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ELECTRON RANGE COMPUTATIONAL TOOL FOR ARBITRARY MATERIALS OVER A WIDE ENERGY RANGE

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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.

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 rest, depositing their charge. At very low energies where only single inelastic collisions are likely to occur, this becomes synonymous to the ***inelastic mean free*** path (IFMP). The range and the electron IMFP are two common ways to parameterize electron interactions with materials

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.

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).[1]

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 along with its ability to estimate the electron range for most arbitrary materials with no free parameter—based solely on the material parameters. This model is given as:

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

II. Microsoft Excel Tool

The **Microsoft Excel Worksheet** is a multipage worksheet which calculates the IMFP and electron range for 246 materials as well as 10 user input custom materials. The data are presented in both tabular and graphical format as shown in Figs. 1 and 2.

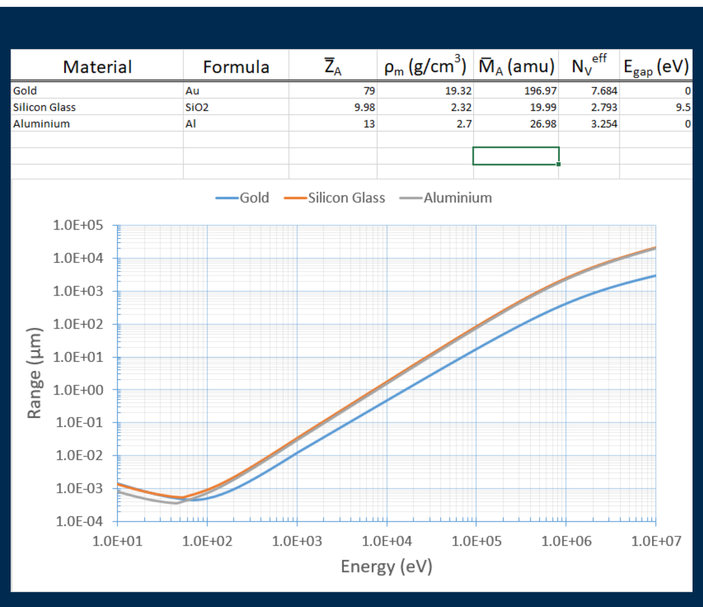

Fig. 1. The material table and graph for the *Excel* sheet. The table includes the used material properties along with the fitting parameter N_v. Gold, Silicon Glass and Alumina are shown as example materials.

The worksheet is organized into several tabs including the *Information, Graphs and Data, Custom Material, Material Data, Range Calculation* and *IMFP Calculation* tabs. The *Graphs and Data* tab is the primary tab for user interaction. Custom materials can be input into the sheet using the *Custom Material* tab, which can then be accessed from the *Graphs and Data* tab.

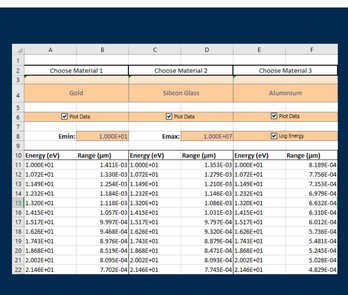

Fig. 2. The material select and tabular data for the Excel Worksheet.

