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Scattering Cross Sections in Argon from Electron Transport Parameters

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Abstract

Previously determined experimental drift velocities v_{dr} and ratios of lateral diffusion coefficient to mobility D_T/μ have been refitted directly with a three parameter modified effective range theory (MERT) representation of the S wave phase shift, a one parameter fit to the P wave phase shift and fixed higher partial wave phase shifts. The MERT representation now extends to $1 \cdot 0$ eV, a threefold extension of the energy range of the MERT fit reported by Milloy *et al.* (1977). The total cross section derived from the phase shifts is also reported, together with the differential cross section at $1 \cdot 0$ eV which is compared with a previous experimental determination.

Milloy *et al.* (1977) derived the momentum transfer cross section for electron–argon collisions in the energy range 0–4 eV using their measurements of the transport parameters (Milloy and Crompton 1977; Robertson 1977). These authors incorporated modified effective range theory (MERT) to remove some of the uniqueness problems associated with the derivation of cross sections from transport parameters.

Recently a small error in the reported values of D_T/μ has been discovered (Milloy and Crompton 1982) which was caused by an error in the calibration of the pressure gauge used in the measurements. The discovery of this error has led us to repeat the previous analysis to redetermine the cross section from the corrected data. Although the small error in the D_T/μ data makes very little difference to the derived cross section we show that it is possible to extend the MERT fit to $1 \cdot 0$ eV, that is, to an energy about three times larger than the limit set by Milloy *et al.* (1977). Thus we are able to give the MERT parameters from which the cross sections (differential, total, or momentum transfer) can be calculated over this somewhat larger energy range.

The procedure has been detailed previously (O'Malley 1963; Milloy and Crompton 1977; O'Malley and Crompton 1980). We use the MERT formula for the phase shifts

$$\eta_0 = -Ak\{1+(4\alpha/3a_0)k^2\ln(ka_0)\} - (\pi\alpha/3a_0)k^2 + Dk^3 + Fk^4\,, \tag{1}$$

$$\eta_1 = (\pi/15)\alpha k^2\{1-(\varepsilon/\varepsilon_1)^{\frac{1}{2}}\}\,, \tag{2}$$

$$\eta_L = \pi\alpha k^2/\{(2L+3)(2L+1)(2L-1)a_0\}\,, \tag{3}$$

where k is the wave number, related to the energy ε (in eV) by $\varepsilon = 13\cdot605(ka_0)^2$, and a value of $\alpha = 11\cdot08\,a_0^3$ (Miller and Bederson 1977) was used. The momentum transfer cross section is given in terms of the phase shifts as

$$\sigma_{\mathrm{m}} = \frac{4\pi}{k^2}\sum_{L=0}^{\infty}(L+1)\sin^2(\eta_L - \eta_{L+1})\,. \tag{4}$$

The substitution into equation (4) of values of η_1, η_2 and higher order phase shifts η_L calculated from equations (1), (2) and (3) respectively enables v_{dr} or D_{T}/μ to be calculated at a particular value of E/N. This involves substituting values of σ_{m} into the integrals for the distribution function $f(\varepsilon)$, the drift velocity v_{dr}, and the ratio of the lateral diffusion coefficient to mobility D_{T}/μ (see Huxley and Crompton 1974). Thus values of v_{dr} and D_{T}/μ can be calculated as a function of E/N with the parameters A, D, F and ε_1 being the only variables.

Table 1. Effect of varying the upper energy limit

Upper limit (eV)	Chi (%)	A (a_0)	D (a_0^3)	F (a_0^4)	ε_1 (eV)
0·5	0·9	−1·492	64·3	−77·3	0·884
1·0	0·9	−1·488	65·4	−84·3	0·883
1·5	0·9	−1·489	65·0	−82·9	0·881
2·0	1·4	−1·493	64·4	−79·6	0·877
3·0	4·4	−1·501	63·0	−73·6	0·871
5·0	6·5	−1·502	62·7	−73·1	0·870

