2018

Electron Range Computational Tool for Arbitrary Materials Over a Wide Energy Range

Gregory Wilson
Utah State University

JR Dennison
Utah State Univesity

Anne C. Starley
Utah State University

Electron Range Computational Tool for Arbitrary Materials Over a Wide Energy Range

Gregory Wilson, Anne Starley, and JR Dennison

***Abstract*—A continuous, simple, composite, piecewise formula is used to calculate the approximate electron range in materials (10^{-9} m to 10^{-2} m) over an extended energy span (<10 eV to >10 MeV). This model is applicable to a wide array of conducting, semiconducting, insulating, elemental, compound, and composite materials using tabulated values of a single empirical free parameter, termed the effective number of valence electrons, N_V^{eff}. It can also be applied to arbitrary materials which have no available range data using a predictive formula for N_V^{pre}, requiring only the material composition, mass density and bandgap energy. A user-friendly computational has been implemented for *Microsoft Excel* and as a self-contained *HTML/JavaScript* application which can be used in any modern browser. The resulting range data calculations can be exported in both graphical and tabular formats, along with the used material properties. Use of the tool is described, along with the results of several sets of computational studies designed to illustrate the use and versatility of the tool.**

***Index Terms*—Electron scattering, materials, range, space environment interactions, spacecraft charging.**

I. Introduction

The electron range in materials, *R*, describes the maximum distance electrons of an initial incident energy can travel through a material before they lose all of their kinetic energy and come to a rest, depositing their charge. At very low energies where only single inelastic collisions are likely to occur, this becomes synonomous to the inelastic mean free path (IFMP). The range and the electron IMFP are two common ways to parameterize electron interactions with materials.[1-3]

An approximate range expression has been developed by merging well known semi-empirical models for the interaction of electrons with materials in different energy regimes by employing the continuous slow down approximation (CSDA) and constant loss approximation (CLA), as well as an extension of the IMFP of electrons to multiple scattering; details of the model are provided in [3] with a summary of the basic equations outlined in Appendix I.

Using these approximations, a continuous, simple, composite, piecewise formula—with a single empirical free parameter, termed the effective number of valence electrons, N_V^{eff}— approximates the range over a large length scale (10^{-9} m to 10^{-2} m). Estimation of the range over an extended energy span (<10 eV to >10 MeV), particularly at lower energies where few inelastic collisions occur before electrons stop, is an important advantage for this model over other range models[1].

The ability to estimate the electron range for most arbitrary materials with no free parameters—based solely on the material elemental composition and mass density plus an estimate of the mean energy of the primary inelastic collisional losses from the plasmon or bandgap energies—is the other most important advantage of the present model. Using the NIST database,[1] N_V^{eff} was numerically determined for 246 conducting, semiconducting, insulating, elemental, compound, and composite materials. Agreement of the model presented here with available databases of electron interactions are within <20% for almost all of these materials over the full energy range, and are generally much less than 20% with the largest discrepancies at high relativistic energies and low energies.[4] For materials not in the database, a predictive formula was developed for N_V^{pre}, where agreement between N_V^{pre} and N_V^{eff} for materials in the database is generally well within ~10% which again leads to maximum discrepancies for the range of ≤ 20%.[5]

This paper describes two computational tools which have been developed to make this model and database more readily available and to extend its applicability. The first tool is a *Microsoft Excel* worksheet and the second is an *HMTL/JavaScript* webpage hosted by Utah State University's Materials Physics Group[6].

II. Microsoft Excel Worksheet

The *Microsoft Excel* worksheet is a multipage worksheet which calculates the electron range and IMFP for 246 materials using a database of materials properties and values of N_v^{eff} determined from fits to the NIST databases.[1,2] The worksheet also allows 10 user input custom materials for which N_v^{pre} is determined by user input materials information. The calculated range data are presented in both tabular and graphical format (see Fig. 1).

The worksheet is organized into several tabs including the *Information*, *Graphs and Data*, *Custom Material*, *Material Data*, *Range Calculation*, and *IMFP Calculation* tabs. All user-customizable fields are denoted with an orange fill, as shown in Figs. 1 and 2. Cells without orange fill should not be changed without a clear understanding of inner workings of the worksheet.