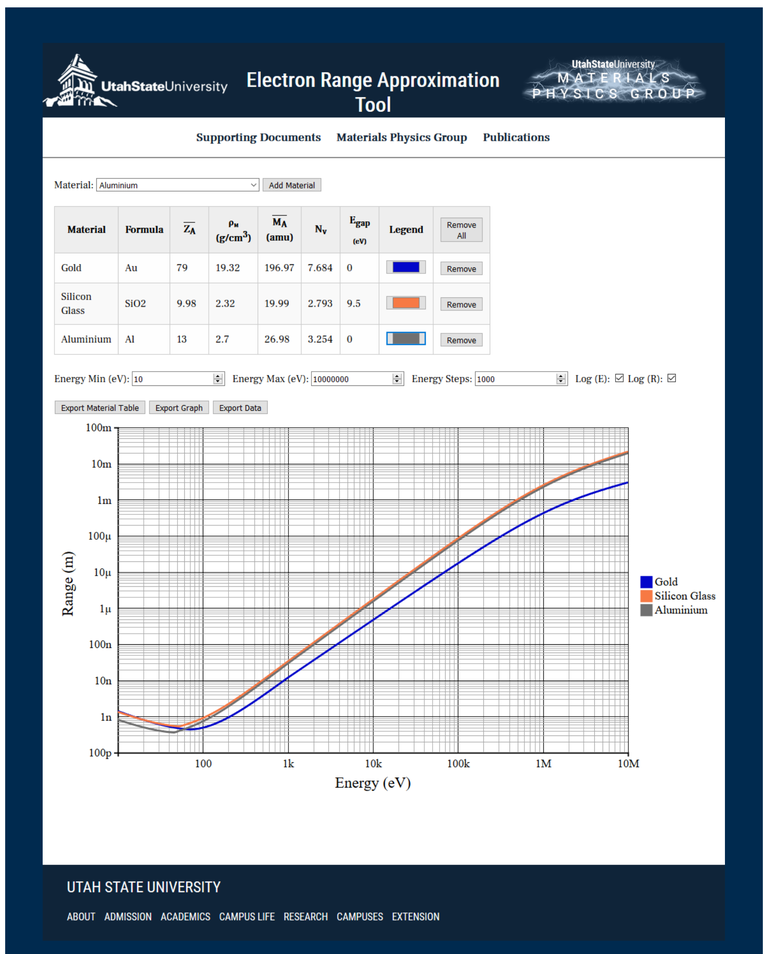

Fig. 3. *HTMl/JavaScript Range Tool*. Au, SiO_2 and Al are shown as example materials. The page consists of the *Material* drop down box to select the material, *the Material Table*, the *Energy Range Input* boxes, the *Export* buttons and the *Graph*.

III. HTML/JavaScript Tool

The **HTML/JavaScript webpage**[4] is an online tool which calculates the electron range for 246 materials as well as any number of custom materials. The webpage consists of two different pages, the *Electron Range Approximation Tool* page and the *Supporting Documents* page. The webpage provides the ability to add or remove any number of materials, plotting them on the graph and listing them in a table with the material properties and fitting parameter, N_v^{eff} (see Figs. 3 and 4).

Material	Formula	$\bar{Z}_A$	ρ_M (g/cm^3)	$\bar{M}_A$ (amu)	N_V	E_{gap} (eV)
PEEK	C21H18)3	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	1.513	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	4.748	4.11

Fig. 4. *The Material Table* shows a list of the currently graphed materials along with the relevant material properties The *Legend* column of the *Material Table* allows users to customize the color of the trace of a specific material as shown in Fig. 3.

For custom materials, $\bar{Z}_A$ and $\bar{M}_A$ can be calculated by clicking the *Calculate* button. This brings up a periodic table, where the number atoms of each element in the chemical formula can be entered . The other required parameters are ρ_M and E_{gap}. N_v can be predicted automatically by entering 0 into the *Input Box*.

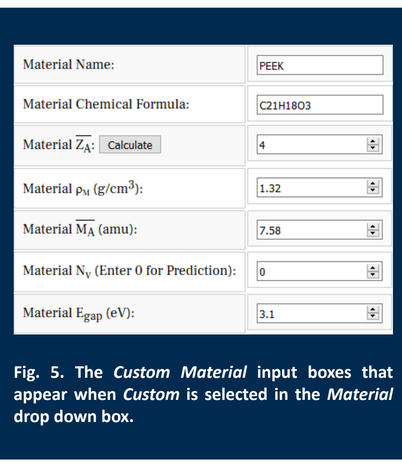

Fig. 5. The *Custom Material* input boxes that appear when *Custom* is selected in the *Material* drop down box.

After graphing selected materials, data can be ***exported*** in several formats:

- *Material Table Export* exports a tab-delimited text file, *Material Table*
- *Graph* exports as a .png image file.
- The range data in a tab-delimited text file can be imported into *Microsoft Excel* or any other program that can handle tab delimited text files such as *IGOR, MatLab* or *MathCad*.

