SRIM-Based Numerical Fitting and Comparison with PSTAR for Proton Stopping Power in Al, Cu, and Pb

Wafaa N. Jasim.

Department of Physics, College of Education for Women, University of Kufa, Najaf,Iraq

Abstract. In this research, we conducted a theoretical study to calculate the stopping power of protons in aluminum, copper, and lead for energy ranges between 0.2 and 2.0 MeV. We used SRIM 2013 software to extract the stopping power values, and then numerically fitted these values using MATLAB 2015 to obtain a semi-empirical stopping power equation that describes the behavior of the stopping power with energy. The results of the proposed equation were compared with standard PSTAR data, and the comparison showed good agreement within acceptable deviation limits for most energy points. These results confirm the validity of the equation in representing the stopping power of protons in the studied materials and its potential use in radiation shielding applications and modeling charged particle-matter interactions.

Keywords: Stopping power, protons, SRIM, PSTAR, semi-empirical equations, MATLAB, numerical fitting.

I. Introduction

When radiation consisting of charged particles interacts with matter, the stopping power is the fundamental quantum that describes the loss of kinetic energy of a charged particle per unit path length. Mathematically, it is expressed as dE/dx, representing the rate of energy loss of the particle as it passes through the medium. The primary mechanism for energy loss of heavy charged particles in the low and medium energy ranges is the ionization and excitation of the atoms in the medium. This results from the Coulomb interaction between the incident particle and the electrons of the material. This occurs when attractive or repulsive forces between the charged particle and the electrons lead either to ionization (the release of some electrons from the atoms) or excitation (raising them to higher energy levels without releasing any electrons).

These interactions are concentrated near the path of the incident particle[1].The first theoretical model for the loss of energy of charged particles penetrating matter was Bohr's classical stopping formula in 1913.In this model, energy transfer was divided into a nuclear component and an electronic component, according to classical scattering theory[2]. Bethe's theory followed, describing the stopping power of alpha particles and establishing itself as an important physical method. Additionally, Bohr's theory was used to encompass the extent of fission fragments, but subsequent attempts to establish the stopping power laws for heavy ions were built upon Bethe's theory rather than Bohr's [3]. Bethe's formula is:

$$-\frac{dE}{dx}=\frac{4\pi {Z_1}^2 e^4}{mv^2} NZ_2\, ln\left(\frac{2mv^2}{I(1-\beta^2)}\right)-\beta^2 \ldots\ldots(1)$$

Where:

m, e: represent the charge and mass of the electron, respectively.
v: represents the velocity of the incident particle.
Z1 and Z2: are the atomic numbers of the incident particle and the target, respectively.
I: is the ionization potential of the target material in eV.
: represents the ratio between the velocity of the incident particle and the speed of light [4].

The equation for stopping power (1) can be written as follows:

$$-\frac{dE}{dx}=NS_e=\frac{4\pi {Z_1}^2 e^4}{mv^2} NZ_2 L(x,Z_2)\ \ldots\ldots(2)$$

Where N represents the atomic density of the medium and Se is the atomic stopping power, L(x,Z2) represents the stopping number which depends on the target material (Z2) and the velocity of the incident particle v, where:

$$x=\frac{v^2}{Z_2 v_o^2}\ \ldots\ldots(3)$$

v_o : Electronic speed[5,6]. The role of stopping power is highlighted by its reference to the properties of the material through which the particle passes, while the energy loss per unit length of the particle's path describes what happens to that particle during its passage. This is because the stopping power depends on the properties of the material and the type and energy of the incident particle. The production of an ion pair requires a specific and constant amount of energy, and during ionization, the ionization density along its path is directly proportional to the stopping power [7]. Studying stopping power and energy loss plays a vital role in evaluating and measuring radiation effects. By studying these factors, the effects of radiation resulting from these interactions and the energy deposited in the target material can be determined.

