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Calculation of electron inelastic mean free paths (IMFPs) VII. Reliability of the TPP-2M IMFP predictive equation†

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We report comparisons of electron inelastic mean free paths (IMFPs) determined from our predictive IMFP equation TPP-2M and reference IMFPs calculated from optical data. These comparisons were made for values of the parameter N_v (the number of valence electrons per atom or molecule) that we have recommended and those that were recommended in a recent paper by Seah *et al.* (*Surf. Interface Anal.* 2001; 31: 778). The comparisons were made for eight elemental solids (K, Y, Gd, Tb, Dy, Hf, Ta and Bi) and two compounds (KBr and Y_2O_3) for which there were appreciable differences in the recommended N_v values from the two sources and for which optical data were available for the IMFP calculations. The average of the root-mean-square (RMS) deviations for the ten materials between IMFPs from the TPP-2M equation with our N_v values and the reference IMFPs was 11.0%, whereas the corresponding average with the Seah *et al.* N_v values was 20.2%. The larger average in the latter comparison was mainly due to large (>20%) RMS deviations for four materials (K, Hf, Ta and KBr). For the other six materials, the RMS deviations with the Seah *et al.* values of N_v were similar to those with our values of N_v. Based on the comparisons for these ten materials, we believe that it is preferable to use our values of N_v in the TPP-2M equation.

KEYWORDS: AES; XPS; inelastic mean free path; TPP-2M equation

INTRODUCTION

The electron inelastic mean free path (IMFP) is a key material parameter in Auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS), as well as in other techniques involving electron scattering or emission at solid surfaces.[1,2] This parameter together with the experimental configuration affects the surface sensitivity of AES and XPS measurements[3] and is needed for modeling of signal electron transport.

We previously reported calculations of electron IMFPs from experimental optical data for 27 elemental solids, 15 inorganic compounds and 14 organic compounds, as well as analyses of these results.[4–9] The optical data were checked for internal consistency using two sum rules,[10] and these checks revealed that the available data for the group of elements and the group of organic compounds were more reliable than for the group of inorganic compounds. We therefore analyzed IMFPs for the groups of elements and organic compounds to derive an equation, designated TPP-2M, that could be used to estimate IMFPs for other materials.[8]

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The TPP-2M predictive equation for the IMFP, λ, as a function of electron energy, E (in eV), is

$$\lambda = \frac{E}{E_p^2[\beta \ln(\gamma E) - (C/E) + (D/E^2)]} \quad (\text{in Å}) \tag{1a}$$

$$\beta = -0.10 + 0.944(E_p^2 + E_g^2)^{-1/2} + 0.069\rho^{0.1} \tag{1b}$$

$$\gamma = 0.191\rho^{-1/2} \tag{1c}$$

$$C = 1.97 - 0.91U \tag{1d}$$

$$D = 53.4 - 20.8U \tag{1e}$$

$$U = N_v\rho/M = E_p^2/829.4 \tag{1f}$$

where $E_p = 28.8(N_v\rho/M)^{1/2}$ is the free-electron plasmon energy (in eV), N_v is the number of valence electrons per atom (for elemental solids) or molecule (for compounds), ρ is the density (in g cm^{-3}), M is the atomic or molecular weight and E_g is the bandgap energy (in eV).

We point out that the value of N_v discussed here should not be identified with the chemical valence of an element. For some elemental solids (e.g. the alkali metals), our recommended value of N_v (1 in this case) is indeed the same as the valence. In contrast, our recommended value of N_v for halogens (7 in this case) is very different from the valence. The term E_p in Eqn (1), a function of N_v, originated from an analysis of the Bethe[11] equation for inelastic electron scattering in matter.[4] The fact that a given element may have different chemical valences in different compounds (or even at a surface and in the bulk) is therefore of no consequence in determining values of N_v for use in the TPP-2M IMFP predictive equation.

We have discussed the appropriate choice of values for the parameter N_v in Eqn (1) for different elemental solids and have indicated out that there can be ambiguity in choosing a value of this parameter for some elements.[4–7,12] The value of N_v is normally computed from the number of electrons in the valence band for the particular solid. For example, in an elemental solid such as Al there are three valence electrons and $N_v = 3$, whereas in a compound such as Al_2O_3 there are six valence electrons from the Al and eighteen valence electrons from the oxygen so that $N_v = 24$. Ambiguity in the choice of N_v arises for certain elemental solids in the Periodic Table that occur after those elements in which an atomic subshell is filled. There is then a large change in N_v and electrons that were formerly in the valence band now occupy a subshell with a 'small' binding energy (BE). The question then arises as to how large this 'small' BE can be, so that the subshell does not contribute significantly to the IMFP. For example, elemental copper has ten 3d electrons and one 4s electron in its valence band, and so we expect $N_v = 11$ for Cu. For the neighboring element Zn in the Periodic Table, there are two 4s electrons in the valence band and the ten 3d electrons have an average BE of $\sim$10 eV.[13] For the two following elemental solids in the Periodic Table, Ga and Ge, the numbers of electrons in their valence bands are three and four, respectively, whereas the average BEs of the ten 3d electrons are $\sim$18.7 eV and 29.7 eV, respectively.[13] Although the ten 3d electrons are clearly contributing to the strength of inelastic scattering (more precisely, to the energy-loss function or the differential inelastic scattering cross-section for energy losses of between 0 eV and about 50 eV, the energy-loss region that has a large contribution to the total inelastic-scattering cross-section) in copper, they have a progressively weaker influence as the BE increases with atomic number (i.e. for Ga, Ge and the following elemental solids).

