

Mean excitation energies of atoms using the local plasma approximation

This content has been downloaded from IOPscience. Please scroll down to see the full text.

1988 J. Phys. D: Appl. Phys. 21 1125

(<http://iopscience.iop.org/0022-3727/21/7/012>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 140.113.38.11

This content was downloaded on 28/04/2014 at 20:15

Please note that [terms and conditions apply](#).

Mean excitation energies of atoms using the local plasma approximation

C J Tung†, R L Shyu† and C M Kwei‡

† Institute of Nuclear Science, National Tsing Hua University, Hsinchu, Taiwan, Republic of China

‡ Department of Electronics Engineering, National Chiao Tung University, Hsinchu, Taiwan, Republic of China

Received 27 January 1988

Abstract. Mean excitation energies of atoms have been calculated based on a local plasma approximation. A treatment for atomic shell-wise contributions to the mean excitation energy has been established. The effect of plasma damping was included by an empirical approach. Electron density distributions of atoms have been obtained using the Hartree–Fock–Slater model. Results of this work are compared with those of the detailed matrix element evaluations.

1. Introduction

The mean excitation energy, I , is a crucial parameter in the Bethe theory (Bethe 1930, 1933) of stopping power for charged particles. Its determination relies to a great extent on theoretical calculations because experimental measurements are extremely difficult (ICRU 1984). Among the theoretical methods, the oscillator strength approach (Dehmer *et al* 1975, Inokuti *et al* 1981) and the local plasma approximation (LPA) (Lindhard and Scharff 1953, Chu and Powers 1972, Tung and Watt 1985) are the two most popular ones. The former approach is a direct evaluation of transition matrix elements for the full photo-absorption spectra. Although it is believed this approach can be quite accurate, it is not particularly attractive because of the tedious computation of detailed dipole oscillator strength distributions. On the other hand, the LPA utilises a simple inhomogeneous electron gas model which requires only electron density distributions. Because of its simplicity, LPA retains the competitive position.

Even though LPA is useful, previous development of the model suffers the weakness of an undetermined parameter γ . Lindhard and Scharff (1953) in their establishment of the LPA have argued that the value of γ lies between 1 and $\sqrt{2}$, depending on the atomic number. This argument was based on an assumption that the single electron revolution frequency was approximately equal to the free electron plasma frequency at any position of the electrons in an atom. As we have shown (Tung and Kwei 1985, Kwei and Tung 1986), this assumption was unrealistic because of the constant value of the quantum mechanical revolution energy as compared with the space varying plasma energy for any subshell of an atom. In addition, the correlation of

electron densities from different subshells altered the effective plasma energy as determined by Lindhard and Scharff. Finally, the plasma damping effect neglected previously plays a notable role in the determination of mean excitation energies.

In this paper, we will first derive a formula for the mean excitation energy using the LPA from first principles. Effective plasma energies in this work are determined from correlated electron density distributions of individual subshells. We will then show that the equivalent expression in the previous LPA is a special case of this formula under certain assumptions. Further, we will include the plasma damping effect by an empirical approach. Finally, we will present and discuss mean excitation energies calculated in this work and compare the results with those obtained using the oscillator strength method.

Note that all equations and quantities in this paper are expressed in atomic units unless otherwise specified.

2. Local plasma approximation

The basic idea taken by the LPA is a concept of an inhomogeneous electron gas associated with the electron density distribution of an atom. In this approximation, the plasma oscillation of the electron cloud plays an equally important role as the revolution of electrons in contributing to the dynamic response of the atom. The gross response function of a weakly interacting atomic system is described by its energy loss function, i.e. the imaginary part of the negative inverse dielectric function. For an atom composed of several subshells of different binding energies, the dielectric

function is given by (Raether 1980)

$$\varepsilon(W) = 1 + \sum_{(W > W_i)} \frac{W_{pi}^2}{W_i^2 - W^2 + i\Gamma_i W} \quad (1)$$

where $W_{pi} = (4\pi n_i)^{1/2}$, n_i , W_i and Γ_i are, respectively, the free electron plasma energy, the electron density, the binding energy and the plasma damping coefficient associated with the i th subshell.

