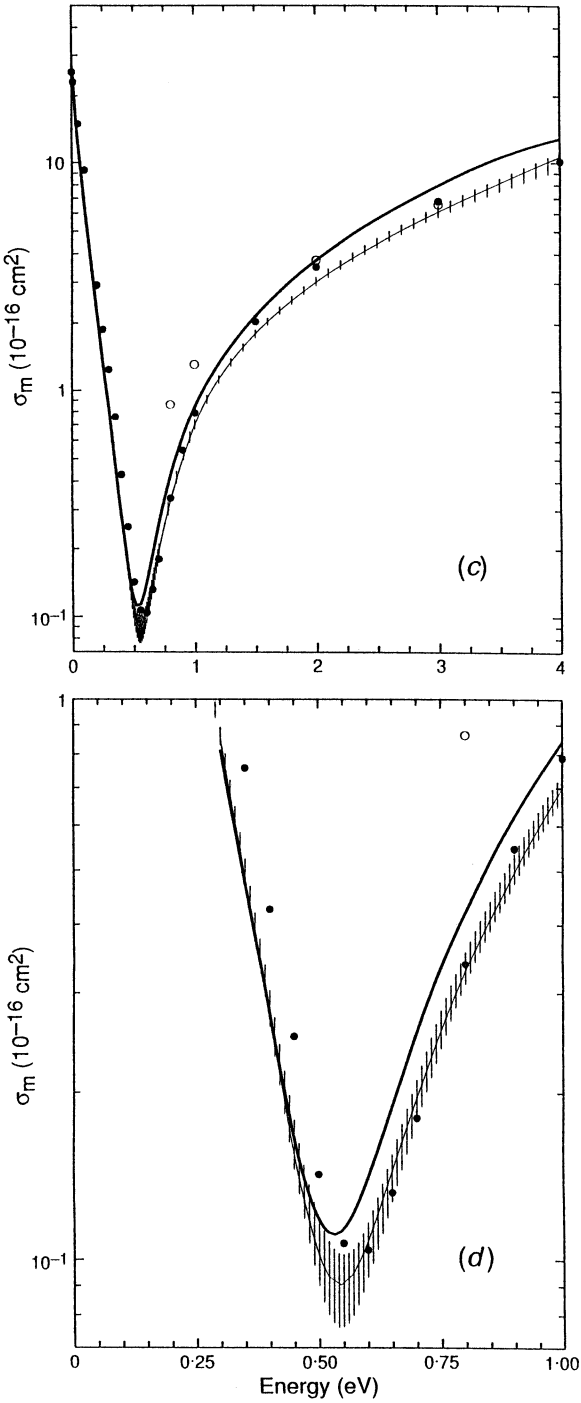

Fig. 1*c*. Present momentum transfer cross section for krypton 0–4 eV. The present σ_m (with uncertainty band) is compared with the theoretical work of Mimnagh *et al.* (thick solid curve), Baluja *et al.* (•) and Sienkiewicz and Baylis (○).

Fig. 1*d*. Detail of the momentum transfer cross section for krypton 0–1 eV. The legend is the same as for Fig. 1*c*.

cross section in Figs 1*c* and 1*d* are the result of *ab initio* calculations. It can be seen from Figs 1*a* and 1*b* that the present cross section has a significantly deeper Ramsauer–Townsend minimum ($0{\cdot}0902\times10^{-16}$ cm^2 at 0·54 eV) than any other derivation. Note also that, not unexpectedly, the uncertainty in the present cross section is largest in this region. Measurement of values of D_T/μ for pure krypton, rather than hydrogen–krypton mixtures, may have a significant impact on the total uncertainty because of the higher sensitivity to the Ramsauer–Townsend minimum and the absence of the uncertainties due to the hydrogen admixture. Unfortunately such measurements pose a number of experimental problems (Elford *et al.* 1992) and the only published data for this coefficient, those of Koizumi *et al.* (1986), are subject to significant error (see England and Elford 1988). Another experiment currently in progress (Schmidt 1992), which measures the drift velocity and components of the diffusion tensor for electron swarms in similar mixtures to those studied here, but in crossed electric and magnetic fields, may ultimately serve to decrease the uncertainty in the derived σ_m. A direct test of a given momentum transfer cross section, which is free from most

