

AN ANALYSIS OF THE CROSS-SECTIONS FOR THE
IONISATION OF INNER-SHELL ELECTRONS BY ELECTRONS

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ABSTRACT

A theoretical analysis by a two parameters formula of the experimental cross-sections for ionisation of inner-shell electrons by electrons shows that the data for all the elements might be fitted with a single value for each of the parameters.

A review article has been recently devoted to an analysis of the cross-sections for the ionisation of inner-shell electrons by electrons¹. From a comparison with the experimental data it has been shown that the various theoretical formulae proposed to explain the phenomenon do not fit accurately the data near the threshold where the Coulomb field and the structure of atom disturb the motion of the primary electron.

Another formula was proposed² (Fabre 1949) long time ago the purpose of which was to take the influence of this field into account in order to explain the shape of the ionisation cross-section even near the threshold.

This formula reproduces quite well the ionisation cross-section for some gases like H², He, Ne, Ar, Kr and Xe. The ionisation of sodium vapour is surprisingly well reproduced and the ionisation cross-section of the K-shell electrons of Ag is also well fitted.

We intend now to extend this analysis to more recent works that deal with the ionisation of inner-shell electrons.

We expect to obtain results at least as good as those we got for Ag.

For a shell of quantum numbers (n,l) populated by Z_{nl} electrons each bound by an energy E_{nl} , the formula proposed for the single-ionisation cross-section in which one electron of the (n,l) shell is knocked out is :

$$\sigma_{nl}(E) = \frac{6.511}{E_{nl}^2} \frac{Z_{nl}}{k_{nl}} \frac{\text{Log } U_{nl}}{U_{nl} + \chi_{nl}} \cdot 10^{-16} \text{ cm}^2, \quad (E_{nl} \text{ in eV}), \quad (1)$$

where $U_{nl} = E/E_{nl}$.

The quantity $k_{nl} E_{nl}$ is the average energy lost by the primary electron of energy E and $\chi_{nl} E_{nl}$ is the energy gained by this electron penetrating into the atomic field in the vicinity

of the (n,l) -shell electron with which it interacts.

We expect χ_{nl} to be of the order of unity and $k_{nl} > 1$.

The maximum of the cross-section is determined by χ . The next table shows the position U_m of the maximum of the cross-section in terms of χ as given by $\chi = U_m(\text{Log } U_m - 1)$:

U_m	2.72	3.2	3.4	3.6	3.8	3.9	4.	4.2	4.4	4.6	4.8	5
χ	0	0.52	0.76	1.01	1.27	1.40	1.54	1.82	2.12	2.42	2.73	3.03

The maximum of the experimental cross-section appears for $U_{nl}=4$ which corresponds to $\chi = 1.5$. Our calculation does not distinguish (except by the binding energies) between the various shells, and so the value of k is supposed to be approximately the same for all shells. If this assumption is correct, then the maximum cross-section $\sigma_{nl}(4 E_{nl})$ ($U_m=4$) when plotted against E_{nl} in a double logarithmic scale should exhibit a straight line of slope -2. This has been observed⁸. Unfortunately the errors on the absolute cross-sections do not enable one to obtain a definite value for k . It is only possible to show that k lies between 1 and 2.

In order to obtain a more accurate evaluation of k , it is necessary to study in detail the cross-section as a function of E .

The very simple expression (1) enables one to check easily its validity by plotting

$$\frac{6.51 Z_{nl}^2}{E_{nl}^2 \sigma_{nl}(E)} \text{ Log } U_{nl} \cdot 10^{-14} \quad \text{against } U_{ln} \quad (2)$$

where $\sigma_{nl}(E)$ is the experimental cross-section. If our calculation holds, we expect to get a straight line enabling one to determine the two parameters k_{nl} and χ_{nl} .

Following the discussion of Powell¹ about the accuracy of the experimental data, we decided to choose those of Glupe and Melhorn³ of Glupe⁴ and of Bekk⁵ for C, N, O and Ne and also those of Pockman et al.⁶ for Ni and of Hind and Ziegler⁷ for Al to be compared with the formula (1) for K shell ionisation.

