Barkas and Bloch corrections dependent to electronic energy loss calculation

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Abstract:

In this research the energy loss was calculated theoretically by using modified Bethe-Bloch theory. Protons and alpha particle stopping power were calculated in the liquid composition such as blood($C_{11}H_{10}N_3O_{75}Na_2S_2Cl_3K_2$), water(H2O) and solid elements such as (Cu,Au) by using Bragg's Rule for compounds. Also programming the equations by using (MATLAB) language. the values of Bloch's and Barkas corrections of energy range (0.25-1000)MeV had been calculated. The calculations were compared with the experimental data of the SRIM 2012 This comparison showed a good agreement with the experimental data.

Keywords: Phthalocyanine, Substrate temperature, Grain size, crystalline, Nano rods.

اعتماد تصحيحات باركز وبلوخ لحساب فقدان الطاقة الالكترونية

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الخلاصة

في هذا البحث تم حسب فقدان الطاقة نظريا بأستخدام نظرية بيث-بلوخ المعدلة وحسبت قدرة الايقاف للبروتونات وجسيمات الفا في مركبات سائلة مثل الدم $(C_{11}H_{10}N_3O_{75}Na_2S_2Cl_3K_2)$ والماء $(C_{11}H_{10}N_3O_{75}Na_2S_2Cl_3K_2)$ وعناصر صلبة مثل الذهب والنحاس (Cu, Au) بأستخدام قاعدة براك للمركبات وبرمجت المعادلات بأستعمال لغة الماتلاب ،حيث حسبت تصحيحات بلوخ وباركز عند مدى الطاقة (O.25-1000) فورنت الحسابات مع النتائج العملية لبرنامج واظهرت توافق جيدا.

الكلمات المفتاحية: قدرة الايقاف ، عدد الايقاف ،تصحيح باركز ،تصحيح بلوخ.

1. Introduction

The electronic stopping power had been calculated for many years because of its direct application in problems concerning material damage, ion beam analysis and plasma physics. The theoretical treatment of the stopping power in atomic collisions has been greatly improved over the latter decades[1] Bichsel compared experimental and theoretical values of the Barkas equation for proton (p), antiproton (P'), alpha Particle(α) and Lithium ions. For a gold absorber, existing theories of Baraks term L_1 do not provide a great approximation for the experimental data. The Bloch term

L₂ is used without any modifications. [2] Sigmund and Schinner have shown that the difference between the stopping power on a swift charged particles penetrating through matter and there anti-particles (Barkas correction). has been calculated theoretically as a function of velocity and projectile-target combination [3].

2. Stopping Power

A charged particle moving through a material exerts Coulomb effect on many atoms simultaneously. Every atom has many electron with different ionization and excitation potentials. As a result of this, the moving charged particle interacts with a tremendous number of electrons-millions. Each interaction has its own probability for occurrence and for a certain stopping power. It is impossible to calculate the stopping power by studying individual collision. Instead, an average energy loss is calculated per unit distance travelled. The calculation is slightly different electrons or positrons than for heavier charged particles like p, d, and a particle, for the following reason Relative calculation of the energy loss of charged particles with kinetic energies below a few MeV/u is required in Monte Carlo simulation for stopping power processes and the accurate estimate of their ranges in matter[4]. The energy loss of penetrating through matter number of scattering governed by a processes such as[5]:-

- 1) Excitation and ionization of target electron.
- 2) Electron capture.
- 3) Projectile excitation and ionization.

The theoretical work about the dierential stopping power of charged particles in matter has been started by Bohr

as a classical formula at non-relativistic velocities[6]

$$-\frac{dE}{dx} = \frac{4\pi Z_1^2 Z_2 e^4}{m_e v^2} L_{Bohr}$$
 (1)

where

$$L_{Bohr} \approx ln \left(\frac{Cm_e v^3}{|z_1 e^2| w} \right)$$

Bethe obtained a similar expression from a quantum mechanical approach but wrote L_{Bethe} in terms of an average excitation energy (I) as[7]

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

The formalism of Bethe–Bloch theory of energy loss, including various modifications, has been described extensively in several investigations[8]

$$\begin{split} \frac{dE}{dx} &= \frac{4\pi Z_2 Z_1^2 e^4}{m_e v^2} N \left[ln \frac{2m_e c^2 v^2}{1-\beta^2} - \beta^2 - ln I \right. \\ &\left. + L_{Bloch} \right] \end{split} \tag{3}$$

$$\beta = v/c$$
 where

$$L_{Bloch} = L_0 + Z_1 L_1 + Z_1^2 L_2$$

Where L_0 is the Born correction, Z_1L_1 is Barkas effect, which comes due to the polarization and $Z_1^2L_2$ is Bloch effect.