Similar considerations apply to other elements in the Periodic Table as valence subshells are filled and become core levels. Although the IMFP from Eqn (1) depends on N_v in a complicated way through the values of E_p, β, C and D, the IMFP value for some elemental solids and compounds fortunately does not depend sensitively on the choice of N_v.[4–7,12] For example, we analyzed the extent to which IMFPs calculated from an earlier version of TPP-2M depended on N_v, E_p, ρ and E_g as each of these parameters was varied in turn over a substantial range while the other parameters were fixed at their known values for Al, Au, Al_2O_3 and GaAs.[5,7] Although the results vary with material, a change in the value of N_v by 50% from the known values will typically lead to a change of <15% in the derived IMFPs. This test, made with the TPP-2 predictive IMFP equation developed earlier,[5] is expected to be a reasonable guide to the performance of the TPP-2M equation. Although the TPP-2M equation has a different expression for β than that given for the TPP-2 equation, both equations give closely similar values of IMFPs for the elemental solids and inorganic compounds considered in Refs 4–6. Examples will be presented here of the extent to which IMFPs depend on the choice of N_v in the TPP-2M equation.

In Table 1 we show the values of N_v for each element that we have recommended in previous papers[4–8] or that have been recommended in a NIST IMFP database;[14] these N_v values will be referred to hereafter as the TPP values. For the rare-earth elemental solids, the values of N_v have been determined from the sum of the number of valence electrons for the solid state, either two or three as discussed by Netzer and Matthew,[15] and the six 5p electrons that contribute strongly to the energy-loss function.[16] (J. A. D. Matthew, personal communication). Although the 5p electrons for the rare-earth elements have binding energies of 18–27 eV,[17] they have been included in the calculation of N_v because of the strong 5p–6d excitations that occur close to the threshold energy for excitation (i.e. the BE)[16] (J. A. D. Matthew, personal communication). The number of 4f electrons, which increases with atomic number through the rare-earth series, has not been included in the N_v calculation. Although these 4f electrons have binding energies of <9 eV,[18] their orbitals are highly localized and they contribute weakly to the energy-loss function because of the substantial 'delayed onset' in plots of the photo-absorption cross-section versus photon energy.[16] Similar delayed onsets have been found in plots of the yields of $N_{6,7}$VV Auger electrons in Au, Pb and Bi as a function of incident electron energy.[19]

Seah, Gilmore and Spencer (hereafter denoted SGS) recently reported an analysis of Auger electron intensities for 61 elemental solids and of photoelectron intensities for 58 elemental solids (in AES and XPS experiments, respectively).[20] These intensities were compared with predicted intensities for which the TPP-2M equation was used to obtain the IMFPs for the relevant elements and electron energies. Seah *et al*. found systematic differences between the experimental and predicted intensities from which they concluded that there was either an error in their intensity measurement procedure or a systematic error in IMFPs from the TPP-2M equation. The latter possible systematic error was associated with the choice of N_v in Eqn (1). Seah *et al*. found that the systematic differences between the measured and calculated intensities could be minimized by computing N_v from the number of electrons with BEs of $\leq$28 eV; for the lanthanide series, they recommended that the number of 4f electrons for each element be included. Table 1 shows the values of N_v recommended by Seah *et al*.[20] (M. P. Seah and I. S. Gilmore, personal communication).

Figure 1 is a plot of the N_v values from Table 1 versus atomic number, Z. For 45 of the 75 elemental solids for which there are both TPP and SGS recommendations of N_v, there is no difference in the N_v values from the two sources. We also note that, of the remaining 30 elements, Seah *et al*. measured and analyzed AES or XPS data for all elements except F, K, Rb and Cs.

We report here comparisons of IMFPs calculated from the TPP-2M equation for eight elemental solids (K, Y, Gd, Tb, Dy, Hf, Ta and Bi) for which there were significantly different

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Table 1. Values of N_v recommended by the present authors (TPP) and by Seah *et al.*[20] (SGS) for the indicated elemental solids and values of the atomic number Z

