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The Momentum Transfer Cross Section for Krypton

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Abstract

A form of modified effective range theory (MERT) has been used to analyse drift velocity data for both pure krypton and molecular hydrogen–krypton mixtures. The present momentum transfer cross section reproduces the data to within 4% for pure krypton and to within 1·0% for the H_2–Kr mixtures.

1. Introduction

Previous determinations of the momentum transfer cross section σ_M have been performed by Hunter *et al.* (1988) and England and Elford (1988) from drift velocity v_{dr} measurements in pure krypton and H_2–krypton mixtures respectively. Koizumi *et al.* (1986) have also derived σ_M from measurements of the ratio D_T/μ (where D_T is the transverse diffusion coefficient, μ is the electron mobility equal to v_{dr}/E, and E is the electric field strength). There have also been determinations of the momentum transfer cross section by Frost and Phelps (1964) and Hoffman and Skarsgard (1969), however these older measurements can be regarded as being superseded by the more modern experiments. Buckman and Mitroy (1989) also derived a momentum transfer cross section for krypton by doing a modified effective range theory (MERT) analysis (O'Malley *et al.* 1962; O'Malley 1963) of (beam) total elastic cross section data, but the large uncertainties inherent in the MERT analysis make this σ_M of limited use.

One problem these determinations of the momentum transfer cross section have in common is that σ_M is determined by manual adjustment of a trial cross section until satisfactory agreement is reached between experimental transport coefficients and transport coefficients computed via a Boltzmann analysis. This process imposes no constraints upon the actual shape of the cross section, which can take any form consistent with transport coefficients that conform with experiment. The potential problem with this approach is best illustrated by an examination of the σ_M of England and Elford (1988) in the region of the cross section minimum. This cross section is depicted in Fig. 1 (dashed curve) and is compared with an attempt to fit it with a MERT expression for the phase shifts (solid curve) in the region from 0 to 1·0 eV. The MERT cross section has a sharper and deeper minimum and could not

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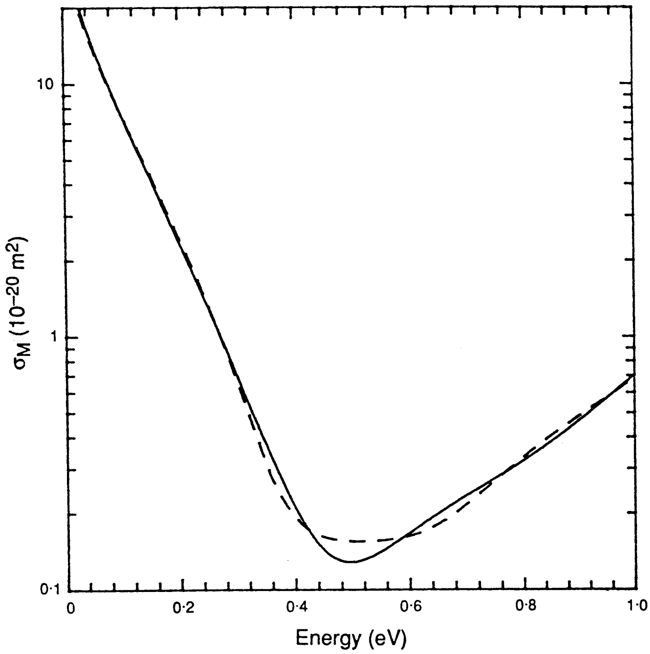

Fig. 1. Comparison of the momentum transfer cross section of England and Elford (1988) (dashed curve) and that resulting from an attempt to fit this data with a cross section derived from a six-parameter MERT expression (solid curve) for the phase shifts.

reproduce the broad shallow minimum of England and Elford. Since MERT is a very general theory in which short range scattering events are described by adjustable parameters, it is surprising, to say the least, that a MERT expansion with six free parameters could not provide an adequate description of this cross section. While it is possible that the inability of MERT to reproduce the shape of the England and Elford cross section is due to a limitation with MERT, it is more likely that it is the shape of the England and Elford cross section that is unphysical. This has serious implications since one of the reasons for doing an experiment with a krypton–H_2 mixture was that the mixture data should have more sensitivity to σ_M in the region of the minimum than an experiment using pure krypton. Another indication that something may be wrong with the England and Elford σ_M is provided by the fact that this cross section does a poor job (5–8% discrepancies) of reproducing the drift velocity data for pure krypton at E/N values less than $0 \cdot 03$ Td (corresponding to mean energies less than $0 \cdot 6$ eV). Similarly, England and Elford have pointed out that the σ_M of Hunter *et al.* does not reproduce their drift velocity data to within experimental error, although in this instance the discrepancies are smaller and do not exceed 3%.