3. Barkas correction

Barkas correction has been interpreted as a polarization effect in the stopping material depending on the charge of the projectile. It shows as the second term (proportional to Z_1^3) in the implied Born expansion of the stopping power[9].

The Ashley correction led to a term in Z_1^3 for the energy transfer to distant collisions. They suggested for the high velocity limit a form [10]:-

$$L_1 = \frac{\chi F_{ARB}(b/X^{1/2})}{Z_2^{1/2}X^{3/2}}$$
 (4)

Where
$$X = \frac{v^2}{Z_2 v_0^2} = \frac{(137\beta)^2}{Z_2}$$

$$b = \eta \chi Z_2^{1/6}$$

The term χ is a free – electron gas parameter which corrects for binding forces .

Jackson and McCarthy gave a function which can be approximated to better than $\pm 3\%$ by [11]

$$Z_1 L_2 = \frac{B_0 Z_1}{v^2} \left[g - h \ln(V + X^2) \right] / Z_2^{\frac{1}{2}}$$
 (5)

$$V = \frac{v}{v_0 Z_2^{1/2}}$$

Where $1 \le V \le 10$, v_0 is the Bohr velocity and for $X^2 = 2$ at g=0.477, h=0.1385, while $X^2 = 3$ at g=0.607, h=0.175. Jackson and McCarthy suggest a different minimum impact parameter $a_w = (2m_e\hbar w)^{1/2}$

Ashley et.al led to a term in Z_1^3 for the energy transfer to distant collisions. They suggested for the high velocity limit a form[12]

$$Z_1 L_1 = \frac{3\pi Z_1 e^2 \omega}{2mv^3} \ln \left(\frac{v}{1.7a_\omega \omega} \right)$$
 (6)

where v is the velocity of the projectile, ω is the free electron gas plasma frequency.

4. Bloch correction

L_{Bloch} is the stopping number and the standard expression of Bloch's formula is given by the following equation [13]:

$$L_{Bloch} = L_{Bethe} + \Delta L = \ln \frac{2m_e v^2}{I} + Re[\Psi_{(1)} - \Psi_{(+iz_1 v_0/v)}]$$
(7)

where I denotes the mean excitation energy of a target atom, ψ the digamma function, and Re is the real part.

With
$$y = \frac{Z_1 v_0}{v} = \frac{Z_1}{137\beta}$$

For y > 1, eq.(7) becomes [53]

$$Z_1^2 L_2 = -y^2 \sum_{i=1}^{\infty} [j(j^2 + y^2)]^{-1}(8)$$

But when y < 1, eq.(7) becomes

$$Z_1^2 L_2 = \sum_{j=1}^{\infty} (-1)^j \, \xi(2j + 1) y^{2j}$$
 (9)

where ξ represents Rieman function

Eq. (7) needs shell and Barkas corrections at low velocities and density and relativistic corrections at high velocities. The Bloch theory can thus also be seen as a correction to the Bethe theory in respect of more distant collisions and we can write the Bloch stopping number in two forms [6],

$$L_{\text{Bloch}} = L_{\text{bethe}} - 1.202 \left(\frac{Z_1 v_0}{v}\right)^2$$
 (10)

$$L_{Bloch} = L_{Bohr}$$

$$-\frac{1}{2} \left(\frac{v}{Z_1 v_0}\right)^2$$
 (11)

in the limit of high v and low Z_1e .

From a practical viewpoint of calculating accurate stopping powers, Bichsel has proposed a simple parameterization of the Bloch correction which accurately fits a large range of high velocity stopping results [9].

$$Z_1^2L_2 = -y^2 [1.202 - y^2 (1.042 - 0.855 y^2 + 0.343 y^4)]$$
 (12)

where
$$y = z_1 \alpha / \beta (\alpha = 1/137)$$

where the velocities is low, the value of $Z_1^2L_2 \rightarrow -0.58$ - ln(y), and thus the Bloch effect provides and For high velocities,

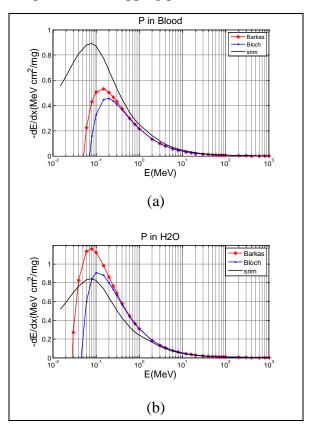
 $Z_1^2L_2 \rightarrow .-1.2 \text{ y}^2$. As will be shown in the next section, this term is Always quite small.

