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Effect of the Tow Approximations of Lindhard on Energy Loss Fluctuation (Straggling) of Diclusters Hydrogen Ions at Low Velocities with No Damping

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Abstract: ***In this search, we study straggling of dicluster with no damping at low velocities. We use (Na,k,Cs) as targets mediums based on an electron gas model. This work discusses effect of wigner-sitz radius (density parameter rs) and internuclear distance (r12) on stopping power. The results show the linear behavior of the energy loss with the ion velocity obtained under the free electron gas (FEG) and linear dielectric formalism. This search gives detail studying about straggling at different adverbs and effect of different parameters. A program in matlab has been written for execute.***

Keyword: dicluster, straggling, low velocity

1. Introduction

A heavy ion passing through a target of certain thickness will suffer a number of collisions with the atoms and electrons of the target. In each collision it will transfer a certain amount of energy to the target atom and electron. Because the collisions are discrete and random, statistical fluctuation is expected in the number of collisions. [1, 2] The present study is concerns with the deposition of electronic energy by slow molecules and clusters in matter (less or Fermi velocity (vF)). [3, 4] We can studies variance from stopping power because of the statistical nature for the stopping power quality. The threshold effect is very important to describe the energy loss and straggling in a single crystal in channeling they found a mass effect between channeled protons and deuterons, in the relative straggling values: increasing mass yields higher relative straggling [5, 6].

2. Lindhard Dielectric Function

The Lindhard function [7] gives in a self-consistent way an exact expression of the dielectric constant for a non-relativistic free electron gas of high density at zero temperature. In the low energy limit, within the Random Phase Approximation (RPA) for the dielectric constant, the loss function can be written as follows:

$$\in(\vec{k},\omega) \cong \in_1(\vec{k}) + i\in_2(\vec{k},\omega) \qquad (1)$$

$$\text{or} \quad \frac{1}{\in(k,\omega)} = \frac{1}{\in_1(k) + i\in_2(k,\omega)} \qquad (2)$$

The imaginary part of $\frac{-1}{\in(\vec{k},\omega)}$ can be obtain by multiplying and dividing Eq. (2) by its conjugate.

Therefore the $\mathrm{Im}\left[\frac{-1}{\in(k,\omega)}\right]$ can be written as:

$$\mathrm{Im}\left[\frac{1}{\in(\vec{k},\omega)}\right] = \frac{\in_2(\vec{k},\omega)}{\in_1^2(\vec{k}) + i\in_2^2(k,\omega)} \qquad (3)$$

From Nagg et al. [8] we have that:

$$\left.\begin{aligned} \in_1(\vec{k}) &= C(\vec{k})f_1(\vec{k}) + 1 \quad \text{for arbitrary } \vec{k} \\ \in_2(k) &= C(\vec{k})\frac{\pi\omega}{2kk_F} \quad \text{for } k \le 2k_F \end{aligned}\right\} \qquad (4)$$

Where

$$\left.\begin{aligned} f_1(\vec{k}) &= \frac{1}{2}\left[1 + \frac{4k_F^2 - k^2}{4k.k_F}\ln\left|\frac{k+2k_F}{k-2k_F}\right|\right] \\ C(\vec{k}) &= \frac{4k_F}{\pi k^2} \end{aligned}\right\} \qquad (5)$$

The approximation of the dielectric constant at low velocities ($v<v_f$)

2.1 The First Approximation $f_1(\vec{k})$:

For $\in(\vec{k},\omega)$ an approximation is made to Eq. (3), if $\in_1(\vec{k}) >> \in_2(\vec{k},\omega)$, therefore,

$$\mathrm{Im}\left[\frac{-1}{\in(\vec{k},\omega)}\right] \approx \frac{\in_2(k,\omega)}{\in_1(k)} \qquad (6)$$

Using the first approximation method to $f_1(\vec{k}) = 1$ then, equation (6) becomes:

$$\mathrm{Im}\left[\frac{-1}{\in(\vec{k},\omega)}\right] = \frac{C(\vec{k})\left[\frac{\pi\omega}{2kk_F}\right]}{[C(\vec{k})+1]^2} = \frac{2\omega}{k^3\left[\frac{4k_F}{\pi k^2}+1\right]^2}$$

$$= \frac{2k\omega}{(k^2+k_D^2)^2} \quad \text{for } k \le 2k_F \qquad (7)$$

$$\text{Where } k_D^2 = \frac{4k_f}{\pi} \qquad (8)$$

2.2 The Second Approximation to $f_1(\vec{k})$:

A good approximation to straggling of energy loss values obtained numerically by using the full (RPA) dielectric response function has been proposed by Lindhard and

