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Calculation of the energy deposited on the surface of C_{60} molecule resulting from the fall of the fast Si^+ ions using the Beth - Bloch equation

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ABSTRACT

The energy deposition of slow Si^+ *ions interacting with* C_{60} *molecule is determined theoretically, by using Bethe–Bloch equation which is applied at high energy. The obtained result is compared with Local Density Approximation equation at the energy (0.5 MeV) and found good agreement between the two formulas. The behavior of energy deposition with the atomic numbers has been calculated. Stopping number for both equations has been compared too.*

Keywords: Energy deposition, stopping power, Energy loss

INTRODUCTION

The energy deposition of a swift particle in matter per unit path $(-dE/dx)$, referred to as the stopping power of the material, has been made in the context of a model where energy transferred from ion projectile to the electron ,and to a lesser extent , to the nuclei of the target material [1,2]. The energy loss rate (stopping power) of matter for energetic particles is of recurring interest in physics, the understanding of the slow down of these particles is of great fundamental and applied physics relevance [3]. The high velocity ions are passing through a matter is usually assumes two major simplifications in stopping theory: (1) the ions are moving much faster than the target electrons and fully stripped of its electrons, (2) the ions are much heavier than the target electrons [4]. The transferred energy occurs from energetic projectile to surface electrons and nucleus, fraction of this energy is deposited to electronic degree of freedom. The deposited energy is partly spent for ionization (binding energy of electrons and their kinetic energy) and excitation the target atoms. However, some part of the deposited “electronic energy” is transferred to the vibration degree of freedom (i.e. to the internal energy of the molecular ion) [4, 5]. Most studies used Local Density Approximation (LDA) equation to calculate the electronic energy loss; it was introduced by Lindhard [4]. The Lindhard treatment is a many –body self-consistent treatment of an electron gas responding to a perturbation by a charged particle. It naturally includes the polarization of the electrons by the charged particle and the resultant charge screening and the plasma density fluctuations. It treats smoothly both individual electron excitation and collective plasmon excitation without separate 'distant' and 'close' collision processes. Lindhard's approach to the interaction of particle with a free electron gas makes the following assumption:

- The free electron gas consists of electrons at zero temperature (single electrons are described by plane wave) on a fixed uniform positive background with overall charge neutrality.

- The initial electron gas is of uniform density.
- The interaction of the charged particle is a small perturbation on the electron gas.
- All particles are non-relativistic.

Under this assumption Lindhard and Scharff in recent study were suggested considering each volume element of the target atom independently as an electron gas of uniform density that is equal to the electron density of the atom.

In this work the Bethe –Bloch equation has been used to calculate the deposition energy (which applied at high energy limit) and compared it with LDA equation at the primary energy (0.5 MeV) for the incident ion. The behavior of energy deposition as a function of atomic number has been found it .The bethe stopping number and LDA stopping number have been comported.

In this study, the use of equation Beth - Bloch to calculate the residual energy resulting from the fall of the ions on the surface of silicon particle in carbon energy ---- After a closer the following: as density scatterometer are the same density of electrons. The result was compared with the equivalent density approximation spot. System was considered atomic unit in our calculations.

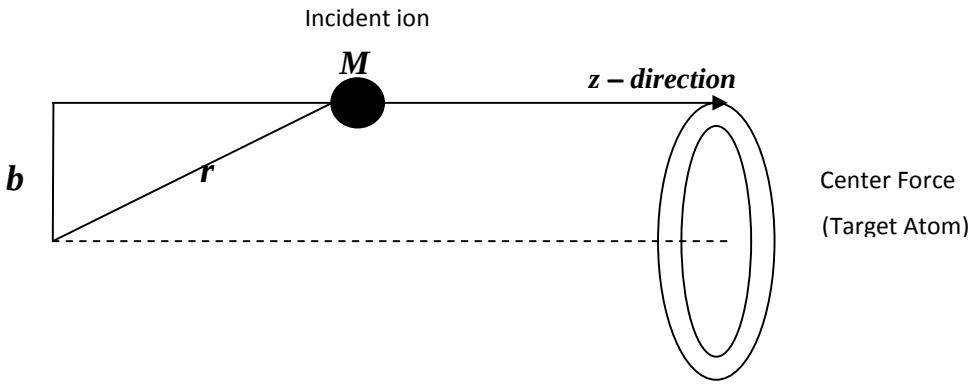
2. Mathematical description of Local Density approximation and Bethe –Bloch equation:

2.1-Local Density Approximation:

The electronic energy loss can be described by the following equation [6, 10]:

$$\frac{dE}{dz} = \frac{2\pi Z^2}{\upsilon^2} \rho(r)\, L(\rho(r), \upsilon) \qquad (1)$$

Where Z , υ and r are the charge , velocity and position of the incident ion, measured from center C_{60} molecule , $\rho(r)$ is electron density and it is given by the analytical expression[11,12]:



$$\rho(r) = 0.146 \exp\left(-\frac{(r-6.6)^2}{2.7}\right) \qquad (2)$$

Fig.(1) represent collision incident ion at an impact parameter b with target atom.

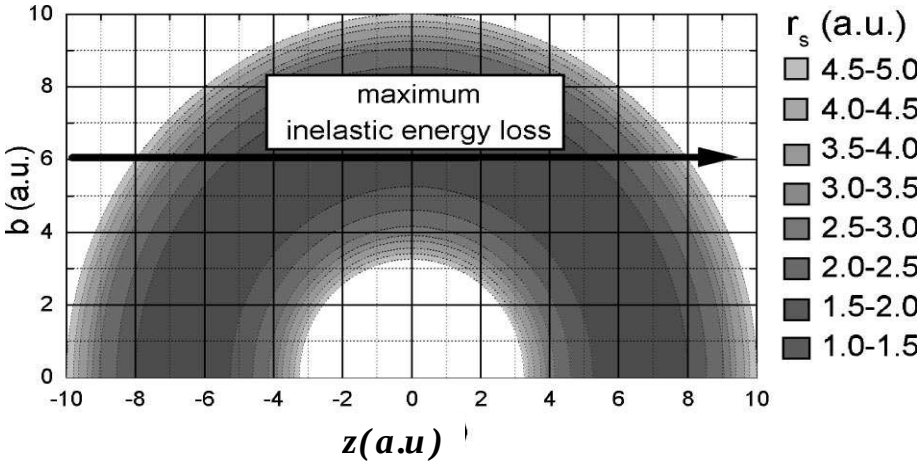


Fig.(2) Contour plot showing the electron density of the C_{60} experienced by the projectile along its path at different impact parameters[6]. The electron density is expressed by the density parameter $r_s = (\frac{4}{3}\pi\rho(r))^{-1/3}$ [13].

Where $r = \sqrt{b^2 + z^2}$, b represent the impact parameter, z is the direction of the incident ion (see fig.(1)) , in the fig. (2) at $(z = 0)$ the incident ion enter in the maximum inelastic energy loss region . $L(\rho(r), v)$ is the stopping number

$$L(\rho(r), v) = \ln(\frac{2v^2}{\omega_p(r)}) - \frac{3}{5}(\frac{v_F(r)}{v}) \qquad (3)$$

$v_F(r)$ is the Fermi velocity, $v_F(r) = [3\pi^2\rho(r)]^{1/3}$ with plasma frequency $\omega_p(r) = [4\pi\rho(r)]^{1/2}$, the deposition energy $E_d(b)$ calculated by integration of eq.(1) along the direction of incident ion ($z-axis$):

$$E_d(b) = \frac{2\pi Z^2}{v^2}\int_{-\infty}^{\infty}\rho(r)\,L(\rho(r), v)\,dz \qquad (4)$$

$$E_d = \frac{2\pi}{\pi b_\circ^2}\int_0^{b_\circ} b\,E_d(b)\,db \qquad (5)$$

2.2 Bethe –Bloch equation:

Consider energetic ion passing through surface target has the charge $(Z_1 e)$, moving at velocity, v with impact parameter b . There are two basic approaches used to evaluate a particles's energy loss to target electrons. These are Bohr approach, which is dependent on the impact parameter between the particle's trajectory and target nucleus, and the Bethe approach which depends on the momentum transfer from the particles to target electrons.