The *Information* tab acts as a front end to the worksheet with links to information on how to use the worksheet,

This work was supported by a Utah NASA Space Grant Consortium Fellowship.

Greg Wilson is a PhD student at Utah State University, Logan, UT 84322 USA. (e-mail: GregDWilson@gmail.com).

JR Dennison is a Professor of Physics with the Materials Physics Group, Utah State University, Logan, UT 84322 USA. (e-mail: JR.Dennison@usu.edu).

(a)

	A	B	C	D	E	F
1						
2	Choose Material 1		Choose Material 2		Choose Material 3	
3						
4	Gold		Silicon Glass		Aluminium	
5						
6	☑ Plot Data		☑ Plot Data		☑ Plot Data	
7						
8	Emin:	1.000E+01	Emax:	1.000E+07	☑ Log Energy	
9						
10	Energy (eV)	Range (μm)	Energy (eV)	Range (μm)	Energy (eV)	Range (μm)
11	1.000E+01	1.411E-03	1.000E+01	1.353E-03	1.000E+01	8.189E-04
12	1.072E+01	1.330E-03	1.072E+01	1.279E-03	1.072E+01	7.756E-04
13	1.149E+01	1.254E-03	1.149E+01	1.210E-03	1.149E+01	7.353E-04
14	1.232E+01	1.184E-03	1.232E+01	1.146E-03	1.232E+01	6.979E-04
15	1.320E+01	1.118E-03	1.320E+01	1.086E-03	1.320E+01	6.632E-04
16	1.415E+01	1.057E-03	1.415E+01	1.031E-03	1.415E+01	6.310E-04
17	1.517E+01	9.997E-04	1.517E+01	9.797E-04	1.517E+01	6.012E-04
18	1.626E+01	9.468E-04	1.626E+01	9.320E-04	1.626E+01	5.736E-04
19	1.743E+01	8.976E-04	1.743E+01	8.879E-04	1.743E+01	5.481E-04
20	1.868E+01	8.519E-04	1.868E+01	8.471E-04	1.868E+01	5.245E-04
21	2.002E+01	8.095E-04	2.002E+01	8.093E-04	2.002E+01	5.028E-04
22	2.146E+01	7.702E-04	2.146E+01	7.745E-04	2.146E+01	4.829E-04

(b)

Material	Formula	$\bar{Z}_A$	ρ_m (g/cm^3)	$\bar{M}_A$ (amu)	N_V^{eff}	E_{gap} (eV)
Gold	Au	79	19.32	196.97	7.684	0
Silicon Glass	SiO2	9.98	2.32	19.99	2.793	9.5
Aluminium	Al	13	2.7	26.98	3.254	0

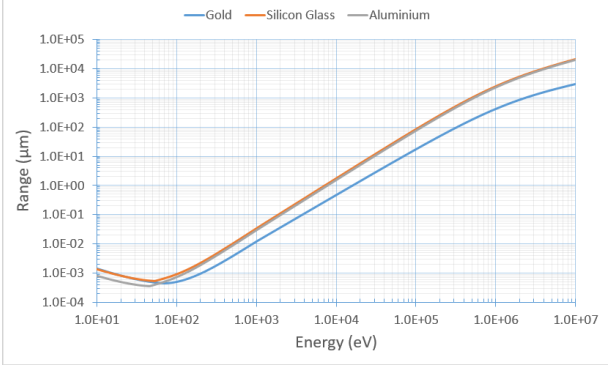

Figure 1. (a) Left side of the *Graphs and Data* tab. This includes a drop-down list of three different materials, check boxes to include each data set in the output, energy range settings, and a tabular list of the data. (b) Right side of the *Graphs and Data* tab. This includes lists of the material properties of the selected materials, as well as a customizable graph of the data.

the theoretical basis for the model and its development, and supporting references for this and related range models.