Winther [9]. Expanding the function $f_1(\vec{k})$ and then, $f_1(\vec{k})$ up to the second order in $\vec{k}$ and then, $f_1(\vec{k})$ becomes [10].

$$f_1(\vec{k}) = 1 - \frac{1}{3}\left(\frac{\vec{k}}{2\vec{k}_F}\right)^2 \quad (9)$$

The imaginary part of the (RPA) dielectric loss function is given by inserting Eqs. (3-5) and Eq. (9) into Eq. (2) as follows:

$$\mathrm{Im}\left(\frac{-1}{\in(\vec{k},\omega)}\right) \cong \frac{\frac{4\vec{k}_F}{\pi k^2}\frac{\pi\omega}{2\vec{k}.\vec{k}_F}}{\left\{1+\left[1-\frac{1}{3}\left(\frac{\vec{k}}{2\vec{k}_F}\right)^2\right]\times\left(\frac{4\vec{k}_F}{\pi k^2}\right)\right\}^2}$$

$$\cong \frac{2\omega}{k^3\left(1-\frac{1}{3\pi\vec{k}_F}+\frac{4\vec{k}_F}{\pi k^2}\right)^2} \quad (10)$$

Let the constants $\left[\Pi^2 = 1 - \frac{1}{3\pi\vec{k}_F} \text{ and } k_D^2 = \frac{4\vec{k}_F}{\pi}\right]$

then Eq. (10) becomes

$$\mathrm{Im}\left(\frac{-1}{\in(\vec{k},\omega)}\right) \approx \frac{2\omega}{k^3\left(\Pi^2+\frac{k_D^2}{k^2}\right)^2}$$

$$\approx \frac{2\vec{k}\omega}{\left\{\Pi^2 k^2 + k_D^2\right\}^2} \quad (10a)$$

3. Fluctuation in Dicluster Energy Loss

Straggling is a complex issue in general. For penetrating atomic ions, fluctuations in energy loss are governed by the statistics of energy-loss processes and charge-changing events. The former dominates far light ions and hinge on close collision. Therefore, the processes giving rise to the enhanced stopping power of light molecular ions must be less efficient with regard to straggling [10]. On the other hand, charge-exchange straggling goes as the square of the stopping power [11] and may, therefore, become relatively more important for molecular than for atomic ions.

The width of the energy-loss spectrum of transmitted particles must be affected by the orientation dependence of molecular stropping powers. To the extent that a penetrating molecule retains approximately its initial orientation, this contribution to the width will be proportional to the mean energy loss. The square of the width will then depend quadratically rather than linearly on the layer thickness and should, therefore, not be considered as a contribution to straggling [12].

If a beam of charged particles, with energy (E), transmitted through a target of thickness (Δx), the variance (straggling) can be defined as follows [13]

$$\Omega = \sqrt{\left\langle(\Delta E - \langle\Delta E\rangle)^2\right\rangle} = \sqrt{\left\langle\Delta E^2\right\rangle - \langle\Delta E\rangle^2} \quad (11)$$

Where ΔE is the energy loss of the charged particle when it passes through the target and <ΔE> is the average energy loss of the same charged particle. The square root in Eq. (11) is called standard deviation (Ω) in energy loss (ΔE) from its mean <ΔE>.

