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Studying of electronic Stopping Power of Proton in many compounds

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Abstract

In this study, the stopping power of proton was examined in many polymers that are often found in daily life, including Lexan, Acrylic, Nylon, Kapton, Paraffin wax, Polystyrene, and Toluene in the energy range of (1-100000) KeV. Ziegler equations were utilized for three of the aforementioned energy areas. Using the data from the SRIM 2013 software and the PSTAR data, the stopping power of these compounds was also estimated, and the findings were compared with the data acquired from the derived Ziegler equations. Their compatibility was clearly evident.

1. Introduction:

Stopping power is an important quantity in the field of materials physics and is used extensively in the microelectronics industry. It refers to the ability of a material to stop charged particles, such as ions, as they pass through it. The stopping power of ions inside materials is typically calculated using computer simulations, such as molecular dynamics simulations, and can be affected by factors such as the local electronic environment inside the material and the nonlinear results from density functional theory [1]. In the medical field, stopping power can be used to calculate the range of protons in biological human body parts, which is important for radiation therapy treatment planning[2]

A charged particle moving rapidly through matter loses energy primarily by ionizing and exciting atoms. An important goal of theoretical understanding of these processes is the prediction of the average rate of energy loss of the particle per unit distance traveled as a function of the particle's energy. This fundamental quantity is called the stopping power of the material for that particle. It is often denoted by the symbol (-dE/dx)and expressed in the units MeV/cm. Dividing the stopping power by the density ρ of the material gives the closely related mass stopping power,(- dE/ρdx) which can be expressed in MeV.cm^2/g[3] The stopping power is the most important parameter of the energy loss process of energetic ions that is passing through matter. The energy loss of heavy ions is complicated because of the charge-exchange effect which leads to charge-state fluctuations . The electronic stopping is caused by the interaction of ions with the target bound electrons. The lost energy of the ions penetrating the material can occur due to several processes excitation and ionization of the target atoms, the capture of the electron, ionization or excitation of the projectile [4]

Stopping power is defined as loss of energy per distance in the target material which can be written as (-dE/dx) which is depending on the projectile charge and also on the target matter. The study of stopping power is one of the subjects which takes a large space in the study of physics scientists. These studies were theoretical and experimental by using different methods [5] .

can be calculated by using Bethe equation (quantum mechanics)[5, 6]

$$-\frac{1}{\rho}\frac{\mathrm{dE}}{\mathrm{dx}} = \frac{4\pi Z_1^2 Z_2 e^4 N_A}{m_e c^2 \beta^2 A} L_{\mathrm{Bethe}} \qquad \dots\dots\dots \quad (1)$$

Where $\beta = \frac{v}{c}$

$$-\frac{1}{\rho}\frac{\mathrm{dE}}{\mathrm{dx}} = 0.30707\,\frac{Z_1^2 Z_2}{\beta^2 A} L_{\mathrm{Bethe}} \qquad \dots\dots\dots \quad (2)$$

Where $\frac{4\pi e^4 N_A}{m_e c^2} = 0.30707$

$$L_{\mathrm{Bethe}} = \ln\left[\frac{2m_e c^2 \beta^2}{1-\beta^2}\right] - \beta^2 - \ln I \qquad \dots\dots\dots \quad (3)$$

Where:

m_e: electron rest mass.

v : velocity of the particle.

Z_1: charge of the particle.

Z_2: charge of target

e : electron charge

I: Ionization potential

2. Ziegler Semi empirical Electronic Stopping Power

The sum of the stopping power as a result of interactions with the target electrons $\left(-\frac{1}{\rho}\frac{dE}{dx}\right)_{tot}$ and the nuclear stopping power $\left(-\frac{1}{\rho}\frac{dE}{dx}\right)_{e}$ as a result of the interactions with the target nuclei [7] $\left(-\frac{1}{\rho}\frac{dE}{dx}\right)_{n}$.

$$\left(-\frac{1}{\rho}\frac{dE}{dx}\right)_{tot} = \left(-\frac{1}{\rho}\frac{dE}{dx}\right)_{e} + \left(-\frac{1}{\rho}\frac{dE}{dx}\right)_{n} \quad \dots\dots\dots \quad (4)$$

At high energies, the equation becomes:

$$\left(-\frac{1}{\rho}\frac{dE}{dx}\right)_{tot} \approx \left(-\frac{1}{\rho}\frac{dE}{dx}\right)_{e}$$

Nuclear stopping power is expressed by the following equations[7]:

$$\left(-\frac{1}{\rho}\frac{dE}{dx}\right)_{n} = \frac{8.462\, Z_1 Z_2 A_1 S_n(\varepsilon)}{(A_1+A_2)(Z_1^{0.23}+Z_2^{0.23})}$$ (Nuclear stopping power in units eV(10^{15} atoms/cm^2))

