Stopping power of heavy ions at low velocity $v \le v_o z_1^{2/3}$

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ABSTRACT

In the present work, a theoretical investigation for the interaction of heavy ions like Ar, O and Li in different targets Ar, Kr and N at the low velocity region $v \le v_o z_1^{2/3}$ has been investigated by using Lindhard and Scharff [1] formula for electronic interaction. The interactions of stopping power at low velocity, shows the curvature of increment vary from one interaction to another and fitted with sigmoid function. Also the increment is not linear as given in Lindhard formula for electronic interaction. Therefore, effective charge is important in the low velocity region. Good agreement is achieved with SRIM-software [2]. The mathematical formulas, found in the present work, where solved numerically and programed by writing a computer program in (Fortran-90) language with more than one subroutines.

Keywords: stopping power, low velocity, Sigmoid function, effective charge.

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1. INTRODUCTION

Heavy charged particles passing through matter are usually slowed down by electronic collisions and nuclear collisions [3]. Lindhard [3] devided heavy ions stopping into three regions as shown in figure (1):

Region 1: corresponds to the high velocity region where the stopping power dE/dR decreases with decreasing velocity.

Region 2: an intermediate velocity region $2v_o z_1 > v \ge v_o z_1^{2/3}$ (where v_o is the Bohr velocity in Hydrogen atom and equal to $e^2/\hbar \approx 2.185 \times 10^6$ m/s), includes the maximum stopping.

Region 3: a low velocity region $v \le v_o z_1^{2/3}$ where the nuclear stopping cross-section mechanism is dominating, while the electronic contribution decreases with decreasing ion velocity.

Lindhard and Scharff [1] proven for heavy ions that the electronic stopping cross sections are proportional to v at speeds up to ~ ($v_{TF} = v_o Z_1^{2/3}$). This was shown to be corroborative by range measurements with fission fragments [4]. This assertion showed by two studies in 1966 that was only approximately [5]:

(i) Fastrup et al., [6] could match experimental results for electronic stopping cross section (S_e) with several ions on Carbon at $v \le v_o$ by a relation ($S_e \propto E^p$), where the coefficient (p) in several cases differed virtually from (p = 1/2).

(ii) For heavy ions like Bromine and Iodine at ($v > v_0$) , Brown and Moak, [7,8] found, a linear velocity dependence but with an apparent threshold.

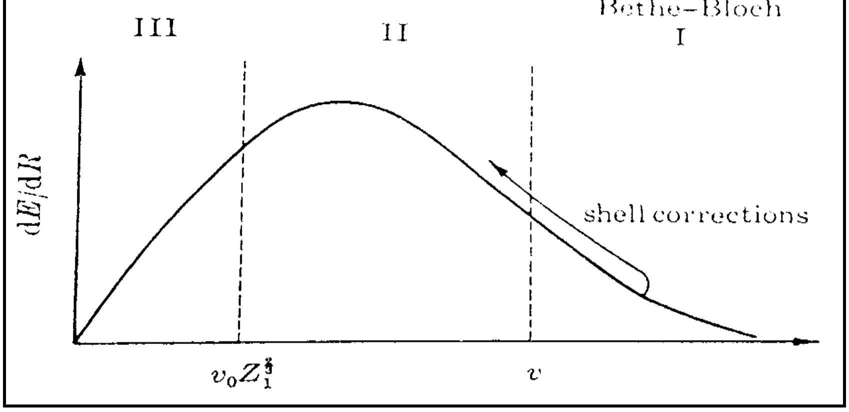


Figure 1 Shows regimes of heavy ions stopping [3].

In the present work, Sigmoid function [9] has been used, whose graphs are "S-shaped" curves, is a mathematical function refers to the special case of the logistic function as shown in figure (2).

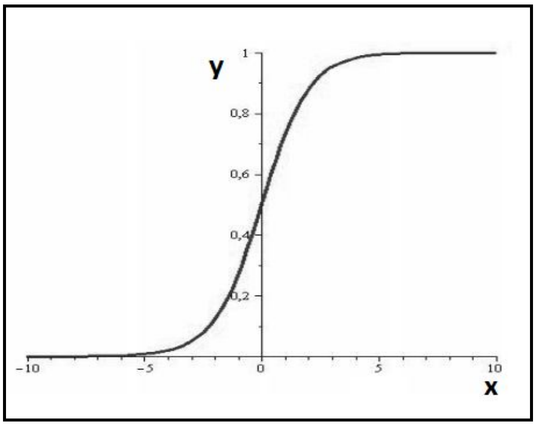


Figure 2 shows the variation of the Sigmoid function (y) given in equation (1) vs (x=log10(EMev/u1)) [9].

$$y = a + (1-a)/\{1 + \exp[-(x-b)/c]\} \qquad (1)$$

Where a= base (low energy limit), $x = \log_{10}\left(E_1/u_1\right)$, u_1 is the atomic number of projectile, E is the energy in MeV, c=width (transition from the low to the high energy region) and is centered at b= $(y_{min}+y_{max})/2$.