The *Graphs and Data* tab (Fig. 1) is main worksheet where user interaction occurs. This tab includes three drop-down lists where three different materials can be selected. Below each drop-down list is a check box which turns the data export for each material on or off. The material properties are then displayed in a table to the right, as shown in Fig. 1(b). The range data are presented in two formats which can be copied and pasted into other applications for further use by the user: (i) a tabular format and (ii) a graphical format (When pasting the graph into another *Microsoft* program, use the *Picture* option.).

Any formating properties of the graph can be readily changed according to user preferences using *Excel* options . The energy range for calculations and plotting can also be customized by editing the values in cells B8 and D8, which will automatically adjust the graph axes to fit the data. The *Log Energy* checkbox in cell E8. automatically changes the graph between a Log-Log plot

	A	B	C	D	E	F	G
1	Material Name			Sodium Chloride	PEEK	Deuterated PI	Tin-Rich ITO
2	Formula			NaCl	$C_{22}H_{14}O_5$	$C_{22}H_5D_5N_2O_5$	$(In_2O_3)_{0.904}(SnO_2)_{0.096}$
3	ρ_m (g/cm^3)			2.165	1.32	1.42	6.8
4	E_{gap} (eV)			8.75	3.1	2.32	4.11
5	Z	$\bar{M}$ (amu)	Element				
6	1	1.008	H		18	5	
7	2	4.003	He				
8	3	6.968	Li				
9	4	9.012	Be				
10	5	10.81	B				
11	6	12.01	C		21	22	
12	7	14.01	N			2	
13	8	16.00	O		3	5	60.638
14	9	19.00	F				
15	10	20.18	Ne				
16	11	22.99	Na	1			
17	12	24.31	Mg				
18	13	26.98	Al				
19	14	28.09	Si				
20	15	30.97	P				
21	16	32.07	S				
22	17	35.45	Cl	1			
23	18	39.95	Ar				
24	19	39.10	K				
54	49	114.8	In				36.17
55	50	118.7	Sn				3.191
109	1	2.014	H-2			5	
110	1	3.016	H-3				
111	2	3.016	He-3				
112	6	13.003	C-13				
113	6	14.003	C-14				
114	7	15	N-15				
115	8	17.999	O-18				
116	1	1	Custom 1				
117	1	1	Custom 2				
118		Totals Atoms		2	42	39	99.999
119		Z: Mean Atomic Number		14	4	4.897435897	24.1700817
120		M: Average Atomic Weight		29.22	7.579857143	9.673846154	55.01350714

Figure 2. The Custom Material tab in the Excel worksheet. Examples are shown for sodium chloride, PEEK, partially deuterated LDPE, and tin-rich ITO.

and a Linear-Linear plot and changes the spacing of the 200 energy values calculated from linear to logrithmic.

The *Custom Material* tab is used to input custom matieral properites and determine the number-weighted Mean Atomic , $\bar{Z}$, and Average Atomic Weight, $\bar{M}$, for up to 10 custom materials. $\bar{Z}$ and $\bar{M}$ are calculated for a custom material by entering the number of atoms of each element (rows 6 to 108) from the material's chemical formula. For example, in column D of Fig. 2, sodium chloride (NaCl) is entered as a custom material, with the name in cell D1, the chemical formula in cell D2, the mass density in cell D3, the bandgap in cell D4, and 1 in cells D16 and D22 for Na and Cl respectively. Cells D119 and D120 list the calculated values of 14 for $\bar{Z}$ and 29.22 for $\bar{M}$. Calculations and plots for custom material can then be selected from one of the three drop-down boxes in the *Graphs and Data* tab. Note, the custom materials are found at the bottom of the list and not in alphabetical order. Values for the relative number of atoms for a material can also be entered as percentages; see an example for tin-rich indium-tin oxide (ITO) in column G of Fig. 2. Specific isotopes of elements (rows 109-115 for deuterium (D), tritium (T), He^3, C^{13}, C^{14}, N^{15}, O^{18} and rows 116 to 117 for two isotopes) with user-defined atomic numbers and atomic weights can also be selected for custom materials; see an example for partially deuterated polyimide $[C_{22}H_5D_5N_2O_5)_n]$ in column E of Fig. 2.

