Calculations of Electron Inelastic Mean Free Paths from Experimental Optical Data

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Calculations are reported of inelastic mean free paths (IMFPs) for 100–2000 eV electrons in C, Mg, Al, Al_2O_3, Cu, Ag, Au, and Bi from experimental optical data. These calculations require knowledge of the momentum-transfer dependence of the differential scattering cross section; this information was taken from Penn's calculations. The calculated IMFPs agree reasonably with direct calculations and with measured electron attenuation lengths (ALs). Since accurate measurements of ALs are difficult, it is suggested that calculations of the present type are useful if the needed optical data are available. The present approach is also useful for materials (such as the transition and noble metals) for which it is not possible to make a meaningful distinction between valence-electron and core-electron excitations as required in current IMFP calculations. The dependence of the calculated IMFPs on electron energy varied with material and was associated with different spectral distributions of the electron energy-loss function. The trend in the dependence of IMFP on energy was similar to that found in analysis of AL data.

INTRODUCTION

Many calculations of inelastic mean free paths (IMFPs) of low-energy electrons in solids have been reported, as summarized in a recent review.[1] These calculations have been based on different models for describing inelastic electron scattering in solids.

This paper reports simple calculations of IMFPs from experimental optical data. These calculations require one key assumption which introduces some uncertainty into the absolute values of the IMFPs. The calculations, however, were undertaken mainly to compute the dependence of IMFP on electron energy in different materials for which only relative IMFP values are required. Specifically, it was desired to investigate whether materials with qualitatively different electron energy-loss spectra would show different dependences of IMFP on electron energy. Wagner, Davis, and Riggs[2] have recently reported analyses of experimental attenuation length (AL) data as a function of electron energy that show different dependences from material to material. (For a discussion of the difference between IMFP and AL, see the companion paper[3] or Ref. 1.) For some materials, the AL dependences found by Wagner *et al.* corresponded closely to the IMFP dependences expected from theory[4,5] but for others there was disagreement. The present calculations indicate the reason for this apparent discrepancy.

Most IMFP calculations have been based on analyses of the excitations of the valence electrons, for which the cross sections are much greater than those for inner-shell excitations, and it has often been assumed that there is a single mode of valence-electron inelastic scattering (e.g., volume-plasmon excitation).[1] This is a good approximation for those materials which have a simple energy-loss spectrum with a single, dominant peak (the so-called free-electron-like materials). The assumption is not a good approximation for those materials which have more complex energy-loss spectra and for which no unambiguous distinction can be made between excitations from different shells or subshells (e.g., transition metals and alkali halides).[1]

The present IMFP calculations make use of experimental optical data for which no separation is needed between valence- and core-electron excitations. They are based on an approach that has been used previously[6,7] but is extended here to show the calculated dependence of IMFP on electron energy. Calculations have been made for both free-electron-like and non-free-electron-like solids in order to demonstrate the effects of different types of energy-loss spectra on the dependences of AL on energy. The IMFP values, based as they are on experimental optical data, are also of interest for comparison with experimental AL measurements since it is difficult to make the latter measurements with high accuracy.[1]

THEORY

The differential inelastic scattering cross section, per atom or molecule, for energy loss $\Delta E = \hbar\omega$ and momentum transfer q in an infinite medium by an electron of energy E is

$$\frac{d^2\sigma}{d(\Delta E)\,dq} = \frac{me^2}{\pi N\hbar^2 E}\,\mathrm{Im}\left[\frac{-1}{\varepsilon(\omega, q)}\right]\frac{1}{q} \qquad (1)$$

where N is the density of atoms or molecules and $\varepsilon(\omega, q)$ is the complex dielectric constant of the medium.[1,8] Equation (1) is expected to be valid for $E \gg \Delta E$; the extent to which this inequality need be satisfied is discussed elsewhere[1,3,8] and below.

The function $\mathrm{Im}\,[-1/\varepsilon(\omega, q)]$ is known as the energy-loss function and can be obtained experimentally from the distribution of electrons transmitted through thin specimen films as a function of ΔE and of q.[9,10] Data for $\mathrm{Im}\,[-1/\varepsilon(\omega, 0)]$ can be obtained from optical experiments. The dependence of $\mathrm{Im}\,[-1/\varepsilon(\omega, q)]$ on momentum transfer is not well known except for the case of

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plasmon excitation; calculations have also been made of Im $[-1/\varepsilon(\omega, q)]$ for inner-shell excitations in selected atoms.[11]

Equation (1) can be integrated over q to obtain

$$\frac{d\sigma}{d(\Delta E)} = \frac{me^2}{2\pi N\hbar^2 E} \operatorname{Im}\left[\frac{-1}{\varepsilon(\Delta E, 0)}\right] \ln\left[\frac{c(\Delta E)E}{\Delta E}\right] \quad (2)$$

where $c(\Delta E)$ is a parameter, expected to be between approximately 1 and 4, that depends on the q-dependence of $\varepsilon(\omega, q)$. A total inelastic cross section σ_T can be found by integration of (2) over all possible values of ΔE. Since the IMFP $\lambda_T = 1/N\sigma_T$, we can write

$$\lambda_T = \frac{3.325E}{\int_0^{E_{max}} \operatorname{Im}[-1/\varepsilon(\Delta E)] \ln[c(\Delta E)E/\Delta E]\, d(\Delta E)} \text{ Å} \quad (3)$$

where the energy E has been expressed in electron volts and E_{max}, the upper limit for the integration, is less than E.

Determination of absolute values of λ_T from (3) will depend on a suitable choice of the parameter c but since this parameter does not vary greatly from material to material (see below) and appears in a logarithm its value should not be critical. Selection of a value for c with a high degree of confidence is difficult owing to the almost complete lack of experimental data in the range of interest for surface analysis by AES and XPS[3] and the limited theoretical guidance available. One choice is to obtain c from the relation

$$c = \hbar\omega_p \exp(b) \quad (4a)$$

where $\Delta E_p = \hbar\omega_p$ (in eV) is the free-electron bulk plasmon energy and b is a parameter calculated by Penn.[4] Equation (4) is expected to be useful for free-electron-like materials. It is convenient to express c in terms of the average valence-electron spacing r_s as follows:

$$c = 46.9 r_s^{-3/2} \exp(b) \quad (4b)$$

where

$$r_s a_0 = (3/4\pi n_e)^{1/3},$$

a_0 is the Bohr radius, and n_e is the valence-electron density given by

$$n_e = N_v N_a \rho / A \quad (5)$$

In (5), N_v is the number of valence electrons per atom or molecule, N_a is Avogadro's number, ρ is the bulk density, and A is the atomic or molecular weight. Figure 1 is a plot of c as a function of r_s using Penn's data[4] for b for 58 elements. Except for the low-density elements K, Rb, and Cs, c is between 1 and 4.

Values of the parameter c may also be derived from other IMFP calculations such as those of Ashley[12] and of Szajman and Leckey.[13] Another option is to make use of values of c deduced from analyses of experimental AL data.[3]

RESULTS

Equation (3) has been evaluated for eight materials (glassy carbon, Mg, Al, Al_2O_3, Cu, Ag, Au, and Bi) for which evaluated experimental optical data exist over a wide range of photon energies, typically at least 1 to 2000 eV.[14,15] Values of Im $[-1/\varepsilon(\Delta E)]$ have been calculated from $\varepsilon(\Delta E)$.

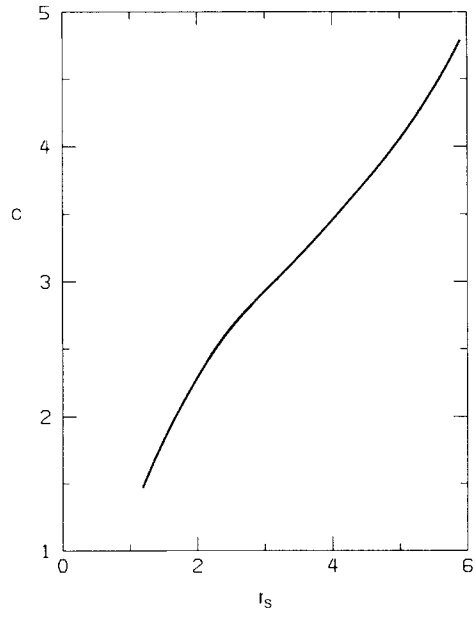

Figure 1. Plot of the parameter c as a function of average valence-electron spacing r_s from Penn's data[4] for his parameter b (4).