A1, A2 The mass number of the charged particle and the target, respectively

Where ε is Reduced ionic energy

$$\varepsilon = \frac{32.53 A_1 A_2 (\frac{E}{M_1})}{Z_1 Z_2 (A_1 + A_2)(Z_1^{0.23} + Z_2^{0.23})} \quad \dots\dots\dots \quad (5)$$

When the energy is $E \leq 30$keV we use the following equation[8]

$$\left(-\frac{1}{\rho}\frac{dE}{dx}\right)_{n} = \frac{\ln(1 + 1.1383\varepsilon)}{2(\varepsilon + 0.01231\varepsilon^{0.212} + \varepsilon^{0.5})} \quad \dots\dots\dots \quad (6)$$

Ziegler was able to calculate the electronic stopping power at the same units[9]

$$\left(-\frac{1}{\rho}\frac{dE}{dx}\right) = A_1 E^{1/2} \qquad at \quad E(1-10)keV \quad \dots\dots\dots \quad (7)$$

As for energies (10-999) keV, use the following equation

$$\left(\frac{-dE}{\rho dx}\right)^{-1} = \left(\frac{-dE}{\rho dx}\right)_{\text{low}}^{-1} + \left(\frac{-dE}{\rho dx}\right)_{\text{high}}^{-1} \quad \dots\dots\dots \quad (8)$$

$$\left(\frac{-dE}{\rho dx}\right)_{low} = A_2 E^{0.45} \quad \dots\dots\dots \quad (9)$$

$$\left(\frac{-dE}{\rho dx}\right)_{high} = \left(\frac{A_3}{E}\right) \ln\left(1 + \left(\frac{A_4}{E}\right)\right) + (A_5 E) \quad \dots\dots\dots \quad (10)$$

As for energies (999-100000) keV

$$\left(\frac{-dE}{\rho dx}\right) = \left(\frac{A_6}{\beta^2}\left(\frac{\ln(A_7\beta^2)}{1-\beta^2}\right) - \beta^2 - \sum_{i=0}^{4} A_{i+8}\left(\ln E^i\right)\right) \quad \dots\dots\dots \quad (11)$$

Ziegler managed to summarize the experimental data for the stopping power of the proton for many elements and within a wide range of energies, and in order to find the values of the elements, a group of researchers compared the curves with the available experimental data to reach the coefficients[10].

Results And Discussions

The Ziegler equations have been used to theoretically calculate the electronic stopping power of charged protons affecting many polymers-Lexan, acrylic, nylon, Kapton, paraffin wax, polystyrene and and toluene-in the energy range (1-100000) KeV. The information from the 2012 SIRIM program, the PSTAR data, and the results of the Ziegler equations were compared, and the following schemes are also shown in the following figures :