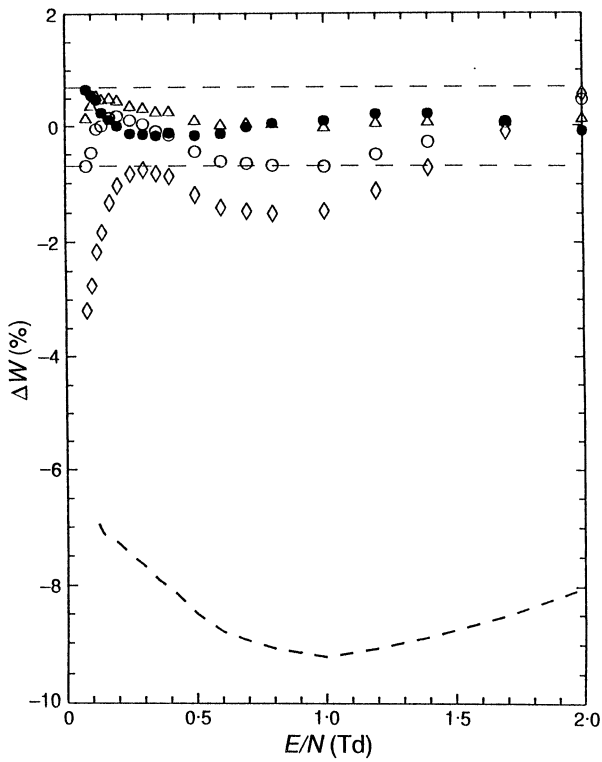

Fig. 2. Difference curve for drift velocities in a 0·467% hydrogen–krypton mixture at 293 K. The differences (see text) between the values predicted by solution of the Boltzmann equation using the present Kr σ_m and the measured values of England and Elford (•) are compared with differences calculated using the Kr σ_m of Mitroy (○), England and Elford (△), Hunter *et al.* (◇) and Mimnagh *et al.* (– –). The stated experimental error (0·7%) is indicated by horizontal dashed lines.

of the uncertainties involved in the derivation described above, is to test the consistency of the transport coefficients predicted by the given cross section against the experimental data. In the present case W and D_T/μ values for a 0·4673% hydrogen–krypton mixture were chosen as a test. Figure 2 shows the differences between calculated and experimental values for the drift velocity, for the cross sections shown in Fig. 1. The fact that three of the cross sections—the present ones and those of England and Elford (1988) and Mitroy (1990)—give differences which lie within the estimated experimental uncertainty quoted for the data (≈0·7%) is not surprising, since in each case these data were used in the derivation of the cross section and the differences merely indicate the goodness of fit achieved. The fact that these three cross sections differ considerably, yet still give good agreement with the drift velocity data indicates the lack of uniqueness that may occur when only drift velocity data are used in the derivation.

The importance of using D_T/μ values in the determination of σ_m can be seen from Fig. 3, which shows that of the three cross sections which were