The *Material Data* tab includes a table which lists all of the 246 materials for which N_V^{eff} has been determined from fits to the NIST databases, along with the requried material properties and parameters for the model. At the bottom of the material list is a set of 10 rows for custom materials carried over from the *Custom Material* tab along with their material properties, fitting constants, and model parameters. Columns H through R shows calculated values for intermediate model values based on formulas listed in Appendix I.

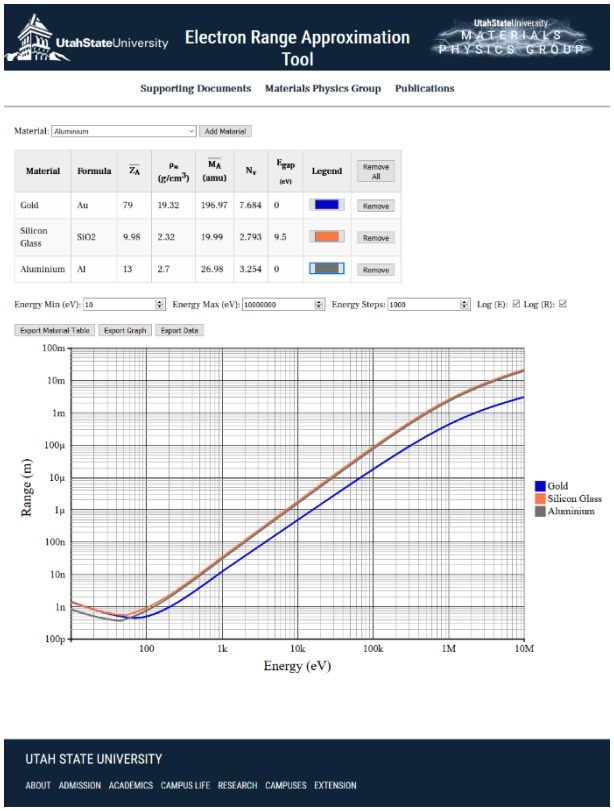

Figure 3. The *HTML/JavaScript* webpage. At the top of the page is the *Material* drop-down box. Just to the right of the drop-down box is the *Add Materia*l button. Just below those is the *Material Table*. Below those are the *Energy Input Boxe*s and below these are the *Data Export* buttons. The *Graph*, rendered by an HTML Canvas using D3.js, takes up the rest of the webpage.

The *Range Calculation* tab calculates the range for all materials listed in the *Material Data* tab (246 NIST materials and 10 custom materials) for the energies specfied in column B using the parameters found in the *Material Data* tab. The energies specified in column B are determined by the E_{min} and E_{max} values and the Log Energy checkbox found on the *Graphs and Data* tab.

The *IMFP Calculation* tab lists the calcualted IMFP data values from the TPP-2M equation, as described in [3,7], for all materials listed in the *Material Data* tab. The energies used in the calculation are pulled from the *Range Calculation* tab.

III. HTML/JAVASCRIPT WEBPAGE

The *HTML/JavaScript* webpage is an online tool which calculates the electron range for 246 NIST materials as well as any number of custom materials. The webpage consists of two different pages, the *Supporting Documents* and the *Electron Range Approximation Tool* page.

The *Supporting Documents* page is nearly identical to the *Information Page* of the *Excel* worksheet. It lists the current version of the Range Tool and the date it was updated, as well as the current supporting documents and references.

The *Electron Range Approximation Tool* page consists of several different parts that allows users to select the data to output and several input boxes for user control.

Material	Formula	$\overline{Z_A}$	ρ_M (g/cm^3)	$\overline{M_A}$ (amu)	N_v	E_{gap} (eV)	Legend	Remove All
Gold	Au	79	19.32	196.97	7.684	0		Remove
Silicon Glass	SiO2	9.98	2.32	19.99	2.793	9.5		Remove
Aluminium	Al	13	2.7	26.98	3.254	0		Remove

Figure 4. The *Material Table* which includes the material name, formula, atomic number, density, atomic mass, effective number of valence electrons and band gap. The table also includes the *Legend*, which allows you to change the line color in the graph and a column with buttons to remove the material from the table and graph.