A measure of fluctuations for a dicluster may be found by computing Ω in Eq. (11) (the variance of energy loss about the mean loss). If the energy loss experienced by a charged entity in traversing a target of small thickness, then Ω2 given into Eq. (11) indicates that the brackets indicate an average over the probability distribution of energy losses [13]. The appropriate probability distribution of energy losses for the case of diclusters penetrating a valence electron gas may be obtained from the following equation $S_c = (Z_1^2 + Z_2^2)S_S + 2Z_1Z_2S_{corr}(r_{12})$ where Sc,Ss and Scorr refers to the cluster. To reach an expression for the energy losses distribution, one must recognize that the quantum of energy corresponding to the frequency ω is ħω. Then the probability that the spherically averaged dicluster should lose a quantum of frequency is (ω), while traversing the path length is (dx) [14].

$$\left\langle\frac{dP}{d\omega}\right\rangle = dx\left\{\begin{array}{l}(Z_1^2+Z_2^2)\frac{2e^2}{\pi v^2}\int_{\omega/v}^{\infty}\frac{dk}{k}\mathrm{Im}\left[\frac{-1}{\in(k,\omega)}\right]+\frac{4Z_1Z_2e^2}{\pi v^2}\\ \int_{\omega/v}^{\infty}\frac{dk}{k}\frac{\sin(k.r_{12})}{kr_{12}}\mathrm{Im}\left[\frac{-1}{\in(k,\omega)}\right]\end{array}\right\} \quad (12)$$

Note that the second term in Eq. (12) may be negative under some conditions. This is related to the fact that the wake of the leading ion may deliver energy to the trailing ion. The first term of Eq. (12) originates from the reaction of each wake on its causative ion. The second term describes the distribution of energy loss (or gain) of one ion due to the wake of the other. By taking into account the fact that contributions to the straggling form these two mechanisms of energy transfer must be statistically independent of one another by [14]:

$$\Omega^2 = \Omega_s^2(\mathrm{v}) + \Omega_{corr}^2(\mathrm{v}, \mathrm{r}_{12})$$

Where

$$\Omega_s^2/dx = \frac{2e^2}{\pi v^2}\int_0^{\infty}\frac{dk}{k}\int_0^{k.v}d\omega\,\omega^2\,\mathrm{Im}\left[\frac{-1}{\in(k,\omega)}\right](Z_1^2+Z_2^2) \quad (13)$$

is the straggling parameter of the single particle and

$$\Omega_{corr}^2/dx = \frac{2e^2}{\pi v^2}\int_0^{\infty}\frac{dk}{k}\frac{\sin(k.r_{12})}{k.r_{12}}\int_0^{k.v}d\omega\,\omega^2\,\mathrm{Im}\left[\frac{-1}{\in(k,\omega)}\right](2Z_1Z_2) \quad (14)$$

By choosing an appropriate form to the $\mathrm{Im}\left[\frac{-1}{\in(k,\omega)}\right]$, one can solve Eqs. (13, 14)

4. Straggling by using 1st Approximation at Low Velocity

Using the first order approximation (f1(k) =1) with $\in_1(\vec{k}) >> \in_2(\vec{k})$, one can determine the single and correlated straggling in energy loss of dicluster ions . By inserting the dielectric function in 1st approximation, which is described in Eq. (7) into Eqs. (13, 14), the energy straggling for both branches (single and correlated) are obtained:

$$\Omega_s^2 / dx = \frac{2e^2}{\pi v^2}\int_0^{2k_F}\frac{dk}{k}\int_0^{k.v} d\omega\ \omega^2 \frac{2k\omega}{(k^2+k_D^2)^2}(Z_1^2+Z_2^2)$$

$$=\frac{4e^2}{\pi v^2}(Z_1^2+Z_2^2)\int_0^{2k_F}\frac{dk}{(k^2+k_D^2)^2}\int_0^{k.v}\omega^3 d\omega$$

$$=\frac{e^2(Z_1^2+Z_2^2)v^2}{\pi}\int_0^{2k_F}\frac{k^4\,dk}{(k^2+k_D^2)^2} \qquad (15)$$

and the correlated part of the variance in energy loss which is given in Eq. (14).

$$\Omega_{corr}^2 / dx = \frac{4e^2Z_1^2Z_2^2}{\pi v^2}\int_0^{2k_F}\frac{dk}{k^2}\frac{\sin(kr_{12})}{r_{12}}\int_0^{k.v} d\omega.\omega^2.\frac{2k\omega}{(k^2+k_D^2)}$$

$$=\frac{2e^2Z_1Z_2v^2}{\pi}\int_0^{2k_F}\frac{k^3}{(k^2+k_D^2)^2}\frac{\sin(kr_{12})}{r_{12}}dk \qquad (16)$$

When $\lim_{r12\to 0}\frac{\sin(k.r12)}{k.r12}$ and the cluster behaves as a single ion. Also when $\lim_{r12\to\infty}\frac{\sin(k.r12)}{k.r12}$ and there will be no vicinage effect. This equation can programming by using matlab program and got the results.