2. THEORETICAL PART

The present work is a theoretical investigation for a stopping power of heavy ions at low velocity region $v \le v_o z_1^{2/3}$, and their connection to the basic problem of quasi-elastic collisions between ions and atoms.

The most familiar formula of the stopping cross section in this region is given by Lindhard and Scharff [1],

$$S_e = \xi_e 8\pi e^2 a_o . \frac{Z_1 Z_2}{Z} . \frac{v}{v_o} , \qquad v \le v_1 = v_o Z_1^{2/3}, \qquad (2)$$

Where ξ_e is a constant approximately equal to $Z_1^{2/3}$, $a_o = \hbar / me^2$, and $Z^{2/3} = Z_1^{2/3} + Z_2^{2/3}$. This equation shows that S_e increases linearly with (v) while according to experimental data the electronic stopping cross section (S_e) at $v \le v_o z_1^{2/3}$ increases with v in different form of curvature as shown in figure (3).

Bethe equation for high velocity and Lindhard equation for low velocity summarized by Anderson and Ziegler [11] in one semi-empirical equation which can be applied for the light and heavy elements,

$$\frac{1}{S_e} = \frac{1}{S_{Low}} + \frac{1}{S_{High}} \qquad (3)$$

This equation can be expressed in different formats according to the ranges of energy that used and the type of incident particle as follows [12]:

1. For protons (p) at an energy range from (10 KeV) to (1 MeV), and for alpha particles (α) at an energy range from (1 KeV) to (10 MeV) so (S_{high} , S_{low}) take the following form :-

$$S_{Low} = A_1 (1000\, E)^{A_2} \qquad (4a)$$

$$S_{High} = \frac{A_3}{E} \ln\left(1 + \frac{A_4}{E} + A_5 E\right) \qquad (4b)$$

Where (E) is the energy in (MeV) units, A_1, A_2, A_3, A_4, A_5 is the absolute fitting parameters which can get it directly for protons from [12] and for alpha particles from [13].

2. For protons (p) at an energy range from (1 MeV) and above

$$S_e = \frac{A_6}{\beta^2}\left[\ln\left(\frac{A_7+\beta^2}{1-\beta^2}\right)-\beta^2-\sum_{i=0}^{4}A_{i+8}(\ln E)^i\right] \qquad (5)$$

