Bloch correction at high velocity

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Abstract:-

One of the needs of various accelerators to stimulate recent developments in calculating the energy loss of charged particles in matter is heavy ion ionization energy loss. Bloch incorporates Bethe and Bohr theory in a very transparent way. Thus, Bloch found the bridging formulation between the classical Bohr impact – parameter approach, and the quantized Bethe momentum transfer approach to energy loss. In this paper, the behavior of Bloch correction of protons in Aluminum (Al) and Gold (Au) has been studied as well as Bloch correction have also been measured of protons and alpha particles in Nitrogen (N). We have described an implementation of Bloch correction to stopping power (dE/dx) in order to take into account the deviations from the Bethe theory at (non – relativistic) and (relativistic) velocities as well as the effects at ultra – relativistic velocities. Bloch correction is expressed in terms of the transport cross section for electron – ion scattering and dependence on the scattering phase shifts.

1. Introduction:-

The electronic energy loss has been studied for many years because of its direct application in problems concerning material damage, ion beam analysis and plasma physics. The theoretical treatment of the energy loss in atomic collisions has been greatly improved over the last decades[1]. Stopping power, i.e. energy loss of energetic particles per unit length in matter, has been studied experimentally and theoretically since the beginning of the 20^{th} century because of its wide application area, such as ion implantation, fundamental particle physics, nuclear physics, radiation damage, radiology, and structure analysis of solid target by Rutherford backscattering spectroscopy[2]. The slowing down of energetic ions in matter is dominated by momentum exchanging collision with electrons. The theory of this venerable subject was formulated early on by Bohr [3]and Bethe[4]. The first classical calculation of the energy loss of energetic particles was made by Bohr[3], while the first quantum mechanical treatment was done by Bethe[4]. This latter theory of stopping power is particularly accurate when the projectile's velocity is sufficiently high. It was modified by Bloch[5], and it was shown that at relativistic velocities a Mott correction for spin changing collisions was required[6]. Lindhard and Sorensen performed exact quantum mechanical calculations on the basis of the Dirac equation to produce values for the average energy loss and straggling which are stated to be accurate for any value of projectile charge[7].

2. Stopping power:-

The mean ionization energy loss of charged particles heavier than electrons is given by the Bethe expression[8]

$$-\frac{1}{\rho}\frac{dE}{dx} = 4\pi N_a r_e^2 mc^2 \frac{Z_1^2 Z_2}{A_1 A_2}\frac{1}{\beta^2}L(\beta)$$

(1)

$L(\beta)$ is the ionization logarithm and presented in the following form

$$L(\beta) = L_0(\beta) + \sum_i \Delta L_i$$

(2)

$L_0(\beta)$ = ln $\left(\frac{2mc^2\beta^2\gamma^2}{I}\right) - \beta^2 - \frac{\delta}{2}$
(3)

Where

γ = $(1 - \beta^2)^{-1/2}$ is the Lorentz factor

$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2}$ is the classical electron radius

$\beta = \frac{v}{c}$ is the speed of the particle relative to c

Z_1 and A_1 are the charge and mass of the projectile (in a. m. u.)

Z_2 and A_2 are the charge and mass of the target material

I and δ are the mean excitation energy and density correction, respectively.

N_a is Avogadro's number

When neglecting all the corrections ΔL_i and dealing only with the $L_0(\beta)$, eq.(1) is referred to as the Bethe equation. The corrections ΔL_i are to take into account the deviations from the Bethe theory for ions at both low and high energies[8]. This is the form derived originally from the quantum perturbation theory, and the first two terms are typically called the Bethe result. The third terms is the density effect. We will refer to L_0 as the Bethe result inclusive of the density effect[9].

At high energies, the electronic stopping is determined by Bethe's or Bohr's treatment[10]. The decisive point is whether or not the problem can be treated by classical theory. This is possible for large values of Bohr's parameter[11].

$K = \frac{2Z_1 v_0}{v} = 2\eta$

In the quantum mechanical limit K □ 1 Bethe’s formula based on a first order perturbation treatment gives the high – energy expression in the non relativistic case valid for light ions[10]

$L_{Bethe} = \ln \frac{2mv^2}{I}$
(4)

Once notes that the condition for quantum can not be expected to hold for slow projectiles or projectiles of high atomic number. In this case the logarithm in eq.(4) is replaced by Bohr’s expression[10]

$L_{Bohr} = \ln \frac{C\,m\,v^3}{Z_1 e^2 \omega}$
(5)

$C = 2e^{-\gamma} = 1.1229$; $\gamma = 0.5772$ is (Euler’s constant)

The major difference is that Z_1 enters into the argument of the logarithm, and therefore, influences the position of the stopping maximum. ω is a characteristic frequency of each electron level of the target atom, since the derivation is performed for a harmonic oscillator[10].