Since neither of these cross sections are entirely satisfactory, a Boltzmann analysis of both sets of data has been performed. In order to alleviate the non-uniqueness problems in the region of the cross section minimum a form for the momentum transfer cross section derived from MERT has been used in the energy range for 0–7 eV. In most respects the methods used for the present work are similar in concept to those adopted by Haddad and O'Malley (1982) in their analysis of transport data for pure argon.

2. Details of the Calculation

The form of MERT adopted for this work was described by Buckman and Mitroy (1989) in their analysis of low energy total cross sections. Accordingly only a brief recapitulation of the particular form of the expression used for krypton need be given here. The s-wave, p-wave and d-wave phase shifts are modelled by the following expressions:

$$\tan\eta_0 = -Ak\{1+(4\alpha_d/3)k^2\ln(k)\}-(\pi\alpha_d/3)k^2+Dk^3+Fk^4\,, \tag{1}$$

$$\tan\eta_1 = a_1\,\alpha_d\,k^2 - A_1\,k^3+(b_1\,\alpha_d^2+c_1\,\alpha_q^2)k^4+Hk^5\,, \tag{2}$$

$$\tan\eta_2 = a_2\,\alpha_d\,k^2 - (b_2\alpha_d^2+c_2\,\alpha_q^2)k^4+A_2k^5\,, \tag{3}$$

where α_d is the dipole polarisability of the atom, α_q is the 'effective' quadrupole polarisability, k is the wave number, A is the scattering length, and D, F, A_1, H and A_2 are additional fitting parameters. The phase shifts for the higher partial waves with electron angular momentum $l>2$ are given by (Ali and Fraser 1977)

$$\tan\eta_l = a_l\,\alpha_d\,k^2+(b_l\,\alpha_d^2+c_l\,\alpha_q)k^4\,. \tag{4}$$

The coefficients a_l, b_l and c_l are given by

$$\begin{aligned} a_l &= \frac{\pi}{(2l+3)(2l+1)(2l-1)}\,,\\ b_l &= \frac{\pi\{15(2l+1)^4-140(2l+1)^2+128\}}{\{(2l+3)(2l+1)(2l-1)\}^3(2l+5)(2l-3)}\,,\\ c_l &= \frac{3a_l}{(2l+5)(2l-3)}\,. \end{aligned} \tag{5}$$

In terms of the phase shifts, the momentum transfer cross section is

$$\sigma_M = \frac{4\pi}{k^2}\sum_l (l+1)\sin^2(\eta_l-\eta_{l+1})\,, \tag{6}$$

All the formulae here are given in terms of atomic units ($e=\hbar=m_e=1$), although cross section results will be reported in units of Å^2 as a function of energy in eV. For this work a value of 16·744 a.u. (Dalgarno and Kingston 1960) was used for the dipole polarisability and a value of 8·0 a.u. for the effective quadrupole polarisability was derived by combining the non-adiabatic dipole term (Dalgarno and Kingston 1960) and the adiabatic quadrupole polarisability (McEachran *et al.* 1979).

There are two different, though related reasons for which MERT analyses are undertaken. Firstly, the aim can be to fit a cross section and then derive information about individual partial wave phase shifts. The other purpose is merely to have a convenient and accurate functional form with which to describe the behaviour of the cross section as a function of energy. The criteria imposed upon the validity of the MERT expansions which are used purely as fitting tools can be less stringent than those designed to extract information about phase shifts (Buckman and Mitroy 1989). For instance, the particular form of MERT adopted here is able to reproduce the theoretical momentum transfer cross sections of McEachran and Stauffer (personal communication 1987) and Stauffer *et al.* (1986) with a maximum error of 5%. The maximum error occurred near the cross section minimum, and away from the minimum MERT was much more accurate. Similar considerations are relevant to the work by Haddad and O'Malley (1982) in which a four-parameter expression for the phase shifts was used to define the momentum transfer cross section between 0 and 1 eV. In spite of the fact that this is beyond the range of validity of a single parameter form for the p-wave phase shift (Buckman and Mitroy 1989), the resulting functional form for the transfer cross section is sufficiently flexible to describe this cross section without any significant loss in accuracy,