3. For alpha particles (α) at an energy range from (1 MeV) and above

$$S_e = Exp\left(A_6 + A_7 EE + A_8 EE^2 + A_9 EE^2\right) \qquad (6)$$

Where E is the energy in MeV

$$EE = \ln\frac{1}{E} \qquad (7)$$

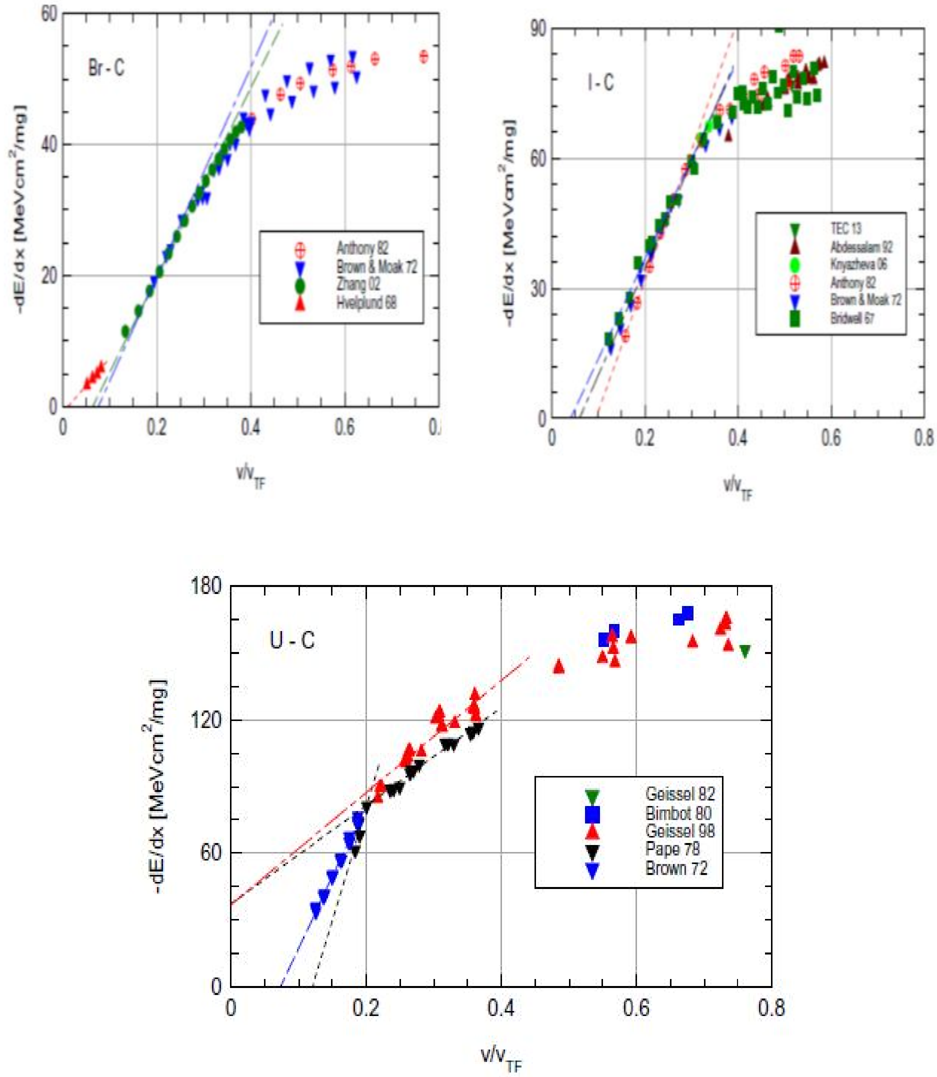


Figure 3 Measured stopping power for C on Br, I and U ions. Stippled straight lines and dotted are extrapolation from experimental data [10].

The stopping cross section (S) assumed to be depends on the square of the effective charge [14] i.e. $S \propto Z_1^{*2}$.
The incident ion effective charge (Z_1^*) is usually expressed by the incident ion charge (Z_1) and the effective charge parameter γ, $Z_1^* = Z_1\gamma$ Where $\gamma = 1 - e^{-v_r}$ and $v_r = v / v_o z_1^{2/3}$ [15].
Therefore, one can calculate the stopping cross section for different heavy ions (Hi) in terms of effective charge at a certain velocity and in the same target. If one of these ions chosen to be Helium ion (He) then,

$$\frac{S_{Hi}}{S_{He}} = \left(\frac{Z^*_{Hi}}{Z^*_{He}} \right)^2 \tag{8}$$

Helium ion has been used as a basis in the present work because its stopping powers are usually being better known than proton stopping powers.

Thus,

$$\frac{S_{Hi}}{S_{He}} = \left(\frac{Z_{Hi}}{2} \right)^2 \left(\frac{v_{Hi}}{v_{He}} \right)^2 \tag{9}$$

And,

$$\frac{\left(S_{HI} / Z^2_{Hi}\right)}{\left(S_{He} / 4\right)} = \left(\frac{v_{Hi}}{v_{He}} \right)^2 \tag{10}$$

Equation (10) is equivalent to equation (1).

From historical review and according to SRIM software [2] the stopping power varies look like Sigmoid function which is given in eq. (1) [16].

This curvature is fitted either with a two or three parameters method, where the three parameters a, b and c depending on Z_1:

1-Two parameters fit: if one takes the prediction of Lindhard and Scharff equation (2) and then rewrite this equation for Helium and heavy ion as follows:-

$$\left(\frac{S_{Hi}}{S_{He}} \right) = \frac{Z_{Hi}^{1/6} 8 \pi e^2 a_o \cdot \dfrac{Z_{Hi} Z_2}{(Z_{Hi}^{2/3} + Z_2^{2/3})^{3/2}} \cdot \left(\dfrac{v}{v_o} \right)}{Z_{He}^{1/6} 8 \pi e^2 a_o \cdot \dfrac{Z_{He} Z_2}{\left(Z_{He}^{2/3} + Z_2^{2/3}\right)^{3/2}} \cdot \left(\dfrac{v}{v_o} \right)},$$

$$= \left(\frac{Z_{Hi}}{2} \right)^{7/6} \left[\frac{\left(2^{2/3} + Z_2^{2/3}\right)}{\left(Z_{Hi}^{2/3} + Z_2^{2/3}\right)} \right]^{3/2} \tag{11}$$