3. Bloch correction (ΔL_{Bloch}):-

Bloch indicated the exact scattering amplitude (but non – relativistic) should be adopted for collisions with small impact parameter, and derived a correction which is called (Z_1^4) correction term[12]

$$\Delta L_{Bloch} = Z_1 L_2 = \psi(1) - Re\psi\left(1 + i\frac{Z_1 v_0}{v}\right) \quad (6)$$

Here, $\psi(x) = d \ln \Gamma(x) / dx$ is the digamma function, v_0 is the Bohr velocity and with $y = \frac{Z_1 v_0}{v}$, eq.(6) becomes

$$\Delta L_{Bloch} = Z_1 L_2 = \psi(1) - Re\psi(1 + iy) \quad (7)$$

To bridge the gap between the Bethe's quantum mechanical and Bohr's classical formula. This term is mainly originated in the close collision with small scattering angle which is important for low velocity ions[12]. Eq.(6) may be solved as a chain

$$\Delta L_{Bloch} = Z_1 L_2 = -y^2 \sum_{n=1}^{\infty} [n(n^2 + y^2)]^{-1} \qquad \text{for } y>1 \quad (8)$$

$$\Delta L_{Bloch} = Z_1 L_2 = \sum_{n}^{\infty} (-1)^n \xi(2n + 1) n\, y^2 \qquad \text{for } y<1 \quad (9)$$

Where n=1, 2, 3, …… and ξ is the Rieman function

From a practical viewpoint of calculating accurate stopping powers, Bichsel has proposed simple parameterization of the Bloch correction which accurately fits a wide range of high velocity stopping data[13,14]

ΔL_{Bloch} = $Z_1 L_2$ = $-y^2$[1.202 − y^2(1.042 − 0.855y^2 + 0.343y^4)]
(10)

For low velocity, the value of(ΔL_{Bloch}) becomes

ΔL_{Bloch} → 0.58 − ln(y)
(11)

And thus the Bloch correction provides the transition to the classical stopping formula of Bohr.

For high velocities, i. e. y → 0, the value of (ΔL_{Bloch}) becomes

ΔL_{Bloch} = $-1.202y^2$
(12)

This term is usually quite small.

According to Bloch, the stopping cross section of an atom is determined by the following expression for the stopping number[5]

L_{Bloch} = L_{Bethe} + ΔL_{Bloch}

L_{Bloch} = $\ln\frac{2mv^2}{I} + \psi(1) - Re\psi\left(1 + i\frac{Z_1 v_0}{v}\right)$
(13)

When Bloch correction(ΔL_{Bloch}) is added to (L_{Bethe}), one arrives at the Bohr stopping formula at the low – velocity end. ΔL_{Bloch} reduces to the Bohr logarithm

eq.(5) at low projectile speed and at high projectile speed, ΔL_{Bloch} goes to zero[3].

Figure (1) shows the results of Bloch correction as a function of energy for protons in different targets Al(Z_2=13) and Au(Z_2=79) which are calculated from eq.(10) at high velocity. In this figure, the Bloch correction of protons is the same in two target and no variation with Z_2 because it is independent on the target and this is mathematically clear as shown in eq.(10). From the figure, the Bloch correction decreases with increasing the energy and becomes quite small and approaches to zero at very high velocity.

Figure (2) shows the percent contribution of Bloch correction to stopping number as a function of energy for protons in different targets Al(Z_2=13) and Au(Z_2=79) which are calculated from eq.(10) at high velocity. From the figure, the percent of Bloch correction decreases with increasing the energy and becomes small at high velocity and the Bloch correction for Al target contributes less than 1% for all energies above (10MeV) while for Au target it contributes less than 1% for all energies (15MeV), therefore there is a divergence in values at low velocities and an convergence in values of percent contribution of Bloch correction at high velocities. The percent Bloch correction in Al target is larger than that of Au target because the targets are different and for each one a specific atomic number and there are a number of corrections to the stopping number for each target.

Figure (3) shows the results of Bloch correction as a function of energy for different incident particles(protons and alpha particles) in N target which are calculated from eq.(10) at high velocity. In this figure, the Bloch correction for protons is different from that for alpha particles and they have larger values than that of alpha particles because the Bloch correction is dependent on the projectile and its atomic number (Z_1) and this is mathematically clear as shown in eq.(10) . From the figure, the Bloch correction decreases with increasing the energy and becomes quite small and approaches to zero at very high velocity.