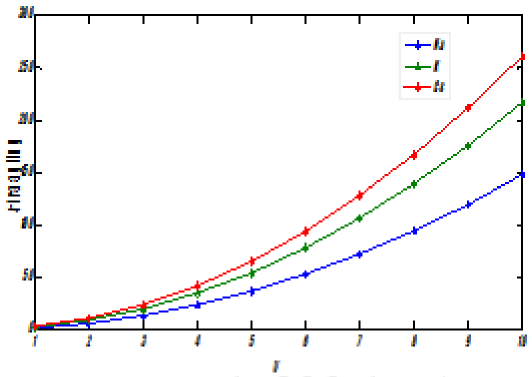

Figure 1: Shows the dicluster ion as single ion at low velocity in 1st approximation.

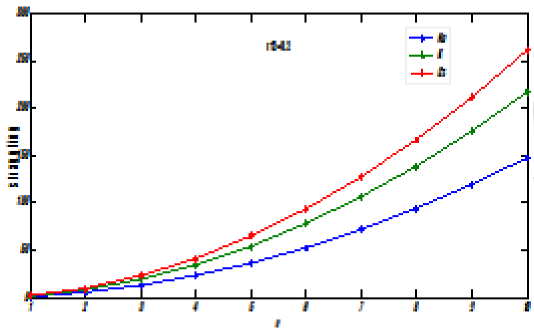

Figure 2: straggling of dicluster hydrogen ion at low velocity (single and correlated) when r_{12}=0.2 in 1st approximation

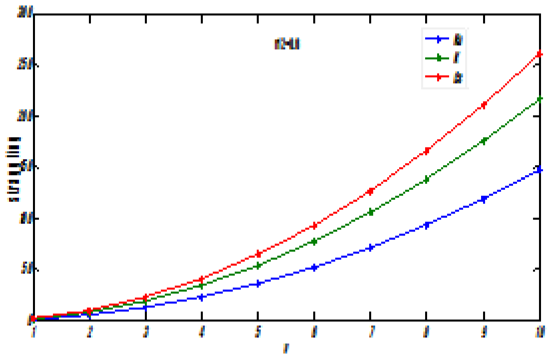

Figure 3: straggling of dicluster hydrogen ion at low velocity (single and correlated) when r12=0.6 in 1stapproximation

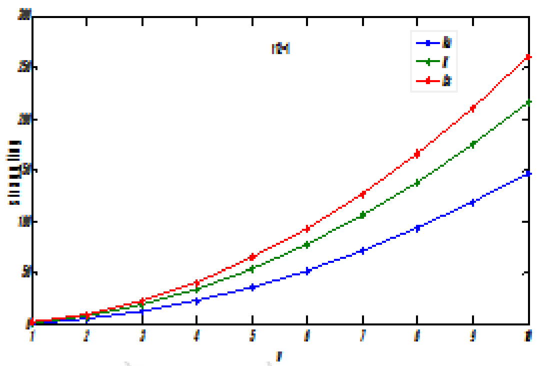

Figure 4: straggling of dicluster hydrogen ion at low velocity (single and correlated) when r12=1 in 1st approximation

5. Straggling by using 2nd approximation at Low Velocity

Now to discuss the variance at low velocity ions with no damping (γ→0)by using the second approximation which is presented by Lindhard [7]. By substituting Eq. (10a) into the straggling of a single charges projectile expression, Eq. (13), one can get:

$$\Omega_s^2 / dx = \int_0^{\infty}\frac{d\vec{k}}{\vec{k}}\int_0^{\vec{k}.\vec{v}}\omega d\omega\frac{2\vec{k}\omega}{\Pi^4\left[k^2+(k_D/\Pi)^2\right]^2}\left(z_1^2+z_2^2\right)$$

$$=\frac{2\left(z_1^2+z_2^2\right)v^3}{3\Pi^4}\int_0^{2\vec{k}_F}\frac{k^3d\vec{k}}{\left[k^2+(k_D/\Pi)^2\right]^2} \qquad (17)$$