Consequently, the energy loss function may be written as (Tung and Kwei 1985, Kwei and Tung 1986)

$$\text{Im}\left[-\frac{1}{\varepsilon}\right] = \sum_i \frac{(\bar{W}_{pi}^2 - W_i^2)W\Gamma_i}{(W^2 - \bar{W}_{pi}^2)^2 + W^2\Gamma_i^2} \quad (2)$$

where the resonant or effective plasma energy, \bar{W}_{pi} , is a solution of the equation

$$\prod_i (W_i^2 - \bar{W}_{pi}^2) + \sum_i \left[W_{pi}^2 \left(\prod_{j \neq i} (W_j^2 - \bar{W}_{pi}^2) \right) \right] = 0. \quad (3)$$

If we neglect the plasma damping, i.e. taking $\Gamma_i = 0$, equation (2) becomes

$$\text{Im}\left[-\frac{1}{\varepsilon}\right] = \frac{\pi}{2} \sum_i \frac{\bar{W}_{pi}^2}{\bar{W}_{pi}} \delta(W - \bar{W}_{pi}) \quad (4)$$

where $\bar{W}_{pi}^2 = 4\pi\bar{n}_i = \bar{W}_{pi}^2 - W_i^2$.

Substituting equation (4) into the equation for mean excitation energy (Fano 1963)

$$\ln I = \frac{2}{\pi W_p^2} \int W \ln W \text{Im}\left[-\frac{1}{\varepsilon}\right] dW \quad (5)$$

we obtain

$$\ln I = \sum_i \frac{4\pi\bar{n}_i \ln \bar{W}_{pi}}{4\pi n} \quad (6)$$

where $n = \sum n_i$, \bar{n}_i and \bar{W}_{pi} are varying with the radial distance, r , from the nucleus of an atom. Averaging equation (6) over the entire space, we get

$$\ln I = (1/Z) \sum_i \int 4\pi r^2 \bar{n}_i(r) \ln \bar{W}_{pi}(r) dr. \quad (7)$$

Equation (7) is the formula for mean excitation energies of the LPA. It will be shown below that the equivalent formula in the previous LPA is a simplification of (7) under certain assumptions.

For convenience, we may rewrite (7) as

$$\ln I = (1/2Z) \sum_i \int 4\pi r^2 \bar{n}_i(r) \ln \bar{W}_{pi}^2(r) dr. \quad (8)$$

Lindhard and Scharff argued that the free electron plasma energy, W_{pi} , was approximately equal to the electron revolution energy, W_i . Following this argument, we obtain

$$\ln I = (1/2Z) \sum_i \int 4\pi r^2 \bar{n}_i(r) \times \ln(\bar{W}_{pi}^2(r) - W_i^2 + W_{pi}^2(r)) dr. \quad (9)$$

Because the function $4\pi r^2 \bar{n}_i(r)$ is sharply peaked and the function $\bar{W}_{pi}^2(r) - W_i^2 + W_{pi}^2(r)$ is only important in the peaked region, it is not significantly different to write equation (9) as

$$\ln I = (1/2Z) \sum_i \int 4\pi r^2 \bar{n}_i(r) \times \ln\left(\sum_i (\bar{W}_{pi}^2(r) - W_i^2 + W_{pi}^2(r))\right) dr. \quad (10)$$

To demonstrate the above description, we plot the functions $4\pi r^2 \bar{n}_i(r)$ and $\bar{W}_{pi}^2(r) - W_i^2 + W_{pi}^2(r)$ in figures 1 and 2 for a fluorine atom. It is clear that the replacement of equation (9) by equation (10) generates only a minor difference in evaluating $\ln I$.

Now, applying the sum rule

$$\int_0^\infty W \text{Im}\left[-\frac{1}{\varepsilon(W)}\right] dW = \frac{\pi}{2} \sum_i W_{pi}^2 \quad (11)$$

to equation (2), we find

$$\sum_i (\bar{W}_{pi}^2 - W_i^2) = \sum_i \bar{W}_{pi}^2 = W_p^2 \quad (12)$$

and

$$\sum_i 4\pi r^2 \bar{n}_i(r) = \sum_i 4\pi r^2 n_i(r) = 4\pi r^2 n(r). \quad (13)$$

Combining equations (10), (12) and (13), we get

$$\ln I = (1/Z) \int 4\pi r^2 n(r) \ln(\gamma W_p(r)) dr \quad (14)$$

where $\gamma = \sqrt{2}$, as suggested by Lindhard and Scharff.