This equation is equivalent to the parameter (a) given in eq. (1)

$$(y - a) = (1 - a) / \{1 + \exp[-(x - b)/c]\},$$

$$\left(\frac{1 - a}{y - a} \right) = 1 + \exp[\ -(x - b)/c],$$

And,

$$\exp[\ -(x - b)/c] = \left(\frac{1 - a}{y - a} \right) - 1 = \frac{1 - y}{y - a},$$

Therefore, by taking the logarithm

$$-(x - b)/c = \ln \left(\frac{1 - y}{y - a} \right),$$

$$\frac{b}{c} - \frac{x}{c} = \ln \left(\frac{1 - y}{y - a} \right) \tag{12}$$

This equation is equivalent to the straight line equation

$$Y = A + bX \tag{13}$$

Where

$$Y = \ln \left(\frac{1 - y}{y - a} \right), \qquad A = \frac{b}{c} \qquad \text{and} \qquad B = -\frac{1}{c}$$

And by using the linear square method one can get the coefficients b and c.

2- Three parameters fit: Newton – Raphson Method [17] has been used here to find the parameters of Sigmoid function a, b and c. Newton – Raphson Method is used to find the roots of nonlinear algebraic equation. This method depends on Taylor series expansion for nonlinear functions.

Lifschitz and Arista illustrated that in a linear–linear plot versus speed, stopping cross sections takes an S-shaped curve starting with a linear portion at the low-velocity end, followed up by an interval with positive curvature, a quasilinear region and, finally, a bend-over to negative curvature towards the stopping peak. The stopping cross sections may show a positive curvature after an initial straight-line behavior because of increasing contributions of inner target shells, increasing the ion charge and variations in dynamic screening [10].

Equation (2) indicates that S_e directly proportional with velocity υ , but we need to investigate the curvature of increased either positive or negative.

This means is to apply equation (3) for an incident charged particle on a target should be taken into the consideration the effective charge of Z_1 .

3. RESULTS AND DISCUSSION

There are many theoretical predictions for total stopping cross-section (electronic and nuclear) of heavy ions in various absorbers, they are Bohr (1948) [18], Firsov (1959) [19], Lindhard and Sharff (1961) [1] and Lindhard et al. (1963) [4]. Each of these theories may be applied in a certain absorber, Bohr theory (1948) [18] can be applied for light absorbers, Firsov theory can be applied for median and heavy absorbers and Lindhard theory can be applied for all absorbers. Lindhard theories were taken in the consideration in the present work.

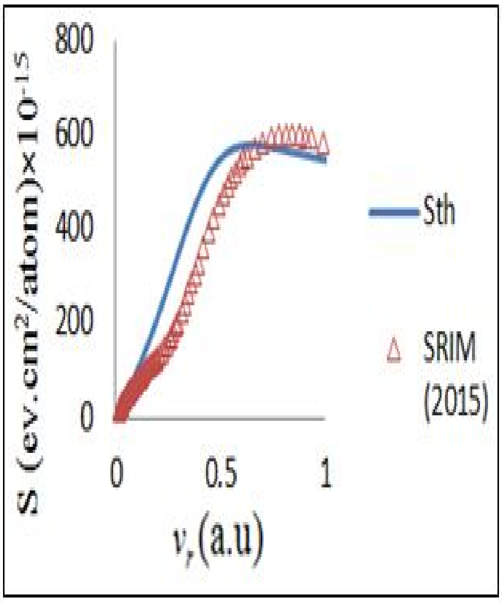
Fig (4) Shows a comparison between the stopping cross-section given by Lindhard equation (2) taking into the consideration the effective charge Z^* and results from SRIM program [2] for Ar, Li and O ions in N, Ar and Kr-targets, good agreement are achieved with software SRIM-2015 presented by Ziegler.

Fig (5) shows the two parameters fit from Sigmoid equation (1) and y that represents to $\left(S_{SRIM}/Z_1^2\right)/\left(S_{He}/4\right)$ where S_{SRIM} is the stopping power of SRIM program [2].