We have explicit integration of eq. (17) in matlab program

To calculate the straggling in 2nd approximation for the two correlated ions we substitute Eq. (10a) into Eq. (17) as follows:

$$\Omega_{corr}^2 / dx = (2z_1z_2)\int_0^{\infty}\frac{d\vec{k}}{\vec{k}}\int_0^{\vec{k}.\vec{v}}\omega d\omega\frac{2\vec{k}\omega}{\Pi^4\left[k^2+k_D^2/\Pi^2\right]^2}\frac{\sin(\vec{k}.\vec{r}_{12})}{\vec{k}.\vec{r}_{12}}$$

$$=\frac{2}{3}\frac{v^3}{\vec{r}_{12}\Pi^4}(2z_1z_2)\int_0^{2\vec{k}_F}\frac{k^2d\vec{k}}{\left[k^2+k_D^2/\Pi^2\right]^2}\sin(\vec{k}.\vec{r}_{12}) \qquad (18)$$

The correlated straggling can be solved numerically in program written in matlab, linking and executing.

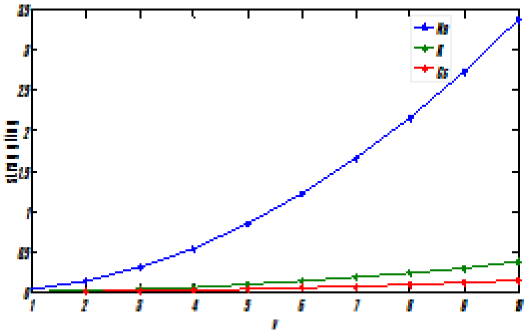

Figure 5: Shows the dicluster ion as single ion at low velocity in 2nd approximation.

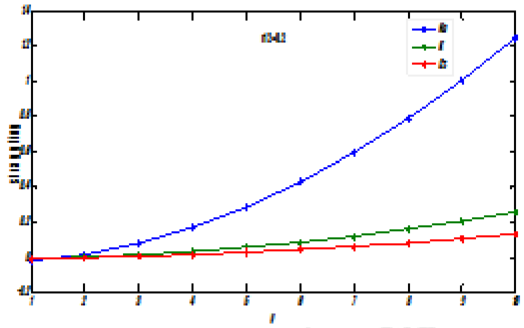

Figure 6: straggling of dicluster hydrogen ion at low velocity (single and correlated) when r12=0.2 in 2nd Approximation

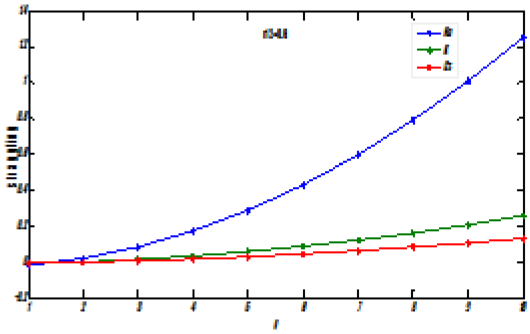

Figure 7: straggling of dicluster hydrogen ion at low velocity (single and correlated) when r12=0.6 in 2^{nd} approximation.

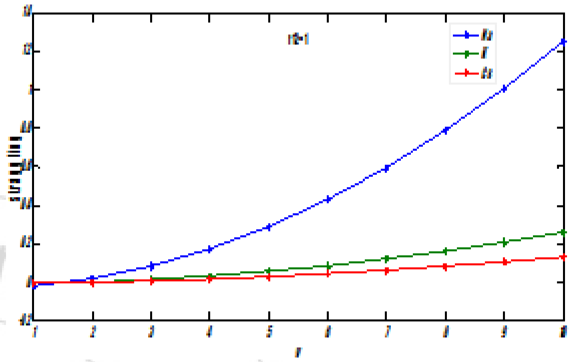

Figure 8: straggling of dicluster hydrogen ion at low velocity (single and correlated) when r12=1 in 2nd approximation.