The first figure shows a (2) type plot for N and O. The experimental points are well distributed along a straight-line for values of U_K ranging from 1.5 to about 25. All the points lie on the line within the experimental errors.

The straight line enables one to determine the two parameters k_K and χ_K . The experimental data are all consistent with the same value $\chi_K = 1.32$ for both elements.

Figure 2 shows the relative experimental cross-section for the K shells of C, N, O and Ne in terms of $U_K = E/E_K$, together with the theoretical curve for $\chi = 1.32$, normalised to one at the maximum.

The total error of the experimental relative cross-sections does not exceed $\pm 2\%$. Our curve is everywhere in agreement with experiment.

From the absolute cross-sections given in references 3, 4, and 5, one gets the following values for k_K :

Element	C	N	O	Ne
k_K	1.18	1.15	1.21	1.23

Following Glupe and Melhorn³, we estimate the total errors of the absolute cross-sections to be $\pm 5\%$ leading to an error of ± 0.06 in k_K . A single value $k_K = 1.18$ is therefore consistent with the experimental data for these four elements. The reported experiments^{3,4,5} on C, N, O and Ne were obtained by an Auger-electron-yield method with gaseous targets.

The K-shell ionisation for Al⁶ and Ni⁷ that we intend to study now have been obtained by an x-ray-yield method. The (2) type plot for both elements are on a straight line. The figure 3 shows the theoretical cross-section $E_K^2 \sigma_K(E)$ obtained by using $k_{Al} = 1.16$, $\chi_{Al} = 0.60$ and $k_{Ni} = 1.32$, $\chi_{Ni} = 0.73$.

It is worth noticing that the values of χ for this kind of experiment seem to be consistent with each other but not with those obtained by the Auger-electron-yield method. The rather larger value of k_{Ni} may proceed from an underestimate of the magnitude of the total cross-section by about 10 %.

The experimental data on L-shell ionisation are far less accurate than for the K-shell :

i) the cross-sections $E_{L_{2,3}}^2 \sigma_{L_{2,3}}(E)$ plotted against of $U_{L_{2,3}} = E/E_{L_{2,3}}$ are not as close together as for the K-shell for various studied atoms

ii) the two experiments on Ar^{9,10} do not agree in magnitude by a factor 2.

The figure 4 shows the ionisation cross-section (normalised) in the L_{2,3} shells obtained by Vrakking and Meyer⁸ for S, P, and Cl as a function of $U_{L_{2,3}} = E/E_{L_{2,3}}$. The theoretical curve with the same normalisation is in agreement with the experimental points for the same single value of $\chi = 1.32$ that fits the K-shell ionisation. But the absolute magnitudes of $\sigma_{L_{2,3}}$ at the maximum ($U_{L_{2,3}} = 4$) vary as $E_{L_{2,3}}^{-1,68}$ which differs from the E_K^{-2} behaviour for the K-shell. Therefore the parameter $k_{L_{2,3}}$ for the L_{2,3} shell cannot be a constante (as it was for the K-shell), but rather a smooth function of $E_{L_{2,3}}$. Nevertheless this last result does not seem to be corroborated by the x-ray absorption data (see Powell¹).

We have also investigated the data of Christofzik⁹ which agree with the theoretical curve shown in Fig. 5 for the rather large value $\chi_{L_{2,3}}(Ar) = 2.15$.

The errors on the absolute cross-section which range from $0.730 \cdot 10^{-16} \text{ cm}^2$ to $0.897 \cdot 10^{-18} \text{ cm}^2$ for $U_{L_{2,3}} = 16$ introduce

an uncertainty in $k_{L_2}(\text{Ar}) = 1.22 \pm 0.12$. This value in contrast to those obtained by Vrakking and Meyer is consistent with the K-shell data ($k_K = 1.18$).