Having decided to use the MERT form to describe the low energy behaviour of the cross section we could then automate the determination of σ_M. The Boltzmann equations, in the two-term approximation, were solved at values of E/N for which experimental v_{dr} data existed and the root mean square difference of the calculated and experimental drift velocities was minimised by adjusting the MERT parameters using standard nonlinear optimisation techniques. The individual data points for both the pure and mixture data were all given the same weighting during the fitting. The parameter A_2 was not permitted to vary during the minimisation procedure. It was fixed at a value of $4\cdot2$ for reasons discussed by Buckman and Mitroy. At energies larger than $1\cdot0$ eV an average of the numerically tabulated cross sessions of Hunter *et al.* and England and Elford was taken and linear interpolation used to determine σ_M at energies other than at the tabulated grid points. A smoothing procedure was used for energies between $0\cdot9$ and $1\cdot0$ eV to partially eliminate any kinks in going from the MERT defined σ_M to the numerically tabulated σ_M.

The percentage differences between the calculated values and the experimental data are shown in Fig. 2. The fit to the data of Hunter *et al.* (stars) is within the quoted error limits for all values of E/N except those at $0\cdot025$ to $0\cdot035$ Td, where discrepancies of 2% to 4% occur. It should be mentioned that the cross section of Hunter *et al.* also gave similar discrepancies at these values of E/N. Also shown in Fig. 2 are the difference curves for two Kr–H_2 gas mixtures (triangles and circles). The largest discrepancy was less than $1\cdot0$%, which is larger than the error tolerance quoted by England and Elford ($0\cdot7$%) and is also much larger than the maximum discrepancy ($0\cdot35$%) given by the England and Elford cross section for the same transport data. However, the result is as good as can be expected, since the use of cross sections for H_2 which are not known exactly can be expected to induce errors up to 1%.

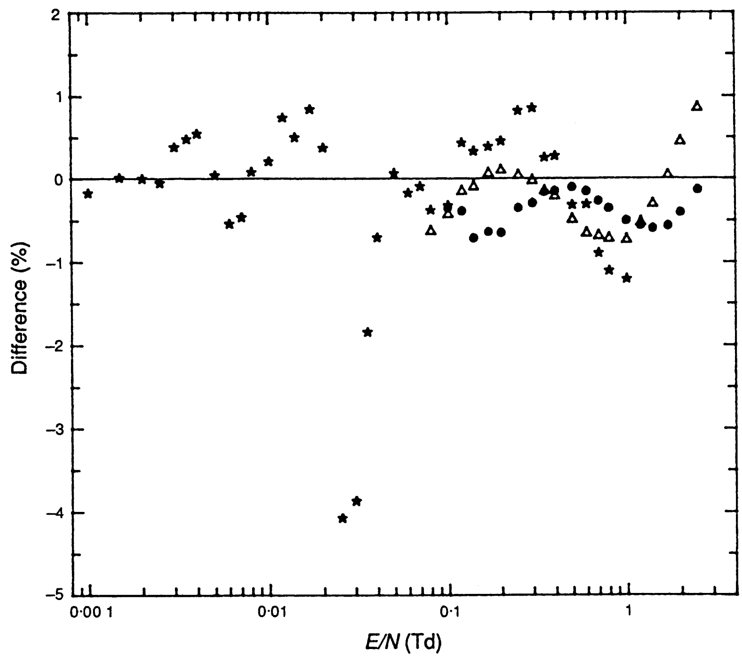

Fig. 2. Percentage differences between calculated and experimental drift velocities using the krypton momentum transfer cross section derived in this work. Differences with the pure krypton data (Hunter *et al.* 1988) (stars), and the 0·4673% (triangles) and 1·686% (circles) H_2–Kr mixtures (England and Elford 1988) are shown.

In Table 1 we give the momentum transfer cross section that was derived from the fit to the transport data. The MERT parameters used to compute the cross section in the energy region from 0 to 1·0 eV are also given. This momentum transfer cross section is depicted in Fig. 3 and compared with the cross sections of Hunter *et al.* and England and Elford. The present cross section has a deeper and sharper minimum than both these previous cross sections.

The present cross section does a poor job of reproducing the D_T/μ measurements of Koizumi *et al.* (1986). At E/N values below 0·1 Td the present σ_M predicts values that exceed experiment by as much as 40%. This result can probably be ascribed to the presence of impurities in the Koizumi *et al.* experiment since the admixture of even a very small impurity of two common gases (H_2 and N_2) leads to a swarm with a greatly reduced mean energy. This is consistent with the fact that the Koizumi *et al.* D_T/μ data are smaller in magnitude than those predicted by the present σ_M.