Bloch evaluated the differences between the classical (Bohr) and quantum-mechanical (Bethe) approaches for particles with velocities much larger than the target electrons. Thus

Bloch found the bridging formulation between the classical Bohr impact –parameter approach, and the quantized Bethe momentum transfer approach to energy loss in the fallowing equation which called Bethe –Bloch equation [4]:

$$\frac{dE}{dz} = \frac{4\pi Z_1^2 Z_2 e^4}{m\upsilon^2} L_\circ^{Bethe}(\upsilon)\, n \qquad (6)$$

n represents the scattering density, m is the mass of the ion, e is electron charge and Z_1, Z_2 are atomic numbers of incident ion and target atoms respectively. To find the deposition energy as an approximation n is replaced by $\rho(r)$ and then by integrating over direction of incident ion, one gets

$$E_d(b) = \frac{4\pi Z_1^2 Z_2 e^4}{m\upsilon^2} L_\circ^{Bethe}(\upsilon) \int_{-\infty}^{\infty} \rho(r)\, dz \qquad (7)$$

The average value of E_d is estimated from the following [9]:

$$E_d = \frac{2\pi}{\pi b_\circ^2} \int_0^{b_\circ} b\, E_d(b)\, db \qquad (8)$$

$L_\circ^{Bethe}(\upsilon)$ is the Bethe stopping number (including relativistic terms:

$$L_\circ^{Bethe}(\upsilon) = \ln\left(\frac{2m_e\upsilon^2}{I_\circ}\right) - \ln(1-\beta^2) - \beta^2 - \delta/2 \qquad (9)$$

As usual $\beta = \upsilon/c$ where c is light velocity and δ is the density correction term which corrects the relativistic polarization effect when projectile velocities become comparable to projectile rest mass [13, 14].

$I_\circ$ is the averaged excitation potential ($I_\circ \cong 10\, Z_2\ eV$). In this study consider $(b = 10\ \ a.u)$ [8] and $(-R_p \le z \le R_p)$ have been used. R_p Is projectile range [15].

$$R(nm) = \frac{6E_\circ(KeV)}{\rho_t(gm/cm^3)} \frac{(Z_1^{(2/3)} + Z_2^{(2/3)})}{Z_1 Z_2} \frac{m_1}{(m_1+m_2)m_2} \qquad (10)$$

$$R_p = \frac{R}{\left(1 + \frac{m_2}{2m_1}\right)}$$

Where R is the ion range and ρ_t is the mass density of target surface.

RESULTS AND DISCUSSION

Numerical solution of equations (5) and (8) be clear in Fig (3), one can note the difference between the two peaks. In the current study we note the shift of the peak by (1.5 a.u) because of the different equations used to calculate the energy deposited.

The widths of curve of LDA equation is greater than the ones of the Bethe-Bloch equation since the integral in the first equation over two quantities ($\rho(r), L(\rho(r), \upsilon)$) while in the second equation over one quantity ($\rho(r)$). The area under the two curves (i.e. total energy deposition) is differing by about 26%, for any value of impact parameter where the peak occurs at $(b \cong 6.3\ a.u)$. The correction term does not have an effect on the value of the energy deposits. Figures (4) represents the change of energy deposited with the atomic number increases upwards and have oscillating behavior with him, this means that the projectile found the average density of electrons. Energy deposited by light ions ($1 < Z < 8$) are small because of their small mass and therefore able to penetrate the surface and as a result not lose energy, while the heavy ions ($30 < Z < 70$) have a high value of the energy

deposited. Fig. (5) represent the behavior of Bethe stopping number in comparison with LDA stopping number as a function of ion velocity. Generally the stopping number (L) increases with the ion velocity. The two quantities almost equal each other at high velocities, if we extended the range of the velocity we'll find the Bethe stopping number become greater than LDA stopping number. The Bethe stopping number varies $(0 \leq L_{\circ}^{Bethe} \leq 9.8)$ more than LDA stopping number. Its has positive value for this range of the ion velocity, below this range the stopping number has negative value.

In the present work, the primary energy $(E_{\circ})$ of the incident ion is $(1.34\ MeV)$, above this value the numerical solution program is terminate because the second term of equation (8) going to infinite value. The stopping number increases with the ion velocity, the Bethe and LDA stopping numbers having same values at high velocities.