CONCLUSION

- The analysis of the experimental data shows that
- i) the value of the parameter $\chi = 1.3$ fits the shape of the ionisation cross-section of inner-shell electrons obtained by Auger-electron-yield method for most of the elements
 - ii) a single value of the parameter $k = 1.18$ is consistent with the experimental data for the K-shell, but the uncertainty about the absolute cross-sections¹ do not enable one to rule out the possibility to extent this value to the other shells.

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FIGURE CAPTIONS

- Fig.1 : The experimental values of the expression $\frac{13. \text{Log } E/E_K}{E_K^2 \sigma_K(E)} 10^{14} \text{ (cm-eV)}^{-2}$ are plotted in terms of the reduced energy E/E_K for O and N . They lie along straight lines to the accuracy of the experimental data.
- Fig.2 : Relative experimental ionisation cross-sections for the K-shell of C, N, O and Ne as a function of primary electron energy E (in units of E_K). The normalised theoretical curve fits the experimental data for $\chi = 1.32$.
- Fig.3 : Experimental values of $\sigma_K E_K^2$ for Al and Ni. For the theoretical curve the values of the parameters are $\chi_{Al} = 0.6$, $k_{Al} = 1.16$ and $\chi_{Ni} = 0.73$, $k_{Ni} = 1.32$.
- Fig.4 : Ionisation cross-section (normalised) in the $L_{2,3}$ shells of S, P and Cl as a function of reduced energy $E/E_{L_{2,3}}$. The normalised theoretical cross-section is plotted for $\chi = 1.32$.
- Fig.5 : Normalised ionisation cross-section in the $L_{2,3}$ shell for Ar. The normalised theoretical curve is drawn for $\chi = 2.15$.