The term $c(\Delta E)$ in (3) has been assumed to be independent of ΔE. Equation (3) has been evaluated for each material with c given the values 0.65, 1, 2, and 4. The latter three values for c were selected to encompass the likely range of values of c (Fig. 1) in order to find the extent to which λ_T values depended on c. The lowest value of c (0.65) was chosen to simulate empirical values obtained from analyses of AL[3] and inner-shell ionization cross-section data.[11] In addition, λ_T values were calculated with the value of c for each material calculated by Penn[4] [4].

Figures 2-9 show results of the calculations of λ_T that were made for electron energies from 100 to 1000 eV, in 100 eV increments, and for $E_{max} = E$. These figures show values of λ_T for 0.65, 1, 2, and 4 that were obtained with the optical data of Hagemann *et al.*[14] Figures 2(a)-9(a) show the calculated IMFP values as a function of electron energy on linear scales to indicate the extent to which the λ_T values depend on c and also to show how the curvature of the $\lambda_T - E$ plots depends on c. Even with the extreme values chosen for c (0.65 and 4), the calculated values of λ_T varied by less than ±50% for $E = 200$ eV, less than ±30% for $E = 1000$ eV, and less than ±25% for $E = 2000$ eV from the average values of λ_T found in the eight materials for these limiting values of c at each density.

Figures 2(b)-9(b) show the same calculated values of λ_T as a function of electron energy on logarithmic scales. These plots show fits to the empirical AL relation proposed by Wagner *et al.*[2]

$$\lambda = kE^m \quad (6)$$

The solid lines in Figs 2(b)-9(b) are linear least-squares fits of the calculated λ_T values to (6) over the electron energy ranges where the plots were judged to be sufficiently linear. The figures show the least-squares

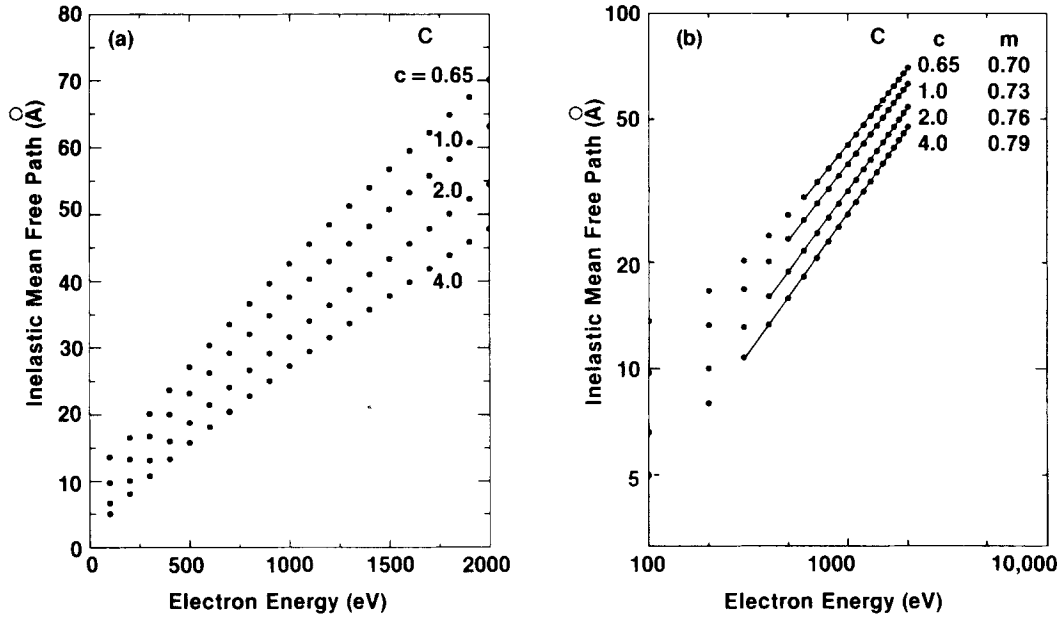

Figure 2. Plot of values of inelastic mean free paths as a function of electron energy for glassy carbon calculated from the optical data of Hagemann *et al.*[14] using (3) with $c=0.65$, 1, 2, and 4 on (a) linear and (b) logarithmic scales. The solid lines indicate linear least-squares fits to (6) for selected electron energy ranges. The derived values of the exponent m in (6) are indicated for the corresponding values of the parameter c.

values of the exponent m for the indicated values of the parameter c. The derived values of m decrease slightly as c is decreased, and the energy range over which the plots in Figs 2(b)-9(b) are linear decreases as c decreases.

Figures 10 and 11 show values of λ_T as a function of electron energy for the eight materials calculated with the Penn[4] values of c. These values are plotted on linear scales in Fig. 10 and on logarithmic scales in Fig. 11. The lines in Fig. 11 indicate fits to (6) and the derived values of m are shown together with the Penn values of c. The plots in Fig. 11 were considered to be linear over the electron energy ranges of 600-2000 eV for Cu, Ag, and Au, and 500-2000 eV for C, Al, and Al_2O_3, and 400-2000 eV for Mg.

Smith *et al.*[15] have re-analyzed the optical data for aluminum and have proposed new values for $\varepsilon(\omega, 0)$ which better satisfy the optical sum rules than the data of Hagemann *et al.*[14] IMFP values for Al were computed with the optical data of Smith *et al.* and it was found that the λ_T values were less than those found with the Hagemann *et al.* data by less than 5%. There were negligible changes in the derived values of the exponent m.

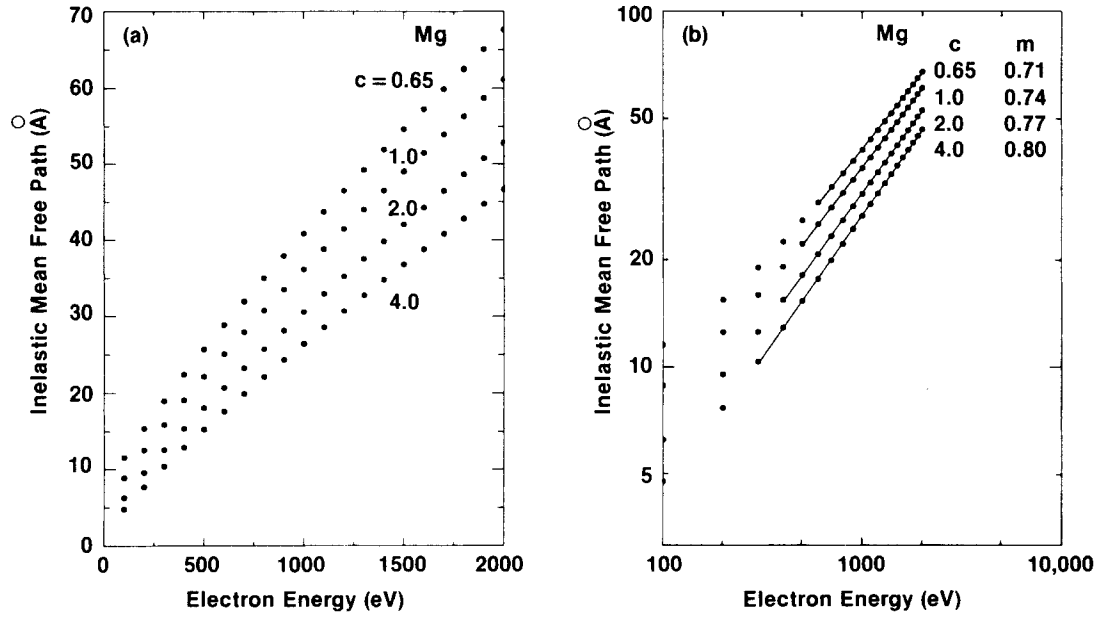

Figure 3. Plot of calculated IMFP values for Mg as a function of electron energy on (a) linear and (b) logarithmic scales. See caption to Fig. 2.

