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Ionisation cross sections of P, S, Cl, K and Ca for protons and alpha particles between 0.6 and 2.8 MeV

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Abstract. Ionisation cross sections for protons incident on P, S, Cl, K and Ca and for alpha particles on Cl and Ca have been obtained from experimental x-ray production cross sections for collision energies between 0.6 and 2.8 MeV. Systematic comparisons of all existing theories with the present results and previous ones at the same scaled projectile velocity are also shown.

1. Introduction

The recent collections of experimental cross sections for ionisation by collisions with ions (Rutledge and Watson 1973, Gardner and Gray 1978) show a relative lack of experimental data for collisions of protons and, particularly, alpha particles with targets with $15 \leqslant Z \leqslant 20$. In this region, in fact, there are measurements for only $Z = 18$ (Ar).

The purpose of this work was partially to overcome this deficiency and also to compare experimental results with the most recent theories of atomic collision processes, including, in particular, the perturbed stationary states (PSS) model and its corrections (Basbas *et al* 1973, 1978).

The experimental apparatus is the same as that of Milazzo and Riccobono (1976) and Magno *et al* (1979). Since the elements considered here have low-energy characteristic x-ray lines (<4 keV), a precise determination of x-ray silicon detector efficiency is very important. We have put the x-ray detector under vacuum in order to avoid errors coming from an incorrect estimate of the x-ray absorption in air.

The detector Be window has been shielded with a mylar film to stop the particles scattered from the target entering the detector. The mylar thickness has been measured by weighing (9.8 mg cm^{-2}).

From an accurate existing study of the problem of Si(Li) detector efficiency (McGeorge *et al* 1973) we know that for low-energy x-rays the efficiency values given by theory agree, within limits which are acceptable for the present work, with the values measured by different techniques. Therefore the efficiency has been theoretically calculated considering the cumulative effect of absorption from the various absorbing layers that the x-rays have to cross before reaching the detector active layer (these calculations are based on the factory data). They had been done separately for K_α and K_β lines for each element because the silicon K absorption edge and gold M edges are present in the region of these x-ray energies. The K_α and K_β x-ray lines have been only partially resolved, so their relative intensities have been taken from the literature (Bambynek *et al* 1972). The calculated values for the efficiency are shown on table 1.

Table 1. Calculated efficiency coefficients for Be window, Au thickness and Si dead layer for the x-ray lines listed in the first row.

Element	Line	Be	Au	Si
P	K_α	0.720	0.945	0.886
P	K_β	0.760	0.952	0.898
S	K_α	0.807	0.850	0.915
S	K_β	0.839	0.872	0.927
Cl	K_α	0.866	0.864	0.937
Cl	K_β	0.891	0.883	0.947
K	K_α	0.933	0.912	0.965
K	K_β	0.948	0.922	0.971
Ca	K_α	0.952	0.927	0.973
Ca	K_β	0.963	0.941	0.979

2. Theoretical models

We have compared our experimental results with the values given by all existing theoretical models.

The semiclassical model or SCA values (Bang and Hansteen 1959, Hansteen and Mosebekk 1970, 1973) have been calculated with Hansteen *et al*'s (1975) tables.

The ionisation cross sections given by the binary encounter approximation (BEA) (Garcia 1970, McGuire *et al* 1973, Hansen 1973) and by the plane-wave Born approximation (PWBA) (Merzbacher and Lewis 1958, Basbas *et al* 1973) have been extracted from the Milazzo *et al* (1979) tables.

For the perturbed stationary states model (PSS) (Basbas *et al* 1973, 1978, Hill and Merzbacher 1974) and its possible corrections, we referred to Basbas *et al* (1978), computing theoretical cross section values corrected for the binding and polarisation effects (PSS (BP)). We have neglected all the corrections to the different models mentioned earlier for typical phenomena of low-energy and high-Z target collisions.

