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Compilation and Comparison of Electron Penetration Ranges as a Function of Effective Number of Valence Electrons

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Abstract

The continuous-slow-down approximation (CSDA) is used to create a simple composite analytical formula to estimate the range or maximum penetration depth of bombarding electrons into traditional materials including conductors, semiconductors, and insulators. This formula generates an approximation to the range using a single fitting parameter, N_v, described as the effective number of valence electrons. This applicability of the formulation extends to electrons with energies from <10 eV to >10MeV. These calculations are of great value for studies of high electron bombardment, such as electron spectroscopy or the vacuum of space. A list comprised of 187 materials has been collected that greatly extends the applicability of this model. Several key material constants were compiled for each material, including the atomic number, atomic weight, density, and band gap. To determine the single fitting parameter, N_v, the model was then fit to existing data from the ESTAR and IMFP databases (2, 3) compiled by NIST. Comparison of N_v with the materials constants from this large database of materials was made, which could possibly lead to the prediction of N_v for materials which have no supporting data.

Introduction

High energy electrons exist in large abundance in extraterrestrial space, and can wreak havoc on satellite and other technological materials that are placed in their paths. Damage to electronics and weakening of physical materials are results of electron embedment. Figure 1 is a visual representation of electron penetration given specific incident energies; the side view clearly shows that the electrons penetrated a fixed distance into the material. The plastic material used in this experiment was has melted in the areas of discoloration and damaged physically due to an electrical discharge across the embedded electrons. It is therefore logical to assume that there is a clear danger to materials from this phenomenon. It is therefore in our best interests to protect entities or systems from the damages associated with abundant electron radiation. Determining the depth that an energetic electron penetrates into any given surface has traditionally been found using experimental data. This source of data acquisition has limits in the amount of samples that can be processed in a given time and the sheer number of materials that exist for testing. It seems logical that a formulation to determine the range of depths would be preferable to further experimentation. Previous work has been done by Wilson and Dennison to determine a formulation that performs this

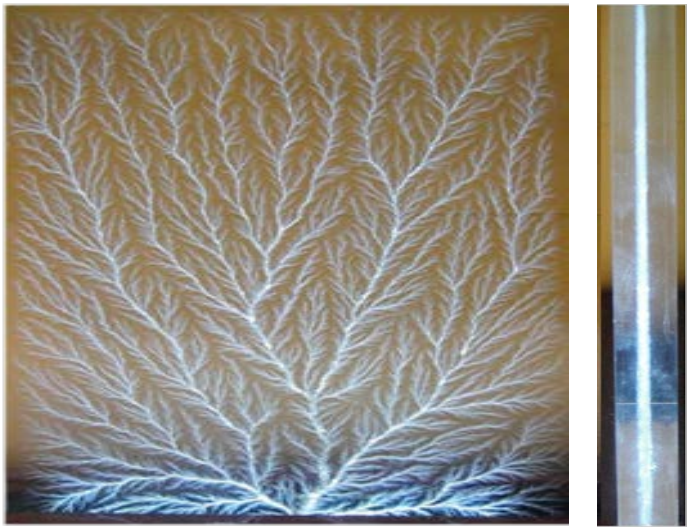


Fig. 1. Front (Left) and side (Right) views of a Lichtenberg discharge tree. The white line (Right) indicates the narrow distribution of deposited charge from a ~1 MeV electron beam at R≈3 mm in a PMMA

task (4, 5). They were successful in their pursuits and they found that the depth of electron embedment in a given material is associated with a single parameter N_v, the number of valence electrons associated with molecules of the material. The goal of this research was to extend the scope of their research to further encapsulate a wide variety of materials, then to compare these materials to one another in a hope to further improve the accuracy of the formulation. It took longer to compile the material than was originally expected, and comparisons were few but useful.

Methods

The number of valence electrons, N_v, for a given material is determined by fitting a simple composite analytic expression, developed to approximate the electron range as tabulated in two standard National Institute of Standards and Technology (NIST) databases. The ESTAR database was used for the high energy (10 keV to 10 MeV) range and the IMFP database was used for the low energy (10 eV to 2 keV) range. Figures 2 shows an example of a finalized fitting process for a specific material, for more detail on fitting procedures and range formulation consult Wilson's text.