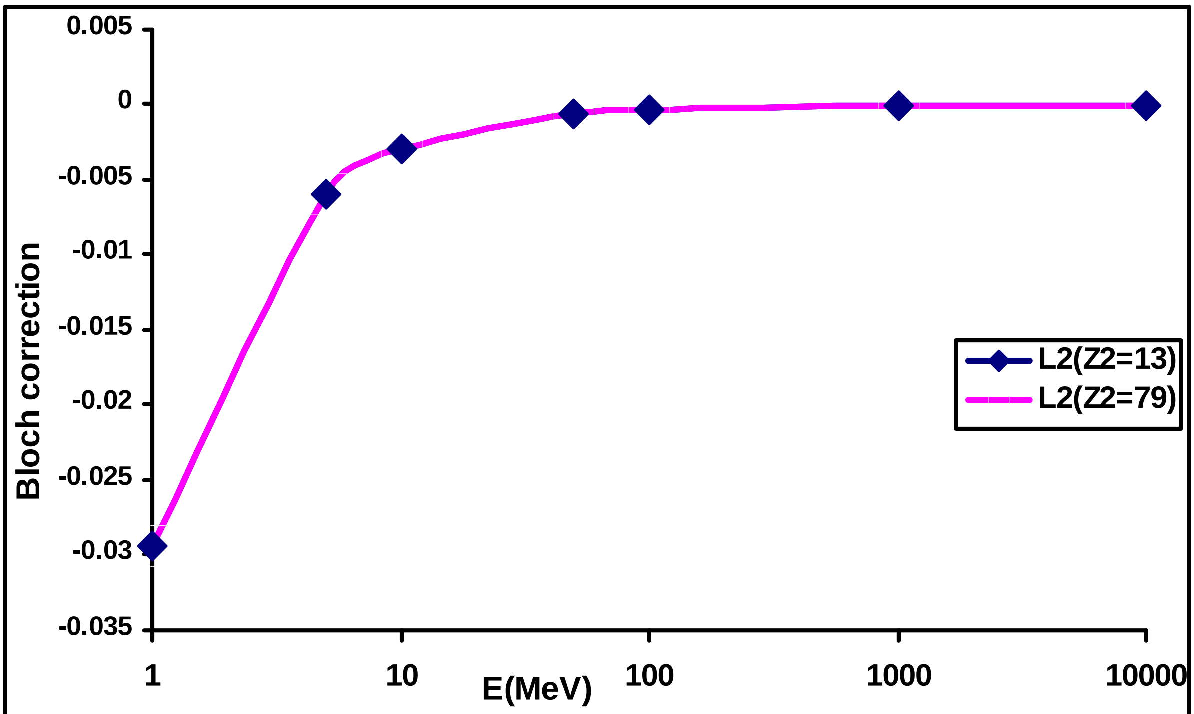


Fig.(1) Bloch correction at high velocity for protons in Al(Z2=13) and Au(Z2=79)

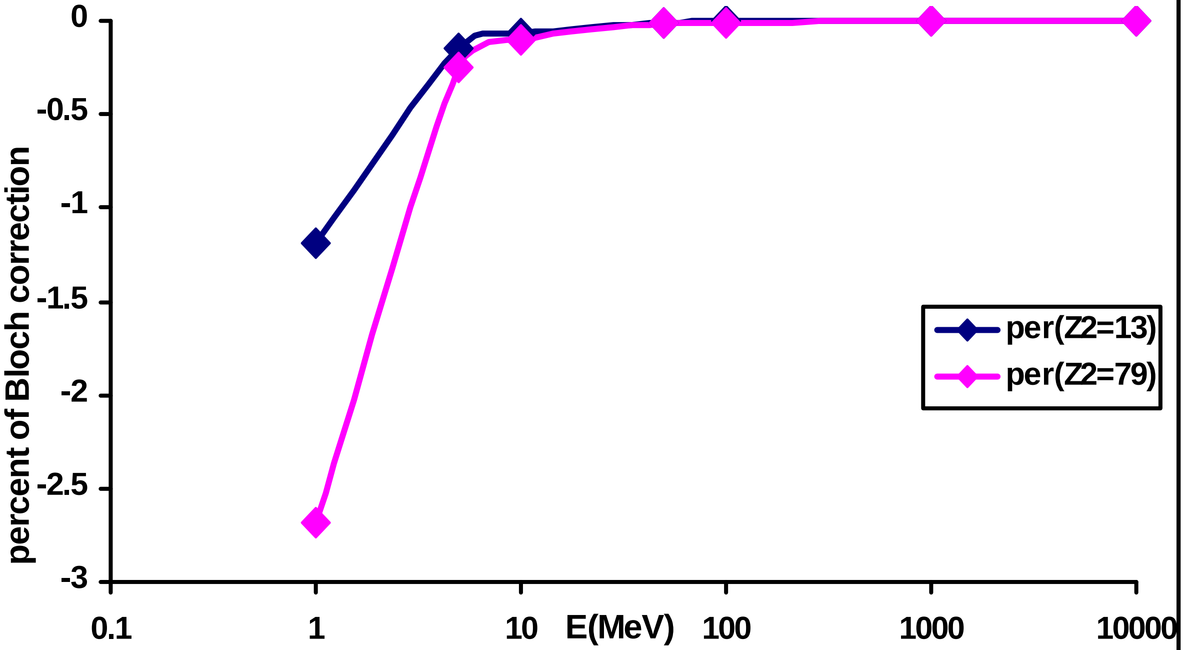


Fig.(2) Percent contribution of Bloch correction to stopping number at high velocity for protons in Al (Z2=13) and Au (Z2=79)