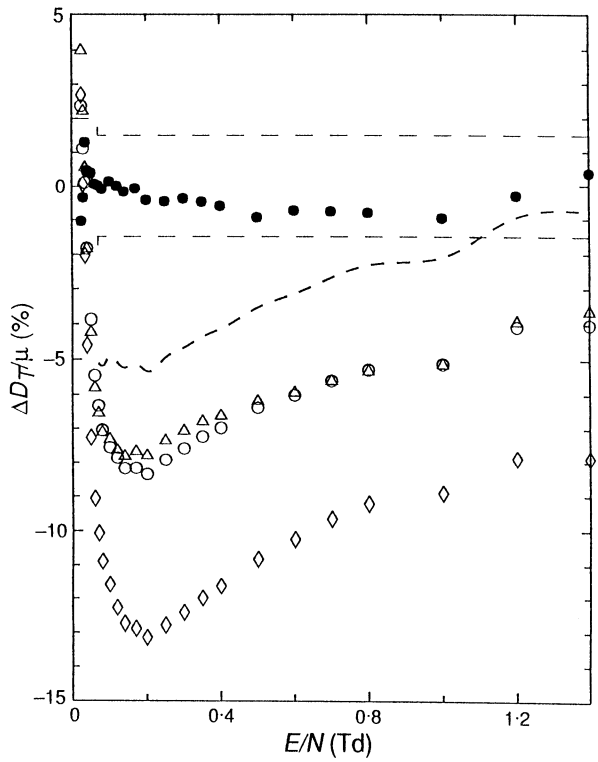

Fig. 3. Difference curve for D_T/μ in a 0·467% hydrogen–krypton mixture at 295 K. The differences (see text) between the values predicted by solution of the Boltzmann equation using the present Kr σ_m and the measured values of England and Elford (•) are compared with differences calculated using the Kr σ_m of Mitroy (○), England and Elford (△), Hunter *et al.* (◇) and Mimnagh *et al.* (– –). Note the different scale with respect to Fig. 2. As in Fig. 2, dashed lines define the acceptable limits of the differences.

consistent with the drift velocity data, only the present one is consistent with the experimental D_T/μ values.

The scattering of electrons by krypton has attracted a good deal of theoretical interest (Yau *et al.* 1980; Sin Fai Lam 1982; McEachran and Stauffer 1984, 1988; Fon *et al.* 1984; Bell *et al.* 1988; Baluja *et al.* 1991; Sienkiewicz and Baylis 1992; Mimnagh *et al.* 1993). Relativistic effects are expected to be significant in theoretical descriptions of electron scattering from krypton, as evidenced by the early work of Sin Fai Lam (1982) and the differences between the non-relativistic and relativistic cross sections of McEachran and Stauffer (1984 and 1988 respectively), in which the same scattering potential was used. The polarisation potential used in both the McEachran and Stauffer calculations included no dynamic effects and retained only the dipole contribution. In their most recent calculation (Mimnagh *et al.* 1993, non-relativistic) a more complete polarisation potential, which included higher multipole contributions as well as dynamic effects, was used. This new cross section (which is significantly different from either of their previous non-relativistic or relativistic calculations), although in better agreement with the present determination than any other theoretical cross section, is still outside the estimated uncertainty of the present work. The cross section of Baluja *et al.* (1991) was obtained by a non-relativistic calculation which assumed a simple model for exchange and polarisation. Their cross section is in significant disagreement with the present cross section at energies below that of the Ramsauer–Townsend minimum.

The recent calculations of the differential cross section for krypton of Sienkiewicz and Baylis at 0·8, 1, 2 and 3 eV were integrated to obtain σ_m and are plotted in Figs 1*c* and 1*d*. The significant disagreement with the present σ_m indicates that although a Dirac–Fock approach has been used, the treatment of polarisation using a model potential retaining dipole and quadrupole terms only is inadequate.

The consistency of the theoretical cross sections with the experimental data was tested in the same way as previous derivations from experimental data (i.e. through solution of the Boltzmann equation). Examples of the difference curves for drift velocity and D_T/μ using the cross section of Mimnagh *et al.* are shown in Figs 2 and 3. Although this cross section lies close to the present one, it is clearly incompatible with the experimental data and predicts transport coefficients that are uniformly smaller than the data.