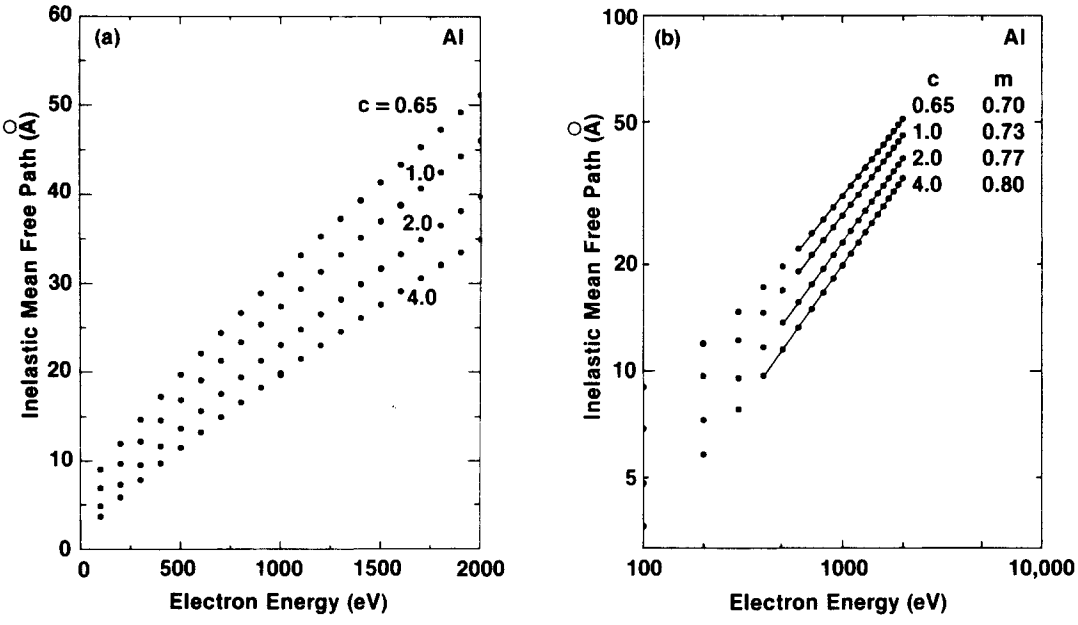

Figure 4. Plot of calculated IMFP values for Al as a function of electron energy on (a) linear and (b) logarithmic scales. See caption to Fig. 2.

COMPARISON OF PRESENT IMFP VALUES WITH OTHER RESULTS

We present comparisons of the IMFP values computed from (3) with other IMFP calculations and with AL measurements to demonstrate that reasonable results have been obtained. Figures 12–16 show comparisons of IMFP calculations and AL measurements for Al, Au, Ag, Cu, and Al_2O_3, respectively. The solid line in each panel shows the results of the present IMFP calculations made with the Penn[4] values of c. The short-dashed lines in Figs 12(a)–16(a) indicate the results of Penn[4] and the long-dashed lines give the results of Ashley and Tung.[5] The latter authors have fitted their IMFP calculations to (6) and their values of k and m have been utilized to generate the plotted curves (the slight discontinuities at $E = 400$ eV are due to the different parameter values above and below this energy). The dot-dashed lines in Figs 12(a)–16(a) indicate the proposed universal IMFP relationship of Szajman *et al.*[16]

$$\lambda = 1.8\bar{E}E^{3/4}/E_p^2 \text{ Å} \qquad (7)$$

where $\bar{E}$ is the centroid value of the energy loss function and E_p is the free-electron plasmon energy (with all energies expressed in electron volts). Equation (7) was derived from a calculation of the IMFP for valence-electron excitations[17] and a general estimate of the IMFP

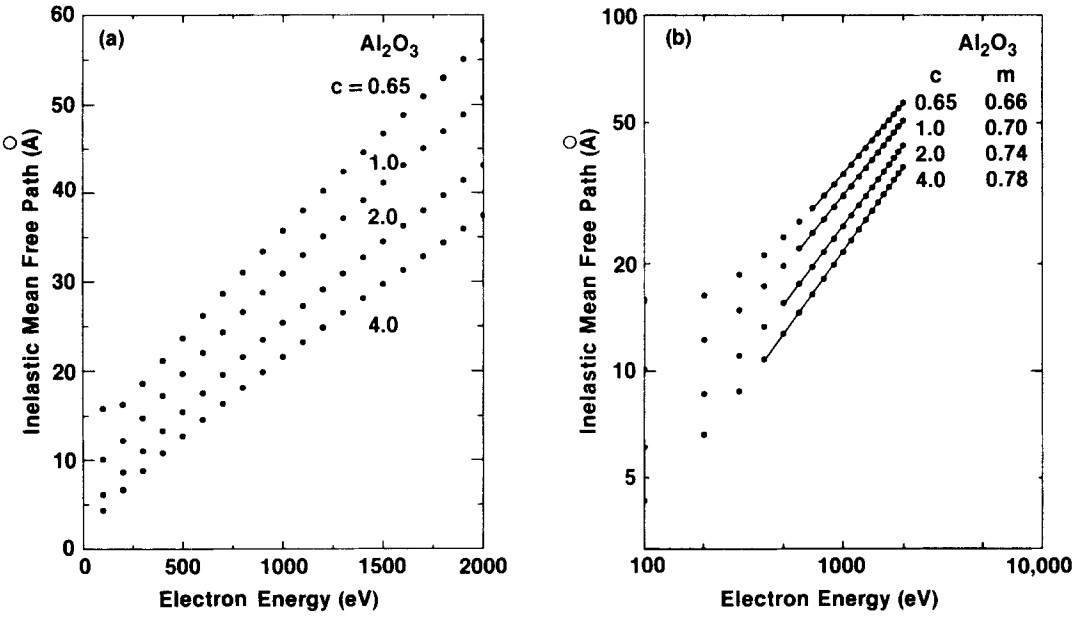

Figure 5. Plot of calculated IMFP values for Al_2O_3 as a function of electron energy on (a) linear and (b) logarithmic scales. See caption to Fig. 2.

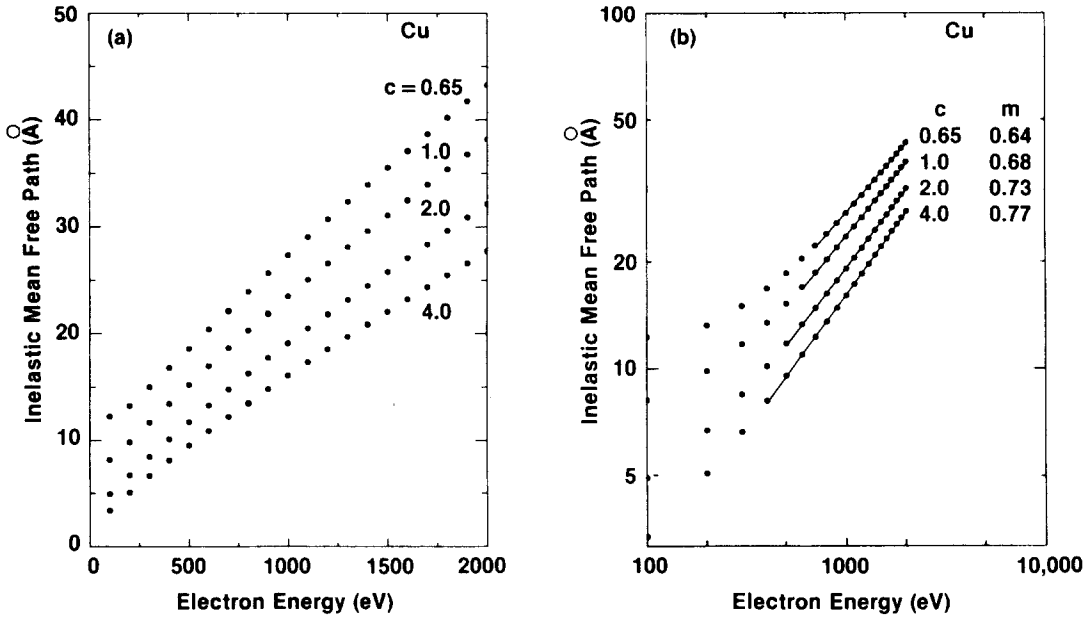

Figure 6. Plot of calculated IMFP values for Cu as a function of electron energy on (a) linear and (b) logarithmic scales. See caption to Fig. 2.