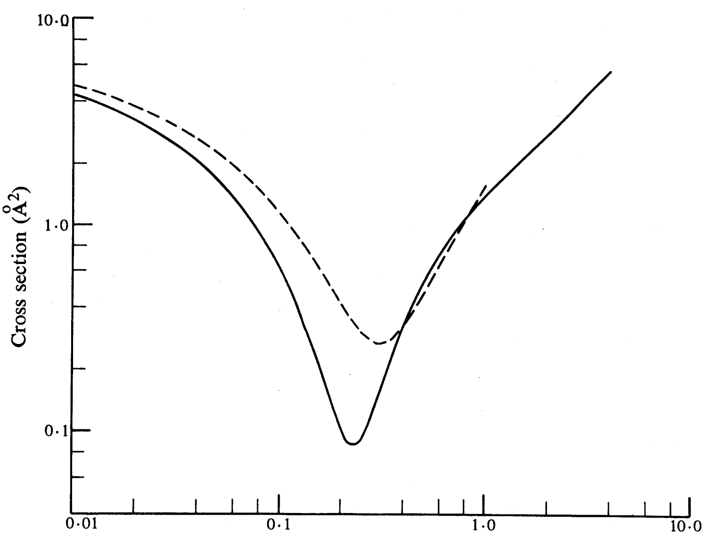

Fig. 1. Momentum transfer (solid curve) and total (dashed curve) cross sections for electron–argon scattering.

In the present work the four parameters were adjusted to obtain the best fit to the 25 values of D_{T}/μ measured at 294 K by Milloy and Crompton (1977) and the 31 values of v_{dr} measured at 89·6 K by Robertson (1977). All 56 data points were given equal significance in the fitting procedure.

We have varied the upper energy limit of the MERT cross section and beyond this limit we have used the tabulated cross section of Milloy *et al.* (1977). The effect of varying the upper energy limit of the MERT cross section is shown in Table 1 where we list this limit together with the value of 'chi' which is minimized during the search procedure. Also listed are the MERT parameters.

It is clear from the tabulated values of chi that using the MERT expansion to energies much higher than 1·0 eV is somewhat questionable. This is verified by the fact that it is the mismatch between the calculated and experimental values of D_T/μ and v_{dr} at the highest values of E/N which makes a significant contribution to the increase in chi.

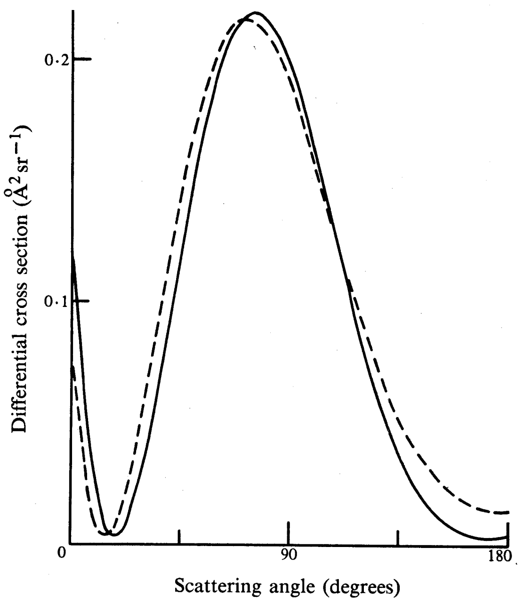

Fig. 2. Comparison of the present result for the differential scattering cross section at 1·0 eV (dashed curve) compared with that (solid curve) of D. Andrick (personal communication).

We have chosen an upper limit on the MERT expansion of 1·0 eV and, using the parameters listed against this limit in Table 1, we have calculated σ_m and σ_T. These data are shown in Fig. 1. Above 1·0 eV the values of σ_m are taken from Milloy *et al.* (1977).

Given the phase shifts one can also calculate the differential scattering cross section. Fig. 2 shows such a calculation at 1·0 eV compared with the results of D. Andrick (personal communication) which were derived from measurements of the angular distributions of scattered electrons at energies from 2 to 20 eV at 1 eV intervals. Each of these distributions was analysed to give the phase shifts, and the energy dependence of each phase shift was fitted to an effective range formula, or a polynomial having the correct theoretical value at zero energy. Cross sections were then calculated from these phase shifts.