To compute the appropriate values of N_v large amounts of data were needed about the specific materials we wished to compare. Included in the required data for each material were its density, atomic weight, atomic number, mean excitation energy, chemical formulation of compounds or elemental stoichiometric ratios of composites, and the atomic weight and number for all constituent elements of the material. Along with these general characteristics the experimental range data acquired from the two NIST databases also had to be compiled and made easily accessible for comparison. Different methods were implemented to acquire these different values, the methods are listed below, and all values were compiled into a Master CSDA Range List for simplicity

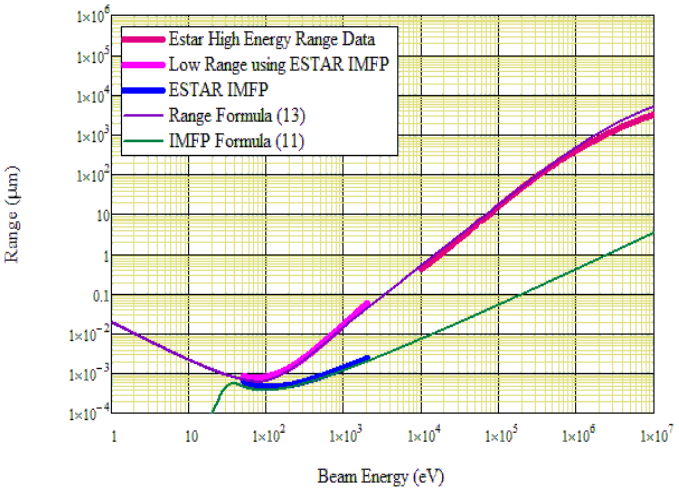


Fig. 2. Comparison of the range formula results to NIST database values for Au

IMFP data was obtained from NIST's downloadable IMFP computer program; this program is limited in its number of constituent materials with experimental data. It contains low energy range data on the majority of the elements that are solid at room temperature, and roughly 50 other commonly found materials. In the program one must select the material in question, the units desired, and a range of energies to compare across. For simplicity the same range of energies were used in compiling IMFP data in order to ease computer aided computation. The IMFP program has the capability to compute IMFP data for materials not already found in its database, further inquiry into this capability could allow for more low energy comparisons to be performed on many previously uncataloged materials.

CSDA range approximation data, for highly energetic electrons, was taken from NIST's online ESTAR database. This data takes into account the relativistic affects of electrons moving with great velocity. The ESTAR database is comprised of 98 of the periodic elements, and several other hundred commonly found materials; including conductors, insulators, semi-conductors, and biological materials. One need only select the desired material, and export the CSDA data to the Master CSDA Range List. Fortuitously, the values for the density, mean excitation energy, and fraction by weight of the constituent elements are also listed for each material. Using atomic weights and atomic numbers found easily in almost any chemistry text one can calculate the atomic weight or number of a compound element by simple summation. This data one can also be extrapolated to find the stoichiometric formula for any compound and its associated fraction by formula of the component elements. Also the majority of these chemical formulas and associated fractions have been conveniently compiled by the Department of Homeland Security. (6)

With all material characteristics compounded in the Master CSDA Range List, these values could be cycled through the MathCad program Wilson 2012 Range Calculator. When the program is ran with appropriate data the result is similar to that shown in Figure 2.

In the Master CSDA Range List additional calculations were made, including calculating the effective nuclear charge and the effective mass number of the materials in the list. The effective nuclear charge is defined as

$Z_{eff} = \sum_i f_i Z_i$.

The effective mass number as

$A_{eff} = \frac{Z_{eff}}{\sum_i f_i \frac{Z_i}{A_i}}$ (7).

f_i is the fraction by weight of the constituent elements given as

$f_i = \frac{n_i A_i^{'}}{M}$,

where n_i is the number of atoms, $A_i^{'}$ is the atomic weight, and M

$M = \sum_j n_j A_j^{'}$,

is the molecular weight of the compound (8).

Tables 1 gives an example of the data associated with a specific material from Master CSDA Range List.

Results

Upon completion of this work a total of 222 materials had been cataloged and plotted. The wide variety of materials illuminates the range formulations applicability across all currently tested material types including conductors, insulators, polymers, metals, and other material types. To

generalize the results of the study for use with materials not included in the NIST databases, a formula to estimate N_v, in terms of common materials parameters is desirable. Comparisons of N_v determined for database materials to several intrinsic properties: density, mean excitation energy, effective atomic weight, and effective atomic number, suggests the following relation: $N_v \propto \rho^{2/3}_m E_m Z_{eff} A^{1/2}_{eff}$. This relation was determined, by graphical comparison (Figure 4) between N_v and the four parameters

ρ_m – Density

E_m – Mean excitation Energy

Z_{eff} – Effective nuclear charge

A_{eff} - Effective mass number

Many properties in a given function do not associate with one another by simple linear relations, thus a power law fit was necessary to determine the relation between a single parameter and N_v.