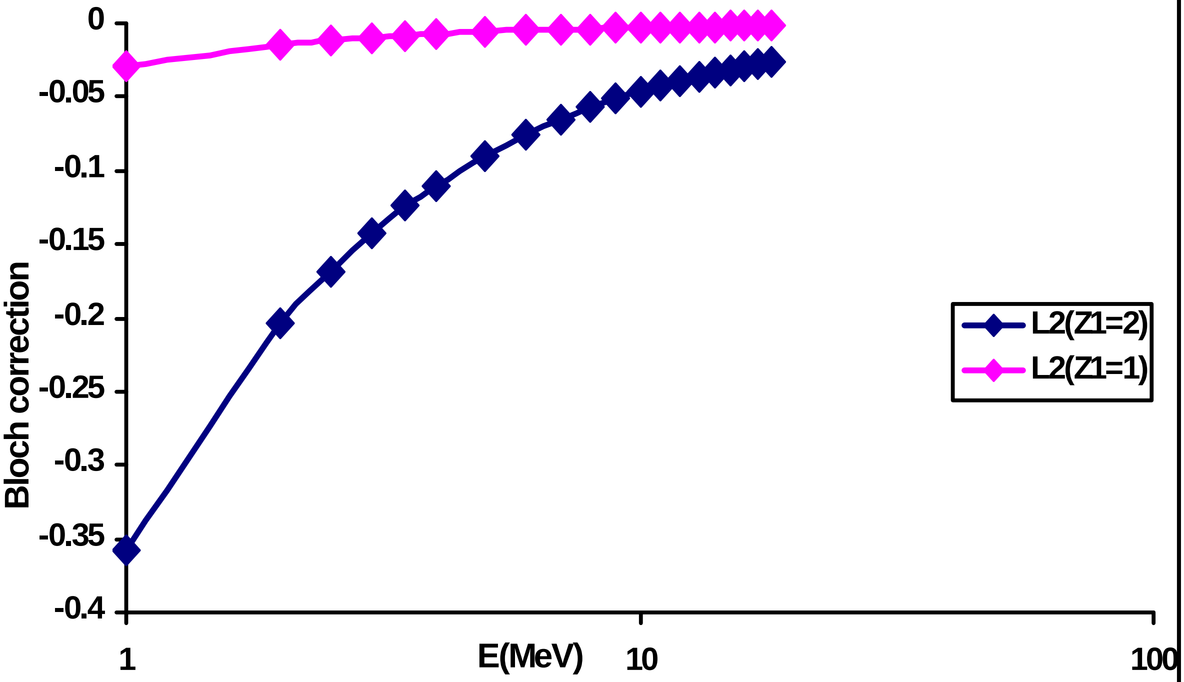


Fig.(3) Bloch correction at high velocity for protons (Z1=1) and alpha particles (Z1=2) in N (Z2=7).

4. Bloch correction and phase shift:-

For a binary collision with a target electron initially at rest, the stopping cross section can be expressed as[7]

$S = mv^2\sigma_{tr}$
(14)

Where the transport cross section σ_{tr} is defined by

$\sigma_{tr} = \int(1 - \cos\theta)\, d\sigma(\theta)$
(15)

θ is the scattering angle in the centre – of – mass system. By using the quantum formalism and depended on the spherical symmetric potential and Legendre polynomials, eq.(15) is written as[7]

$\sigma_{tr}^{qu} = \frac{\lambda^2}{\pi}\sum_{l=0}(l + 1)\, sin^2(\delta_l - \delta_{l+1})$
(16)

$L_{tr} = \frac{\pi^2\sigma_{tr}}{\lambda^2 K^2}$
(17)

Where δ_l is the phase shift and l is the orbital angular momentum quantum number. And by using Rutherford scattering for the phase shift

$\delta_l = arg\Gamma(l + 1 + i) + \frac{K}{2}\ln 2K$
(18)

$(\delta_l - \delta_{l+1}) = arg\left(l + 1 + i\frac{K}{2}\right)$
(19)

Where Γ is gamma function and by supposing that $z = x + iy$, $x = l + 1$, $y = \frac{K}{2}$ and $\theta = \delta_l - \delta_{l+1}$, eq.(19) becomes

$\theta = arg(x + iy)$
(20)

$\sin\theta = \frac{y}{\sqrt{x^2+y^2}}$

$\sin\theta = \frac{(К/2)}{\sqrt{(l+1)^2+(К/2)^2}}$

$sin^2\theta = \frac{(К^2/4)}{(l+1)^2+(К^2/4)}$

$sin^2(\delta_l - \delta_{l+1}) = \frac{(К^2/4)}{(l+1)^2+(К^2/4)}$
(21)

By substituting eqs.(21, 16) into eq.(17),we get the quantum stopping number L_{tr}^{qu} [7]

$L_{tr}^{qu} = \sum_{l=0} \frac{(l+1)}{(l+1)^2+(К^2/4)}$
(22)

The first order perturbation of the quantum stopping number L_{tr}^{qu} when $(К/2) \to 0$

$L_{tr}^{per} = \sum_{l=0} \frac{1}{(l+1)}$
(23)

From the equation above, we can get on Bethe stopping number at high velocities as illustrated in eq.(4) and classically, the stopping number will be in the form [7]

$L_{tr}^{cl} = \int dl \ \frac{l}{l^2+(К^2/4)}$
(24)

After integrating eq.(24), we get on Bohr stopping number at low velocities as illustrated in eq.(5).

After solution the transport cross section σ_{tr} that is given in eq.(16) on the dependence on the quantum formalism by using Legendre polynomial and Rutherford scattering for the phase shift given in eq.(21)[15]

$sin^2(\delta_К - \delta_{К-1}) = \left(\frac{\eta}{К}\right)^2$
(25)

The Bloch correction (ΔL_{Bloch}) at non – relativistic speed, Bloch correction when $\gamma \to 1$ is

$$\Delta L_{Bloch} = \sum_{l=0}^{\infty} \left| \frac{(l+1)}{(l+1)^2 + (K^2/4)} - \frac{1}{(l+1)} \right|$$
(26)

When the Bohr's parameter in eq.(26) is small ($K \ll 1$), the Bloch correction will be given by eq.(12).