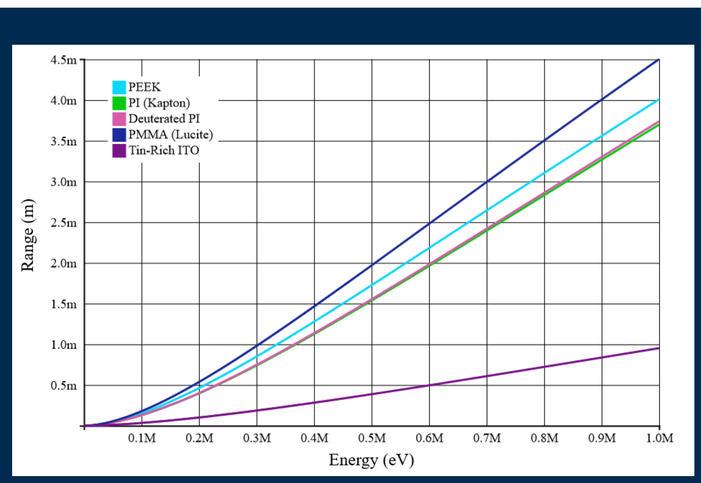

Fig. 6. Plots of the electron range for the materials in Fig. 4 using the online tool.

IV. Range Calculations

The formulas for the electron range model are summarized 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, 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

$$b \equiv \frac{E_{LO}^{1-n}\lambda_{IMFP}(E_{LO})}{E_m\left\{1-\left[1+\left(\frac{E_{LO}}{\frac{N_V}{E_m}}\right)^2\right]^{-1}\right\}} \qquad n \equiv \frac{ln\left[\frac{ln\left\{\left(\frac{e}{\sqrt{2}}\left[\frac{E_{HI}}{N_V E_m}+k\right]\right\}\right\}}{ln\left\{\left(\frac{e}{\sqrt{2}}\left[\frac{E_{LO}}{N_V E_m}+k\right]\right\}\right\}}\right]}{ln[E_{LO}/E_{HI}]}+1$$

with the transition energy constants $E_{LO} \equiv 1\ keV$ and $E_{HI} \equiv 20\ keV$ 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 ħ, 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 expressionswith energies *U*, $E_{m,}$ E_p, and E_{gap} in eV and mass density ρ_m in g-cm^{-3} for

$$\beta \equiv -0.1 + 0.34\,E_m^{-1} + 0.069\,\rho_m^{0.1} \qquad \gamma \equiv 0.191\,\rho_m^{-1/2}$$

$$C \equiv 1.97 - 0.91\,U \qquad D \equiv 53.4 - 20.8\,U \qquad U \equiv {}^{N_v\rho_m}/_{\bar{M}_A}$$

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

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

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 an eV.

VI. Future Work

- We propose to develop a better relativistic approximation for Eq. (1) to improve range predictions well above m_ec^2=0.5 MeV.
- The connection of the electron range with secondary yield is being studied in an attempt to extend the versatility of this model to a predictive secondary electron yield model.
- A detailed paper is being prepared which will detail all of the work and updates that have been done on the model including the predictive formula for N_v^{pre}.
- A second paper is being prepared which details applications and limitations, which will include examples of novel materials.

VII. References

1. Wilson, G., & Dennison, J.R. (2010). Approximation of range in materials as a function of incident electron energy, *IEEE Trans. on Plasma Sci.*, **40**(2), 305-310.
2. T. Quist, B. Moore, G. Wilson and JR Dennison, Electron Penetration Ranges as a Function of Effective Number of Valence Electrons, Utah State University Student Showcase, Logan, UT, April 2013.
3. Anne Starley, Gregory Wilson, Lisa Phillipps and JR Dennison, "Predictive Formula for Electron Penetration Depth of Diverse Materials over Large Energy Ranges," Proceedings of the 14th Spacecraft Charging Technology Conference, Space Research and Technology Centre of the European Space Agency (ESA/ESTEC), (Noordwijk, Netherlands, April 4-8, 2016), 2 pp.
4. Wilson, G., Starley, A., and Dennison, J.R., (2018) http://mpg.physics.usu.edu/range/

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Scan code to access the (right) USU Material Physics Group papers and presentations (left) The HTML/JavaScript Electron Range Tool.