		N_v	
Element	Z	TPP	SGS
H	1	1	
He	2	2	
Li	3	1	1
Be	4	2	2
B	5	3	3
C	6	4	4
N	7	5	5
O	8	6	6
F	9	7	5
Ne	10	8	
Na	11	1	1
Mg	12	2	2
Al	13	3	3
Si	14	4	4
P	15	5	5
S	16	6	6
Cl	17	7	7
Ar	18	8	
K	19	1	7
Ca	20	2	8
Sc	21	3	3
Ti	22	4	4
V	23	5	5
Cr	24	6	6
Mn	25	7	7
Fe	26	8	8
Co	27	9	9
Ni	28	10	10
Cu	29	11	11
Zn	30	12	12
Ga	31	3	13
Ge	32	4	4
As	33	5	5
Se	34	6	6
Br	35	7	7
Kr	36	8	
Rb	37	1	7
Sr	38	2	8
Y	39	3	9
Zr	40	4	4
Nb	41	5	5
Mo	42	6	6
Ru	44	8	8
Rh	45	9	9
Pd	46	10	10
Ag	47	11	11
Cd	48	12	12
In	49	3	13
Sn	50	4	14
Sb	51	5	5
Te	52	6	6
I	53	7	7
Xe	54	8	
Cs	55	1	9
Ba	56	2	8
La	57	3	9
Ce	58	9	10
Pr	59	9	11
Nd	60	9	12
Sm	62	9	14
Eu	63	8	15
Gd	64	9	16
Tb	65	9	17
Dy	66	9	18
Ho	67	9	19
Er	68	9	14
Tm	69	9	15
Yb	70	8	22
Lu	71	9	17
Hf	72	4	18
Ta	73	5	19
W	74	6	6
Re	75	7	7
Os	76	8	8
Ir	77	9	9
Pt	78	10	10
Au	79	11	11
Hg	80	12	12
Tl	81	3	13
Pb	82	4	14
Bi	83	5	15

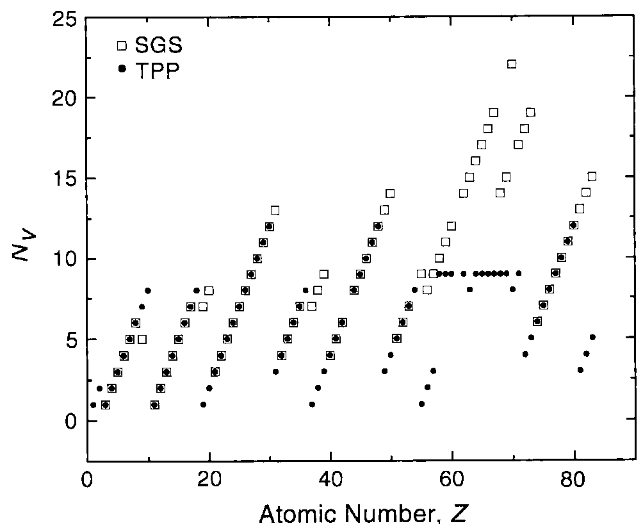

Figure 1. Values of the parameter N_v in Eqn (1) recommended by Seah *et al.*[20] (□) and the present authors (●) as a function of atomic number Z.

values of N_v (Table 1) and for which we had calculated IMFPs from experimental optical data. The latter IMFPs are considered as reference values for each solid, and we make comparisons between these values and the corresponding IMFPs from the TPP-2M equation with the two proposed values of N_v for each solid. We also make similar comparisons for two compounds, KBr and Y_2O_3, for which the N_v values are 8 and 24, respectively, from the TPP values in Table 1 for the constituent elements and 14 and 36, respectively, from the SGS recommendations in Table 1.

RESULTS AND DISCUSSION

Figures 2–11 show plots of IMFPs from experimental optical data (solid lines) for K,[16] Y,[16] Gd,[16] Tb[16] Dy,[16] Hf,[5] Ta,[5] Bi,[5] KBr[16] and Y_2O_3,[16] respectively, for electron energies between 50 and 2000 eV. The long-dashed lines are IMFPs from the TPP-2M equation (Eqn (1)) with our recommended values of N_v, whereas the short-dashed lines are IMFPs from the same equation with the SGS recommendations for N_v. The other material parameters needed for the evaluation of TPP-2M are listed in Table 2.

In order to provide a quantitative description of the results in Figs 2–11, we have calculated percentage deviations between IMFPs calculated from the TPP-2M equation, with the TPP and SGS values of N_v, and the corresponding reference IMFP values at 10 eV intervals between 50 and 200 eV and at 100 eV intervals between 200 and 2000 eV. The root-mean-square (RMS) deviations for each material are shown in Fig. 12. The average of the RMS deviations in Fig. 12 with the TPP values of N_v is 11.0% whereas the corresponding average with the SGS values of N_v is 20.2%.

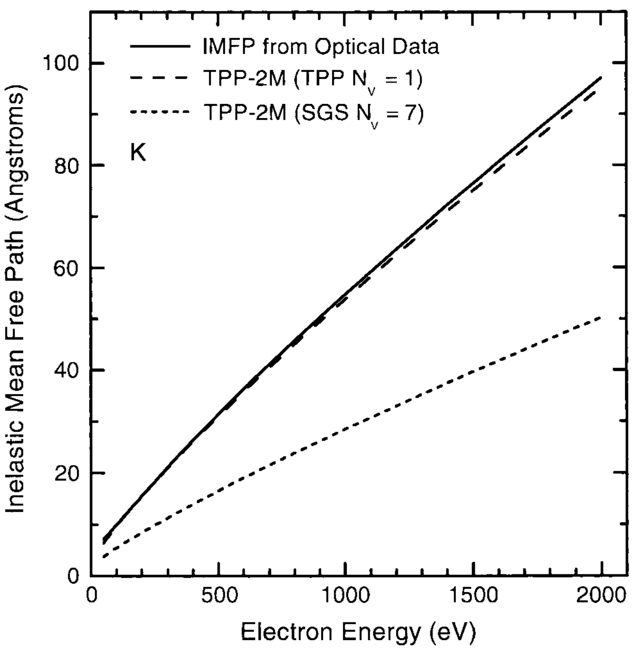

Figure 2. Comparison of IMFPs calculated from experimental optical data (solid line) as a function of electron energy for potassium with IMFPs obtained from the TPP-2M equation (Eqn (1)) with values of the parameter N_v recommended by the present authors (long-dashed line) and by Seah *et al.*[20] (short-dashed line).