for core-electron excitations.[6] The plots of (7) have been obtained from the evaluations reported in Ref. 1 for Al, Cu, Ag, and Au and from $\bar{E} = 24.3$ eV for Al_2O_3.[18]

The dot-dashed lines in Figs 12(b)-16(b) represent evaluations of the empirical AL formulas proposed by Seah and Dench:[19]

(a) For elements,

$$\lambda_m = 538E^{-2} + 0.41(aE)^{1/2} \text{ monolayers} \quad (8a)$$

(b) For inorganic compounds,

$$\lambda_m = 2170E^{-2} + 0.72(aE)^{1/2} \text{ monolayers} \quad (8b)$$

where $\lambda = a\lambda_m$ and a is the average thickness of a monolayer (in nm) given by

$$a^3 = 10^{24}A/\rho n N_a \quad (9)$$

In (9), A is the atomic or molecular weight, n is the number of atoms in the molecule, N_a is Avogadro's number, and ρ is the bulk density (in kg m^{-3}). Also shown in Figs 12(b)-16(b) are results of experimental AL measurements for Al,[20] Au,[21-24] Ag,[25-27] Cu,[28] and Al_2O_3.[29]

Several factors should be considered in comparing the results shown in Figs 12-16. First, the results of Penn,[4] Ashley and Tung,[5] and of Szajman *et al.*[16] are derived from theoretical IMFP calculations. These calculations employ different models for the dominant contribution of valence-electron excitations and different estimates for the effects of core-electron excitations. Second, the present IMFP results are based on experimental optical data and values of the parameter c obtained from theory.[4] While the optical data are

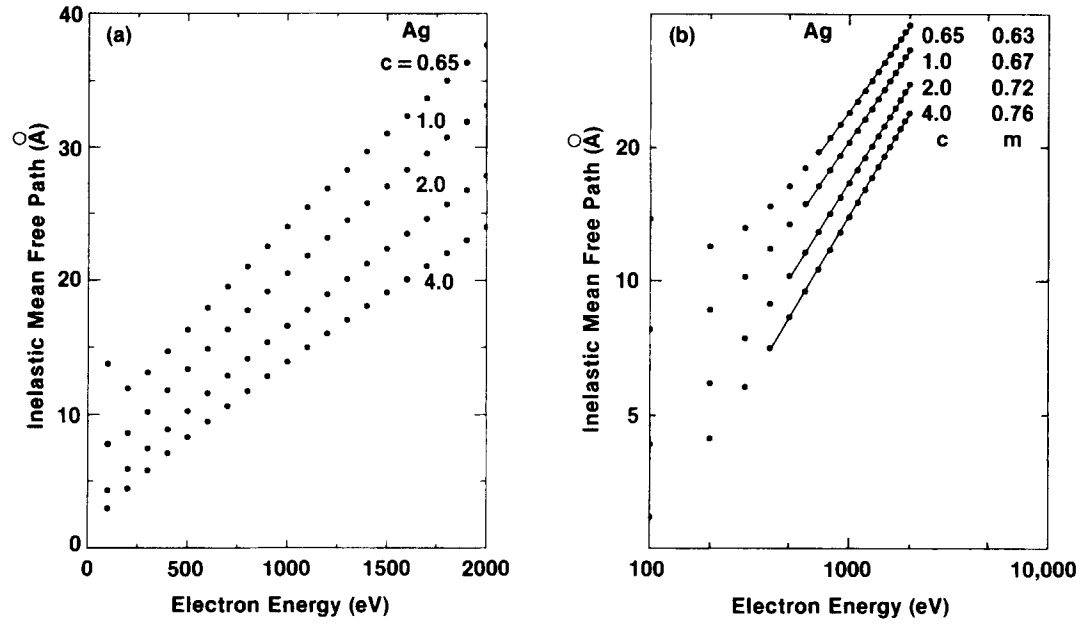

Figure 7. Plot of calculated IMFP values for Ag as a function of electron energy on (a) linear and (b) logarithmic scales. See caption to Fig. 2.

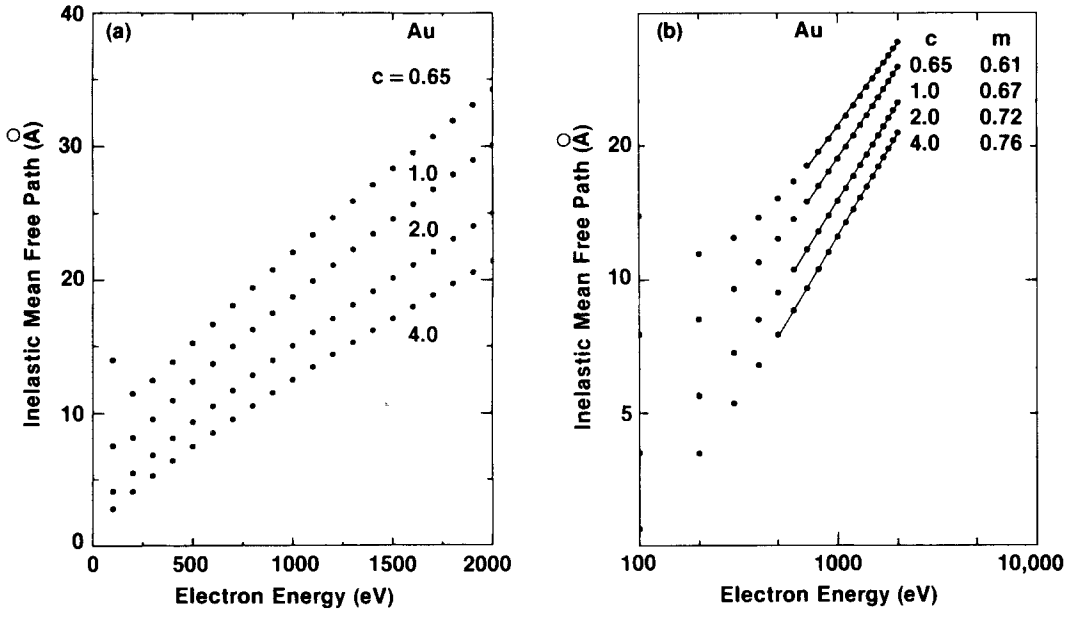

Figure 8. Plot of calculated IMFP values for Au as a function of electron energy on (a) linear and (b) logarithmic scales. See caption to Fig. 2.

believed to be correct to about 5% (in the sense that necessary optical sum rules are satisfied), it is possible that the values of c used may not be correct, particularly for non-free-electron-like materials. In addition, c may in fact be a function of ΔE. No estimate can be made now of the likely uncertainty in λ_T but Figs 2(a)-9(a) indicate that larger variations of c than expected from the likely range of c for all elements (Fig. 1) do not cause appreciable variations in λ_T. Third, experimental AL measurements are difficult;[1] the errors of the AL measurements in Figs 12(b)-16(b) have not been estimated but may be as large as 50-100% for the reasons summarized in Ref. 1. Finally, IMFP and AL values for a given material and electron energy may differ on account of elastic electron scattering (with the IMFP exceeding the AL by about 30%).[1] These factors indicate that the comparisons in Figs. 12-16 should be made only in a semi-quantitative manner.

Figure 12(a) shows IMFP data for Al. The present λ_T values and the results of Penn, Ashley and Tung, and of Szajman and Leckey agree very closely. The AL data of Tracy[20] in Fig. 12(b) are generally slightly less than the present λ_T results. There is a considerable difference for $E > 500$ eV between the present results and that expected from (8a).