5. Conclusions

A momentum transfer cross section for electron scattering from krypton in the range 0–4 eV has been derived from an analysis of drift velocity and D_T/μ data for electron swarms in hydrogen–krypton mixtures. The uncertainty in the derived cross section is a combination of several factors, including the sensitivity of the fitted parameters, the absolute uncertainty in the experimental data and the uncertainty in the cross sections representing the hydrogen admixture. The combination of these factors is an uncertainty of 15–20% at energies in the region of the Ramsauser–Townsend minimum. The present cross section is significantly different from any previous determination, and is the first which successfully predicts all the available swarm data. Amongst the theoretical calculations available, the recent non-relativistic calculation of Mimnagh *et al.* (1993) lies closest to the present cross section over the energy range investigated, although

the predicted transport parameters are uniformly smaller than those measured, over the full range of E/N. A relativistic calculation, using the polarisation treatment of Mimnagh *et al.* rather than the simpler treatment of Sienkiewicz and Baylis, may be sufficient to alter the shape of the cross section sufficiently to improve the level of agreement to within the experimental uncertainties.

Acknowledgments

We acknowledge the considerable contribution that Jim Mitroy has made to this work, through his original code for a two-term solution of the Boltzmann equation. We thank Bob McEachran of the 'York group' for providing us with details of their calculations prior to publication. We are also grateful to Malcolm Elford, Bob Crompton, Steve Gibson and Brenton Lewis for their advice and assistance.

References

Baluja, K. L., Jain, A., Jones, H. W., and Weatherford, C. A. (1991). *Phys. Scripta* **45**, 30.
Bell, K. L., Berrington, K. A., and Hibbert, A. (1988). *J. Phys.* B **21**, 4205.
Brunger, M. J., Buckman, S. J., and Newman, D. S. (1990). *Aust. J. Phys.* **43**, 665.
Brunger, M. J., Buckman, S. J., Newman, D. S., and Alle, D. T. (1991). *J. Phys.* B **24**, 1345.
Buckman, S. J., and Mitroy J. (1989). *J. Phys.* B **22**, 1365.
Crompton, R. W., Elford, M. T., and McIntosh, A. I. (1968). *Aust. J. Phys.* **21**, 43.
Crompton, R. W., and Morrison, M. A. (1993). *Aust. J. Phys.* **46**, 203.
Dalgarno, A., and Kingston, A. E. (1960). *Proc. R. Soc. London* A **259**, 424.
Elford, M. T., Brennan, M. J., and Ness, K. F. (1992). *Aust. J. Phys.* **45**, 671.
England, J. P., and Elford, M. T. (1988). *Aust. J. Phys.* **41**, 701.
England, J. P., Elford, M. T., and Crompton, R. W. (1988). *Aust. J. Phys.* **41**, 573.
Fon, W. C., Berrington, K. A., and Hibbert, A. (1984). *J. Phys.* B **17**, 3279.
Hunter, S. R., Carter, J. G., and Christophorou, L. G. (1988). *Phys. Rev.* A **38**, 5539.
Jain, A. (1991). Personal communication.
Koizumi, T., Shirakawa, E., and Ogawa, I. (1986). *J. Phys.* B **19**, 2331.
McEachran, R. P., and Stauffer, A. D. (1984). *J. Phys.* B **17**, 2507.
McEachran, R. P., and Stauffer, A. D. (1988). Proc. Int. Symp. on Correlation and Polarisation in Electronic and Atomic Collisions (World Scientific: Singapore).
McEachran, R. P., and Stauffer, A. D. (1990). *J. Phys.* B **23**, 4605.
Mimnagh, D. J. R., McEachran, R. P., and Stauffer, A. D. (1993). *J. Phys.* B (submitted).
Mitroy, J. (1990). *Aust. J. Phys.* **43**, 19.
Ness, K. F., and Robson, R. E. (1986). *Phys. Rev.* A **34**, 2185.
O'Malley, T. F. (1992). *J. Phys.* B **25**, 163.
Robertson, A. G. (1972). *J. Phys.* B **5**, 648.
Schmidt, B. (1992). *Comments At. Mol. Phys.* (submitted).
Sienkiewicz, J. E., and Baylis, W. E. (1992). *J. Phys.* B **25**, 2081.
Sin Fai Lam, L. T. (1982). *J. Phys.* B **15**, 119.
Yau, A. W., McEachran, R. P., and Stauffer, A. D. (1980). *J. Phys.* B **13**, 377.

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