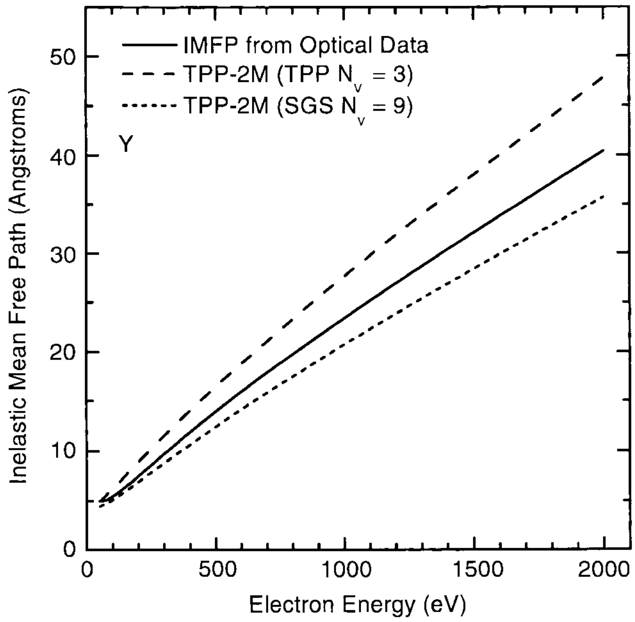

Figure 3. The IMFP results for yttrium (see caption to Fig. 2).

Table 2. Material parameters needed for evaluation of the TPP-2M equation (Eqn (1))

Material	M	ρ (g cm^{-3})	E_g (eV)
K	39.0983	0.89	0
Y	88.90585	4.47	0
Gd	157.25	7.9	0
Tb	158.925	8.23	0
Dy	162.50	8.55	0
Hf	178.49	13.3	0
Ta	180.9479	16.4	0
Bi	208.9804	9.79	0
KBr	119.0023	2.75	6.4
Y_2O_3	225.809	5.033	5.7

We note here that the average RMS deviation of 11.0% with our values of N_v is close to the values found in similar comparisons: 10.2% for the original group of 27 elemental solids that we investigated and 8.5% for our group of 14 organic compounds.[8]

The larger average of the RMS deviations in Fig. 12 for the SGS values of N_v (20.2%) than for the TPP values of N_v (11.0%) is mainly due to the large (>20%) RMS deviations for four materials (K, Hf, Ta, and KBr). For these four materials, the TPP values of N_v give IMFPs that are appreciably closer to the reference IMFPs than the SGS values of N_v. For the other six materials, the average of the RMS deviations with the SGS values of N_v is 10.3%. This average is comparable to that found with the TPP values of N_v for the same materials (11.8%). We thus cannot make a meaningful choice between the TPP and SGS values of N_v for these six materials. We also note that, for the three rare-earth elemental solids considered here, the average RMS deviations are 9.2% and 7.8% for the TPP and SGS values of N_v, respectively; inclusion or exclusion of the 4f electrons in N_v does not make an appreciable difference in the IMFPs from TPP-2M for these materials. For K, Hf, Ta and KBr, however, the TPP values of N_v give IMFPs that are in clearly better agreement with the reference IMFPs than IMFPs obtained from the SGS values of N_v.

We now consider whether the RMS deviations in Fig. 12 might be correlated with uncertainties of the energy-loss functions derived from optical data and in some cases from inelastic electron scattering data that were used to calculate the reference IMFPs.[4–8] Table 3 shows the errors in the f-sum rule and the Kramers–Kronig (KK) sum rule for the energy-loss functions of our materials.[10] The absolute values of the average sum-rule errors for these materials are shown in Fig. 12. The average value of 4.8% for these absolute errors, is comparable to the corresponding value of 5.4% for our original group of 27 elemental solids.[4] We also see from Fig. 12 that the sum-rule errors for K, Hf, Ta and KBr are similar to those for the other materials. In addition, there is no obvious correlation in Fig. 12 between the RMS deviations for the different choices of N_v and the corresponding absolute values of the average sum-rule errors.