The transport cross section σ_{tr} at relativistic speed is given by the equation[16]

$$\sigma_{tr} = \frac{\lambda^2}{\pi} \sum_{l=0} (l+1) \left[\frac{l+2}{2l+3} sin^2(\delta_{-l-1} - \delta_{l-2}) + \frac{l}{2l+1} sin^2(\delta_{l+1} - \delta_l) + \frac{1}{(2l+1)(2l+3)} sin^2(\delta_{l+1} - \delta_{-l-1}) \right|$$
(27)

$$l = \begin{cases} K & for \quad K > 0 \\ -K - 1 & for \quad K < 0 \end{cases}$$
(28)

Eq.(27) may be writer in the form

$$\sigma_{tr} = \frac{\lambda^2}{\pi} \sum_{K=0} |K| \left[\frac{K-1}{2K-1} sin^2(\delta_K - \delta_{K-1}) + \frac{1/2}{4K^2-1} sin^2(\delta_K - \delta_{-K}) \right|$$
(29)

The phase shift at relativistic speed is given by[15]

$$\delta_K = \xi_K - arg\Gamma(s_K + 1 + i\eta) + \frac{\pi}{2}(l - s_K)$$
(30)

The magnitude of the [$arg\Gamma(s_K + 1 + i\eta)$] is given by the equation[17]

$$arg\Gamma(s_K + 1 + i\eta) = \frac{\eta}{2}[(s_K + A + 1/2)^2 + \eta^2] + (s_K + 1/2)\ arctan\frac{\eta}{s_K + A + 1/2} - \eta + arg\left(1 + \sum_{n=1}^{6} \frac{C_n}{s_K + n + i\eta}\right)$$
(31)

By substituting eq.(31) into eq.(30), we get

$$\delta_{K} = \xi_{K} - \frac{\eta}{2}[(s_{K} + A + 1/2)^2 + \eta^2] + (s_{K} + 1/2)\ arctan\frac{\eta}{s_{K}+A+1/2} - \eta + arg\left(1 + \sum_{n=1}^{6}\frac{C_n}{s_{K}+n+i\eta}\right) + \frac{\pi}{2}(l - s_{K})$$

(32) A is a factor = 5

Cn = (76.18009173, -86.50523033, 24.81409827,

-1.231739516, 0.120858003*10-2, -0.536382*10-5)

$$s_{K} = \sqrt{K^2 - (\alpha Z_1)^2}$$

(33)

$$e^{2i\xi_{K}} = \frac{K - i\eta\gamma}{s_{K} - i\eta}$$

(34)

$$tan(\delta_{K} - \delta_{-K}) = -\frac{\eta}{K\gamma}$$

(35)

Where $\alpha = (1/137)$ is the usual fine – structure constant.

$$sin^2(\delta_{K} - \delta_{K-1}) = \left(\frac{\eta}{K}\right)^2\left(1 + \frac{1-(1/\gamma)}{2(K-1)}\right)^2$$

(36)

The Bloch correction(ΔL_{Bloch}) at relativistic speed, Bloch correction when $\gamma \to 0$ is[7]

$$\Delta L_{Bloch} = \sum_{K=-\infty}^{\infty}\left[\frac{|K|}{\eta^2}\frac{K-1}{2K-1}sin^2(\delta_{K} - \delta_{K-1}) - \frac{1}{|K|}\right] + \frac{1}{\eta^2}\sum_{K=1}^{\infty}\frac{K}{4K^2-1}sin^2(\delta_{K} - \delta_{-K}) + \frac{v^2}{2c^2} = \left(\frac{\eta}{K}\right)^2$$

(37) The Bloch correction (ΔL_{Bloch}) at ultra relativistic speed, Bloch correction when $\gamma \to \infty$ is

$$\Delta L_{Bloch} = L_{tr} - L_{tr}^{per}$$

(38)

$$\Delta L_{Bloch} = \sum_{K=-\infty}^{\infty}\left[\frac{|K|}{\eta^2}\frac{K-1}{2K-1}sin^2(\delta_{K} - \delta_{K-1}) - \frac{1}{2|K|}\right] + \frac{1}{\eta^2}\sum_{K=\infty}^{\infty}\frac{K}{4K^2-1}\frac{1}{K^2+(\eta/\gamma^2)} + \frac{v^2}{2c^2}$$

