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Estimation of Velocity Distribution of Aluminum Atom According to Thomas-Fermi Model

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Abstract:

In this paper the velocity of distribution is studded by using Thomas Fermi model for Aluminum atom depending on the Screening function. The input parameter was found by using Screening function that expressed theoretically to estimate stopping force. From the statistical point of view, the Thomas Fermi model gives an opportunity that depends on the atomic number of atoms of target substances.

Keywords: *of Velocity Distribution, Aluminium, Thomas-Fermi Model*

I. INTRODUCTION

For target material compound or element stopping data are entail for predicting the parameter of stopping phenomena and to establish the relationship between compounds and elements when the theoretical and expressional values are available. By using Thomas and Fermi statistical method that of atomic number of atoms that constant the element of target materials [1].

II. THOMAS-FERMI METHOD OF THE ATOM (STATISTICAL)

This method regard the cloud of element like Fermi gas that depends on the density, the minimum total energy of the atom (kinetic and potential) determined the density profile [2, 3]. By assuming the potential energy is similar to classical coulomb energy that distribute in the field of nucleus, while the kinetic energy behaviour according to quantum theory by the relationship between the Fermi wave number and the density of electron.

$$n_e = \frac{K^3(f)}{3\pi^2}$$

Thomas – Fermi method is needed to study the behaviour of atomic parameter. Which depend on the atomic number and the predict table is accounted for these number variations to estimate the potential energy and the kinetic energy of the cloud of electrons in the field of nucleus of the

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neutral atom (z) electrons of nucleus with radius (r) that composed of shell of energy of the clouds of electrons [2]:

$$V_{(E)} = -\frac{9}{19}\frac{z^2 e^2}{r}$$

The kinetic energy can be estimate by:

$$E = \frac{\hbar^2 z^{5/3}}{m r^2}$$

For Thomas model the minimum total energy at:

$$r_{TF} = \frac{\hbar^2}{m e^2 z^{1/3}} = \frac{a_0}{z^{1/3}}$$

a_0 is the Boher radius, by this equation, kinetic, potential and total energy can be estimate for each electron [3]:

$$E_e = \frac{z^{7/3} m e^4}{\hbar^2}$$

The velocity of electron can be derived:

$$\upsilon_e = \frac{z^{2/3} e^2}{\hbar} = z^{2/3}\upsilon_0$$

υ_0 is the velocity of Boher which is $\frac{e^2}{\hbar}$.

The angular frequency can be obtained:

$$\omega_f = \frac{mze^4}{\hbar^3} = \frac{z\upsilon_0}{a_0}$$

From equation (7) the scaling rule can be predicted by Bloch for I-value [2].

$$I = \hbar\omega = z_2 I_0$$

The value of I_0 will be was estimate with the range of 10ev [5], it is necessary to mention that I has the dimension of an energy, it has no scale either $z_2^{\frac{4}{3}}$ or $z_2^{\frac{7}{3}}$, it is important to mentions that the behavior of frequency of I is the same in Both quantum and classical theory, the first shell correction scaling property can be estimate as [5].

$$\Delta L = -\frac{\langle \upsilon_e^2 \rangle}{\upsilon_2} - \frac{\langle \upsilon_e^4 \rangle}{2\upsilon^4} - \frac{5\pi}{3}\frac{\upsilon_0^4}{\upsilon^4} r^3 \rho_e$$

ρ_e is the density of electron [6].

$$-\frac{\upsilon_0^2}{\upsilon^2} = -z_2^4 \left(\frac{\upsilon_0}{\upsilon}\right)^2 \quad (2)$$

We note there is increase the atomic number for stopping materials. Lastly, the Factor of Barkas-Andereson [7]:

$$B_r = \frac{z_1 e^2 \omega_0}{m\upsilon^3} \quad (3)$$

Then we get:

$$B_r = \frac{z_1 z_2 I_0}{m}\frac{\upsilon_0}{\upsilon^3} \quad (4)$$

These relations are very important to assess the effects of various to gather for interpolation. The distribution of velocity for charged particle according to the electron distribution the decreasing the total energy $n_e(r)$ normalized for electron number of the atom, this lead to equation of Thomas-Fermi [9]. (5) (6)

$$\nabla^2(\phi - \phi_r) = \frac{2^{\frac{7}{2}}}{3\pi}\frac{1}{(r_0^3 e)^{\frac{1}{2}}}.(\phi - \phi_r)^{\frac{3}{2}}$$

$$\sigma_0 = \frac{2^{3/2}}{3\pi^2}.\frac{1}{(er_0)^{3/2}} \quad (7)$$

We can reform the equation (13) as:

$$\nabla^2(\phi - \phi_r) = 4\pi\sigma_0 e.(\phi - \phi_r)^{\frac{3}{2}} \quad (8)$$