It is interesting to point out the extent to which IMFPs from Eqn (1) depend on the choice of N_v. Figure 13 shows a plot of ratios of IMFPs at a representative energy, 1000 eV, determined from Eqn (1) with the SGS and TPP values of N_v versus the ratio of these N_v values for the ten materials considered here. Although there is some scatter in the plotted points, we see that the IMFP ratio depends inversely on the N_v ratio. Even for a sevenfold change in the value of N_v (for K), the IMFP changes by less than a factor of two. For the two materials for which the N_v ratio is 3 (Y and Bi), the IMFPs with the SGS N_v values are less than those with the TPP values by 25.1% and 29.4%, respectively. For the five materials for which the N_v ratio is ≤ 2 (Y_2O_3, KBr, Gd, Tb and Dy), the change in IMFPs is <16%. This latter uncertainty is larger than the uncertainty of IMFPs from the TPP-2M equation for our group of 27 elemental solids (10.2%)[5] and for our group of organic compounds (8.5%)[8] but may be sufficiently small for some applications of TPP-2M.

Seah *et al.*[20–24] have actually presented three different recommendations concerning the choice of N_v in Eqn (1). Each recommendation was based on comparisons of experimental and calculated intensities for certain sets of elemental AES and XPS spectra but involved different and increasingly refined procedures for determining peak intensities from the spectra. Initially, they recommended that N_v be computed from the number of electrons with BEs of ≤ 14 eV and that the 4f electrons for the lanthanide series be excluded.[21–23] In another paper, they concluded that N_v should be obtained from the number of electrons with BEs up to a cut-off energy between 14 and 28 eV and that the 4f electrons for the lanthanides be included.[24] Finally, as mentioned previously, they recommended that N_v be determined from the number of electrons with BEs of ≤ 28 eV and that the 4f electrons for the lanthanides be included.[20] In the latter paper, Seah *et al.* also comment that they analyzed a subset of their XPS data with IMFPs obtained from optical data[5] rather than from the TPP-2M equation, and obtained marginally poorer results.

The recommendations of Seah *et al.*[20–24] are valuable because they provide guidance on the choice of N_v from large sets of experimental data that were obtained and analyzed in a consistent manner. As noted earlier, there has been ambiguity in the choice of this parameter for some elemental solids.[4–7,12] It is difficult, however, to develop and apply simple rules for the determination of N_v based on BE considerations alone. For the lanthanide elements in particular, the contributions of the 4f electrons to the IMFP are expected to be weak (because of their strong localization) but the effects of the 5p electrons are much stronger.[16] (J. A. D. Matthew, personal communication). Nevertheless, substantial changes of N_v in the TPP-2M equation do not lead to appreciable changes in the resulting IMFPs, as shown here for Gd, Tb and Dy in Figs 4–6 and for the entire lanthanide series by Seah *et al.*[21] when N_v is ≥ 8.

Tougaard and Jansson[25] reported tests of the consistency and validity of the Tougaard, Shirley and straight-line methods for determinations of peak intensities in XPS from measurements with seven elemental solids (Co, Ni, Cu, Zn, Ag, Pt and Au) and with CuAu, CoNi and

Table 3. Errors in the f-sum rule and the Kramers–Kronig (KK) sum rule used to evaluate the energy-loss function for each material

Material	f-Sum error (%)	KK sum error (%)
K	−6.8	16
Y	1	4
Gd	−5	2.1
Tb	−0.2	6.6
Dy	0.6	−1.1
Hf	−4	−16
Ta	1	3
Bi	6	−2
KBr	−0.8	−4.7
Y_2O_3	4	7.7

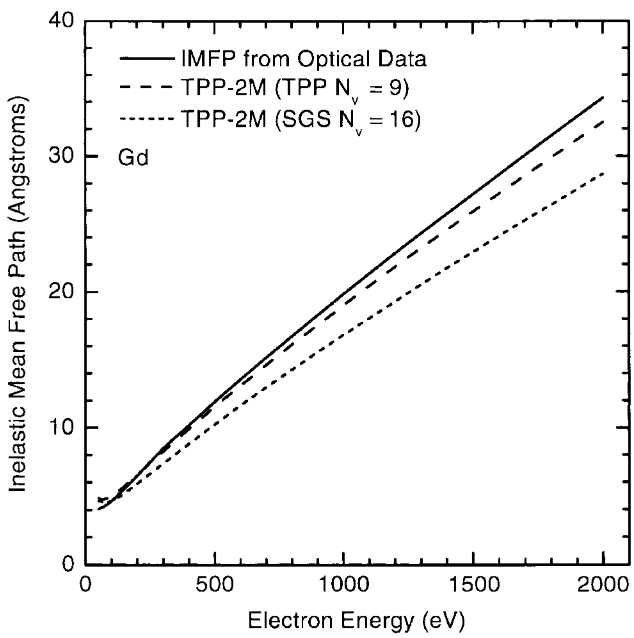

Figure 4. The IMFP results for gadolinium (see caption to Fig. 2).