Consequently, numerous and extensive studies have been conducted on the stopping power and range of heavy and light charged particles using various methods such as inductive, analogical, and experimental approaches. Several mathematical formulas exist to suit each case [8]. This stems from the fact that stopping power is of paramount importance in measuring radiation and is a physical property of the medium. Knowing this property allows us to estimate the necessary dose in radiation therapy. It also has implications in other fields such as radiation physics, chemistry, medicine, and other areas that benefit from studying and understanding the stopping power of a material [9].

II. Results and Discussion:

Since experimental measurement of stopping power is very difficult, we chose the SRIM 2013 program to generate data, and then we performed a fitting of this data using MATLAB 2015 .In other word MATLAB software was used to build a mathematical model and numerically calculate the proton stopping power based on the quasi-empirical equation derived from fitting SRIM data.We use Aluminum, Copper and Lead as aims then we compared the values of stopping power with the results of PASTR program in the range of energy between 0.2-2 MeV .

Table .1: Shows the fitting equation of the proton stopping power in Aluminum (Al), Copper (Cu) and Lead (Pb)for the proton energy range (0.2-2MeV) and values of Correlation coefficient.

Equation fitting of stopping power	Aim of element	Factors of equation	Correlation coefficient
$\frac{dE}{dx} = aE^b + c$	Al	a = 310.5 b = -0.305 c =-133	0.9948
	Cu	a = -891.8 b = 0.06929 c =1013	0.9668
	Pb	a = 181.4 b = -0.1773 c = -116.7	0.986

Table (1) shows the fitting coefficients and correlation coefficient values for the semi-empirical proton stopping power equation used to represent the SRIM results for proton stopping power data in aluminum, copper, and lead. The high correlation coefficient values, 0.9948 for aluminum, 0.9668 for copper, and 0.986 for lead, demonstrate excellent agreement between the proposed equation and the SRIM results. This indicates that the proposed stopping power equation accurately describes the behavior of stopping power change with energy. Within this energy range, electronic stopping is the dominant mechanism, with significant contributions from nuclear stopping at lower energies.

This explains the relatively low correlation coefficient of copper compared to the other selected materials, resulting from the effects of its atomic structure and electron shell. Furthermore, a comparison of the equation results obtained from the current work, based on SRIM data fitting, showed good agreement with standard PSTAR data within the energy range defined in this research, as shown in Tables 2, 3, and 4 below for aluminum, copper, and lead, respectively. The deviations are also within acceptable limits for most energy points, as illustrated in the graphs 1,2and 3, which depict the relationship between the energy of the incident protons on the studied targets and the resulting stopping power. This confirms that the obtained equation can be considered a reliable semi-empirical equation for calculating the proton stopping power of aluminum, copper, and lead.

Table .2: Shows the stopping power of protons in Aluminum (Al) which calculated by SRIM- 2013, PSTAR and this work .

Stopping power in MeV/g/cm² for Aluminum (Al)			
E(KeV)	SRIM-2013	PSTAR	This Work
0.2	373	371.5	374.2
0.3	317.8	321.8	315.2
0.4	279.2	284.4	277.6
0.5	250.8	255	250.5
0.6	228.9	231.6	229.8
0.7	211.5	212.6	213.1
0.8	197.2	196.8	199.3
0.9	185.2	183.5	187.6
1	174.9	172	177.5
1.5	155.8	132.8	141.3
2	110.8	109.5	118.3

Table .2: Shows the stopping power of protons in Copper (Cu) which calculated by SRIM- 2013, PSTAR and this work .

Stopping power in MeV/g/cm² for Copper (Cu)			
E(KeV)	SRIM-2013	PSTAR	This Work
0.2	211.8	205.5	215.3
0.3	195.1	192.6	192.5
0.4	178.8	178.8	176
0.5	164.6	166	163
0.6	152.5	153.8	152.2
0.7	142.1	142.8	142.9
0.8	133.3	133.4	134.8
0.9	125.6	125.3	127.6
1	118.9	118.4	121.2
1.5	94.47	94.5	95.7
2	79.75	79.92	77.3

Table .2: Shows the stopping power of protons in Lead (Pb)which calculated by SRIM- 2013, PSTAR and this work .