Figure 13(a) shows good agreement between the present λ_T data for Au and the three IMFP calculations. There are large variations in reported AL values for Au,

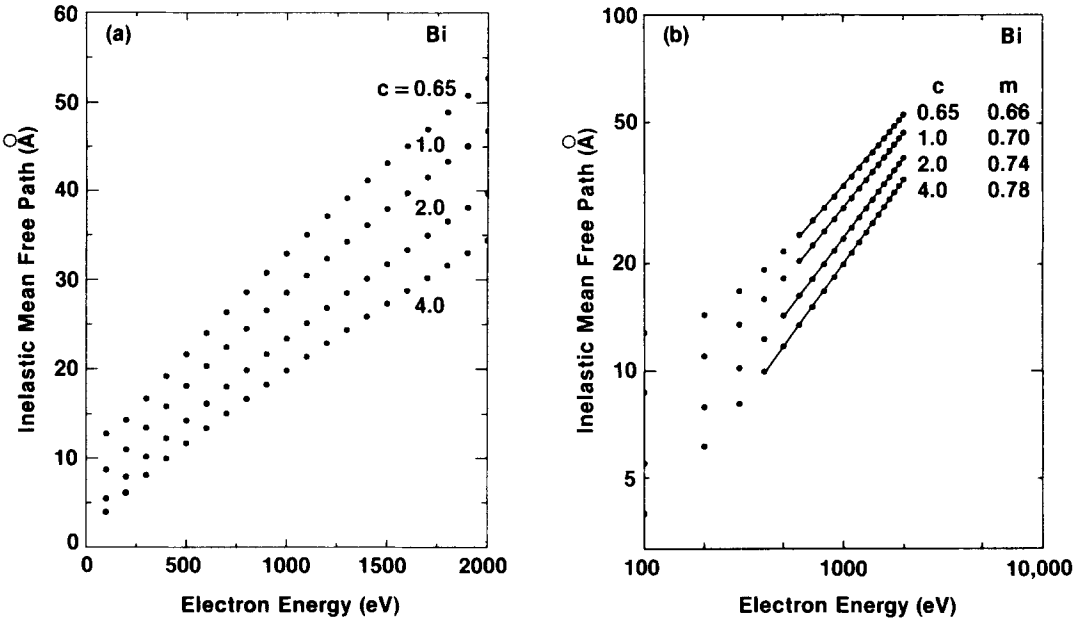

Figure 9. Plot of calculated IMFP values for Bi as a function of electron energy on (a) linear and (b) logarithmic scales. See caption to Fig. 2.

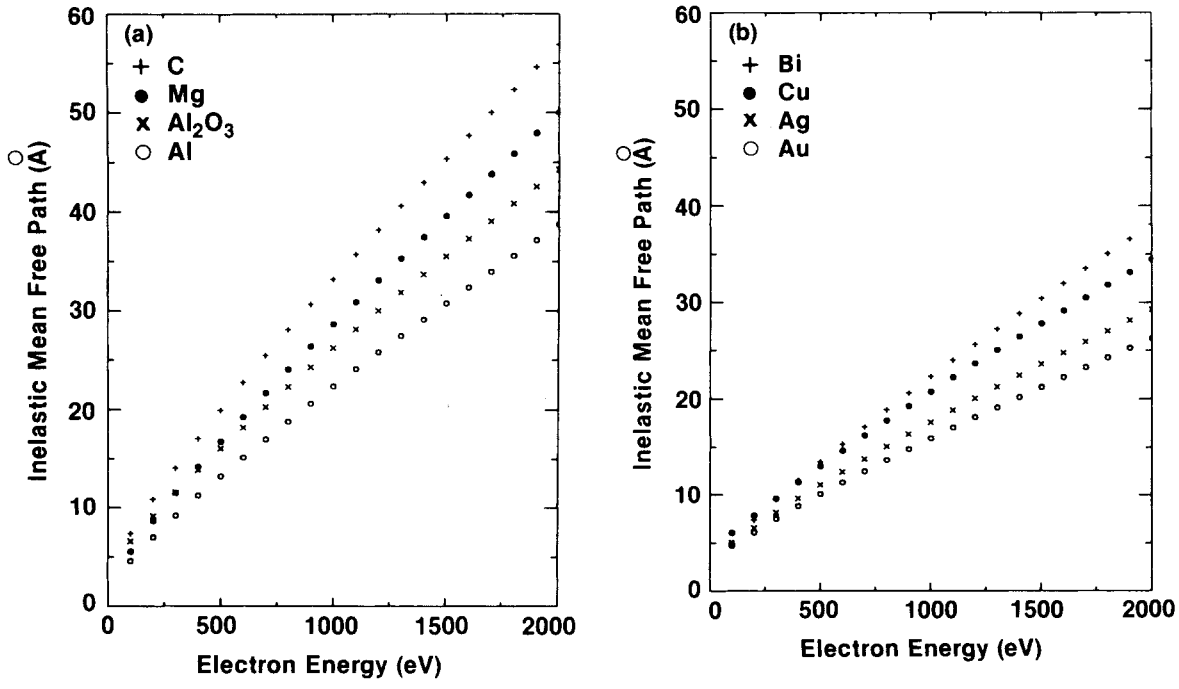

Figure 10. Plot of calculated IMFP values from the optical data of Hagemann *et al.*[14] using (3) and with values of c obtained from the data of Penn[4] using (4). The plots show values of λ_T for (a) C, Mg, Al_2O_3, and Al, and (b) Bi, Cu, Ag, and Au on linear scales.

as shown in Fig. 13(b); these variations are symptomatic of the inaccuracies present in AL data. The present results and the empirical curve of Seah and Dench[19] are of similar magnitudes; both curves appear to be generally consistent with the AL data.

The IMFP results for Ag in Fig. 14(a) are similar but there is a greater spread in the plotted curves than for Al and Au. Experimental AL measurements for Ag in Fig. 14(b), although limited and suggesting different dependences on energy, are generally consistent with the present results and with (8a).

The IMFP calculations for Cu in Fig. 15(a) also differ in magnitude. The experimental AL data[28] for Cu in Fig. 15(b) are close to the values expected from (8a).

Figure 16(a) shows a wide spread in calculated IMFP values for Al_2O_3. The differences in IMFP results are

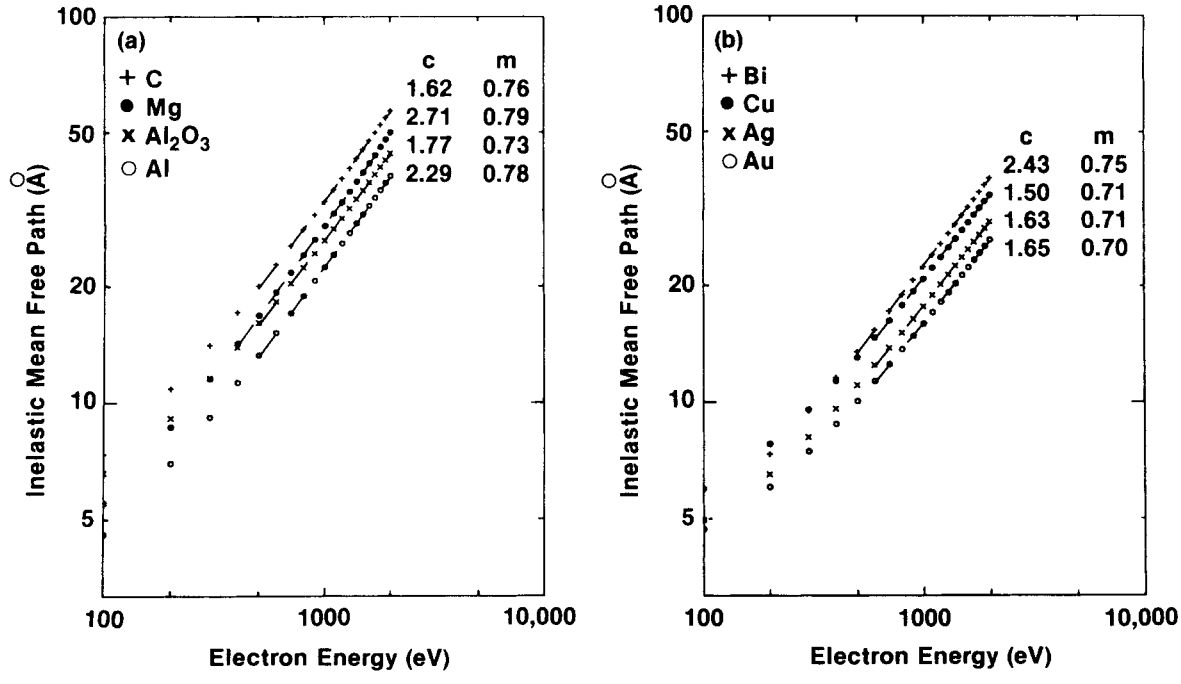

Figure 11. Plots of calculated IMFP values as in Fig. 10 on logarithmic scales. The lines indicate linear least squares to (6). Values of the exponent m are shown together with the value of c obtained from Penn's calculation[4] for each material (4).