In particular, we have neglected both the effect of deflection of the projectile trajectory (Garcia 1970, Basbas *et al* 1973) and the slowing down of the projectile in the nuclear Coulomb field of the target atom (Kunc 1979, Magno *et al* 1979), which with our conditions give corrections of the order of or less than the experimental errors. For the same reasons we have omitted the corrections concerning the relativisitic treatment of the ion–electron collision and the relativistic description of the electronic wavefunctions (Kamiya *et al* 1977).

3. Secondary processes for x-ray production by ion bombardment

We consider here two other competitive ionisation processes which contribute to x-ray production in addition to the ionisation by collision: Coulomb nuclear excitation and charge transfer.

(i) *Coulomb nuclear excitation.* In some cases the effect of Coulomb nuclear excitation followed by internal conversion contributes remarkably to x-ray production (McClelland *et al* 1953, Magno *et al* 1979) and some recent work makes allowance for it (Anholt 1978). In this work, we have neglected this effect because the energy of the first excited nuclear levels of the atoms we studied are, in general, too high (Endt and Van der Leun 1978) to make any appreciable contribution to x-ray production at our bombarding energies.

(ii) *Charge transfer.* Charge transfer processes can also produce electronic holes in the inner shells. However, in general, these processes are more evident when the incident ion charge is higher. Reading and Ford (1980) have recently developed theoretical semi-empirical models to compute charge transfer cross sections. The results of these models are in accordance with one another and with the experimental

Table 2. The experimental values (barns) of the ionisation cross sections for protons on P, S, Cl, K and Ca at the energies listed in the first row. The numbers in brackets are the powers of 10 by which the numbers should be multiplied.

E (keV)	P $\omega_k = 0.060$	S $\omega_k = 0.082$	Cl $\omega_k = 0.0955$	K $\omega_k = 0.138$	Ca $\omega_k = 0.163$
600	2.65 ± 0.40 (+3)	1.89 ± 0.28 (+3)		2.93 ± 0.43 (+2)	1.62 ± 0.24 (+2)
800	5.81 ± 0.87 (+3)	3.60 ± 0.54 (+3)	1.71 ± 0.25 (+3)	6.27 ± 0.94 (+2)	3.47 ± 0.52 (+2)
1000	7.60 ± 1.14 (+3)	4.93 ± 0.73 (+3)	2.76 ± 0.41 (+3)	8.90 ± 1.33 (+2)	5.62 ± 0.84 (+2)
1200	9.32 ± 1.39 (+3)	6.46 ± 0.96 (+3)	2.93 ± 0.44 (+3)	1.30 ± 0.19 (+3)	8.58 ± 1.28 (+2)
1400	1.12 ± 0.17 (+4)	7.84 ± 1.17 (+3)	3.47 ± 0.52 (+3)	1.78 ± 0.26 (+3)	1.11 ± 0.16 (+3)
1600	1.32 ± 0.19 (+4)	9.08 ± 1.36 (+3)	4.38 ± 0.65 (+3)	2.16 ± 0.32 (+3)	1.37 ± 0.20 (+3)
1800	1.52 ± 0.23 (+4)	9.87 ± 1.49 (+3)	5.03 ± 0.75 (+3)	2.47 ± 0.37 (+3)	1.60 ± 0.24 (+3)
2000	1.54 ± 0.23 (+4)	1.07 ± 0.16 (+4)	5.57 ± 0.83 (+3)	3.12 ± 0.47 (+3)	1.80 ± 0.27 (+3)
2200	1.62 ± 0.24 (+4)	1.18 ± 0.17 (+4)	5.72 ± 0.86 (+3)	3.78 ± 0.58 (+3)	2.29 ± 0.34 (+3)
2400	1.61 ± 0.24 (+4)	1.20 ± 0.18 (+4)	5.58 ± 0.84 (+3)	4.03 ± 0.60 (+3)	2.60 ± 0.39 (+3)
2600	1.58 ± 0.24 (+4)	1.26 ± 0.19 (+4)	5.98 ± 0.89 (+3)	4.15 ± 0.62 (+3)	2.60 ± 0.39 (+3)
2800			5.79 ± 0.87 (+3)	4.38 ± 0.66 (+3)	2.80 ± 0.42 (+3)

Table 3. The experimental values (barns) of the ionisation cross sections for alpha particles on Cl and Ca at the energies listed in the first row. Numbers in brackets are powers of 10 by which the numbers should be multiplied.