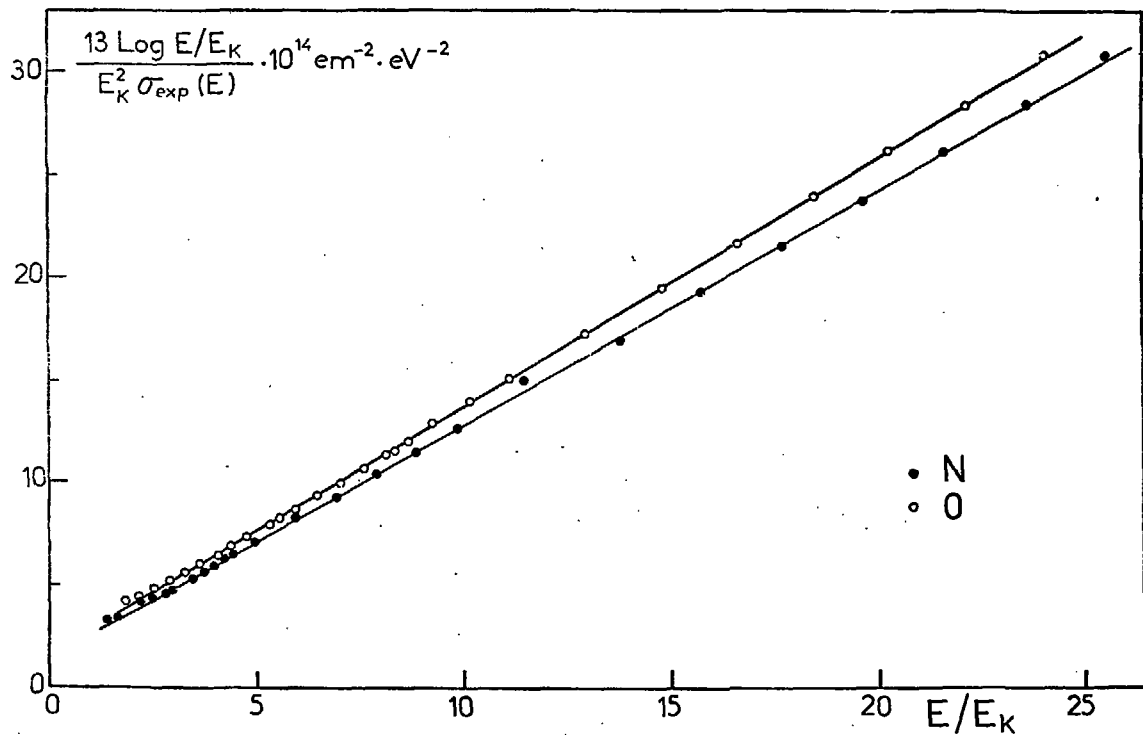


Fig. 1

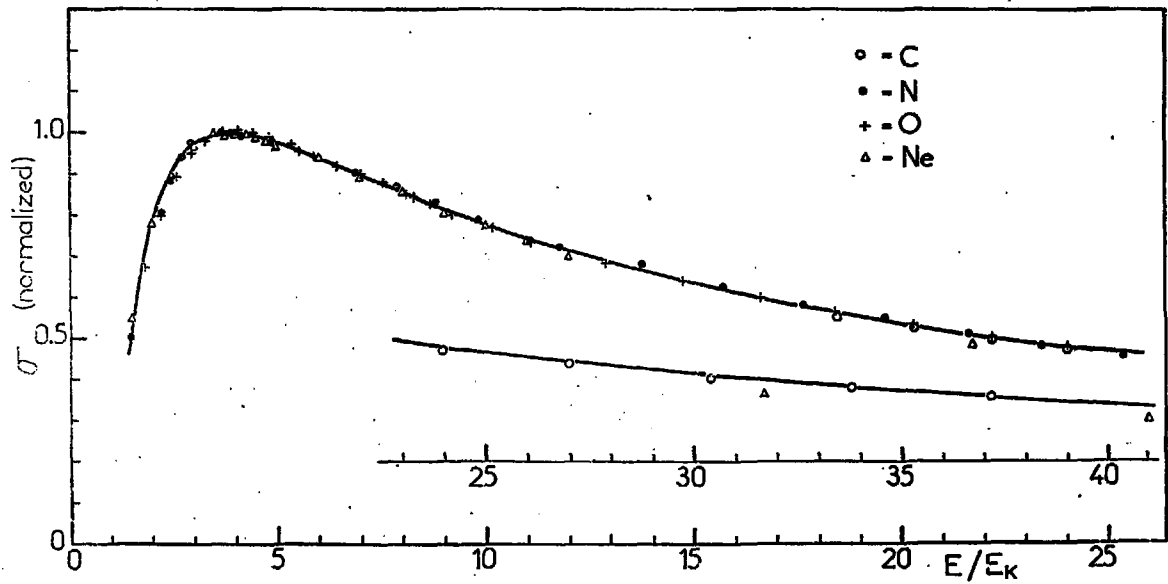
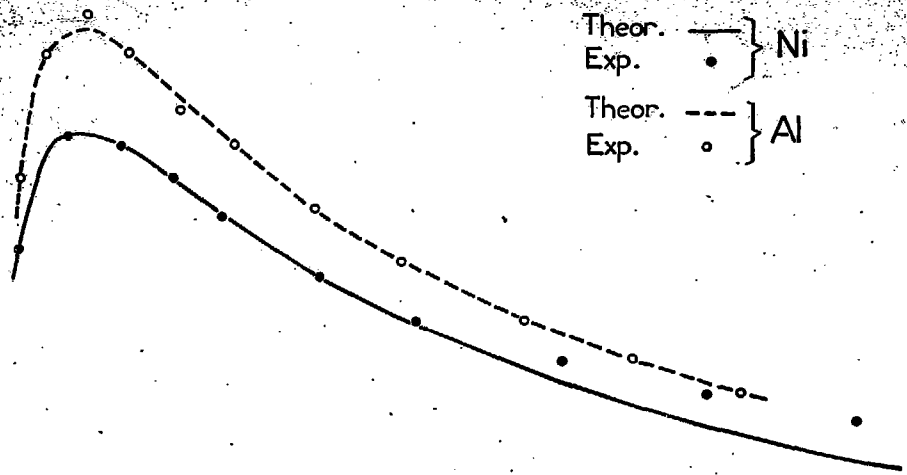