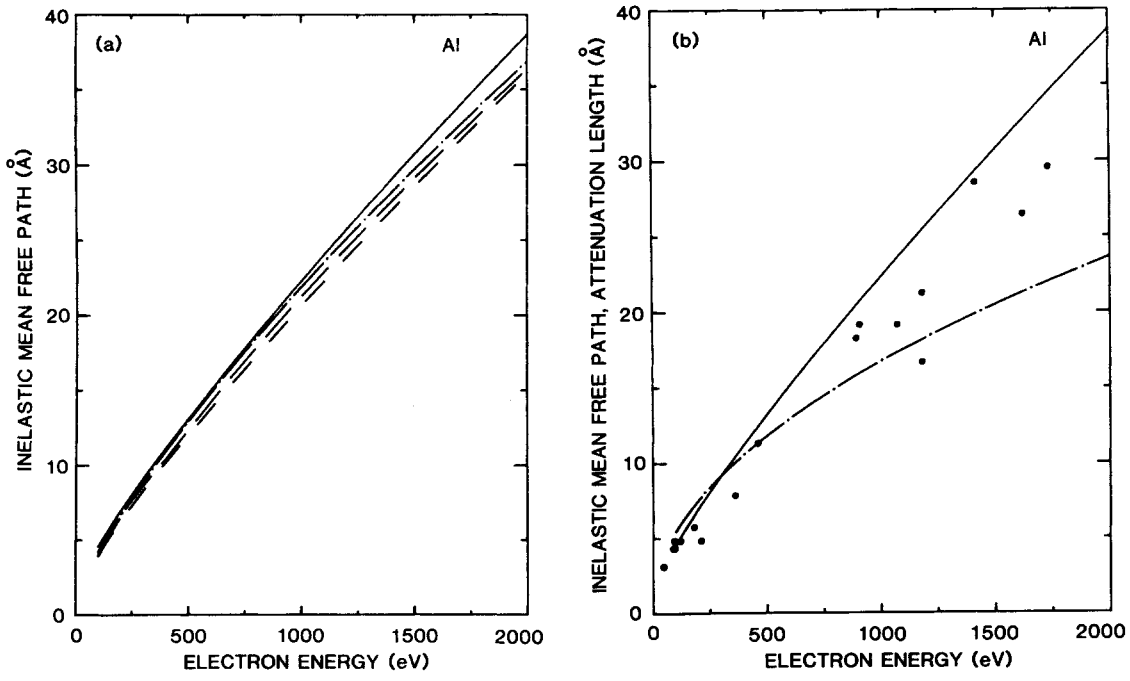

Figure 12. Comparison of IMFP and AL values for Al; (a) comparison of IMFP calculations: ——=present calculation from (13) with the Penn value of c (c=2.29); – – –=result of Penn[4]; — —=result of Ashley and Tung[5]; — · —=result of Szajman *et al.*[16]; (b) comparison of present IMFP calculation (solid line, as in (a)) with AL data; ●=experimental AL data of Tracy[20]; — · —=empirical formula (8a) of Seah and Dench.[17]

surprising, at first, since the energy loss function for aluminum oxide, although broad, consists of a single dominant peak at 24.3 eV that has been identified as a volume plasmon loss.[18] Nevertheless, the oscillator strength for energy losses between 0 and 40 eV is about 11 electrons/molecule, approximately half the number of valence electrons (24). It is surmised that the previous IMFP calculations may have exaggerated the inelastic scattering cross sections by assuming that 24 electrons/molecule contributed to the main loss peak. In Fig. 16(b), the experimental AL values[29] lie considerably below the present λ_T results and the result expected from (8b).

Several conclusions can be drawn from these comparisons. First, there is generally good agreement between the present results for λ_T and IMFP calculations

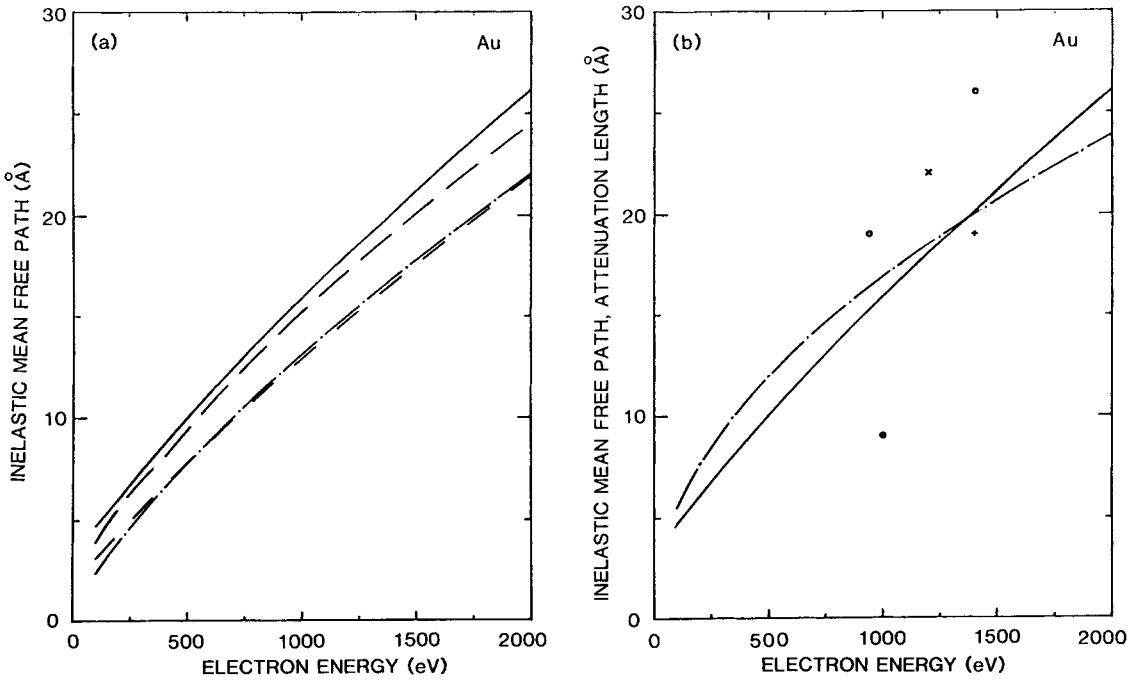

Figure 13. Comparison of IMFP and AL values for Au; (a) comparison of present IMFP calculation (c=1.65), ——, with other results: – – –=result of Penn[4]; — —=result of Ashley and Tung[5]; — · —=result of Szajman *et al.*[16]; (b) comparison of present IMFP calculation (solid line, as in (a)) with AL data: ○=results of Klasson *et al.*[21]; ●=result of Brunner and Zogg[22]; +=result of Henke[23]; ×=result of Baer *et al.*[24]; — · —=empirical formula (8a) of Seah and Dench.[17]