E (keV)	Cl $\omega_k = 0.0955$	Ca $\omega_k = 0.163$
800	1.30 ± 0.19 (+2)	1.48 ± 0.22 (+1)
1000	2.93 ± 0.43 (+2)	3.07 ± 0.46 (+1)
1200	4.94 ± 0.74 (+2)	6.16 ± 0.92 (+1)
1400	7.92 ± 1.18 (+2)	1.08 ± 0.16 (+2)
1600	1.09 ± 0.16 (+3)	1.78 ± 0.26 (+2)
1800	1.59 ± 0.23 (+3)	2.62 ± 0.39 (+2)
2000	2.29 ± 0.34 (+3)	3.77 ± 0.56 (+2)
2200	2.66 ± 0.39 (+3)	5.29 ± 0.79 (+2)
2400	3.11 ± 0.55 (+3)	6.46 ± 0.96 (+2)
2600	4.76 ± 0.71 (+3)	8.64 ± 1.29 (+2)
2800	5.28 ± 0.79 (+3)	1.04 ± 0.15 (+3)

data (Tawara *et al* 1978, Ford *et al* 1979). We have computed the charge transfer cross sections according to directions of Basbas *et al* (1978) which are based on the previous work of Lapicky and Losonsky (1977).

In our case the charge transfer contributions are about 1% at most.

4. Fluorescence yields

During the last ten years much work has been concerned with evaluation of fluorescence yields. The Bambynek *et al* (1972) and Langenberg and van Eck (1979) reviews are especially noteworthy. It is possible to obtain from them reliable ω_k values that the authors derive from the evaluation of experimental measurements and from fitting procedures.