Stopping power in MeV/g/cm² for Lead (Pb)			
E(KeV)	SRIM-2013	PSTAR	This Work
0.2	122.1	126.5	124.6
0.3	110.5	113.5	107.8
0.4	98.99	100.1	96.6
0.5	89.5	89.6	88.4
0.6	81.91	81.46	81.8

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0.7	75.77	75.12	76.5
0.8	70.7	70.15	72
0.9	66.44	66.19	68.1
1	62.79	62.98	64.7
1.5	52.39	52.26	52.1
2	45.5	45.37	43.7

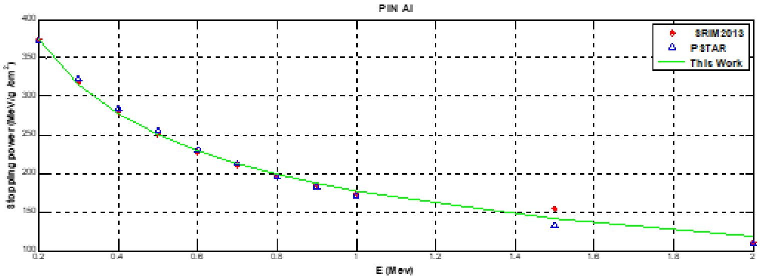

Figure1. The stopping power of Al as a function of proton's energy

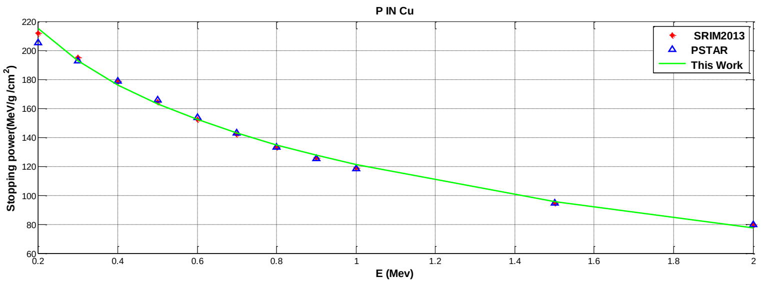

Figure2. The stopping power of Cu as a function of proton's energy

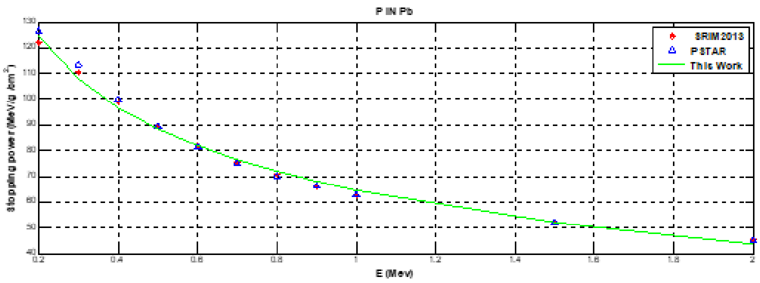

Figure3. The stopping power of Pb as a function of proton's energy

III. Conclusion

To understand the behavior and properties of materials by studying their proton-stopping ability, a semi-empirical equation was developed for the proton-stopping ability of aluminum, copper, and lead within the energy range of 0.2–2.0 MeV. This equation was fitted to SRIM data, yielding correlation coefficients of 0.9948 for aluminum, 0.9668 for copper, and 0.986 for lead. Comparison with the PSTAR database showed good agreement within acceptable deviation limits for most energy points. This demonstrates the accuracy of the proposed model in representing the proton-stopping behavior of these selected elements and confirms the validity of the proposed equation for use in reference and practical applications. These results can be utilized in the fields of medical physics and the design of radiation-resistant and radiation-shielding materials.

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