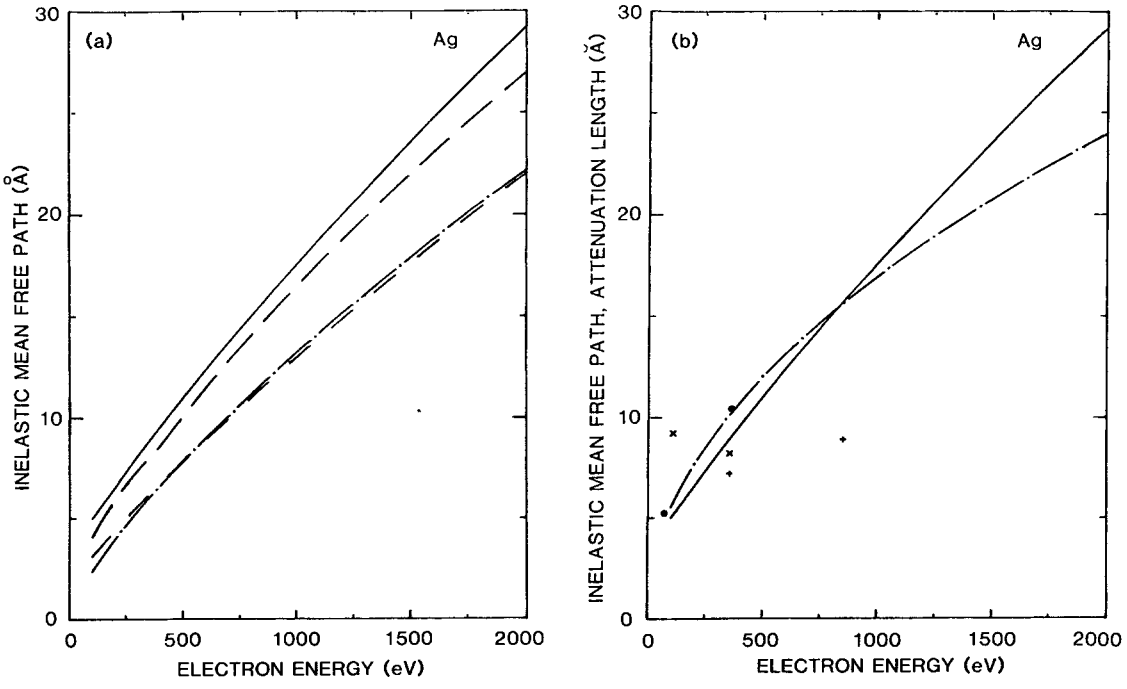

Figure 14. Comparison of IMFP and AL values for Ag: (a) comparison of present IMFP calculation ($c = 1.63$), ——, with other results: – – – = result of Penn[4]; — — = result of Ashley and Tung[5]; — · — = result of Szajman *et al.*[16]; (b) comparison of present IMFP calculation (solid line, as in (a)) with AL data; ● = results of Palmberg and Rhodin[25]; + = results of Jackson *et al.*[26]; × = results of Seah[27]; — · — = empirical formula (8a) of Seah and Dench.[17]

for Al, Au and Ag, but greater differences occur for Cu and Al_2O_3. Second, in all cases, the present λ_T values are larger than the other IMFP results. It is therefore possible that the Penn values of c used here may be systematically low. Third, the present λ_T results are often (but not always) larger than the corresponding AL values in Figs 12(b)–16(b). This observation is consistent with the hypothesis that IMFP values for a given material and energy should exceed AL values on account of elastic scattering. It is, however, possible that this observation may also be associated with the Penn values of c being systematically low. Finally, despite the various uncertainties in the comparisons of results in Figs 12–16, the present λ_T values, based as they are on experimental

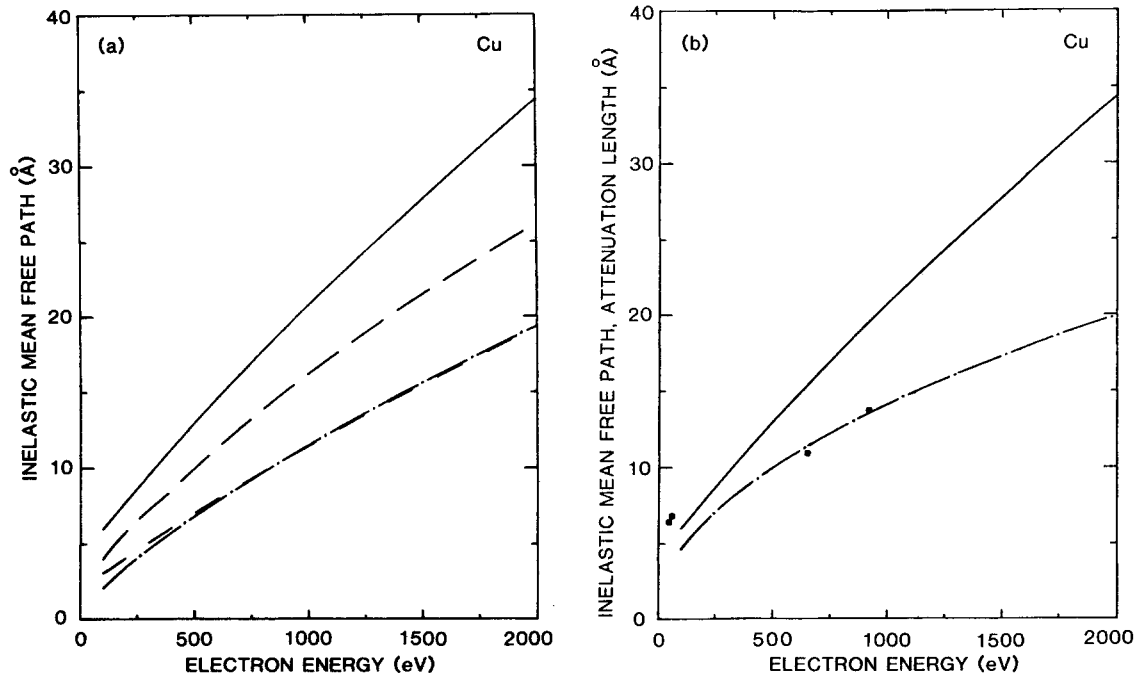

Figure 15. Comparison of IMFP and AL values for Cu: (a) comparison of present IMFP calculation ($c = 1.50$); ——, with other results: – – – = result of Penn[4]; — — = result of Ashley and Tung[5]; — · — = result of Szajman *et al.*[16]; (b) comparison of present IMFP calculation (solid line, as in (a)) with AL data: ● = results of Seah[28]; — · — = empirical formula (8a) of Seah and Dench.[17]

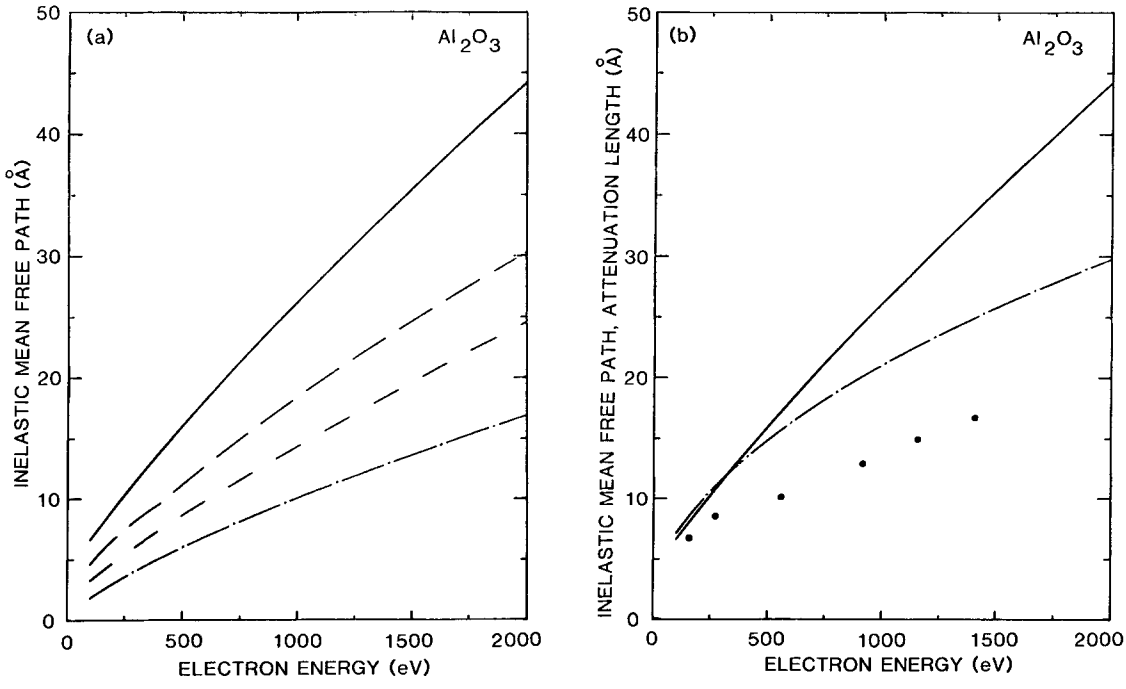

Figure 16. Comparison of IMFP and AL values for Al_2O_3: (a) comparison of present IMFP calculation ($c=1.77$); ——, with other results: – – –=result of Penn[4]; — — —=result of Ashley and Tung[5]; — · —=result of Szajman *et al.*[16]; (b) comparison of present IMFP calculation (solid line, as in (a)) with AL data: ●=results of Battye *et al.*[29]; — · —=empirical formula (8b) of Seah and Dench.[17]