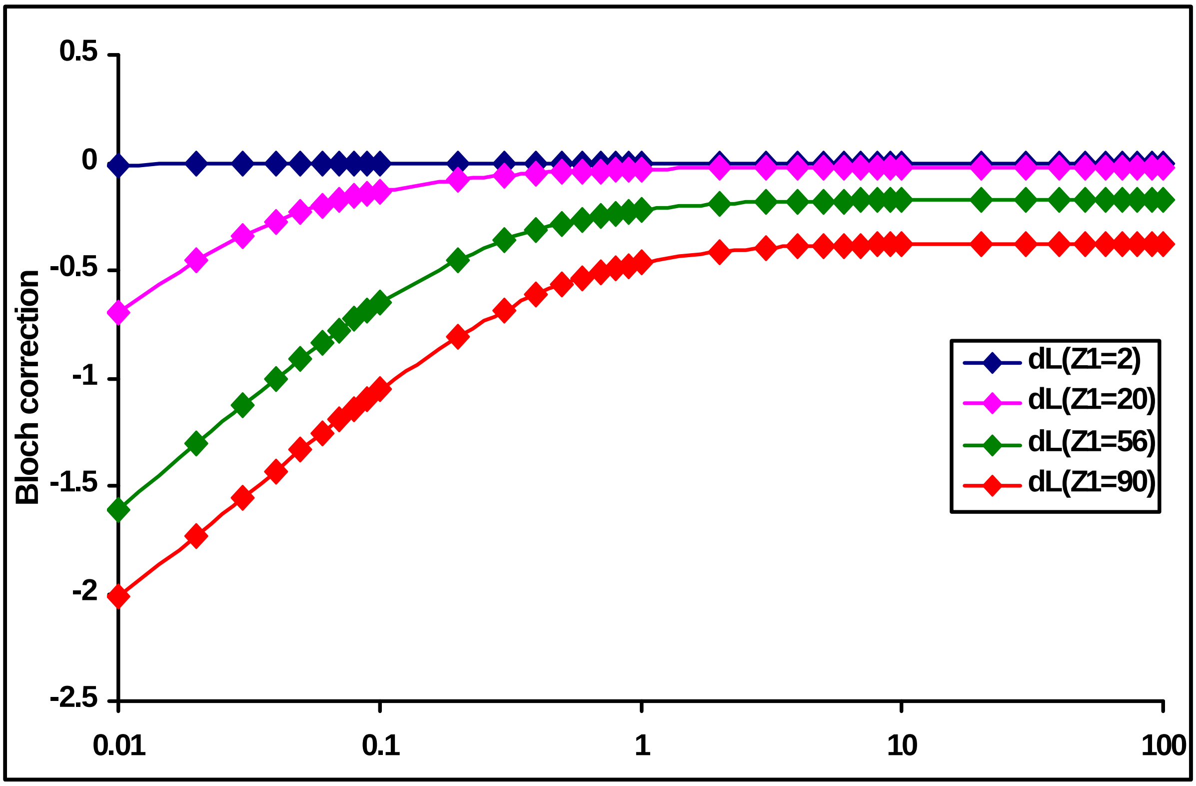
(39)

Figure (4) shows the results of Bloch correction at non – relativistic velocity as a function of energy for different projectile of atomic number(Z_1=2, 20, 56, 90) which are calculated from eq.(26). From this figure, the Bloch correction approaches the classical Bohr stopping number at low velocities especially at high atomic number and for this reason , there is a negative stopping for Bloch correction.

Figure (5) shows the results of Bloch correction at relativistic velocity as a function of energy for different projectile of atomic number(Z_1=2, 20, 56, 90) which are calculated from eq.(37). From this figure, the Bloch correction has a negative values at low velocities but there is an inversion in atomic number at high velocity and positive Bloch correction.

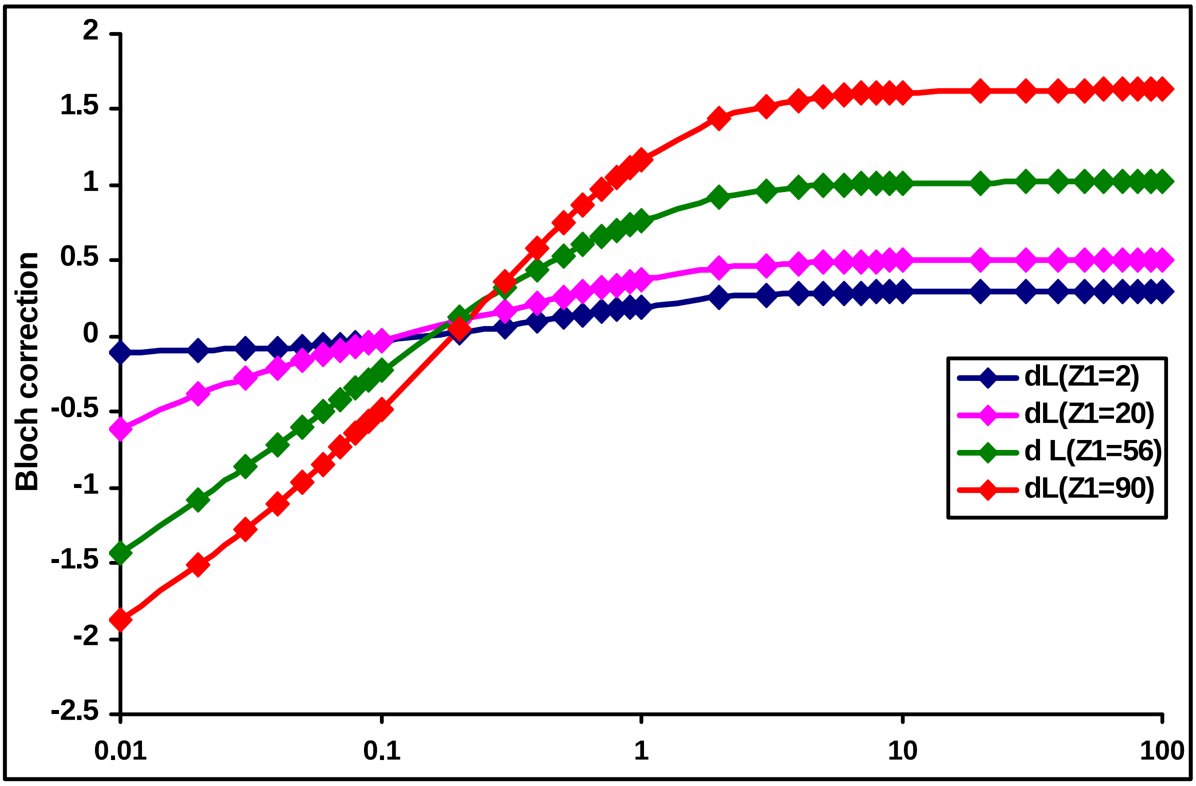
Figure (6) shows the results of difference of Bloch correction at relativistic eq.(37) and non – relativistic eq.(26) velocity as a function of energy for different projectile of atomic number(Z_1=2, 20, 56, 90). From this figure, the Bloch correction at high velocities is independent on the velocity and dependent on the (l) orbital angular momentum quantum number, therefore the difference of Bloch correction at high velocity remains constant.