To begin using the tool, a user selects the desired material by clicking the *Material* drop-down box as shown in Fig. 3. Next, click the *Add Material* button to the right of the drop-down box to add the material to the *Material Table* and the graph. To add multiple materials, simply select another material from the drop-down box and click the *Add Material* button again. This can be done for any number of materials.

The *Material Table* (see Fig. 4) shows the currently graphed materials, along with their key material parameters. The *Legend* column of the *Material Table* allows users to customize the color of the trace of a specific material. The *Remove Material* buttons allows users to either remove a specific material by clicking the corresponding *Remove* button or remove all materials by clicking the *Remove All* button in the header row.

After one or more materials are added to the table and graph, the desired energy range can be customized by changing the *Energy Min (eV)*, *Energy Max (eV)*, and *Energy Steps* buttons. You can also select whether the energy steps are linearly or logarithmically spaced by checking or unchecking the *Log (E)* checkbox. The range of energies that are applicable for this model is ~10 eV to ~10^7 eV. If you select energies outside of this range, the input box will be outlined and red and a warning will popup. The number of energy steps can also be configured, but should generally be less than 10^5 points or the webpage may become unstable. The vertical range axis of the graph can also be changed between linear and logarithmic by unchecking or checking the *Log (R)* checkbox.

After selecting the desired materials to graph, the data can be output in several formats using the three export buttons located directly above the graph. The *Material Table Export* method exports the *Material Table* as a tab-delimited text file. The *Export Graph* method exports the graph as a .png image file. The *Export Data* method exports the range data as a tab-delimited text file that can be imported into *Microsoft Excel* or other analysis or graphing programs compatible with tab-delimited text files.

To input a custom material with the *HTML/JavaScript* online tool, first select *Custom* in the *Material* drop-down box found at the top of the material list. A set of input boxes will appear (see Fig. 5) in input the required material properties. The *Material Name* and *Formula* are entered as text, whereas the other inputs are numeric.

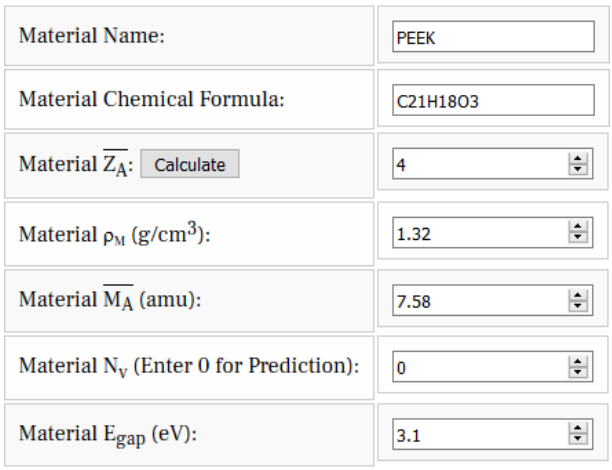

Figure 5. The custom material input boxes. $\bar{Z}_A$ and $\bar{M}_A$ can be calculated by clicking the *Calculate* button which opens a popup window where the chemical formula can be entered, as shown in Fig. 6.

Material $\bar{Z}_A$ and *Material* $\bar{M}_A$ can both be automatically calculated by clicking the *Calculate* button to the right of *Material* $\bar{Z}_A$. This opens a popup window, as shown in Fig. 6. To use this calculator, click on the cell in the periodic table corresponding to an element or isotope listed in the chemical formula and enter the number (or fraction) of atoms for the given element; repeat this for all the elements/isotopes in the material formula. To remove an element from the calculation, simply click on the element and enter 0. When all elements/isotopes are entered, click on the *Ok* button at the bottom right of the popup. Scroll down or maximize the popup window if you cannot see the *Ok* button or some elements are not visible in the popup window. Alternately, you can click the gray area outside the popup to close the calculator and enter the values manually.