Table 1: Explain the Change in the Straggling At Low Velocities by 1st Approximation of Lindhard

v	straggling when r_{12}=0			straggling when r_{12}=0.2			straggling when r_{12}=0.6			straggling when r_{12}=1		
	Na	K	Cs	Na	K	Cs	Na	K	Cs	Na	K	Cs
0.1	1.475966	2.171057	2.60956	1.409666	2.155646	2.601922	1.411702	2.155879	2.602007	1.415495	2.1562999	2.602156
0.2	5.903862	8.684227	10.43824	5.836095	8.668281	10.43028	5.838611	8.668628	10.43042	5.842823	8.6691561	10.43062
0.3	13.28369	19.53951	23.48604	13.21348	19.52267	23.47753	13.21679	19.52321	23.47777	13.2217	19.523916	23.47806
0.4	23.61545	34.73691	41.75296	23.54181	34.71882	41.74369	23.54625	34.71962	41.74406	23.55214	34.720581	41.74448
0.5	36.89914	54.27642	65.23899	36.82109	54.25672	65.22875	36.82698	54.25787	65.22928	36.83412	54.259149	65.22987
0.6	53.13476	78.15804	93.94415	53.05133	78.13638	93.93271	53.05898	78.13795	93.93345	53.06766	78.139622	93.93424
0.7	72.32231	106.3818	127.8684	72.23252	106.3578	127.8556	72.24226	106.3599	127.8566	72.25275	106.362	127.8576
0.8	94.4618	138.9476	167.0118	94.36466	138.921	166.9973	94.37681	138.9236	166.9986	94.38939	138.92628	166.9999
0.9	119.5532	175.8556	211.3743	119.4478	175.8259	211.358	119.4626	175.8292	211.3596	119.4776	175.83246	211.3612
1	147.5966	217.1057	260.956	147.4818	217.0726	260.9376	147.4997	217.0766	260.9395	147.5173	217.08055	260.9415

Table 2: Explain the Change in the Straggling at Low Velocities by 2nd Approximation of Lindhard

v	straggling when r_{12}=0			straggling when r_{12}=0.2			straggling when r_{12}=0.6			straggling when r_{12}=1		
	Na	K	Cs	Na	K	Cs	Na	K	Cs	Na	K	Cs
0.1	0.033777	0.003714	0.001422	-0.02066	-0.00714	-0.00385	-0.019712	-0.00701	-0.00381	-0.01786	-0.006764	-0.003716
0.2	0.135106	0.014857	0.005689	0.017835	0.000938	0.000298	0.018778	0.001061	0.000342	0.020616	0.0013031	0.00043
0.3	0.30399	0.033428	0.012799	0.081999	0.014395	0.007213	0.082928	0.014513	0.007256	0.08474	0.0147482	0.00734
0.4	0.540426	0.059427	0.022754	0.171829	0.033234	0.016894	0.172739	0.033347	0.016934	0.174513	0.0335713	0.017014
0.5	0.844415	0.092855	0.035553	0.287324	0.057455	0.029341	0.28821	0.057562	0.029378	0.289935	0.0577724	0.029451
0.6	1.215958	0.133711	0.051197	0.428485	0.08706	0.044554	0.429341	0.087158	0.044587	0.431007	0.0873516	0.044653
0.7	1.655054	0.181996	0.069685	0.595312	0.122046	0.062533	0.596132	0.122135	0.062561	0.597729	0.1223088	0.062618
0.8	2.161703	0.237708	0.091017	0.787805	0.162416	0.083278	0.788583	0.162493	0.083301	0.7901	0.162644	0.083347
0.9	2.735906	0.30085	0.115193	1.005963	0.208168	0.106789	1.006695	0.208232	0.106806	1.008121	0.2083572	0.10684
1	3.377662	0.371419	0.142214	1.249787	0.259303	0.133066	1.250466	0.259352	0.133076	1.251791	0.2594485	0.133097

6. Conclusion

We have made extensive calculation of straggling, and the numerical results for three solid targets, Na (rs=3.66a.u), K (rs=4.86a.u) and Cs (rs=5.88a.u). These three targets have been chosen because of their frequent use in experiments [15] and also of their different electron densities, where (rs) is a measure of electron density.