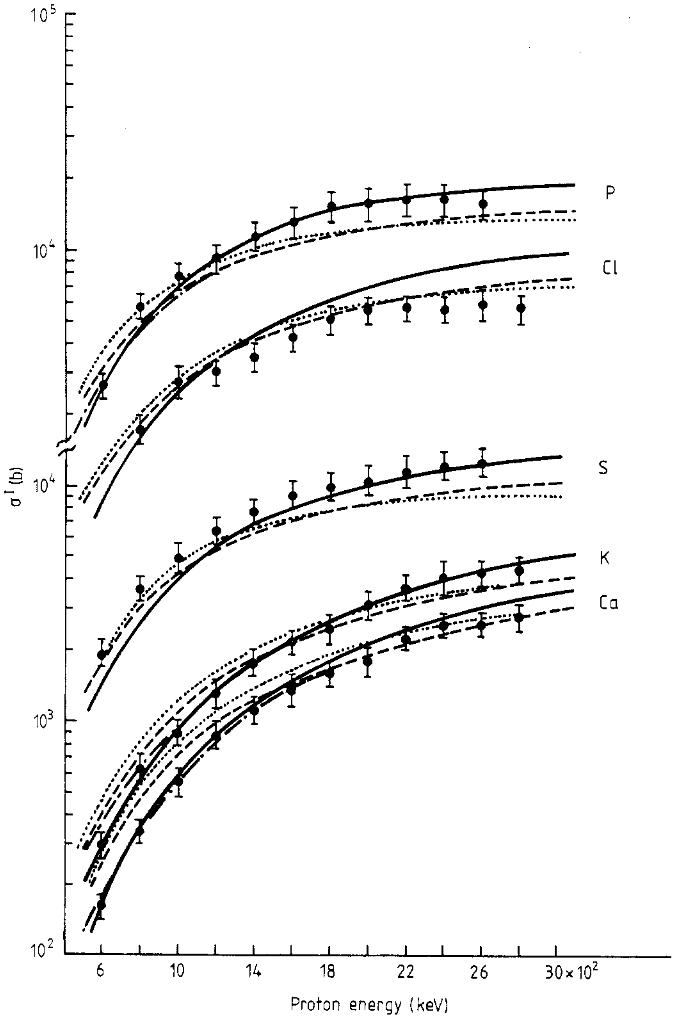

Figure 1. Experimental cross sections for protons on P, S, Cl, K and Ca and the values given by the BEA (——), PWBA (— — —), PSS (BP) (— · — · —) and SCA (· · · · · ·).

There are small discrepancies between the values given which are due to the different ways of evaluating the experimental results. For the elements studied in this work the largest difference is for phosphorus with $\omega_k = 0.0576$ (Langenberg and van Eck) and $\omega_k = 0.060$ (Bambynek *et al*); this difference gives a possible error of 4% in the ionisation cross section.

Multiple ionisation effects can give non-negligible effects on the fluorescence yields (Larkins 1971, Bhalla and Hein 1973). Larkins suggested a simple method to compute the fluorescence yield of an atom with a given hole shell distribution.

Several theoretical and experimental works deal with multiple ionisation processes. Two recent works (Schmiedekamp *et al* 1978, Watson *et al* 1979) give semi-empirical formulae based on current models of collision ionisation which allow the average probability of simultaneous ionisation of the K and L shells, P_L, to be computed. We obtained a maximum value $P_L = 0.02$ for 3 MeV proton collisions with phosphorus for the cases examined in the present work.

Assuming that all the L shell values are in the 2p subshell (Kauffman *et al* 1973, Larkins 1971) we deduced that the ω_k variation from multiple ionisation is always less than 4% and we have neglected it. We note that similar conclusions on this subject were drawn by Basbas *et al* (1978), Gardner *et al* (1979) and Lopes *et al* (1978).

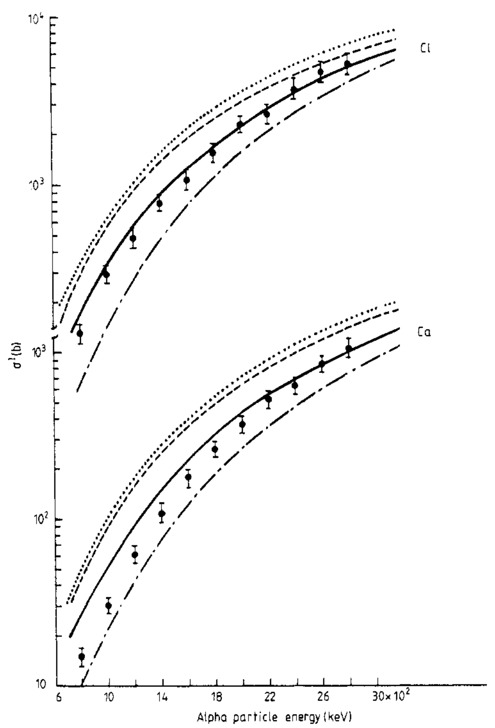

Figure 2. Experimental cross sections for alpha particles on Cl and Ca and the values given by the BEA (——), PWBA (— — —), PSS (BP) (— · — · —) and SCA (· · · · · ·).