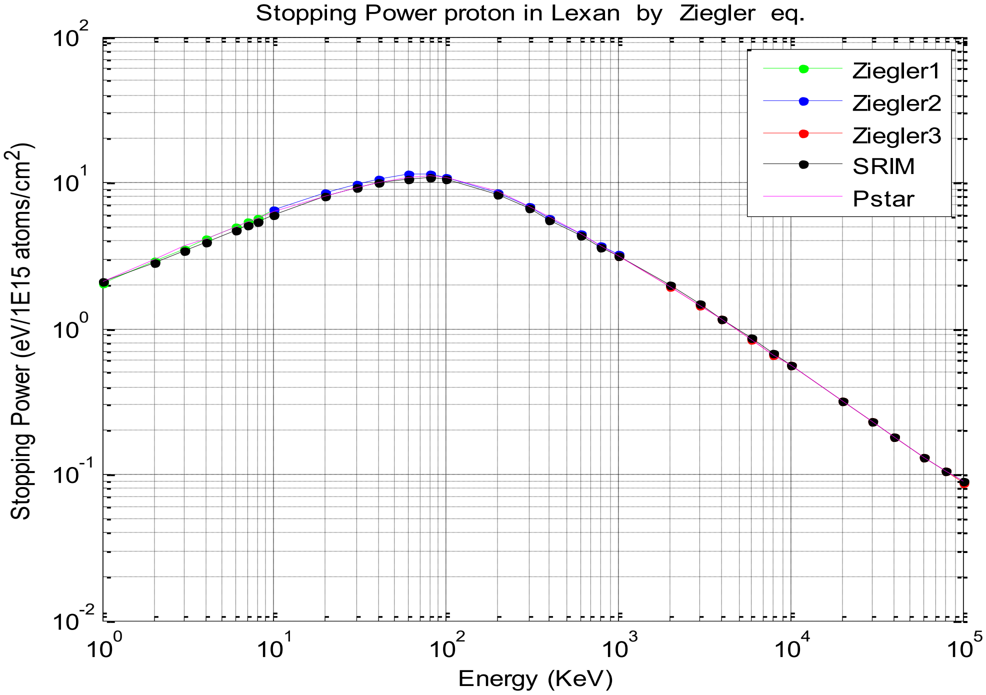

Fig.(1) stopping power for protons in Lexan

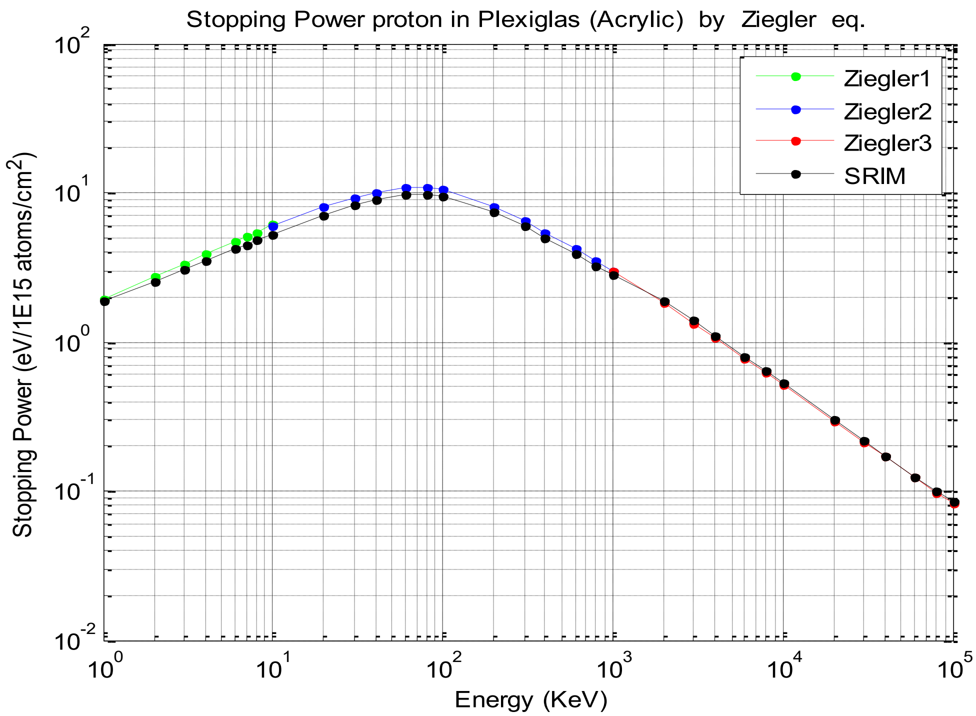

Fig.(2) stopping power for protons in Acrylic

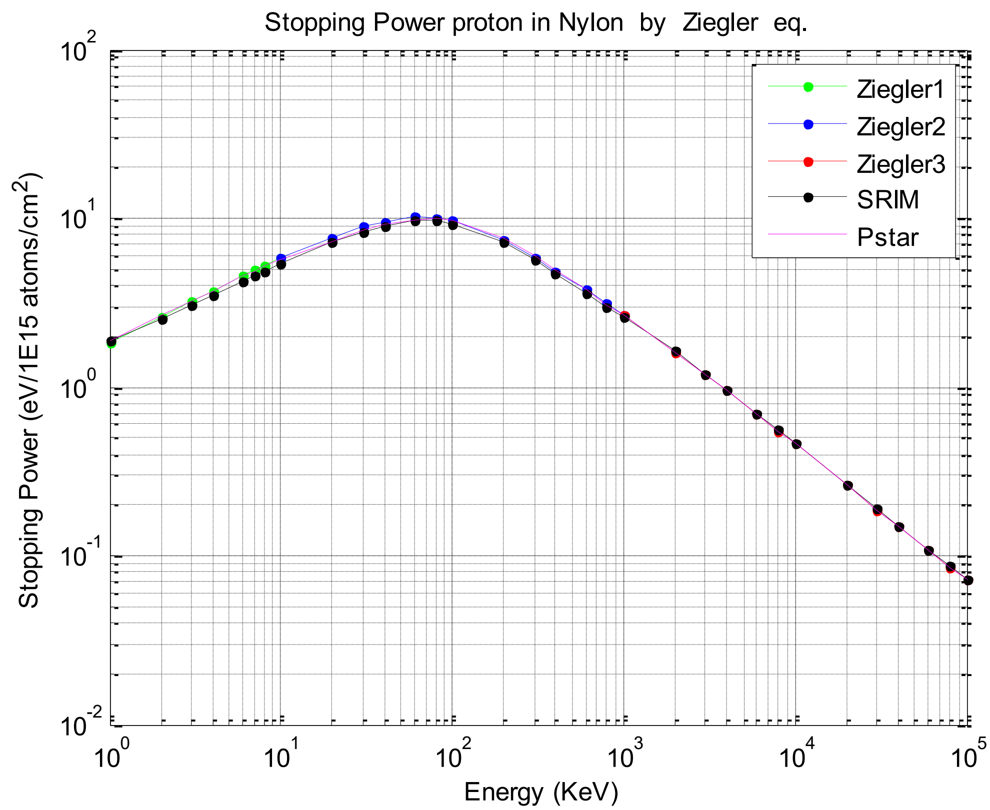

Fig.(3) stopping power for protons in Nylon

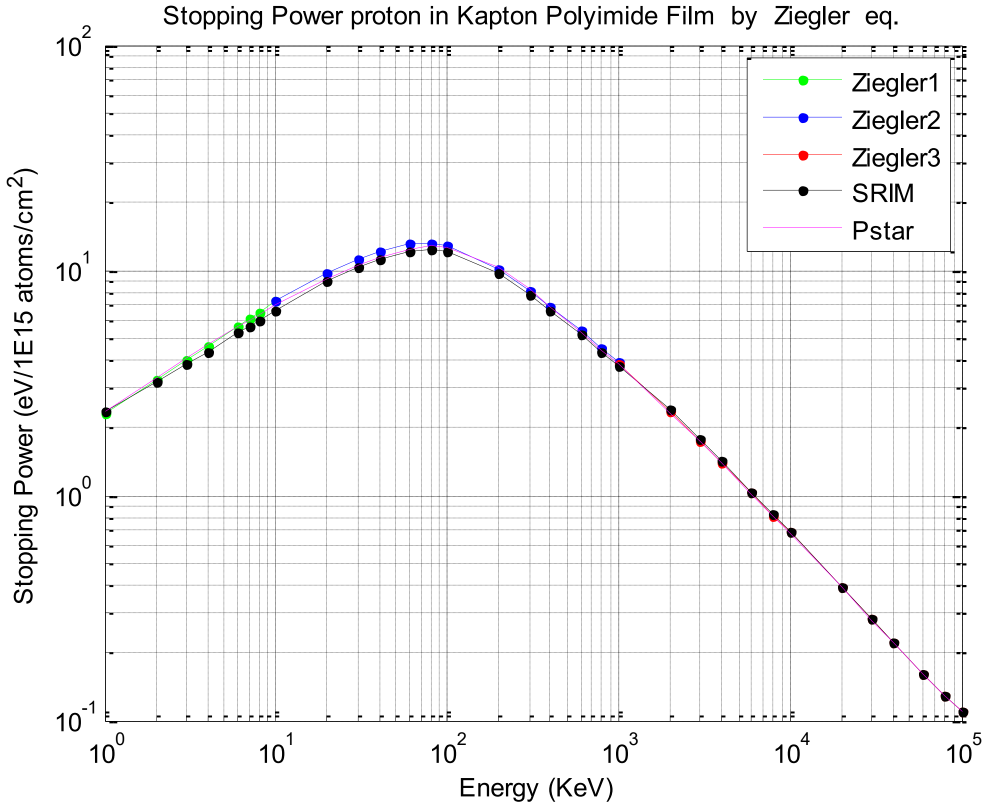