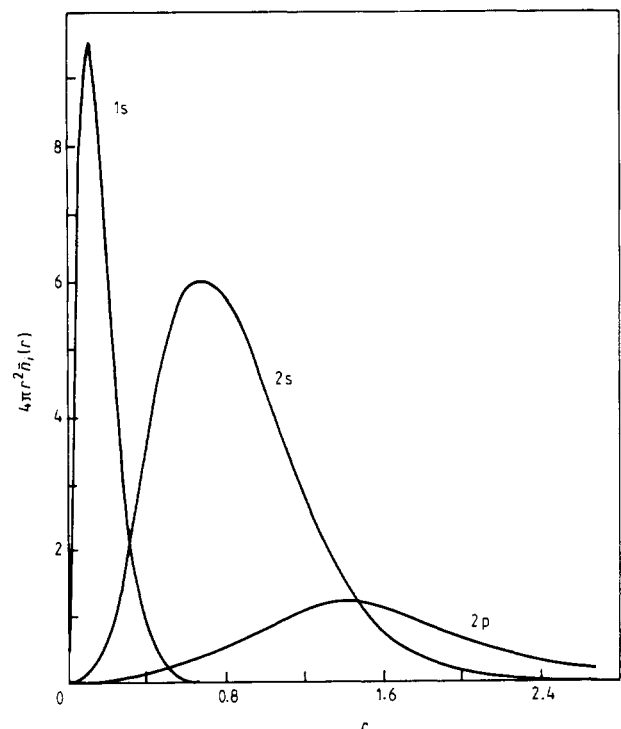


Figure 1. A plot of the function $4\pi r^2 \bar{n}_i(r)$ in the integrand of equation (9) for $i = 1s, 2s$ and $2p$ subshells of a fluorine atom. All quantities are expressed in atomic units.

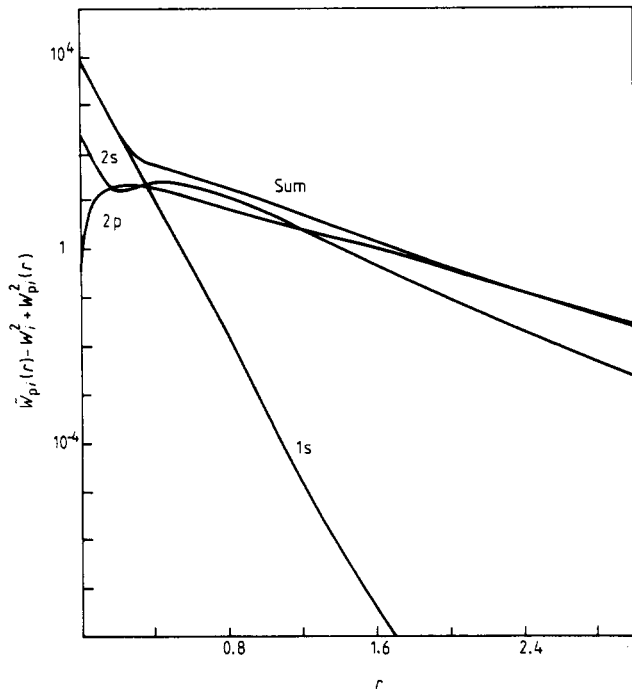


Figure 2. A plot of the function $\bar{W}_{pi}^2(r) - W_i^2 + W_{pi}^2(r)$ in the integrand of equation (9) for $i = 1s, 2s$ and $2p$ subshells of a fluorine atom. All quantities are expressed in atomic units.

Equation (14) is the formula for mean excitation energies in the original LPA.

3. Plasma damping effect

Equation (7) was derived under the assumption of no plasma damping, i.e. via equation (4). To include the effect of plasma damping on the mean excitation energy, we must substitute equation (2) into equation (5). Exact evaluation of the combined equation would require detailed information about the plasma damping coefficient for each subshell of an atom. Since such evaluation greatly reduces the simplicity of the LPA and information on the plasma damping coefficient is seldom available, we propose here an empirical approach which utilises atomic binding energies only.