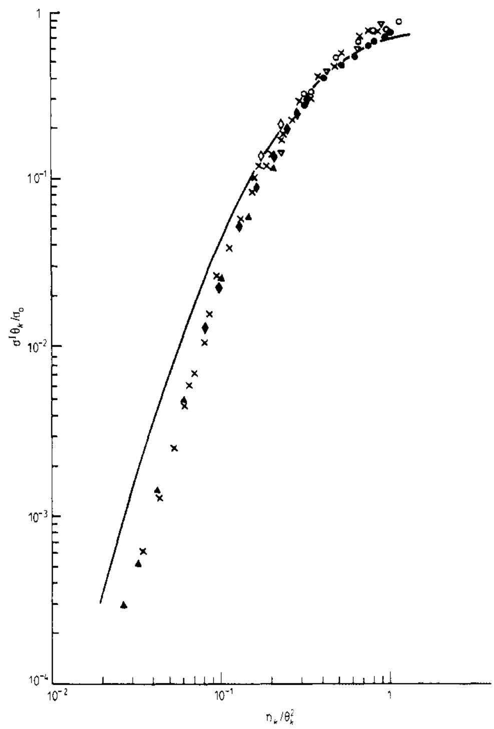

Figure 3. PWBA universal curve plotted against η_k/θ_k^2. σ_0 is given by formula (25) in Basbas *et al* (1973). ○: Bissinger *et al* (1970); ◇: Lopes *et al* (1978); ▽: Hopkins *et al* (1975); ◆: Milazzo and Riccobono (1976); ▲: Langenberg and van Eck (1976); ●: Winters *et al* (1973); ×: this work.

5. Experimental results

We have measured x-ray production cross sections for P, S, Cl, K and Ca at proton energies from 0.6 to 2.8 MeV and for Cl and Ca for alpha particles at the same energies.

Since the efficiency of the Si(Li) detector has been calculated theoretically, we have assigned a 15% error to the quoted values of the ionisation cross sections. These values are reported on tables 2 and 3. For each element we also report the values of ω_k we have used. A first comparison with the predictions of different models is shown in figures 1 and 2. We note that for protons the results of the three quantal theories (PSS, SCA and PWBA) are nearly the same while the BEA theory gives slightly different results. The experimental values of the ionisation cross section are basically in agreement with all the theories. A clearer situation is obtained for alpha particle measurements which are in a range of lower projectile velocities. Here the different theories give appreciably different predictions. The experiments seem to agree better with the BEA results.

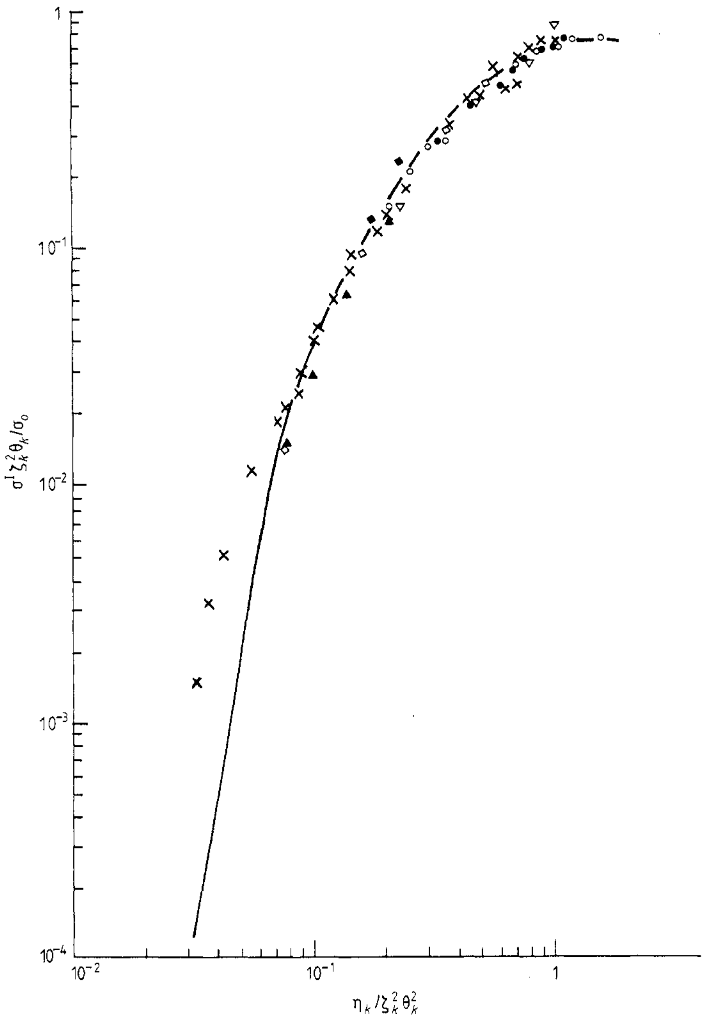

Figure 4. PSS (BP) universal curve plotted against $\eta_k/\zeta_k^2\theta_k^2$. The symbols represent the same work as in figure 3.