Fig.(4) stopping power for protons in Kapton

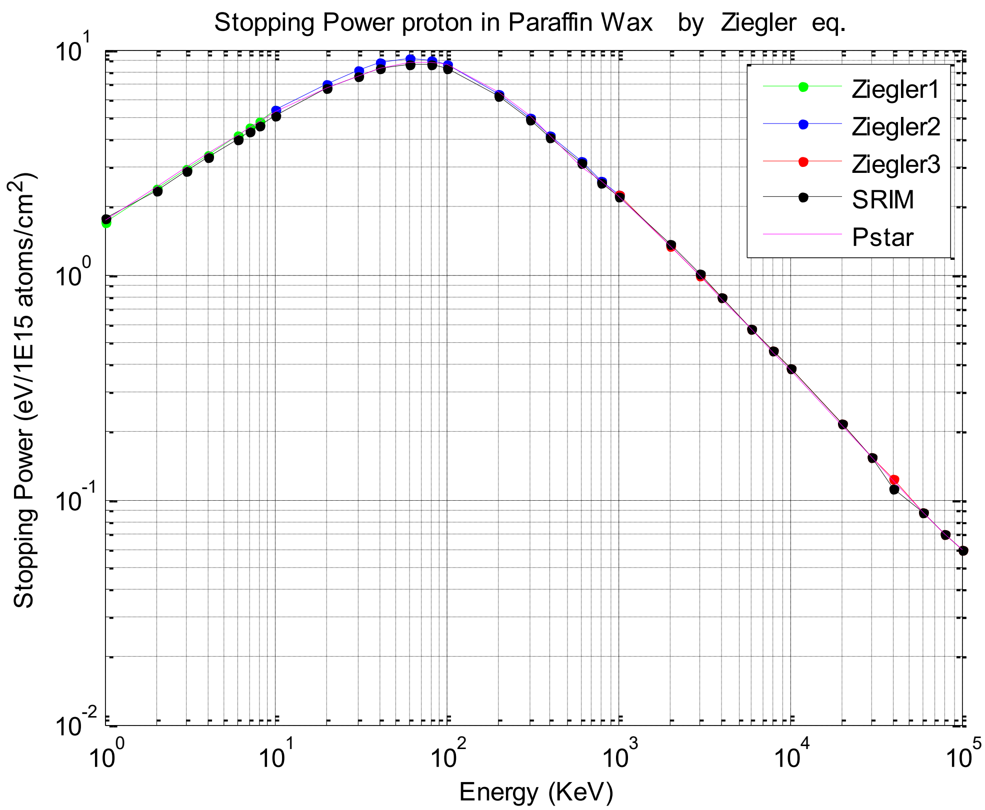

Fig.(5) stopping power for protons in Paraffin wax

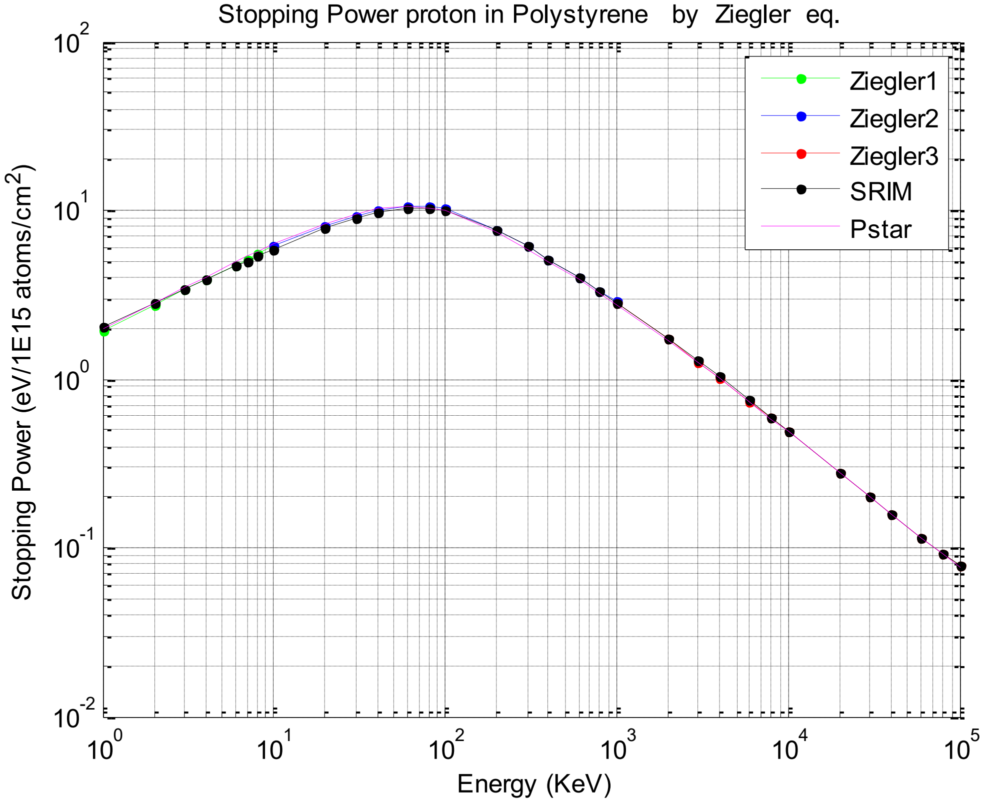

Fig.(6) stopping power for protons in Polystyrene

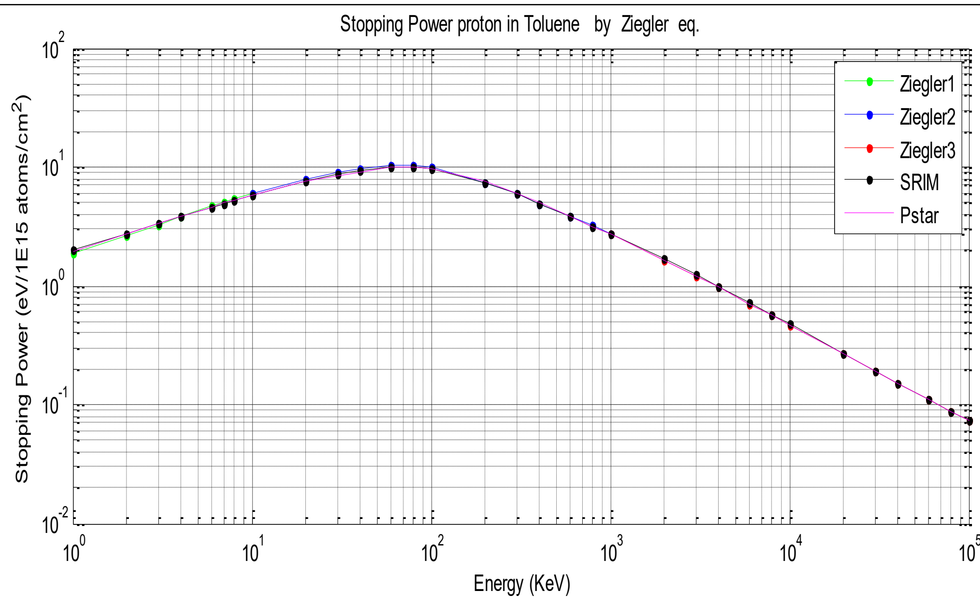

Fig.(7) stopping power for protons in Toluene

We notice from the previous diagrams that the curve extracted using the Ziegler equation fully agrees with the data extracted from the ASHRAM program and the P-STAR data in the three energy regions (1-10,10-1000,1000-100000)KV