The energy loss straggling of partially ionized heavy ions is determined by the stochastic fluctuations of the energy loss in atomic collisions remaining in a fixed charge state, (Collisional straggling) and by influence of charge-state fluctuations (charge-exchange straggling) [16, 17], hence with respect to Figs. (2, 3, 4) which are presenting similar dicluster straggling energy to Figs. (6,7,8) in spite of the difference between them (first and second approximation respectively) where they show a high peak of straggling energy loss localized at the beginning of the internuclear distance domain, if these aspects are discussed from the point of view the effective charge which may be had by the dicluster. As a simple but generic example of a projectile, we have considered a hydrogen dicluster ions (Z1 = Z2 = 1) for which we present theoretical results for the following quantities of physical interest. Fig. (1) show straggling of dicluster hydrogen ion as single ion for three different targets (Na, K and Cs) with no damping (γ→0)in 1st approximation. While the figs. (2, 3, 4) shows straggling of dicluster hydrogen ion (single and correlated) at low velocity in 1st approximation when r12= (0.2,0.6,1) ,respectively. The fig (5) show straggling of dicluster hydrogen ion as single ion for three different targets (Na, K and Cs) with no damping (γ→0) in 2nd approximation. While figs(6,7,8) shows straggling of dicluster hydrogen ion (single and correlated) at low velocity in 2nd approximation when r12=(0.2,0.6,1) ,respectively. While table (1) explain the straggling at low velocities with 1st approximation and table (2) explain the straggling at low velocities with 2nd approximation.

When (r12=0.2 a.u.) the reduce velocity (v) strongly effected on the correlated variance in energy loss, while when distance between two clusters in large (r12≈1a.u.), the relative velocity is approximately independent on the correlated part and the dicluster ions treats as two singly ions. The energy straggling at low velocities (v) is found to be roughly proportional to the velocity of the dicluster ions.

The increasing of internuclear distance and Winger Seitz radius (r_s) has a same relation with straggling of energy loss at low velocities with no damping. This relation is direct proportional. Which means that the increasing in the increase of internuclear distance and Winger Seitz radius (r_s) lead to increasing in straggling. The short enough separator distance between the pair ions permit to the vicinage effect to be active among as great as the number of the surrounding electrons and this off course depends on the density of these electrons which is related conversely with their radius (r_s), however, to get the straggling energy gain rather than loss as in Figs. (2,3,4) according to the dicluster internuclear distance $(r_{12} = 0.2, 0.6, 1)$ in 1st approximation. While the figs. (6, 7,8) show the straggling according to the dicluster internuclear distance $(r_{12} = 0.2, 0.6, 1)$ in 2nd approximation at low velocities.

The effect of the dicluster internuclear distance (r12) on straggling can appear clearly in table (1) and (2) in 1st and 2nd approximation, respectively. These tables shows that the straggling increase with increasing of (r12). In the 2nd approximation the straggling is large from the straggling in 1st approximation which true according to equation $f_1(\vec{k}) = 1$ and equation $f_1(\vec{k}) = 1 - \frac{1}{3}\left(\frac{\vec{k}}{2\vec{k}_F}\right)^2$. This difference can note from compare between table (1) and table (2).

Here two important features are noted: (i) the interference effect becomes negative and this may happen when $\frac{2\bar{v}}{\omega_p} < \vec{r}_{12} < \frac{5\bar{v}}{\omega_p}$ [11] where the electrons excitations of the medium atoms being incoherent to cause increasing projectile energy rather than dissipating it, and vice versa in the case of $\vec{r}_{12} = \bar{v}/\omega_p$ which names resonant or plasmon excitations the highest transfer of projectile energy to the target electrons should happen and this belongs to the coherency of electrons excitations, (ii) The value in the united- atom case $(\vec{r}_{12} = 0)$ takes maximum straggling values where the projectile behaves as a unit charge of $(z_1 + z_2)$ which may increase Coulomb screening or in other ward the stopping power, conversely in the case of $\vec{r}_{12} > 5\bar{v}/\omega_p$ the dicluster should be two separated particles of charge $z_1 e$ and $z_2 e$, where the correlated stopping power would approach to zero[11]. Dicluster could never dissipate energy more than its energy. Therefore, it is clear that the straggling energy loss at low velocity is very little and the depending mechanism to energy transfer is the collective excitation we can note at the low velocities, that appears both interaction components. Especially at small internuclear distance that is required to exhibit the vicinage effect [18]. The latter curve gets characterized board maxima by meeting the two highest actions of the straggling loss energy according to the effect of dicluster projectile velocity, Wigner Seitz radius, and the internuclear distance.

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