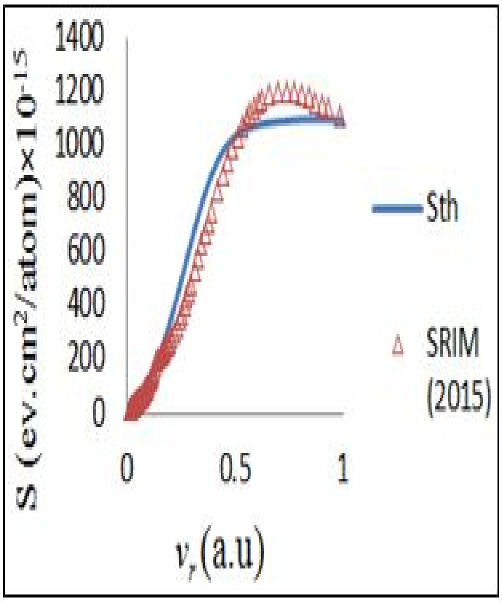
The parameters a, b and c and energy interval from two parameters fit illustrated in table (1)

Fig (6) shows a comparison between the three parameters fit from Sigmoid equation (1), stopping cross-section given by Lindhard equation (2), stopping cross-section given by Lindhard equation (2) taking into the consideration the effective charge Z^* and S SRIM which is the stopping power from SRIM program Ziegler, (2015) for (a) Ar in N, (b) Ar in Ar, (c) Li in Ar, (d) Li in Kr, (e) O in Kr and (f) O in N, at low velocity $v_r \le 1$.

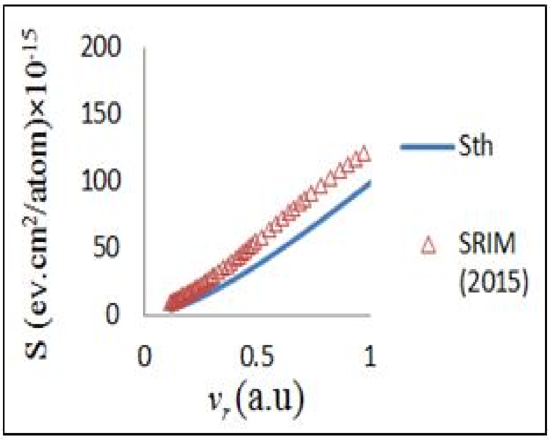
Table (2) shows the parameters a, b and c from Three parameters fit.