Also, the greatest stopping power was at energy (80 KeV) in compounds (Lexan , Acrylic, Kapton, Polystyrene, Toluene)

Also, the greatest stopping power was at energy (70 KeV) in compounds (Nylon, Paraffin wax)

Ziegler's equation of stopping power are divided into three regions :-

1- the first region is the low energy region with energy range of (1-10) KeV and is shown in the following formula:-

S = A1E1/2 ……… (7)

2- the second region of the Ziegler equation for the stopping power with energy range of (10 – 1000) KeV divided into two regions is shown in the following formulas

Low energy equation in the first region as eq. (9)

$$\left(\frac{-dE}{\rho dx}\right)_{low} = A_2 E^{0.45} \quad \dots\dots\dots \quad (9)$$

High energy equation in the second region as eq. (10)

$$\left(\frac{-dE}{\rho dx}\right)_{high} = \left(\frac{A_3}{E}\right) \ln\left(1 + \left(\frac{A_4}{E}\right)\right) + (A_5 E) \quad \dots\dots\dots \quad (10)$$

3- the third region of the Ziegler equation for the stopping power with energy range of (999 – 100000) KeV is shown in eq. (11)

$$\left(\frac{-dE}{\rho dx}\right) = \left(\frac{A_6}{\beta^2}\left(\frac{\ln(A_7\beta^2)}{1-\beta^2}\right) - \beta^2 - \sum_{i=0}^{4} A_{i+8}\left(\ln E^i\right)\right) \quad \dots\dots\dots \quad (11)$$

Where A1,A2,..... A8 is coefficients for stopping of Hydrogen [10].

E (KeV)	Stopping Power (eV/1E15 atoms/cm^2)				
	Lexan			Acrylic	
	Ziegler	SRIM	PSTAR	Ziegler	SRIM
1	2.032E+00	2.090E+00	2.109E+00	1.924E+00	1.865E+00
2	2.873E+00	2.826E+00	2.981E+00	2.720E+00	2.515E+00
3	3.519E+00	3.410E+00	3.652E+00	3.332E+00	3.028E+00
4	4.063E+00	3.899E+00	4.153E+00	3.847E+00	3.459E+00
6	4.976E+00	4.711E+00	5.008E+00	4.712E+00	4.178E+00
7	5.375E+00	5.059E+00	5.374E+00	5.089E+00	4.488E+00
8	5.746E+00	5.380E+00	5.709E+00	5.441E+00	4.775E+00
10	6.424E+00	5.953E+00	6.291E+00	6.083E+00	5.289E+00
20	8.493E+00	7.964E+00	8.140E+00	8.037E+00	7.125E+00
30	9.774E+00	9.159E+00	9.258E+00	9.250E+00	8.246E+00
40	1.058E+01	9.908E+00	1.003E+01	1.002E+01	8.960E+00
60	1.129E+01	1.064E+01	1.091E+01	1.071E+01	9.662E+00
80	1.130E+01	1.076E+01	1.113E+01	1.074E+01	9.774E+00
100	1.096E+01	1.052E+01	1.097E+01	1.044E+01	9.558E+00
200	8.465E+00	8.241E+00	8.729E+00	8.092E+00	7.482E+00
300	6.772E+00	6.595E+00	6.935E+00	6.443E+00	5.972E+00
400	5.710E+00	5.545E+00	5.783E+00	5.407E+00	5.013E+00
600	4.448E+00	4.302E+00	4.453E+00	4.187E+00	3.886E+00
800	3.698E+00	3.584E+00	3.685E+00	3.472E+00	3.245E+00
1000	3.178E+00	3.116E+00	3.160E+00	2.978E+00	2.838E+00
2000	1.936E+00	1.983E+00	1.932E+00	1.812E+00	1.872E+00
3000	1.429E+00	1.462E+00	1.420E+00	1.338E+00	1.382E+00
4000	1.146E+00	1.171E+00	1.149E+00	1.073E+00	1.106E+00
6000	8.351E-01	8.511E-01	8.368E-01	7.816E-01	8.039E-01
8000	6.647E-01	6.764E-01	6.666E-01	6.221E-01	6.388E-01
10000	5.559E-01	5.651E-01	5.575E-01	5.203E-01	5.336E-01
20000	3.172E-01	3.215E-01	3.180E-01	2.969E-01	3.036E-01
30000	2.282E-01	2.311E-01	2.288E-01	2.136E-01	2.182E-01
40000	1.809E-01	1.831E-01	1.813E-01	1.693E-01	1.728E-01
60000	1.310E-01	1.325E-01	1.314E-01	1.226E-01	1.251E-01
80000	1.048E-01	1.060E-01	1.051E-01	9.803E-02	1.000E-01
100000	8.847E-02	8.948E-02	8.880E-02	8.279E-02	8.449E-02