Figure (7) shows the results of Bloch correction at non – perturbative and non – relativistic velocity as a function of energy for different projectile of atomic number(Z_1=2, 20, 56, 90) which are calculated from eq.(39). From this figure, when($\gamma \rightarrow \infty$), the second term in eq.(39) approaches to zero therefore the Bloch correction remains constant at high velocity but when($\gamma \rightarrow 0$), the second term in eq.(39) approaches to infinity in the negative direction.



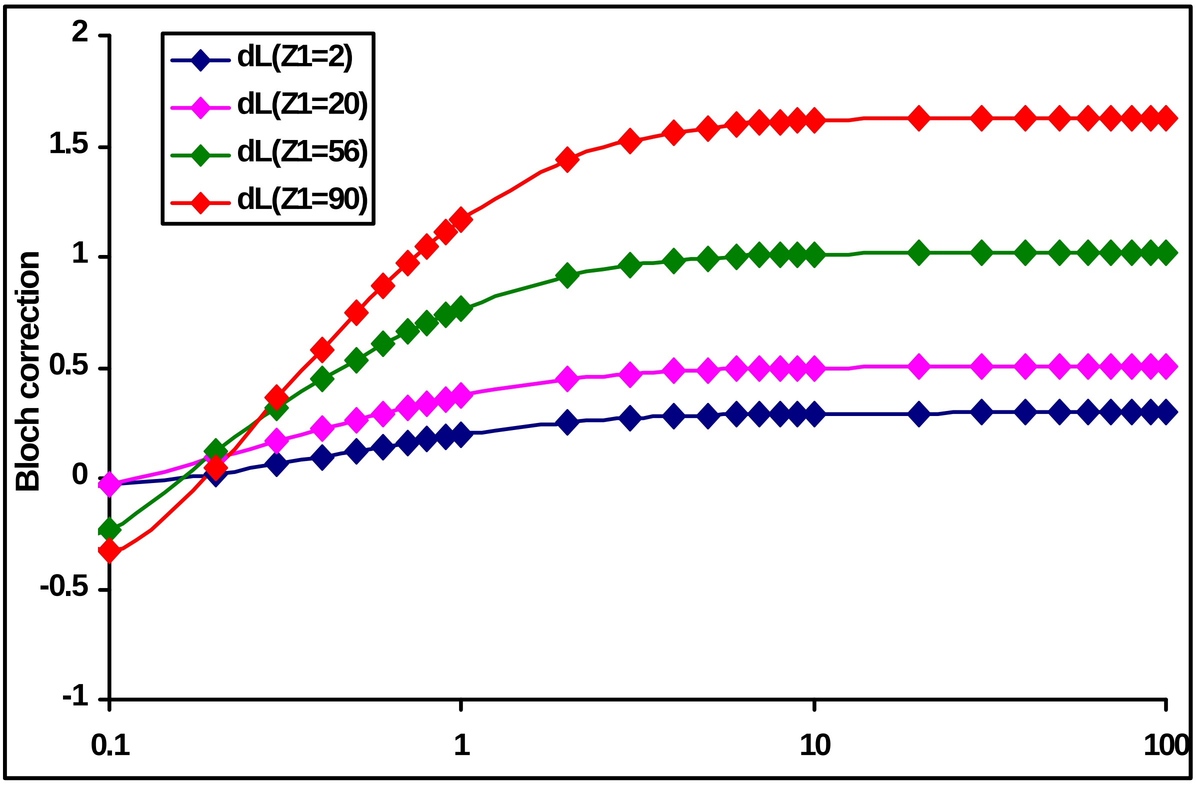
$\gamma - 1$

Fig.(4) Bloch correction at non – relativistic velocity



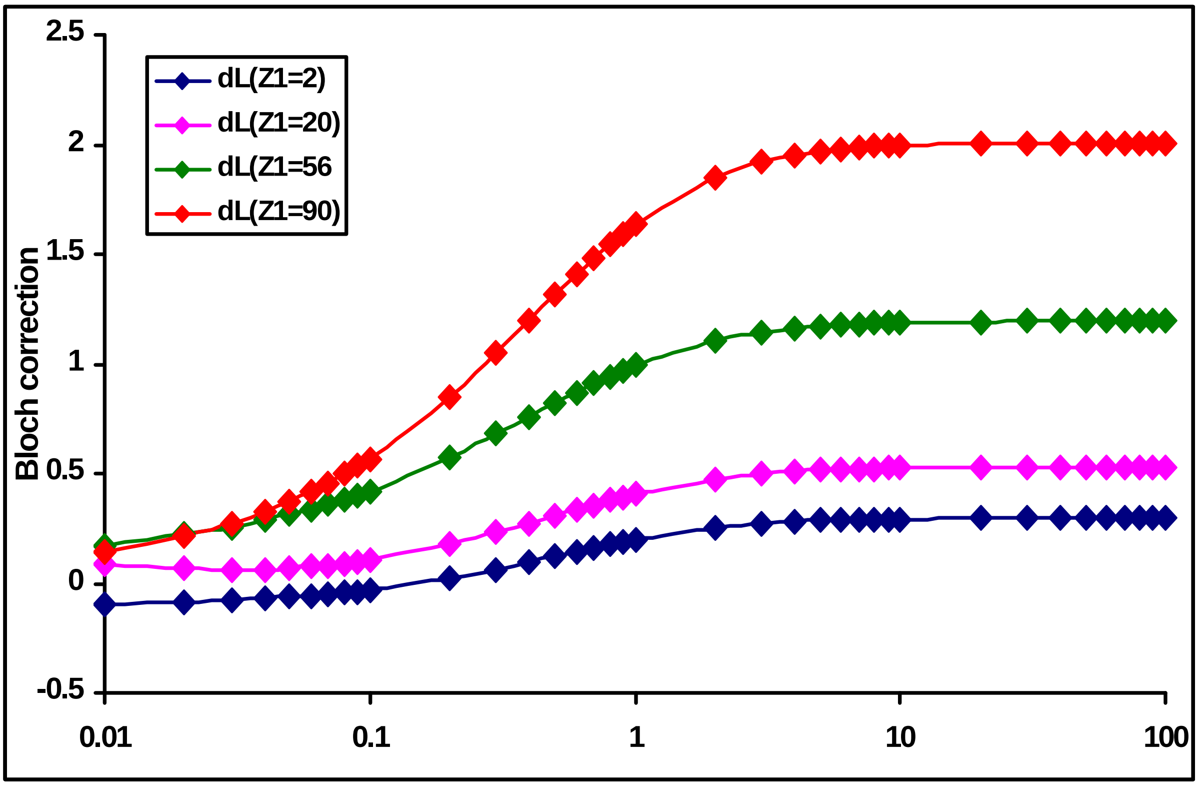
$\gamma - 1$

Fig.(5) Bloch correction at relativistic velocity



$\gamma - 1$

Fig.(6) Difference Bloch correction at relativistic and non relativistic velocity



$\gamma - 1$

Fig.(7) Bloch correction at non relativistic and relativistic velocity

5. Conclusions:-

The main stopping mechanism is the slowing down due to interactions with target atoms through excitations and ionizations of target electrons via Coulomb scattering. The Bethe theory of calculating stopping power of a point charge penetrating through matter at a non – relativistic velocity can be used over a wide energy interval for fast charged particles based on first Born approximation for atomic collision events which it provides a stopping dependent on the square of projectile charge (Z_1e) . Deviations from the (Z_1^2) dependence are especially large at low velocity. For decreasing velocities, high order of (Z_1) terms (Z_1^3 Barkas effect) and (Z_1^4 Bloch correction) dependence in stopping power may be become important. Since the accuracy of this scheme deteriorates with increasing projectile charge and decreasing speed, it seemed reasonable to start at the opposite end, i. e. the classical limit (Bohr theory). Bohr pointed that the regime of validity of classical – orbit models and of quantal perturbation theory are roughly complementary. Bloch evaluated the differences between the classical (Bohr) and quantum – mechanical (Bethe) approaches for particles with velocities much larger than the target electrons. He showed that Bohr's harmonic oscillator approach was valid also in the quantum mechanics of a bound electron if the energy transferred was assumed to be the mean energy loss.