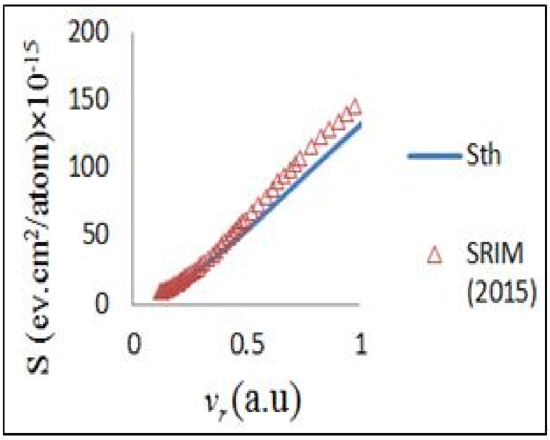
a- Ar in N



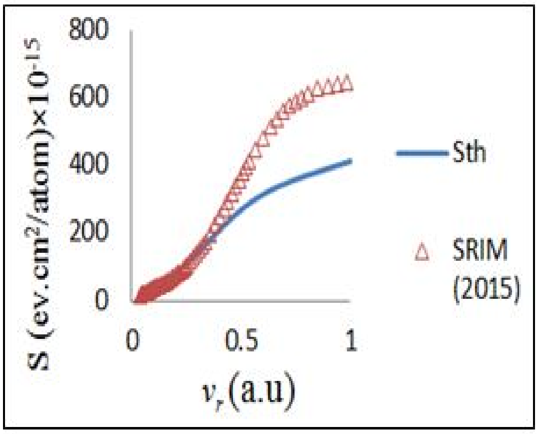
b- Ar in Ar



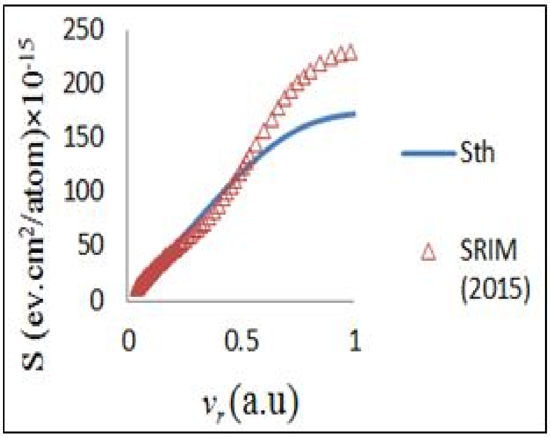
c- Li in Ar



d- Li in Kr

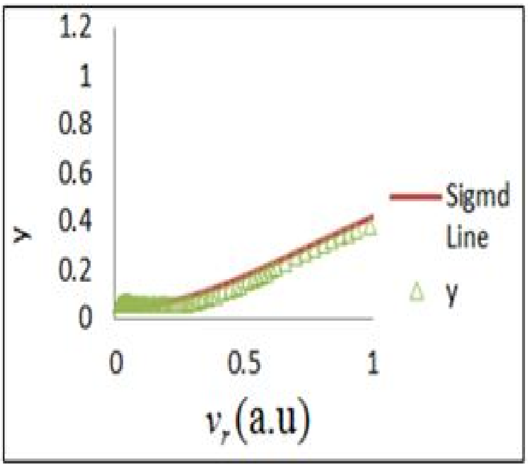


e- O in Kr

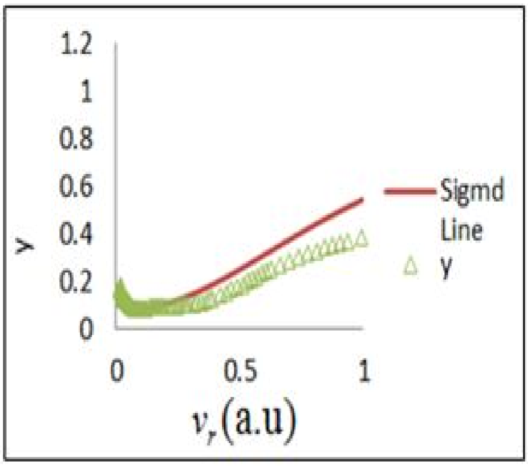


f- O in N

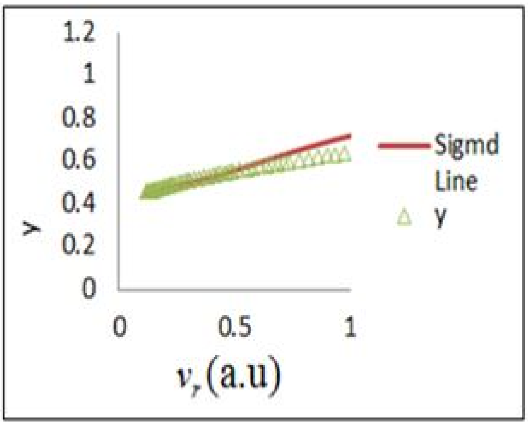
Figure 4 shows a comparison between stopping cross-section given by Lindhard equation (2) taking into the consideration the effective charge Z* and results from SRIM program [2] for (a) Ar in N, (b) Ar in Ar, (c) Li in Ar, (d) Li in Kr, (e) O in Kr and (f) O in N at low velocity $v_r \leq 1$.