To have the *HTML/JavaScript* online tool automatically calculate N_V^{pre} using the predicted method (see Appendix I and Ref. 5), enter 0 in the input box for N_v.

Once all the custom material properties have been entered, click on the *Add Material* button to insert it into the list for analysis and graphing. You can repeat the procedure to add additional custom materials.

IV. Example Application

With newer materials being developed for spacecraft and other applications involving electron fluxes, it is useful to have quick predictive range models. An example of a material with myriad spacecraft applications for which there is no published range data is polyether ether ketone (PEEK). Values of chemical formula, density, and band gap for PEEK [8,9] are listed in Fig. 7 and calculations of $\bar{Z}$ and $\bar{M}$ are listed in Fig. 2, along with data for similar polymers polyimide and PMMA for comparison. As shown in Fig. 8, the electron range for PEEK is predicted to be slightly greater than polyimide and slightly less than PMMA. Similar data and calculations in Figs. 2 and 7 contrast normal polyimide with polyimide with 50% deuterium. Fig. 8 shows the electron range for deuterated polyimide is predicted to be slightly greater than normal polyimide.

An important example of range calculations for non-stochometric materials is indium-tin-oxide (ITO), a heavily doped n-type semiconductor which finds important uses as an optically transparent, electrically conducting ternary oxide alloy glass or ceramic. The optical band gap is largest at 4.20 eV for 5% SnO_2 by weight and reduces to 4.09 eV in the tin-rich (15% SnO_2 by weight) alloy [9]. Data and calculations are listed in Figs. 2 and 7. Fig. 8 shows the electron range for tin-rich ITO is predicted to be slightly greater than normal polyimide at low energies and then becomes slightly less at high energies.

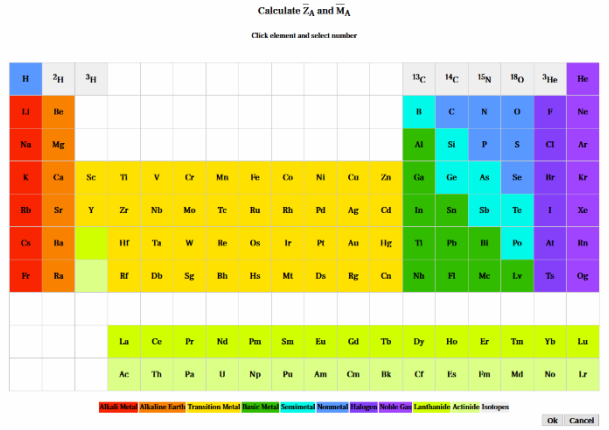

Figure 6. The color coded periodic table for $\bar{Z}_A$ and $\bar{M}_A$ calculation of custom materials. Note additional isotopes in gray cells in the top row of the table.

Material	Formula	$\bar{Z}_A$	ρ_M (g/cm^3)	$\bar{M}_A$ (amu)	N_V	E_{gap} (eV)
PEEK	C21H18O3	4	1.32	7.58	1.089	3.1
PI (Kapton)	C22H10N2O5	5.01	1.42	9.769	1.506	2.32
Deuterated PI	C22H5D5N2O5	5.026	1.42	9.932	1.089	2.32
PMMA (Lucite)	C6H8O2	3.82	1.19	7.149	0.961	3.7
Tin-Rich ITO	(In2O3)0.904(SnO2)0.096	24.17	6.8	55.02	1.089	4.11

Figure 7. Material data for PEEK, normal and partially deuterated polyimide, PMMA, and tin-rich ITO.

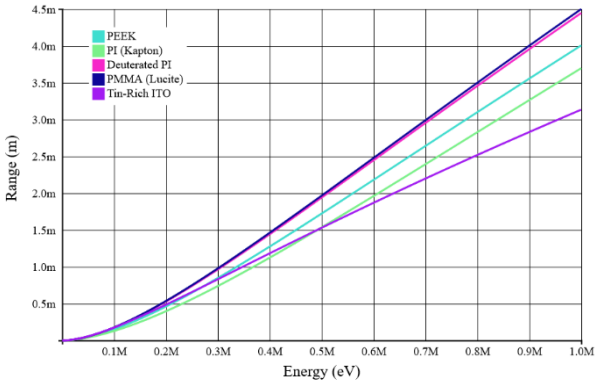

Figure 8. Electron range versus incident energy for PEEK, polyimide, PMMA, and ITO, shown with linear axes.