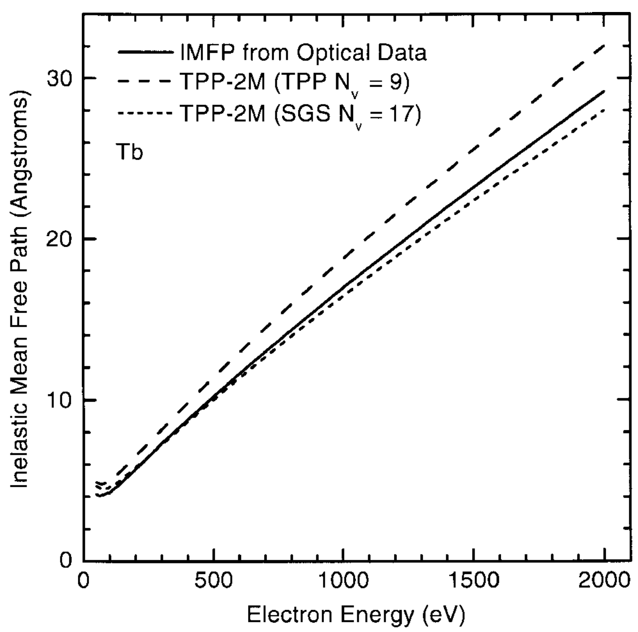

Figure 5. The IMFP results for terbium (see caption to Fig. 2).

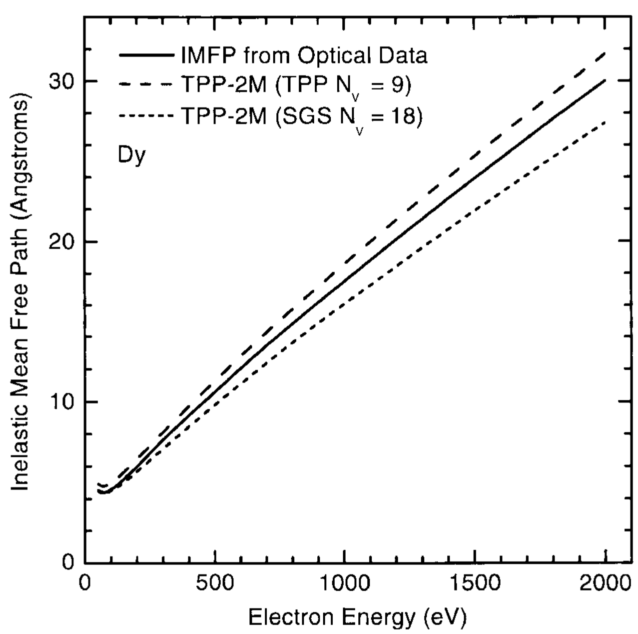

Figure 6. The IMFP results for dysprosium (see caption to Fig. 2).

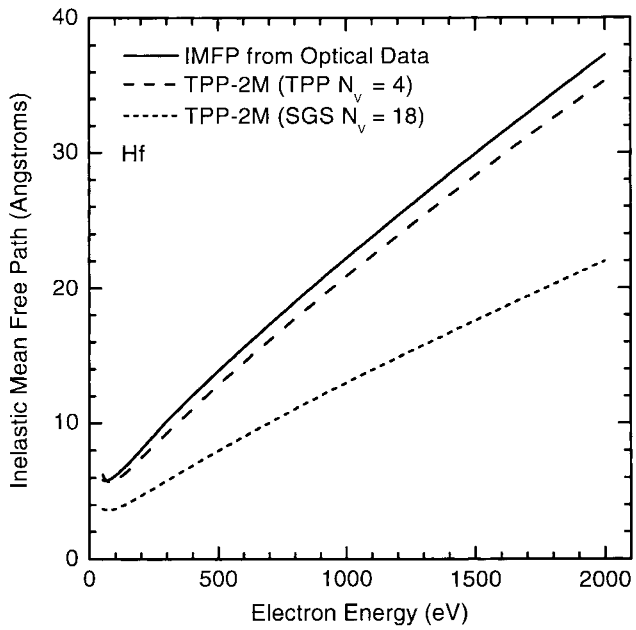

Figure 7. The IMFP results for hafnium (see caption to Fig. 2).

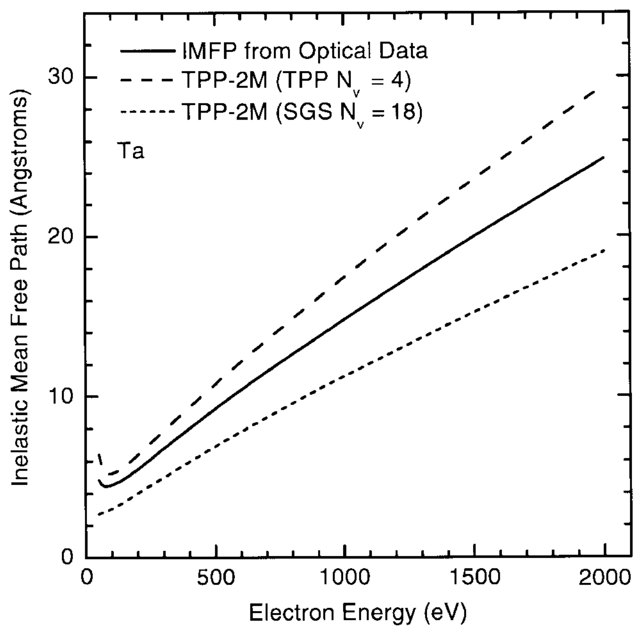

Figure 8. The IMFP results for tantalum (see caption to Fig. 2).