E (KeV)	Stopping Power (eV/1E15 atoms/cm^2)					
	Nylon			Kapton		
	Ziegler	SRIM	PSTAR	Ziegler	SRIM	PSTAR
1	1.856E+00	1.895E+00	1.889E+00	2.299E+00	2.351E+00	2.367E+00
2	2.625E+00	2.555E+00	2.670E+00	3.252E+00	3.169E+00	3.337E+00
3	3.215E+00	3.090E+00	3.263E+00	3.982E+00	3.818E+00	4.099E+00
4	3.712E+00	3.538E+00	3.728E+00	4.599E+00	4.363E+00	4.656E+00
6	4.546E+00	4.280E+00	4.519E+00	5.632E+00	5.268E+00	5.615E+00
7	4.911E+00	4.590E+00	4.866E+00	6.083E+00	5.658E+00	6.023E+00
8	5.250E+00	4.891E+00	5.172E+00	6.503E+00	6.017E+00	6.398E+00
10	5.869E+00	5.415E+00	5.726E+00	7.271E+00	6.661E+00	7.047E+00
20	7.735E+00	7.254E+00	7.179E+00	9.647E+00	8.942E+00	9.133E+00
30	8.877E+00	8.342E+00	8.465E+00	1.114E+01	1.033E+01	1.042E+01
40	9.580E+00	9.000E+00	9.148E+00	1.210E+01	1.122E+01	1.133E+01
60	1.017E+01	9.607E+00	9.850E+00	1.301E+01	1.216E+01	1.242E+01
80	1.013E+01	9.627E+00	9.949E+00	1.311E+01	1.238E+01	1.276E+01
100	9.787E+00	9.343E+00	9.721E+00	1.279E+01	1.218E+01	1.267E+01
200	7.425E+00	7.159E+00	7.546E+00	1.005E+01	9.695E+00	1.026E+01
300	5.860E+00	5.663E+00	5.924E+00	8.102E+00	7.809E+00	8.205E+00
400	4.895E+00	4.729E+00	4.915E+00	6.862E+00	6.592E+00	6.886E+00
600	3.771E+00	3.638E+00	3.768E+00	5.373E+00	5.138E+00	5.340E+00
800	3.117E+00	3.013E+00	3.095E+00	4.482E+00	4.292E+00	4.428E+00
1000	2.669E+00	2.605E+00	2.650E+00	3.854E+00	3.739E+00	3.809E+00
2000	1.615E+00	1.644E+00	1.602E+00	2.362E+00	2.393E+00	2.328E+00
3000	1.188E+00	1.206E+00	1.187E+00	1.748E+00	1.771E+00	1.726E+00
4000	9.516E-01	9.636E-01	9.512E-01	1.405E+00	1.421E+00	1.395E+00
6000	6.918E-01	6.985E-01	6.913E-01	1.025E+00	1.035E+00	1.019E+00
8000	5.499E-01	5.543E-01	5.489E-01	8.169E-01	8.236E-01	8.107E-01
10000	4.595E-01	4.626E-01	4.589E-01	6.838E-01	6.886E-01	6.788E-01
20000	2.616E-01	2.626E-01	2.610E-01	3.910E-01	3.926E-01	3.874E-01
30000	1.880E-01	1.885E-01	1.875E-01	2.816E-01	2.824E-01	2.795E-01
40000	1.490E-01	1.493E-01	1.483E-01	2.233E-01	2.238E-01	2.217E-01
60000	1.078E-01	1.080E-01	1.075E-01	1.618E-01	1.621E-01	1.607E-01
80000	8.614E-02	8.629E-02	8.594E-02	1.294E-01	1.297E-01	1.286E-01
100000	7.272E-02	7.285E-02	7.259E-02	1.093E-01	1.096E-01	1.087E-01