Fig. 2



Theor. — } Ni
Exp. • }

Theor. - - - } Al
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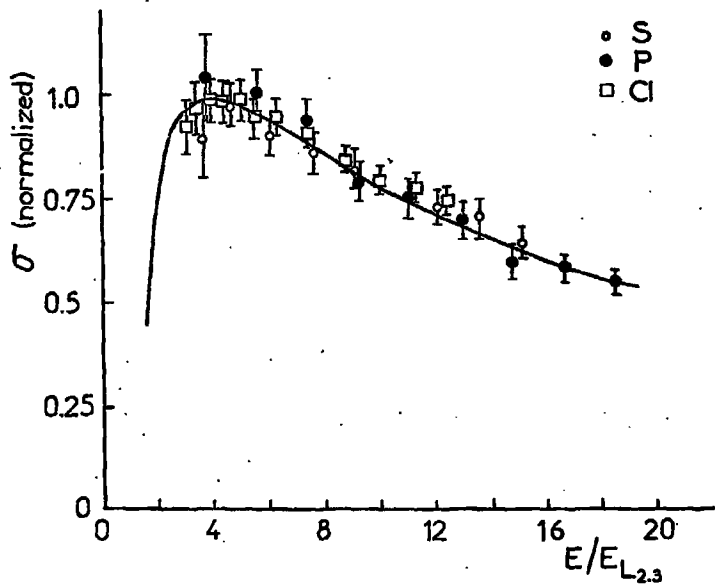


Fig. 4

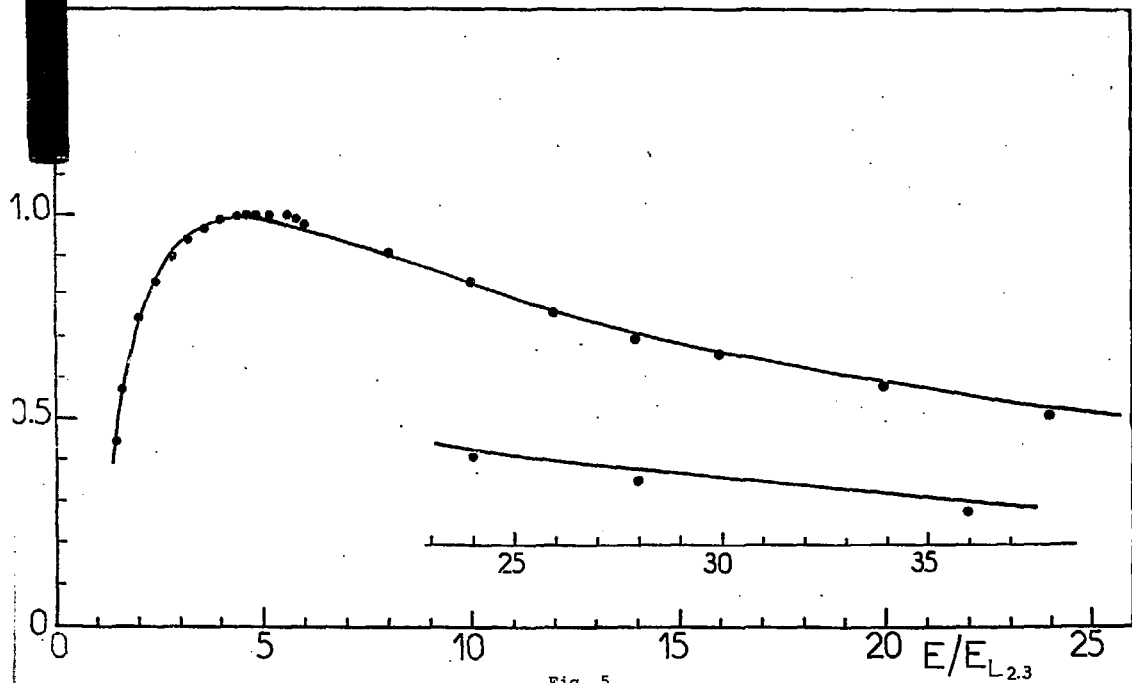


Fig. 5