More general comparisons also including the previous experiments are shown in figures 3–6 where we have related our experimental points to the universal curves given by the PWBA, PSS (BP), BEA and SCA, respectively, and we have reported the comparatively few previous experimental results in the same scaled projectile energy range.

General agreement exists among all the experimental work. Our measurements are situated between 0.34 and 2 for the PWBA and PSS central parameter (Basbas *et al* 1978) $\xi_k = 2\sqrt{\eta_k}/\theta_k$, where $\theta_k = U/Z_k^2R$ (U is the binding energy of the K shell, Z_ke the screened nuclear charge and $R = 13.6$ eV) and η_k is given by formula (3) in the same reference. In figure 3 the PWBA curve is reported as a function of the scaled velocity η_k/θ_k^2.

We see that the PWBA theoretical curve does not fit the experiments for scaled velocity values under 0.5. In this region the Coulomb deflection and binding effect

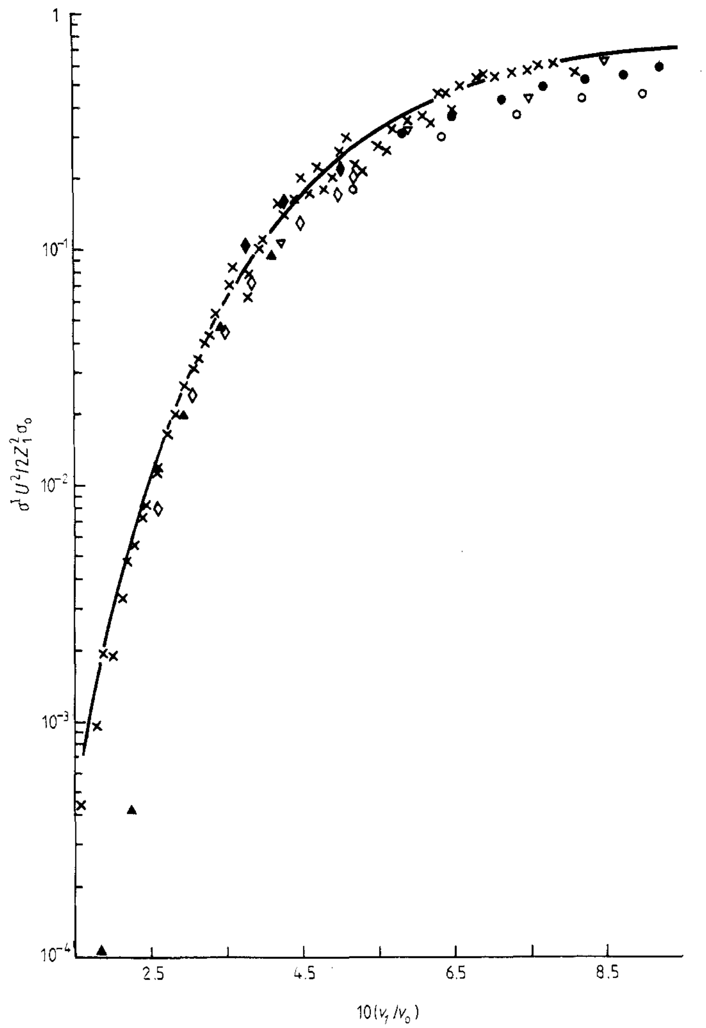

Figure 5. BEA universal curve for K-shell ionisation ($N = 2$) plotted against (v_1/v_0). $\sigma_0 = 6.56 \times 10^{-14}$ cm^2 eV^2, $v_0 = 2U/m_e$. The symbols represent the same work as in figure 3.