E (KeV)	Stopping Power (eV/1E15 atoms/cm^2)					
	Paraffin wax			Polystyrene		
	Ziegler	SRIM	PSTAR	Ziegler	SRIM	PSTAR
1	1.71E+00	1.76E+00	1.74E+00	1.95E+00	2.07E+00	2.01E+00
2	2.41E+00	2.38E+00	2.46E+00	2.75E+00	2.79E+00	2.84E+00
3	2.96E+00	2.88E+00	3.01E+00	3.37E+00	3.38E+00	3.48E+00
4	3.41E+00	3.31E+00	3.44E+00	3.89E+00	3.87E+00	4.02E+00
6	4.18E+00	4.00E+00	4.15E+00	4.77E+00	4.68E+00	4.92E+00
7	4.52E+00	4.30E+00	4.47E+00	5.15E+00	5.02E+00	5.32E+00
8	4.83E+00	4.57E+00	4.75E+00	5.51E+00	5.34E+00	5.69E+00
10	5.40E+00	5.05E+00	5.25E+00	6.16E+00	5.90E+00	6.36E+00
20	7.08E+00	6.72E+00	6.79E+00	8.12E+00	7.85E+00	8.35E+00
30	8.10E+00	7.67E+00	7.68E+00	9.31E+00	8.96E+00	9.49E+00
40	8.70E+00	8.23E+00	8.26E+00	1.00E+01	9.63E+00	1.02E+01
60	9.15E+00	8.67E+00	8.82E+00	1.06E+01	1.02E+01	1.06E+01
80	9.03E+00	8.61E+00	8.85E+00	1.06E+01	1.03E+01	1.04E+01
100	8.65E+00	8.29E+00	8.59E+00	1.02E+01	9.98E+00	9.88E+00
200	6.41E+00	6.23E+00	6.53E+00	7.70E+00	7.69E+00	7.40E+00
300	5.01E+00	4.89E+00	5.07E+00	6.13E+00	6.12E+00	5.87E+00
400	4.17E+00	4.07E+00	4.17E+00	5.15E+00	5.13E+00	5.03E+00
600	3.20E+00	3.11E+00	3.00E+00	4.00E+00	3.96E+00	3.92E+00
800	2.63E+00	2.57E+00	2.60E+00	3.32E+00	3.28E+00	3.24E+00
1000	2.25E+00	2.21E+00	2.22E+00	2.85E+00	2.84E+00	2.78E+00
2000	1.35E+00	1.38E+00	1.34E+00	1.73E+00	1.75E+00	1.70E+00
3000	9.91E-01	1.00E+00	9.81E-01	1.27E+00	1.29E+00	1.25E+00
4000	7.91E-01	8.00E-01	7.83E-01	1.02E+00	1.03E+00	1.01E+00
6000	5.73E-01	5.78E-01	5.71E-01	7.41E-01	7.47E-01	7.24E-01
8000	4.55E-01	4.58E-01	4.49E-01	5.89E-01	5.93E-01	5.82E-01
10000	3.80E-01	3.82E-01	3.78E-01	4.92E-01	4.95E-01	4.85E-01
20000	2.16E-01	2.16E-01	2.14E-01	2.80E-01	2.81E-01	2.77E-01
30000	1.55E-01	1.55E-01	1.54E-01	2.02E-01	2.02E-01	1.99E-01
40000	1.22E-01	1.11E-01	1.22E-01	1.60E-01	1.60E-01	1.58E-01
60000	8.85E-02	8.85E-02	8.75E-02	1.16E-01	1.16E-01	1.14E-01
80000	7.07E-02	7.07E-02	7.03E-02	9.23E-02	9.24E-02	9.12E-02
100000	5.96E-02	5.97E-02	5.93E-02	7.80E-02	7.80E-02	7.72E-02

E (KeV)	Stopping Power (eV/1E15 atoms/cm2) Toluene		
	Ziegler	SRIM	PSTAR
1	1.90E+00	2.03E+00	1.96E+00
2	2.69E+00	2.73E+00	2.76E+00
3	3.29E+00	3.31E+00	3.39E+00
4	3.80E+00	3.79E+00	3.85E+00
6	4.66E+00	4.58E+00	4.64E+00
7	5.03E+00	4.92E+00	4.98E+00
8	5.38E+00	5.23E+00	5.28E+00
10	6.01E+00	5.78E+00	5.82E+00
20	7.92E+00	7.69E+00	7.50E+00
30	9.08E+00	8.78E+00	8.49E+00
40	9.79E+00	9.44E+00	9.15E+00
60	1.04E+01	1.00E+01	9.89E+00
80	1.03E+01	1.00E+01	1.00E+01
100	9.89E+00	9.73E+00	9.78E+00
200	7.46E+00	7.47E+00	7.62E+00
300	5.91E+00	5.93E+00	6.00E+00
400	4.97E+00	4.96E+00	5.02E+00
600	3.85E+00	3.83E+00	3.87E+00
800	3.19E+00	3.17E+00	3.18E+00
1000	2.74E+00	2.73E+00	2.72E+00
2000	1.66E+00	1.68E+00	1.65E+00
3000	1.22E+00	1.23E+00	1.21E+00
4000	9.76E-01	9.86E-01	9.76E-01
6000	7.09E-01	7.15E-01	7.10E-01
8000	5.64E-01	5.67E-01	5.64E-01
10000	4.71E-01	4.74E-01	4.71E-01
20000	2.68E-01	2.69E-01	2.68E-01
30000	1.93E-01	1.93E-01	1.92E-01
40000	1.53E-01	1.53E-01	1.52E-01
60000	1.10E-01	1.11E-01	1.10E-01
80000	8.82E-02	8.83E-02	8.81E-02
100000	7.45E-02	7.45E-02	7.44E-02

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