Given a function of the form

$$y = Ax^B$$

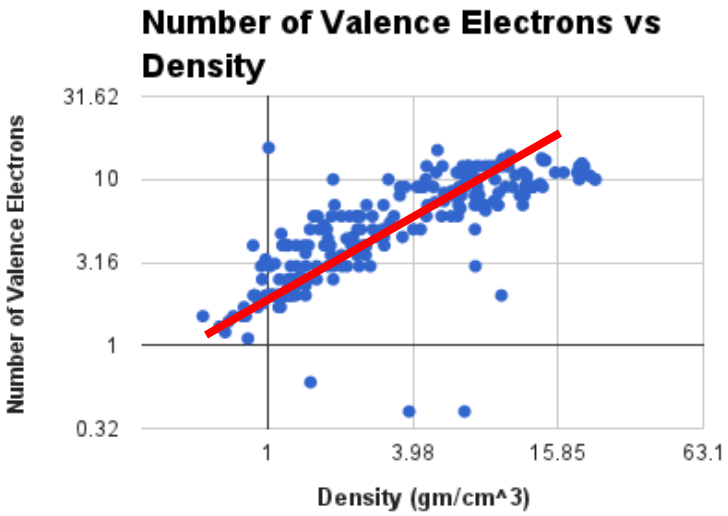
least squares fitting gives the coefficients as

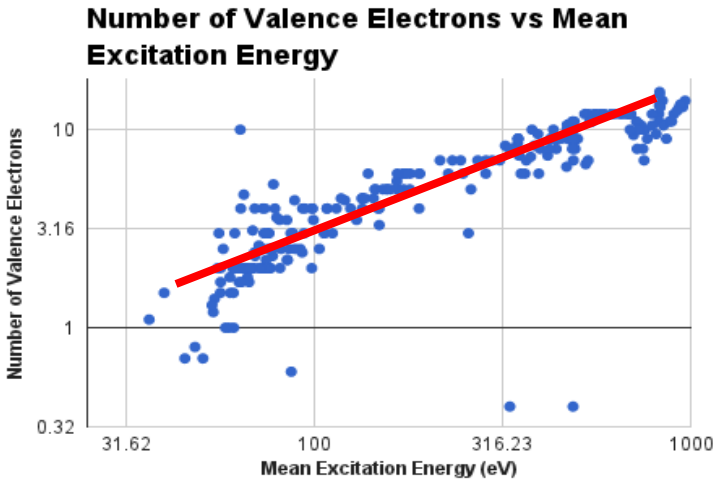
$$b = \frac{n\sum_{i=1}^{n}(lnx_i lny_i) - \sum_{i=1}^{n}(lnx_i)\sum_{i=1}^{n}(lny_i)}{n\sum_{i=1}^{n}(lnx_i)^2 - (\sum_{i=1}^{n} lnx_i)^2}$$

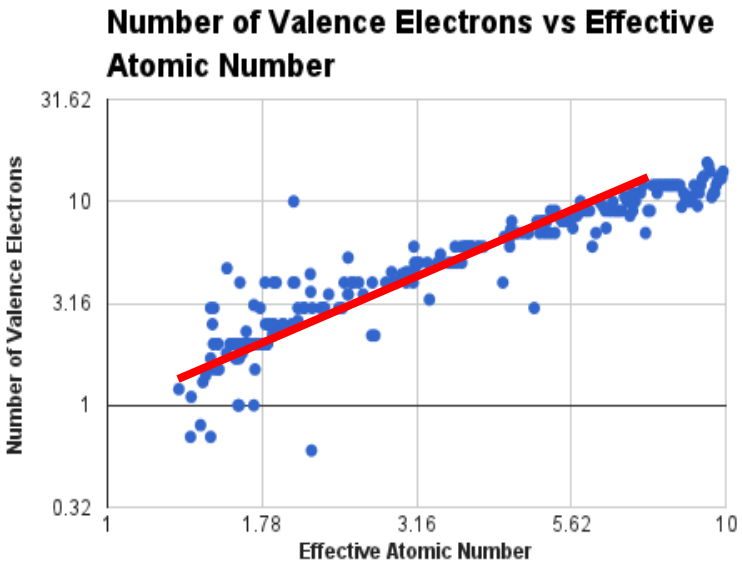
$$a = \frac{\sum_{i=1}^{n}(lny_i) - b\sum_{i=1}^{n}(lnx_i)}{n}$$

where $B = b$ and $A = e^a$ (9).