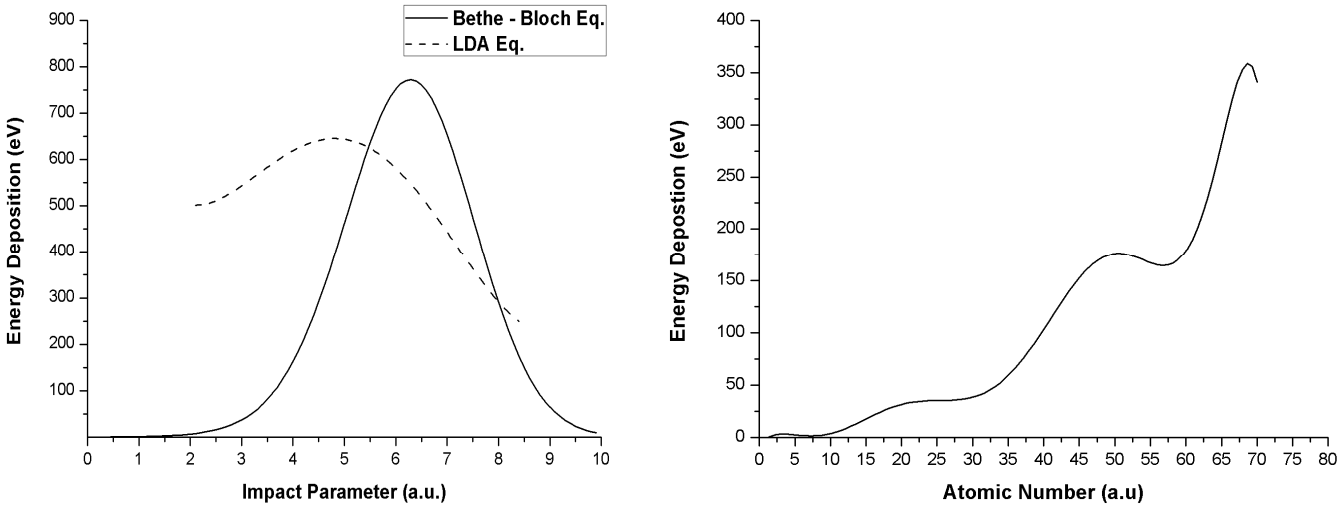


Fig. (4) The deposition energy is displayed as a function of the atomic number at $b = 10\ a.u$ and primary energy ($E_p = 0.5\ MeV$), using surface of C_{60} molecule as a target.

Fig.(3) The deposition energy is displayed as a function of the impact parameter. The (solid line) represent the present study and (dot line) local density approximation (LDA) .

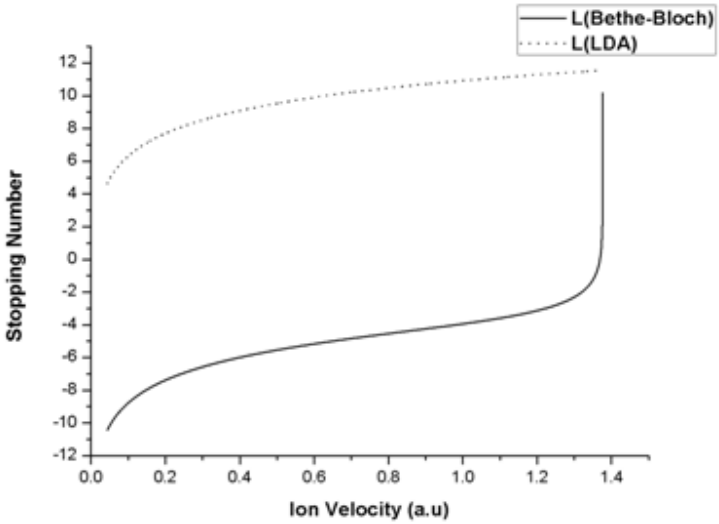


Fig.(5) Represent comparison between of Bethe –Bloch stopping number (solid line) and local density approximation (LDA) stopping number at $(b = 10a.u, z = 10a.u)$ (dot line) .

CONCLUSION

In this research was to test the validity Beth equation to calculate the energy deposited at the low primary energy ($E_{\circ} = 0.5MeV$)and found the following :

We got a good consensus between the energy deposited calculated using the equation of Bethe-Bloch equation and the LDA.

Energy deposited increases with atomic number and have the disposal be patchy and low value for the small ions and high value for the heavy ions.

was the comparison between the stopping number is used by Beth-Bloch and the stopping number is used in the LDA equation, where we found that they are increasing with the velocity of ion and uncompromising when high velocities .

According to these standards Almmattabrp by many researchers conclude that the application of equation Bethe-Bloch possible to calculate the energy deposited at energy about $0.5MeV$.

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