The effect of plasma damping tends to reduce the mean excitation energy determined by (7). This can be understood by rewriting (7) as

$$\ln I = (1/Z) \sum_i \int 4\pi r^2 \bar{n}_i(r) \times \delta(W - \bar{W}_{pi}(r)) \ln W dW dr. \quad (15)$$

The term $4\pi r^2 \bar{n}_i(r) \delta(W - \bar{W}_{pi}(r))$ represents the oscillator strength for excitation energy W in the case of no plasma damping. A sketch of the oscillator strength distribution for a given subshell is made in figure 3. It is seen that in the case of no plasma damping the entire

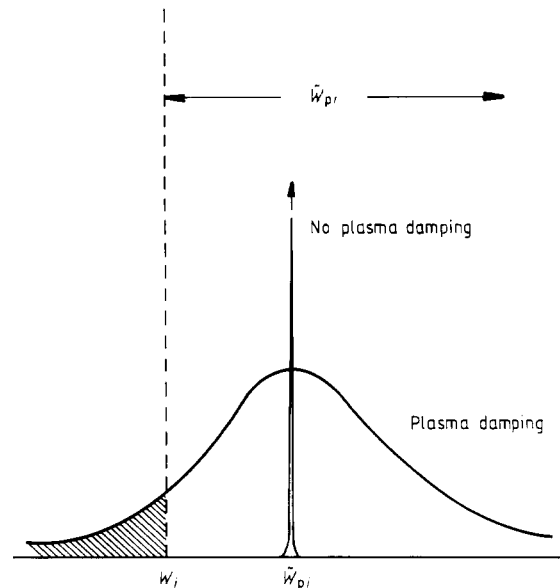


Figure 3. A sketch of the oscillator strength distribution for the i th subshell in an atom. The sharp peak around the effective plasma energy \bar{W}_{pi} is the result neglecting plasma damping. The broad curve is the result taking into account the plasma damping effect. The shaded area represents the oscillator strength distribution where the excitation energy is below the binding energy W_i .

oscillator strength is exhausted in inelastic interactions. However, in the case of plasma damping the shaded portion of the oscillator strength in figure 3 is not used up due to the restrictive condition, $W > W_i$, appearing in equation (1). It is because of this restriction that the contribution to the mean excitation energy from small excitation energies is excluded.

To account for the effect of plasma damping on mean excitation energies, we introduce a modifying factor into equation (7). Let

$$\ln I = (1/Z) \sum_i \int 4\pi r^2 \bar{n}_i(r) \ln(\alpha_i \bar{W}_{pi}(r)) dr \quad (16)$$

where α_i is a plasma-damping-dependent coefficient with a value less than 1. The magnitude of α_i depends on two factors, i.e. Γ_i and W_i . The plasma damping coefficient, Γ_i , controls the width of the oscillator strength distribution sketched in figure 3. Therefore, $\alpha_i \rightarrow 1$ for $\Gamma_i \rightarrow 0$ and $\alpha_i < 1$ for $\Gamma_i \gg 1$. Because the damped oscillator strength distribution peaks around \bar{W}_{pi} where $\bar{W}_{pi} > W_i$ and the damping coefficient is inversely proportional to \bar{W}_{pi} (Kliwer and Raether 1973), the shaded area in figure 3 must be inversely proportional to the binding energy W_i . In other words, α_i approaches 1 for $W_i \rightarrow \infty$ but is a constant value for $W_i \rightarrow 0$. In this work, we assume

$$\alpha_i = 1 - A_i \exp(-B_i W_i) \quad (17)$$

where A_i and B_i are taken as fitting parameters. Equation (17) satisfies the asymptotic behaviour at the two limits and yet keeps a simple form.

4. Results and discussion

Using equation (7) and the Hartree–Fock–Slater electron density distribution (Herman and Skillman 1963), we have calculated the mean excitation energies of atoms of atomic number below 18. The results of I/Z versus Z are plotted in figure 4. For comparison, we have included in this figure the corresponding results of Chu and Powers (1972) using equation (14) and Dehmer *et al* (1975) using the dipole oscillator strength method. It is seen that for $Z > 5$ the results of equation (7) are in better agreement than those of equation (14) with the dipole oscillator strength data. The difference between the results of equation (7) and the dipole oscillator strength method is mainly due to the neglect of plasma damping.

Inspecting equations (16) and (17), we know that the plasma damping effect is more important for smaller binding energies. Let us assume that this effect is only significant for the most weakly bound, or the outermost, subshell. We further assume that mean excitation energies obtained by the dipole oscillator strength method are correct in the sense of the plasma damping effect. To estimate the dependence of the plasma damping effect on the binding energy, we plot in figure 5 the ratio of mean excitation energies calculated by the dipole oscillator strength method (Dehmer *et al* 1975) to those calculated by equation (7) as a function of the binding energy of the outermost subshell.