CuNiMn alloys of various compositions. Selected intensity ratios were compared with those expected from calculated photoionization cross-sections and from IMFPs obtained by Tanuma *et al.*[4] or with the predictive IMFP equation TPP-2.[5] This work showed that the Tougaard method of intensity measurement was superior to the Shirley and straight-line methods. The RMS deviations between the various ratios of measured peak intensities (obtained with the Tougaard method) and the calculated ratios were ~11% for comparisons involving the same solid and ~14% for comparisons involving two solids. These tests, similar in principle but different in detail to the later work of Seah *et al.*,[20–24] indicate that IMFP ratios from Tanuma *et al.*[4,5] are consistent with measured photoelectron intensity ratios for a range of materials, electron energies and data analysis conditions.

Three elemental solids (K, Hf and Ta) and one compound (KBr) have been identified here as materials that give substantially (>20%) smaller IMFPs from the TPP-2M equation with the SGS choices of N_v than the corresponding IMFPs calculated from optical data. Although the optical data used in the IMFP calculations for these four materials is of similar quality to the data used in the IMFP calculations for our group of 27 elemental solids (as judged by the sum-rule consistency checks),[4] further experimental tests with these materials are needed. It would clearly be desirable to obtain independent values of the IMFP by elastic peak electron spectroscopy (EPES).[1,2] It would be desirable also to assess the procedures[21,23–26] used to determine AES and XPS

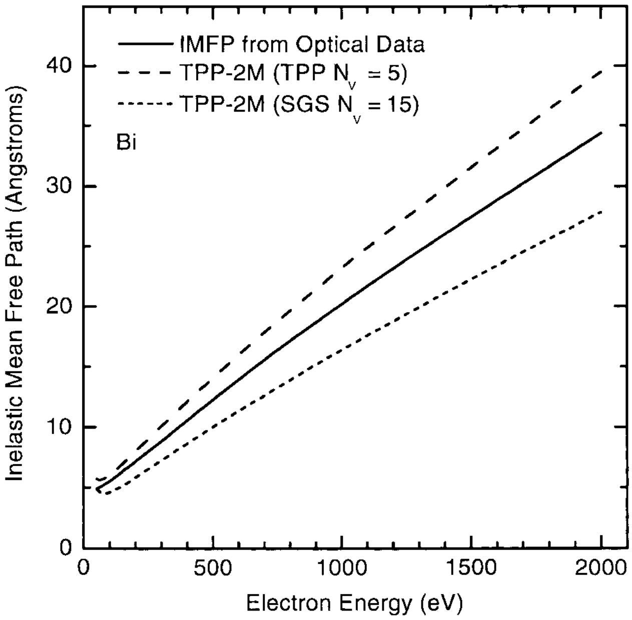

Figure 9. The IMFP results for bismuth (see caption to Fig. 2).

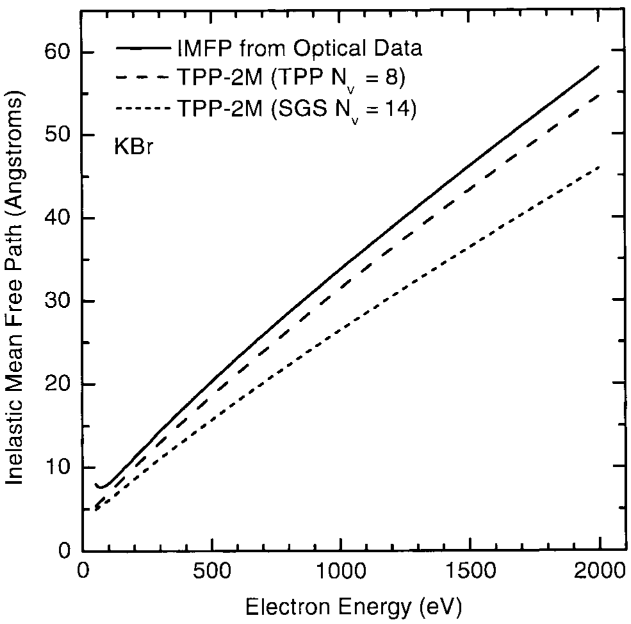

Figure 10. The IMFP results for potassium bromide (see caption to Fig. 2).

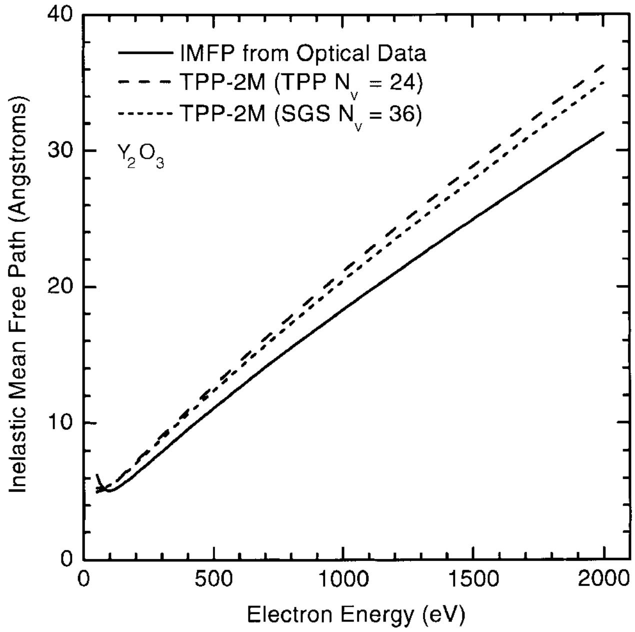

Figure 11. The IMFP results for yttrium oxide (see caption to Fig. 2).