optical data and a theoretical choice of the parameter c, are in reasonable semi-quantitative agreement with other IMFP and AL results. This is clearly reassuring since IMFP calculations on non-free-electron-like materials are difficult and since it is difficult to make AL measurements with high accuracy. While the optical data used here have their uncertainties, the sum rules on $\varepsilon(\omega, 0)$ and $\mathrm{Im}[-1/\varepsilon(\omega, 0)]$ are satisfied to better than 5%.[14,15] It is therefore believed that the principal uncertainty in the present λ_T values arises from uncertainty in the parameter c which, for $E \gg \Delta E$, is derived from the q-dependence of $\varepsilon(\omega, q)$.

The analysis of the dependence on electron energy of AL data in the companion paper[3] indicates that the effective values of c are appreciably less than the Penn values and also that values of the Bethe b parameter (approximately proportional to the integral of $\mathrm{Im}[-1/\varepsilon(\Delta E)]$ over ΔE) are larger than expected from sum-rule considerations. Despite these modifications, the absolute AL values still correspond reasonably well with IMFP calculations (Figs 12–16), but it is clear that more detailed investigations are required of the dependence of λ on E in the energy range of 100–2000 eV where the asymptotic variation of the Bethe equation is not observed.[3]

DISCUSSION

Table 1 lists values of the exponent m of Eq. (6) that have been obtained from least-squares fits to the λ_T values calculated here. Values of m are shown from the calculations with the Penn values of c (Fig. 11) and with $c=0.65$ (Figs 2–9). The table also shows values of m determined from fits to AL data[2,3] and from fits to the IMFP calculations of Ashley and Tung.[5]

The values of m found for the Penn values of c vary with material from a maximum value of 0.786 for Mg to a minimum value of 0.703 for Au. This variation is similar to that found in fits to the IMFP data of Ashley and Tung[5] but is not as large as that deduced from fits to AL data.[2,3] This material dependence of the exponent m is associated with different spectral distributions of the energy-loss function $\mathrm{Im}[-1/\varepsilon(\omega, 0)]$ for different materials. The numerical integrations of (3) lead to

Table 1. Values of the exponent m in (6) for the specified materials. These values have been obtained from fits to AL data for electron energies generally greater than 400 eV (Ref. 2 and 3), from fits to calculated IMFP values for electron energies between 400 and 2000 eV (Ref. 5), and from fits to the present calculated IMFP values with the Penn value of c (Fig. 11) and with $c=0.65$ (Figs 2–9). The fits in the present work were made over an electron energy range that was typically 600–2000 eV. The indicated uncertainties are the probable errors from the least-squares analyses

	m			
	Fits to	Fits to	Present work	
Material	AL data	IMFP data	Penn value of c	$c=0.65$
C			0.758 ± 0.002	0.699 ± 0.003
Mg			0.786 ± 0.002	0.710 ± 0.003
Al	0.78 ± 0.05	0.773	0.778 ± 0.002	0.700 ± 0.003
Al_2O_3	0.54 ± 0.02	0.719	0.735 ± 0.003	0.661 ± 0.003
Cu		0.695	0.714 ± 0.003	0.641 ± 0.004
Ag		0.707	0.715 ± 0.003	0.630 ± 0.004
Au	0.54 ± 0.04	0.688	0.703 ± 0.003	0.614 ± 0.004
Bi			0.754 ± 0.002	0.656 ± 0.003

values of m differing from those expected (0.73–0.78) if there were a *single* dominant energy-loss mechanism.[2]

The Fano plots (fits of experimental AL data to the Bethe equation for inelastic electron scattering) presented in the companion paper[3] indicate that the 'effective' values of c can be much lower than those expected from theory (e.g., the Penn values as presented in Fig. 1). For the free-electron-like metal Al, the effective value of c is in the vicinity of unity while for the non-free-electron-like metal Au, the effective value of c is about 0.18. This trend is qualitatively reasonable since in Al the most probable energy loss is the well-defined volume-plasmon loss of 15 eV. In Au, the energy-loss spectrum is broad and the most probable energy loss is about 40 eV.[8,14] In the electron energy range of 100–2000 eV, it is plausible that the $\lambda_T - E$ dependence will be closer to the expected Bethe dependence for a material with a relatively small energy loss of 15 eV and a sharp loss spectrum than for a material with a larger most probable energy of 40 eV and a broad, extended loss spectrum. Thus, the values of m in Table 1 obtained with the arbitrary choice for c of 0.65 are considered more reasonable for the non-free-electron-like metals Cu, Ag, and Au than those calculated with the Penn values of c. The values of m shown in Table 1 are in semi-quantitative agreement with the results from AL data if cognizance is taken of the likely variation of c, but a more exact comparison will require better knowledge of this parameter. It should also be remarked that significant differences in the values of m determined from AL data and from IMFP data might exist due to the effects of elastic scattering.

SUMMARY

Values of inelastic mean free paths have been computed from experimental optical data for eight materials for electron energies between 100 and 2000 eV. These calculations have been made to examine the dependences of the calculated IMFPs on electron energy in these materials. They also provide an alternative means of obtaining 'experimental' measurements of IMFPs since direct measurements with high accuracy of IMFPs and ALs are difficult in the electron energy range of interest for AES and XPS. The principal limitation in extending the present approach to other materials is associated with the limited data available. Optical data from synchrotron-radiation experiments are increasing and evaluated compilations are becoming available.[30,31] The present approach is also useful for materials such as transition metals and alkali halides for which it is difficult to distinguish valence-electron and core-electron excitations in IMFP calculations.

The IMFP calculations require knowledge of the dependence of the differential inelastic scattering cross section on momentum transfer. There is limited knowledge of this dependence, and it was assumed here that calculations made for free-electron-like materials[4] could be used. This choice was made since the parameter of interest (c in (3)) can be readily determined from the valence-electron density (Fig. 1) and since this parameter does not vary greatly and occurs in a logarithm. Even unrealistically wide variations of this parameter do not greatly affect the computed IMFPs. The IMFP values computed with the free-electron values of c do in fact agree reasonably with IMFP calculations and with AL measurements. More exact knowledge of the parameter c would, however, give more confidence in the computed IMFP values. We note here that empirical values of the parameter c obtained from analysis of AL data are appreciably less than expected from theory.[3] This empirical reduction is approximately compensated (in all the materials examined to date) by an empirical increase in another parameter (b in (3) of Ref. 3) such that measured ALs correspond reasonably to calculated IMFPs in many cases.

The dependence of the calculated IMFPs on electron energy varies from one material to another. This variation is associated with the different spectral distributions of the energy-loss function in different materials. It was convenient to fit the calculated IMFPs to the empirical relation (6) proposed by Wagner *et al.*[2] The range of values of m (a maximum of 0.786 for Mg and a minimum of 0.703 for Au) when the IMFPs were computed with the Penn[4] values of the parameter c is not as large as that found in the analysis of AL data.[2,3] Smaller values of m are found if c is arbitrarily assumed to be equal to 0.65. This choice of c is considered more reasonable for the noble metals on account of their extended energy-loss spectra and leads to values of m ranging from 0.614 to 0.641 for these metals in moderate agreement with the result (0.54 ± 0.04) obtained from analysis of AL data for Au.

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