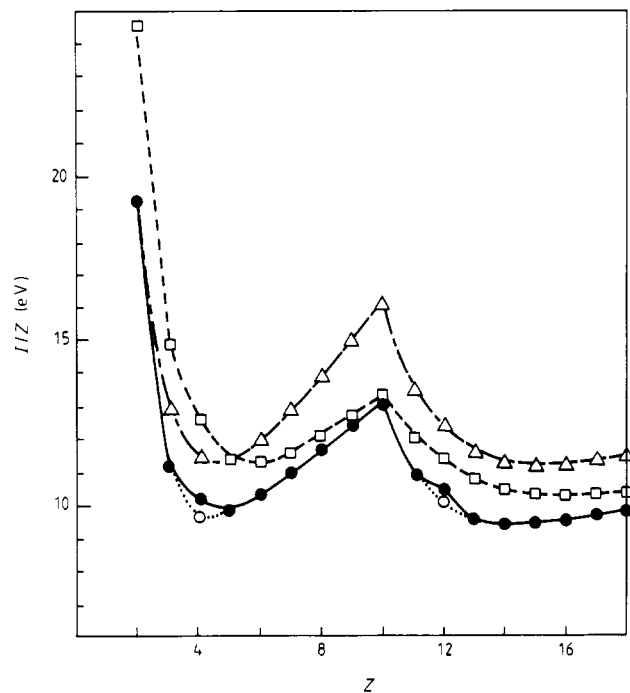


Figure 4. A plot of the mean excitation energy against the atomic number for atoms with $Z = 2$ to 18. The chain curve and triangles present results calculated using equation (14). The broken curve and squares represent results calculated using equation (7). The full curve and full circles represent results calculated using equation (16). The dotted curve and open circles represent results calculated by the dipole oscillator strength method (Dehmer *et al* 1975).

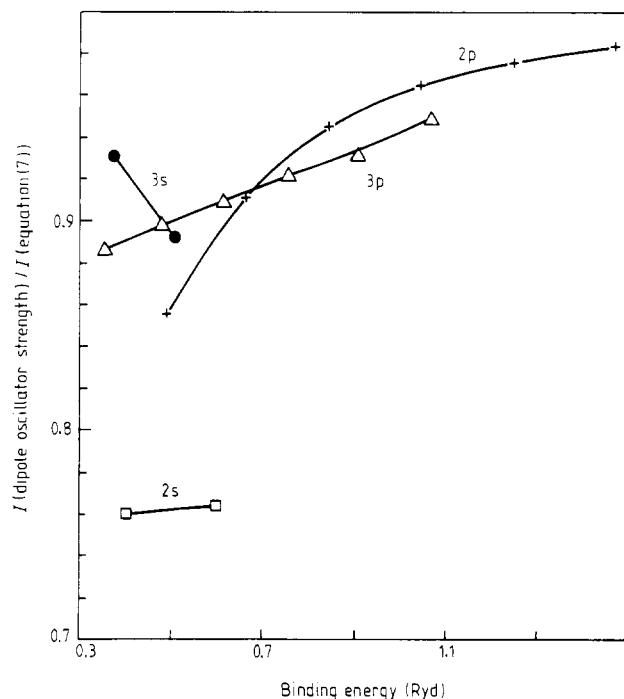


Figure 5. A plot of the ratio of mean excitation energies calculated by the dipole oscillator strength method (Dehmer *et al* 1975) to those calculated by equation (7) as a function of the binding energy of the outermost subshell.

calculated by equation (7) as a function of the binding energy of the outermost subshell. It is found that this dependence varies with the attribution of the outermost subshell. It seems that this dependence for the p subshell is closer to what we expected using equation (17) than that for the s subshell. Recognising the outermost shell-wise dependence of the plasma damping effect, we have chosen different values of the fitting parameters A_i and B_i in (17) for the different outermost subshells. The results of equation (16) for the mean excitation energy including the plasma damping effect are also plotted in figure 4. The fitting parameters A_i and B_i for the outermost 2s, 2p, 3s and 3p subshells are, respectively, 0.34, 0; 0.5, 0.07; 0.4, 0; 0.7, 0.005. The agreement for mean excitation energies between equation (16) and the dipole oscillator strength method is excellent for outermost p subshell atoms. Such agreement for outermost s subshell atoms is somewhat worse due to the poorer application of equation (17). However, the largest deviation for outermost s subshell atoms is only about 5%.