Using these equations the log-log plots and polynomial fits were calculated using excel, further examination will need to be done to evaluate if the intrinsic relations hold to all materials. There are a few statistical outliers that don't quite fit the trend, review needs to be done to determine if this is the result of clerical errors in data collection or if caused by some other as of yet unknown interaction.







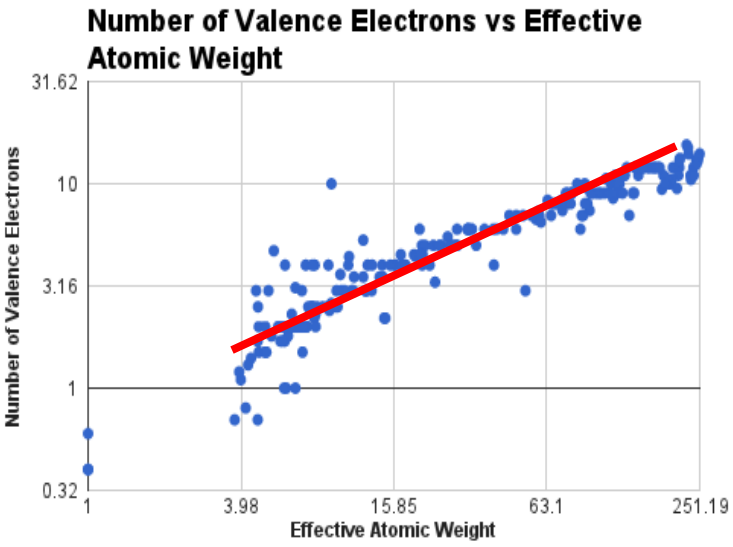


Fig.4. N_v Compared graphically with the four different intrinsic properties in a log-log plot. The red line is the trend line used to determine the between N_v and the intrinsic properties.

Future Work

- Develop a user friendly application to calculate the range verses incident energy for all materials in the database and for other arbitrary materials.
- Develop a general formula to predict values for N_v and the range for arbitrary materials, based on readily available materials properties.
- Obtain IMFP range data for materials not already cataloged.

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Appendix

Material	Aluminum Oxide
Formula	Al2O3
Density (gm/cm^3)	3.97
Mean Excitation Energy (eV)	145.20
Atomic Number	8.00
Atomic Weight	16.00
Fraction by formula	0.60
Fraction by weight	0.47
Atomic Number	13.00
Atomic Weight	26.98
Fraction by formula	0.40
Fraction by weight	0.53
Mean Atomic Number by formula	10
Mean Atomic Number by weight	10.65
Z* (Effective Nuclear charge)	3.139276785
A* (Effective Mass Number)	20.392
	CSDA Range
Energy (MeV)	Alumina (Aluminum Oxide)
1.00E-02	3.35E-04
1.25E-02	4.93E-04
1.50E-02	6.76E-04
1.75E-02	8.84E-04
2.00E-02	1.12E-03
2.50E-02	1.65E-03
3.00E-02	2.26E-03
.....	.....
5.00E+02	7.19E+01
5.50E+02	7.44E+01
6.00E+02	7.67E+01
7.00E+02	8.08E+01
8.00E+02	8.44E+01
9.00E+02	8.76E+01
1.00E+03	9.04E+01
	IMFP Range
Energy (eV)	Alumina (Aluminum Oxide)
50	1.212
50.7	1.185
51.5	1.158
52.3	1.133
53	1.108
53.8	1.084
54.6	1.061
55.4	1.038
56.3	1.016
57.1	0.995
57.9	0.975
.....	.....
1.78E+03	3.222
1.80E+03	3.26
1.83E+03	3.298
1.86E+03	3.337
1.89E+03	3.377
1.91E+03	3.416
1.94E+03	3.457
1.97E+03	3.498
2.00E+03	3.539