corrections must be introduced. PSS (BP) theory, which includes the binding effect, in fact improves the agreement with the experimental points. This is shown in figure 4, where PSS (BP) theory is reported as a function of $\eta_k/\zeta_k^2\theta_k^2$. ζ_k is the projectile velocity-dependent function defined by formulae (37) and (45) of Basbas *et al* (1978). For the smallest values of the scaled velocity η_k/θ_k^2, where we have done some measurements, it seems, however, to overcorrect the PWBA theory since the PSS curve lies under the experimental points. These points correspond to alpha particle measurements. On the other hand, the disagreement between the alpha particle measurements and PSS (BP) is evident from figure 2.

For PSS (BP) theory we agree with Gardner *et al* (1979) that the question of the appropriateness of the calculations is still unresolved. Moreover it should be better understood why a value of 1.5 for the C_k parameter is normally used (Basbas *et al* 1978, Paul 1980a).

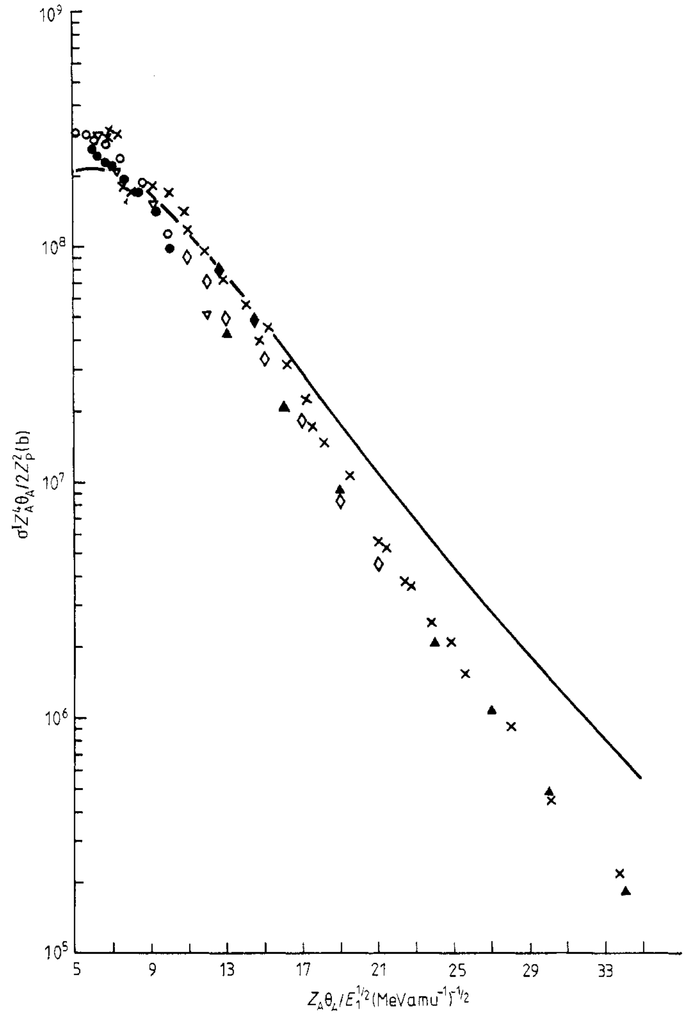

Figure 6. SCA universal curve plotted against $Z_A\theta_A/E_1^{1/2}$. θ_A is given by (8) in Hansteen *et al* (1975), E_1 is the projectile energy in MeV. Z_pe and Z_Ae are the projectile and target charges. The symbols represent the same work as in figure 3.

In figure 5 we see that all the experimental values lie within 20% of the BEA curve. Finally, in figure 6 we show evidence that the SCA model accounts for the experimental results for a rather limited range of scaled energy values, as has already been pointed out by Paul (1980b).

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