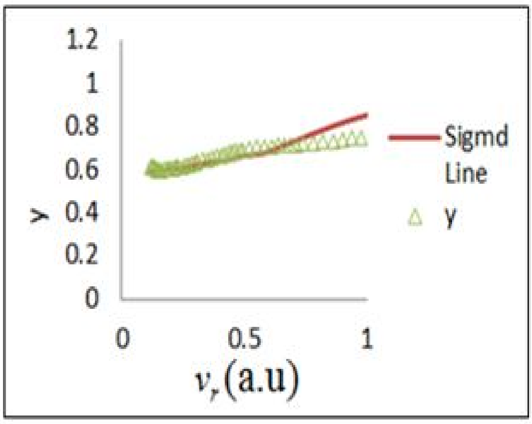
a- Ar in N



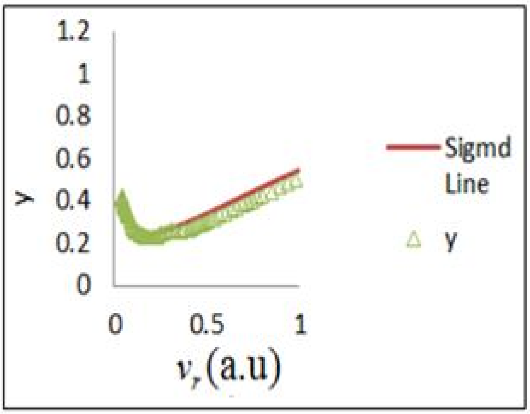
b- Ar in Ar



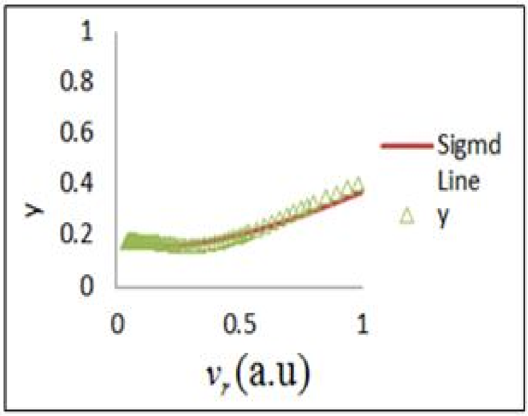
c- Li in Ar



d- Li in Kr

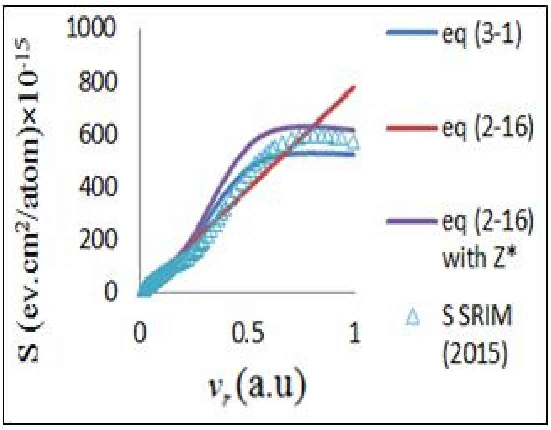


e- O in Kr

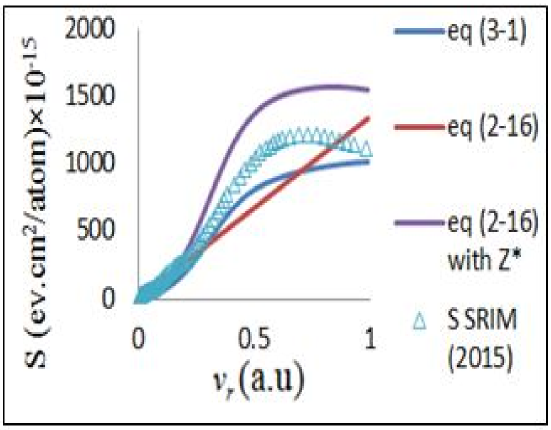


f- O in N

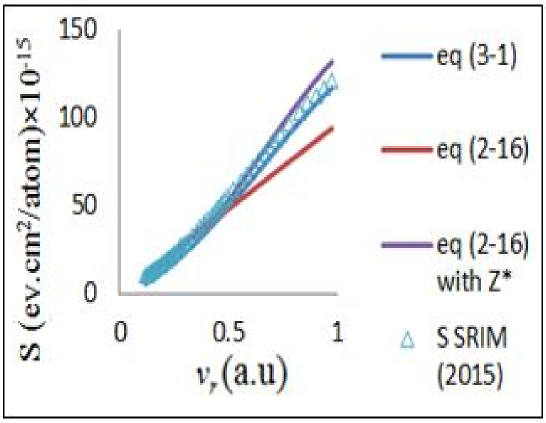
Figure 5 shows for (a) Ar in N, (b) Ar in Ar, (c) Li in Ar, (d) Li in Kr, (e) O in Kr and (f) O in N at low velocity $v_r \leq 1$, a comparison between the two parameters fit from Sigmoid equation (1) and equation (10) and y represents to $\left(S_{SRIM} / Z_1^2\right)/\left(S_{He}/4\right)$ with S_{SRIM} is the stopping power from SRIM program[2].