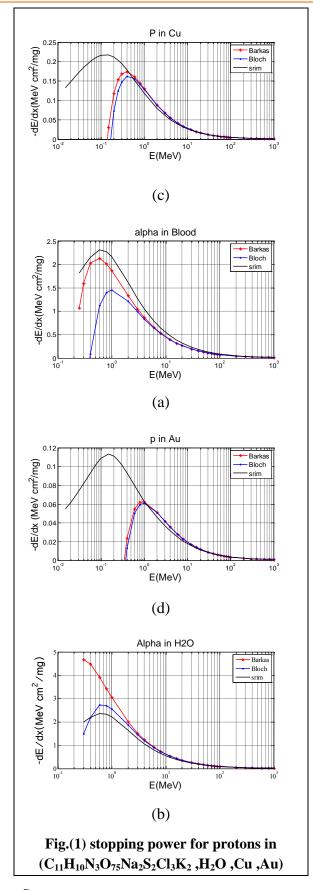
5. Result and Discussion:

Figure (1) shows The electronic stopping power of protons where it studied in composition blood ,water.and elements copper and gold. It also calculated Bethe Bloch modified formula using Bloch and Barkas corrections to indicate energy and the formulas function. equations(6,12). A simple divergance occurs in the beginning of the interval towards the ionization and irritability area(0.25-1)MeV for both corrections for the practical results of SRIM2012. This is due to the Barkas effect on these particles that results from the polarization effect on electrons. But it begins to move away when increasing the speed of projectile(E≥1 MeV), because the two corrections are essential in the high speeds (This occurs in the high speeds). When the medium (blood) liquid, is **Barkas** correction is closer to the practical results than that of Bloch, but when it is (water) liquid, Bloch's is closer. However, when the medium is solid elements, the two corrections are close together, but are rather far from the experimental results, and for 1MeV range, their results converge to be almost identical. In all cases, while increasing the energy, the suspension ability declines whereas the less than 0.08MeV area represents the effect of the nuclear suspension. And, the more than 0.4MeV area represents the nuclear suspension, and the area between these two areas represents the ionization and irritability area.

Figure (2) The electronic stopping power of the Alpha particle was studied in composition (blood and water), and elements (copper and gold). It also calculated Bethe Bloch modified formula using Bloch and Barkas corrections to indicate energy function, and the formulas in equations (6,12).. When projecting

blood with the Alpha particle, we noticed the good convergence at the beginning of the range of Barkas correction from the experimental results of the SIRM2012, and it increasingly rises when widening the used range of energy. When projecting water with the Alpha particle Bloch correction be closer to the experimental results, However, when the medium is solid elements, the two corrections are close together, but are rather far from the practical results, and on the 1Mev range, their results converge to be almost identical. We notice that the nuclear suspension area of the used mediums only appears at the areas less than 1MeV, whereas the nuclear suspension at the area that is greater than 0.7MeV.When the projectile is a proton, the two correction converge, but when the projectile is an Alpha particle, the two corrections diverge. That is, the increase of the atomic number and the mass of the projectile have a vivid impact on the stopping power.





6. Conclusions

1- When calculating the stopping power of the proton and Alpha particles projected on atomic targets such as (Cu, Au) and the other compositions, it was noticed that the stopping power increases as the energy of the projectile rises when it is projected on a certain area until it reaches a certain value. Then, it starts to decrease until it becomes very close to zero on the high energy values.

 $(C_{11}H_{10}N_3O_{75}Na_2S_2Cl_3K_2, H_2O, Cu, Au)$

- 2- The electronic stopping power is proportional with the atomic number of the charged particle, but has an inverse relationship with the atomic number of the medium.
- 3- The two corrections have good and converged results with the practical results.

4- The range of energy used to study the Bloch and Barkas corrections for the heavy particles (0.25 – 1000)MeV is considered good to fulfil Bloch and Barkas's correction formula of the heavy, charged particles used).

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