Lindhard and Scharff have mentioned that the value of γ in equation (14) lies between 1 and $\sqrt{2}$ depending on the atom. Previous applications of the LPA have taken $\gamma = \sqrt{2}$. Although we have proven that equation (14) should be replaced by equation (7), the application of (14) is justified if we let γ be an adjusting parameter. Substituting the results of mean excitation energies obtained by equation (16) into equation (14), we have determined this parameter. Figure 6 is a plot of such a parameter as a function of atomic number. The small

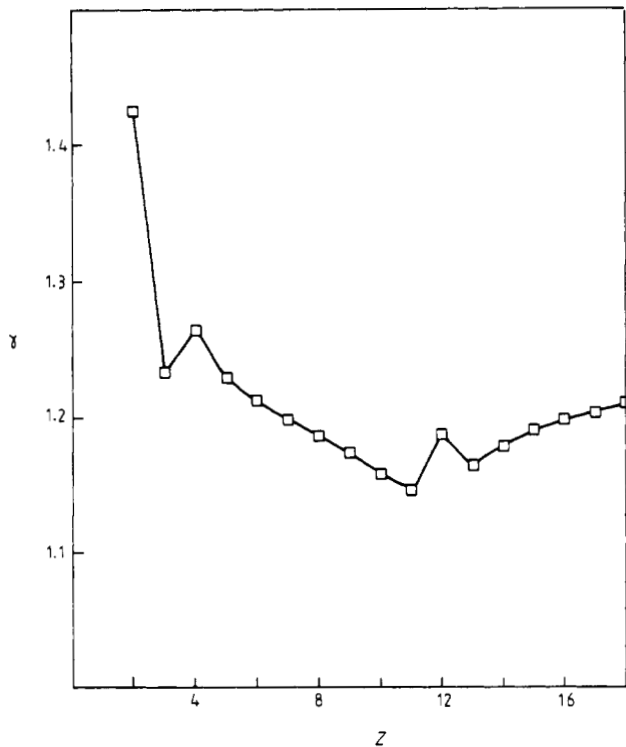


Figure 6. A plot of the parameter γ as determined by substituting the mean excitation energies calculated using equation (16) into equation (14).

'wiggles' appearing at $Z = 4$ and 12 correspond to the outermost s subshell atoms. The value of this adjusting parameter is within the range 1.15 to 1.26 for Z between 3 and 18. In practice, one may choose $\gamma = 1.2$ applying to all atoms. This choice should be better than using $\gamma = 1$ or $\sqrt{2}$.

5. Conclusion

We have studied mean excitation energies of atoms using the LPA. We have shown that the formula for mean excitation energies should be expressed in terms

of the individual contributions by the different subshells in an atom. The effect of plasma damping on the mean excitation energy reduces this energy by an amount depending primarily on the binding energy of the outermost subshell. An empirical approach has been adopted in this work to account for the plasma damping effect. Results of this approach agree very well with the corresponding results of the dipole oscillator strength method. Application of the previous LPA formula is still valid by adjusting the parameter γ . Calculations indicate that the value of γ lies between 1.15 and 1.26 for atomic numbers between 3 and 18.

Acknowledgment

The research was sponsored by the National Science Council of the Republic of China.

References

- Bethe H 1930 *Ann. Phys., Lpz* **5** 325
 — 1933 *Handbuch der Physik* vol 24 (Berlin: Springer) pp 273–560
 Chu W K and Powers D 1972 *Phys. Lett.* **40A** 23
 Dehmer J L, Inokuti M and Saxon R P 1975 *Phys. Rev. A* **12** 102
 Fano U 1963 *Annu. Rev. Nucl. Sci.* **13** 1
 Herman F and Skillman S 1963 *Atomic Structure Calculations* (New York: Prentice-Hall)
 ICRU 1984 *Stopping Powers for Electrons and Positrons, International Commission on Radiation Units and Measurements, Report 37* (Bethesda, MD)
 Inokuti M, Dehmer J L, Baer T and Hanson J D 1981 *Phys. Rev. A* **23** 95
 Kliewer K L and Raether H 1973 *Phys. Rev. Lett.* **30** 971
 Kwei C M and Tung C J 1986 *J. Phys. D: Appl. Phys.* **19** 255
 Lindhard J and Scharff M 1953 *K. Dan. Vidensk. Selsk. Mat. Fys. Medd.* **27** 1
 Raether H 1980 *Springer Tracts in Modern Physics* vol 88 (Berlin: Springer) p 48
 Tung C J and Kwei C M 1985 *Nucl. Instrum. Methods B* **12** 464
 Tung C J and Watt D E 1985 *Radiat. Eff.* **90** 177