V. CONCLUSIONS

The approximate calculations of electron range in materials embodied in the computational user tool described here makes this model more readily accessible. While this model does not extend to extreme relativistic energy for high energy physics applications, the broad range of applicable energies is of particular interest to a

wide array of studies involving energetic electron bombardment, such as electron microscopy and spectroscopy, spacecraft charging, radiation modification of materials, accelerator physics, or electron beam therapy. Another important feature is the applicability of the model to a very broad range of materials which lack existing range data.

Further details of the range model, discussions of the origins and meaning of the model parameters, and how to determine appropriate values are given elsewhere[3,5,10]. The results of several sets of computational studies designed to determine (i) the accuracy of the method over its broad energy range of applicability, (ii) the validity of the algorithm to predict N_v^{pre} and the range for arbitrary materials, and (iii) the sensitivity of the predictive method to the estimates of the mean energy loss are also discussed in these references[5,10,11]. Further work is in progress to extend the model to multilayer ranges, electron yield approximations and predictions, and multilayer electron yield.

REFERENCES

1. National Institute of Standards and Technology (2010). "ESTAR, Stopping Power and Range Tables for Electrons," (physics.nist.gov/PhysRefData/Star/Text/ESTAR.html).
2. National Institute of Standards and Technology (2010). "NIST Electron Inelastic-Mean-Free-Path Database: Version 1.1," (www.nist.gov/data/nist71.htm).
3. Wilson, G., and Dennison, J.R. (2010). "Approximation of range in materials as a function of incident electron energy", *IEEE Trans. Plasma Sci.*, **40**(2), 305-310.
4. Quist, T., Moore, B., Wilson, G. and Dennison, J.R., (2013) "Electron Penetration Ranges as a Function of Effective Number of Valence Electrons", Utah State Univ. Student Showcase, Logan, UT.
5. Starley, A., Wilson, G., Phillipps, L. and Dennison, J.R., "Predictive Formula for Electron Penetration Depth of Diverse Materials over Large Energy Ranges," Proc. 14th Spacecraft Charging Tech. Conf., (ESA/ESTEC), (Noordwijk, Netherlands, April 4-8, 2016), 2 pp.
6. Wilson, G., Starley, A., and Dennison, J.R., (2018) http://mpg.physics.usu.edu/range/
7. Tunuma, S, C.J. Powell and D.R. Penn, (1997), "Calculations of Electron Inelastic Mean Free Paths (IMFPs) VI. Analysis of the Gries Inelastic Scattering Model and Predictive IMFP Equation," *Surf. Inter. Anal.* 25, 25.
8. Ho, J., Olguin, M., and Diaz, C. (2014). "Poly(Aryl -Ether -Ether-Ketone) as a Possible Metalized Film Capacitor Dielectric: Accurate Description of the Band Gap Through *Ab Initio* Calculation", Army Research Laboratory, TR-7160.
9. Kim, H., Gilmore, C. M. (1999). "Electrical, optical, and structural properties of indium-tin-oxide thin films for organic light-emitting devices", *J Appl. Phys.*, **86**(11), 6451-6461.
10. Wilson, G. and Dennison, J.R., "Predictive Electron Range Expression for Extended Energy Ranges", to be submitted.
11. Wilson, G. and Dennison, J.R., "Applications and Limitations of a Predictive Range Expression", to be submitted.
12. Inguimbert, C., Pierron, J., Belhaj, M., & Puech, J. (2016, July). Extrapolated range expression for electrons down to~ 10 eV. *IEEE NSREC Conf*, Jul. 2016.