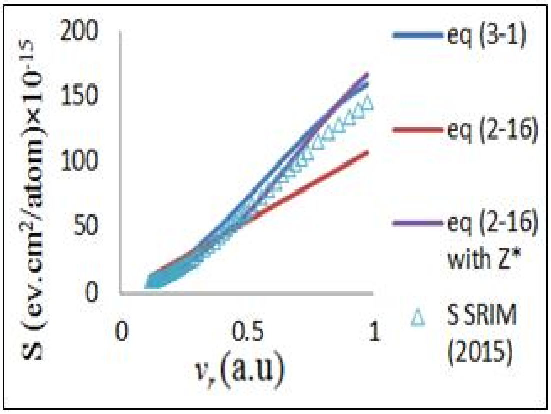
a- Ar in N



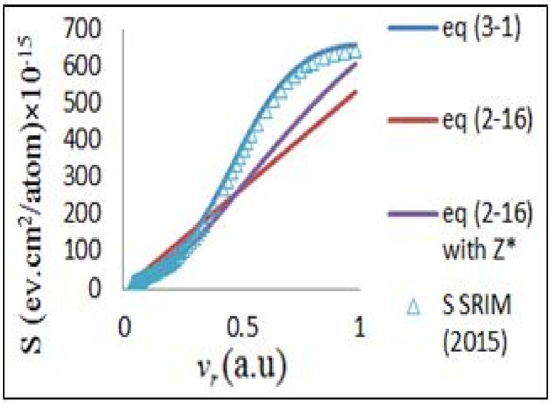
b- Ar in Ar



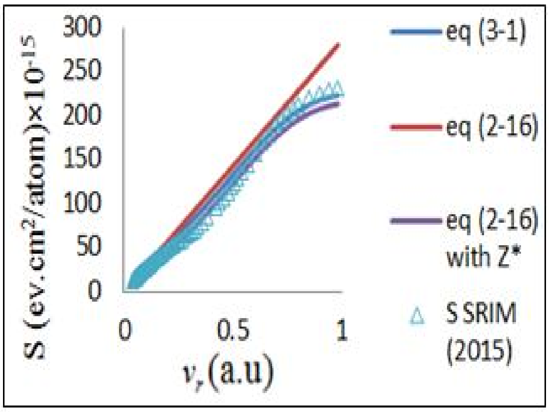
c- Li in Ar



d- Li in Kr



e- O in Kr



f- O in N

Figure 6 shows for (a) Ar in N, (b) Ar in Ar, (c) Li in Ar, (d) Li in Kr, (e) O in Kr and (f) O in N, at low velocity $v_r \leq 1$, a comparison between the three parameters fit from Sigmoid equation (10), stopping cross-section given by Lindhard equation (1), stopping cross-section given by Lindhard equation (1) taking in the consideration the effective charge Z* and S SRIM which is the stopping power from SRIM program [2].

Table 1: The coefficients two parameters fitting of Sigmoid function at different incident projectiles and targets

Z1	**Z2**	**a**	**b (MeV)**	**c (MeV)**	**Energy interval (MeV/u)**
Ar	N	0.045	14.485	4.304	0.0002502 < E < 0.0008133
			26.504	7.277	0.0008758 < E < 0.00035033
			0.252	0.424	0.0037536 < E < 3753.5659180

Ar	Ar	0.77	-5.449	-0.907	0.0002502 < E < 0.0008133
			-5.041	-0.751	0.0008758 < E < 0.00035033
			0.056	0.405	0.0037536 < E < 4003.8037109
Li	Ar	0.655	-5.079	-0.676	0.0014253 < E < 0.0046323
			-1.613	-0.122	0.0049886 < E < 0.0199544
			-1.992	0.483	0.0213797 < E < 6.4139113
Li	Kr	0.583	-4.196	-0.493	0.0014253 < E < 0.0046323
			-1.262	0.347	0.0049886 < E < 0.0199544
			-1.209	0.285	0.0213797 < E < 6.4139113
O	N	0.151	5.008	2.193	0.0006252 < E < 0.0020319
			-8.077	-1.484	0.0021882 < E < 0.0087527
			-0.065	0.346	0.0093779 < E < 3.1259770
O	Kr	0.155	-4.312	-0.523	0.0006252 < E < 0.0020319
			-3.370	-0.274	0.0021882 < E < 0.0087527
			-0.261	0.268	0.0093779 < E < 31. 2597694

Table 2: The coefficients from three parameters fitting of sigmoid function for a various projectiles in various targets

Projectiles (Z1)	Targets (Z2)	Sigmoid coefficients		
		a	b (MeV)	c (MeV)
Ar	N	0.0447	0.37866	0.4315

Ar	Ar	0.0447	0.37335	0.4314
Li	Ar	0.5925	-2.35387	2.3929
Li	Kr	0.5925	-1.67804	2.2141
O	Ar	0.1697	0.07545	3.0720
O	Kr	0.1697	0.13042	4.2737

4. CONCLUSION

From figs. (4, 5, 6) one can say that the variation of stopping power with $v_r = v / v_o Z_1^{2/3} \leq 1$ takes the S-shape or Sigmoid function as given in equation (1) for different type of interaction. The variation is not linear as given in Lindhard and Scharff [1] therefore the effective charge is important at low velocity $v_r = v / v_o Z_1^{2/3} \leq 1$. The form of curvature of interaction is different from one interaction to another and one of future work is to pay attention for more investigation to the shape of curvature for interaction of heavy ions at low velocity, $v \leq v_o z_1^{2/3}$.
The other interesting point is to apply this kind of work on compounds and to see the effects of kind of bonds on the on the variation of electronic stopping power with $v \leq v_o z_1^{2/3}$.
Bohrs formula [18] can be applied for heavy ions at low velocity, at Bohr's parameter $K_P \geq \frac{2 Z_1 v_o}{v} > 1$. Finaly at low velocity region the nuclear interactions is important and can not be neglected especially at velocity $v \leq v_o$.

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