Although we have made the comparison at what we consider to be the upper energy limit of our MERT expansion the agreement between the two results is remarkably good. Unfortunately we cannot extend the comparison to more than one energy, so that this agreement may be fortuitous. Indeed, the comparison at 2·0 eV (outside what we believe to be the valid range of our expansion) is much less satisfactory.

As presented the cross section shows only minor differences from the original cross section of Milloy *et al.* (1977) both within the energy range (0–0·32 eV) of the original MERT fit and outside it. Nevertheless the extension of the MERT representation of the phase shifts to 1·0 eV not only increases the confidence in the cross section in the vicinity of the Ramsauer minimum, since the phase shifts are now derived from a larger body of experimental data, but also increases the range of overlap with experimental data for differential and total cross sections. The largest difference between our cross section and that of Milloy *et al.* is 7% in the region around 0·3 eV. This is due to the small upper limit set for the MERT representation in the earlier work. Elsewhere the maximum difference is of the order of 3%. As expected the small corrections to the values of D_T/μ caused by the error in the pressure gauge calibration (the original cause of this investigation) give rise to no significant changes in the cross section. Fig. 3 presents the differences between the experimental transport coefficients and those predicted with the derived cross sections as a function of E/N.

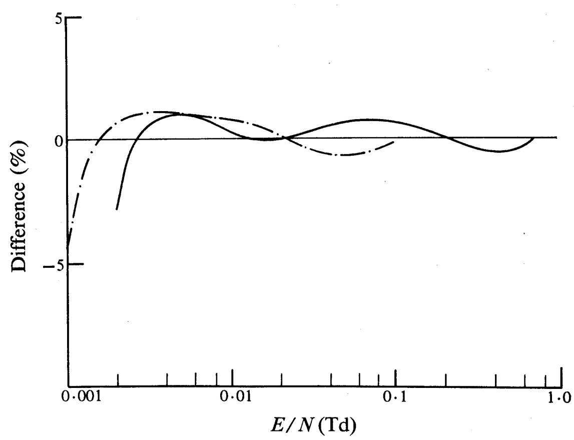

Fig. 3. Differences between the calculated and measured values of D_T/μ at 294 K (dot–dash curve) and v_{dr} at 90 K (solid curve) plotted as functions of E/N. The calculated values of v_{dr} are too low at low E/N.

In summary, we have produced best estimate values of the argon momentum transfer cross section, based on the available transport data, specified in terms of four MERT parameters (the parameters listed against 1 eV in Table 1). There are small changes in the momentum transfer cross section from the original cross section of Milloy *et al.* (1977), due almost entirely to the use of MERT up to a higher energy limit. In addition we give values of the MERT parameters which enable the phase shifts and differential and integral cross sections to be derived over an energy range which overlaps that accessible to experimental determinations of differential and total cross sections.

References

Huxley, L. G. H., and Crompton, R. W. (1974). 'The Diffusion and Drift of Electrons in Gases' (Wiley: New York).

Miller, T. M., and Bederson, B. (1977). *In* 'Advances in Atomic and Molecular Physics', Vol. 13 (Eds D. R. Bates and B. Bederson), p. 1 (Academic: New York).

Milloy, H. B., and Crompton, R. W. (1977). *Aust. J. Phys.* **30**, 51.
Milloy, H. B., and Crompton, R. W. (1982). *Aust. J. Phys.* **35**, YY [present issue].
Milloy, H. B., Crompton, R. W., Rees, J. A., and Robertson, A. G. (1977). *Aust. J. Phys.* **30**, 61.
O'Malley, T. F. (1963). *Phys. Rev.* **130**, 1020.
O'Malley, T. F., and Crompton, R. W. (1980). *J. Phys.* B **13**, 3451.
Robertson, A. G. (1977). *Aust. J. Phys.* **30**, 39.

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