Although any attempt to use the present MERT parameters to construct the total elastic cross section should be treated with scepticism, high confidence can be placed in the derived value of the scattering length. The present value of $-3\cdot387a_0$ almost bisects the values obtained by Hunter *et al.* ($-3\cdot36a_0$) and England and Elford ($-3\cdot43a_0$). The recent analysis by Buckman and Mitroy (1989) of the beam experiment of Buckman and Lohmann (1987) gave a value of $-3\cdot29a_0$, while Weyhreter *et al.* (1988) gave a value of $-3\cdot54a_0$.

Table 1. Present momentum transfer cross section for krypton
The MERT parameters used to define the cross section in the region from 0–0·9 eV are $A=-3\cdot3873$, $D=165\cdot49$, $F=-189\cdot735$, $A_1=13\cdot723$, $H=39\cdot535$ and $A_2=4\cdot2$

Energy (eV)	Cross section (Å^2)	Energy (eV)	Cross section (Å^2)
0·0	40·376	1·80	2·58
0·05	13·288	1·90	2·84
0·10	7·109	2·00	3·11
0·15	4·054	2·20	3·68
0·20	2·349	2·50	4·56
0·25	1·352	2·80	5·66
0·30	0·7637	3·00	6·30
0·35	0·4228	3·30	7·37
0·40	0·2364	3·60	8·48
0·45	0·1468	4·00	9·92
0·50	0·1182	4·40	11·10
0·55	0·1273	4·80	12·60
0·60	0·1589	5·00	13·20
0·65	0·2038	6·00	16·40
0·70	0·2551	7·00	18·40
0·75	0·3099	8·00	20·00
0·80	0·3649	9·00	21·00
0·85	0·4202	10·00	21·00
0·90	0·4737	11·00	21·00
0·95	0·5539	12·00	20·9
1·00	0·6665	13·00	19·4
1·10	0·8920	14·00	17·8
1·15	0·9960	15·00	16·2
1·20	1·111	16·00	14·8
1·25	1·215	17·00	13·6
1·30	1·330	18·00	12·5
1·40	1·570	19·00	11·7
1·50	1·810	20·00	11·0
1·60	2·060	25·00	8·0

4. Conclusions

A momentum transfer cross section for electron scattering from krypton has been derived by using MERT to analyse drift velocity data. The present cross section is close in magnitude to the cross sections of Hunter *et al.* (1988) and England and Elford (1988) at energies where the cross section is large, but significant differences exist at the cross section minimum. Unlike the previous momentum transfer cross sections, the present cross section fits all sets of drift velocity data and should be regarded as superseding these previous determinations. Nevertheless, a careful look at the present cross section (depicted in Fig. 3) reveals minor anomalies in the shape for energies greater than 0·6 eV. This is not surprising since the well known insensitivity of drift velocty data to the cross section in the vicinity of the Ramsauer–Townsend minimum makes it difficult to uniquely define the cross section in this energy region. Hence, an experiment to measure D_T/μ in either pure krypton or a H_2–Kr mixture would be desirable since it would enable a more precise specification of the momentum transfer cross section in the region of the minimum.

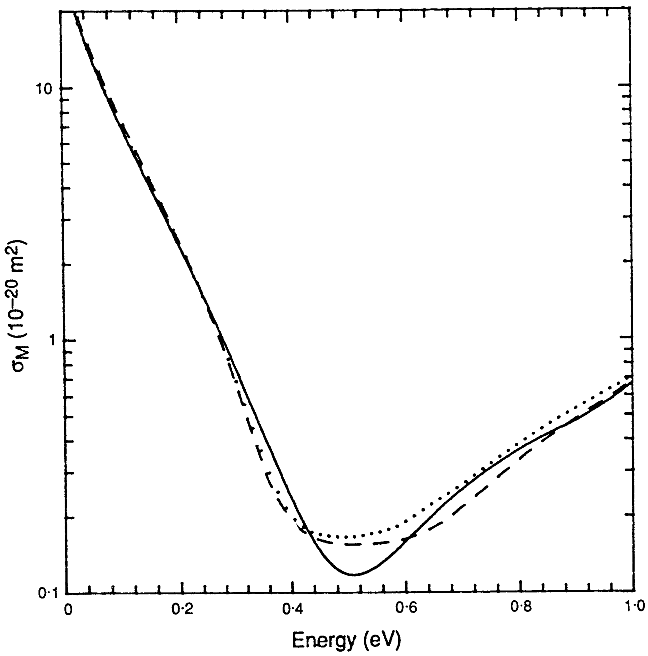

Fig. 3. Present momentum transfer cross section (solid curve) compared with those derived by Hunter *et al.* (dotted curve) and England and Elford (dashed curve) in the energy range from 0 to 1 eV.

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