For light ions (at high velocity and small Bohr's parameter κ), the Bloch correction becomes small and usually approaches to zero and the Bloch stopping number (L_{Bloch}) approaches that of Bethe results eq.(4) but at low velocity, the Bethe theory becomes unphysical because of the negative stopping number, therefore the Bloch correction must be added to Bethe stopping number and arrives at the Bohr stopping number eq.(5) and provides the transition to the classical stopping power. Bloch correction depends upon the projectile and its velocity (energy) and are independent of the sign of the projectile charge (Z_1e). The phase shifts have been added in the calculation of Bloch correction in relativistic and non – relativistic velocities in order to get more exact results. At high velocity, Bloch correction is independent on the velocity therefore the difference of Bloch correction at relativistic eq.(37) and non – relativistic eq.(26) velocity remains constant.

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تصحيح بلوخ عند السرعة العالية

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الخلاصة:-

إن احد الحاجات إلى معجلات متنوعة لتحفيز التطورات الأخيرة في حساب الطاقة المفقودة للجسيمات المشحونة في المادة هي طاقة التأين المفقودة للايونات الثقيلة. قام بلوخ بدمج نظرية بور وبيتا بطريقة واضحة جدا حيث وجد صيغة جسريه بين تقريب بور الكلاسيكي لمعامل الصدم و تقريب بيتا الكمي للزخم الزاوي بالنسبة للطاقة المفقودة. تم في هذا البحث دراسة سلوك تصحيح بلوخ للبروتونات في كل من عنصر الألمنيوم (Al) والذهب (Au) بالإضافة إلى ذلك تم قياس تصحيح بلوخ للبروتونات وجسيمات ألفا في عنصر النتروجين (N). تضمين لتصحيح بلوخ في معادلة قدرة الإيقاف مع الأخذ بنظر الاعتبار الانحراف عن نظرية بيتا في السرع النسبية واللانسبية بالإضافة إلى السرع العالية فوق النسبية. إن تصحيح بلوخ قد تم التعبير عنة بدلالة المقطع العرضي للانتقال لاستطارة ايون – إلكترون وكذلك بالاعتماد على فرق الطور.