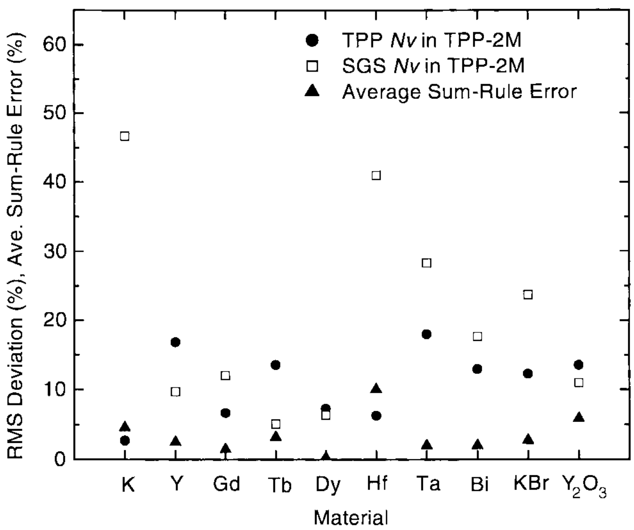

Figure 12. Root-mean-square (RMS) percentage deviation between IMFPs obtained from the TPP-2M equation (Eqn (1)), with the TPP (●) and SGS (□) values of N_v, and IMFPs calculated from experimental optical data for each material considered here. The absolute values of the average sum-rule errors (Table 3) found in the evaluations of the energy-loss functions for each material are also shown (▲).

peak intensities of these materials using the reference IMFPs obtained from optical data as well as independent IMFP measurements when available. Because potassium oxidizes rapidly and it may be difficult to prepare stoichiometric surfaces of KBr, it is suggested that these tests be made with Hf and Ta. Independent determinations of IMFPs by EPES should be made also of those elemental solids in Table 1 for which there are substantial differences in the TPP and SGS values of N_v (e.g. Ca, Ga, Sr, In, Sn, Cs, Ba, Tl and Pb).

SUMMARY

We have investigated the uncertainty in IMFPs derived from the TPP-2M predictive equation (Eqn (1)) associated with different choices of the parameter N_v. We compared IMFPs from this equation using N_v values recommended by us (TPP)[4–8,14] and by Seah *et al.* (SGS)[20] with reference IMFPs calculated from optical data. These comparisons were made for eight elemental solids (K, Y, Gd, Tb, Dy, Hf, Ta and Bi) and two compounds (KBr and Y_2O_3) for which there were appreciable differences in the recommended N_v values (Table 1) and for which optical data were available for the IMFP calculations.

We found that the average of the RMS deviations for the ten materials between IMFPs from Eqn (1) with the TPP

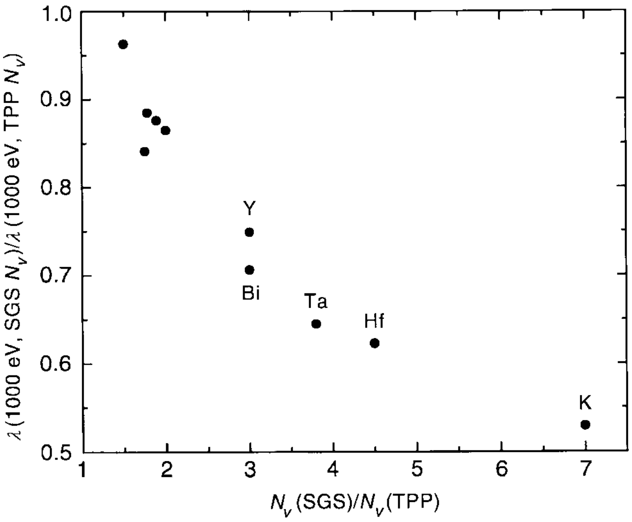

Figure 13. Plot of ratios of IMFPs from Eqn (1) at 1000 eV for the SGS and TPP values of N_v versus the ratios of these N_v values for each material considered here.

N_v values and the reference IMFPs was 11.0% whereas the corresponding average with the SGS N_v values was 20.2%. The larger average for the SGS N_v values was mainly due to large (>20%) RMS deviations for four materials (K, Hf, Ta and KBr). For the other six materials, the RMS deviations with the SGS values of N_v were similar to those with the TPP values of N_v. Based on the comparisons for these ten materials, we believe that it is preferable to use the TPP values of N_v given in Table 1 in the TPP-2M equation. Further experimental tests (particularly for K, Hf, Ta and KBr) are needed of IMFPs calculated from optical data as well as from the TPP-2M equation. Such tests could also be used to assess the procedures used for AES and XPS peak intensity measurements by Seah *et al.*[20]

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