APPENDIX I

The formulas for the electron range model are summarized in this Appendix as:

$$R(E;N_V) = \begin{cases} \left[\frac{E}{E_m}\right]\lambda_{IMFP}(E_m)\left(\frac{1-exp[-1]}{1-exp\left[-\frac{E}{E_m}\right]}\right)^2 & ;E < E_m \\ \left[\frac{E}{E_m}\right]\lambda_{IMFP}(E)\frac{1-exp[-1]}{1-exp\left[-\frac{E}{E_m}\right]} & ;E_m \le E \le E_{LO} \\ bE^n\left(1-\left[1+\left[\frac{\bar{Z}^{0.39}E}{3N_V m_e c^2}\right]\right]^{-2}\right) & ;E > E_{LO} \end{cases}$$

where the intermediate model values are given as

Mean energy loss: $E_m = 2.8\left[(E_p)^2 + (E_{gap})^2\right]^{1/2}$

Effective plasmon energy: $E_p^{eff} = \hbar(N_V {q_e}^2/m_e\varepsilon_0)^{1/2}$

Mean atomic number: $\bar{Z}_A \equiv \sum_i(f_i Z_{A_i})/\sum_i(f_i)$

Mean atomic weight: $\bar{M}_A \equiv \sum_i(f_i M_{A_i})/\sum_i(f_i)$

with atomic fractions f_i which can be determined from the chemical formula for compounds or the chemical fraction for composite materials. The energy-independent power law coefficient and exponent for $E > E_{LO}$ are

$$b \equiv \frac{E_{LO}^{1-n}\lambda_{IMFP}(E_{LO})}{E_m\left\{1-\left[1+\left(\frac{E_{LO}/N_V}{E_m}\right)^2\right]^{-1}\right\}}\frac{1-exp[-1]}{1-exp\left[-\frac{E_{LO}}{E_m}\right]}$$

$$n \equiv \frac{ln\left[\frac{ln\left\{\sqrt{\frac{e}{2}}\left[\frac{E_{HI}}{N_V E_m}+k\right]\right\}}{ln\left\{\sqrt{\frac{e}{2}}\left[\frac{E_{LO}}{N_V E_m}+k\right]\right\}}\right]}{ln[E_{LO}/E_{HI}]}+1$$

with the transition energy constants $E_{LO} \equiv 1000\ eV$ and $E_{HI} \equiv 20000\ eV$ and $k = 0.8$. Physical constants are the electron charge q_e, electron rest mass m_e, speed of light c, permittivity of vacuum ε_0, reduced Planck constant $\hbar$, and Euler's number e. The inelastic mean free path, λ_{IMFP}, is given by the TPP-2M equation[8] as

$$\lambda_{IMFP}(E) = EE_p^{-2}\left[\beta\ ln(\gamma\ E) - CE^{-1} + DE^{-2}\right]^{-1}$$

using the energy-independent TTP-2M expressions for

$$\beta \equiv -0.1 + 0.34\ E_m^{-1} + 0.069\ \rho_m^{0.1}$$

$$\gamma \equiv 0.191\ \rho_m^{-1/2}$$

$$C \equiv 1.97 - 0.91\ U$$

$$D \equiv 53.4 - 20.8\ U$$

$$U \equiv {N_v\rho_m}/{\bar{M}_A}$$

with energies U, $E_{m,}$, E_p, and E_{gap} in eV and mass density ρ_m in g-cm^{-3}

The only fitting parameter for this model is N_v which has been found empirically as N_v^{eff} for many materials through fits to the NIST range database[1] or can be predicted using the formula

$$N_v^{pre} = 5.908(\bar{Z}^{0.222} - 1.162) - 0.111(\rho_m - 0.144\bar{Z})$$

where ρ_m is in g-cm^{-3}. The only required material properties for the model beyond its elemental composition are mass density, ρ_m, and band gap (or similar) energy E_{gap}. If there are no bandgap energy data available, reasonable range results can usually still be obtained if E_{gap} can be approximated to within a few eV and still get. The HUMO/LUMO energy difference can also be used in place of E_{gap} where applicable.