By numerical solving of equation (15) and according to Pissons law, the distribution of electron as relation to the potential:

$$n_e(r) = \sigma_0(\phi - \phi_r)^{\frac{3}{2}}$$

According to the equation (15) we can rewrite the potential of neutral atom as:

$$\phi'_{(r)} = \frac{ze}{r}\phi\left(\frac{r}{r_e}\right)$$

Where:

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$$r_e = \frac{0.8853 r_0}{z^{\frac{1}{3}}}$$

And the density of electron as:

$$n_e(r) = \sigma_0 \left[\frac{ze}{r} \phi_r \left(\frac{r}{r_e}\right) \right]^{\frac{3}{2}} = \frac{32 z^2}{9\pi^2 r_0^3} \left[\frac{r}{r_e} \phi_r \left(\frac{r}{r_e}\right) \right]^{\frac{3}{2}} \quad (19)$$

We can find the distribution of velocity in Atom of inhomogeneous electrons of gas in real and velocity. For $\upsilon \langle \upsilon_f$ the space is:

$$F_{(\upsilon)} = \left(\frac{m}{4\pi\hbar} \right)^3 \quad (20)$$

When $\upsilon \rangle \upsilon_f$ the $F_{(\upsilon)} = 0$. The spatial variable integration leads to normalized to 1 to velocity spectrum:

$$F_{(\upsilon)} \partial^3 \upsilon = \left(\frac{m}{4\pi\hbar} \right)^3 \frac{1}{z} \partial^3 \upsilon = \int_{\upsilon_f} \partial^3 \upsilon \quad (21)$$

Equation (21) could be written as:

$$F_{(\upsilon)} = \frac{1}{3\pi^2 z} \left(\frac{m^3 r_1^3}{\hbar^3} \right)$$

r_1 defined as:

$$n(r_1) = \frac{m^3 \upsilon^3}{3\pi^2 \hbar^3}$$

In unite of dimension.

$$x = \frac{r_1}{r_e} \quad , \quad y = \frac{m r_e \upsilon}{\hbar z^{1/3}}$$

This yield:

$$F_{(\upsilon)} \partial^3 \upsilon = \frac{x^3}{3\pi^2} \partial^3 y = \frac{4}{3\pi} x^3 y^2 \partial y \quad (25)$$

$$y^2 = 1.7706 \frac{\phi_r}{x} \quad (26)$$

The equation (25) can be written as:

$$F_{(\upsilon)} \partial^3 \upsilon = 0.71 x^2 \phi_r \quad (27)$$

The Somerfield 1932 approximation with $\lambda = 0.8034$ is [10]:

$$\phi_r = \left[1 + \left(\frac{x^3}{144} \right)^{\frac{\lambda}{3}} \right]^{-\frac{\lambda}{3}} \quad (18)$$

III. RESULTS AND DISCUSSION

Figure 1 show the behavior of electron density for Aluminum in respect to Fermi model. We can see reversible relationship between $\frac{x}{r}$ on the x-axis and $\frac{n}{z}$ on the y-axis, when the values of $\frac{n}{z}$ decree the value $\frac{x}{r}$ increase. When the value of $\frac{n}{z} \sim 30$, the $\frac{x}{r}$ take value equal to 0.01 as shown below.

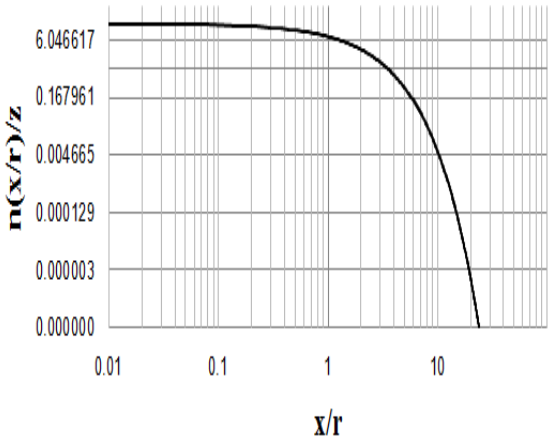

FIGURE 1. Density of electron for Aluminum in respect to Fermi model

Figures 2 and 3 denote the behavior in both large distance $\phi_r(x) = 144/x^3$ and small distance, ϕ_r as exponential.

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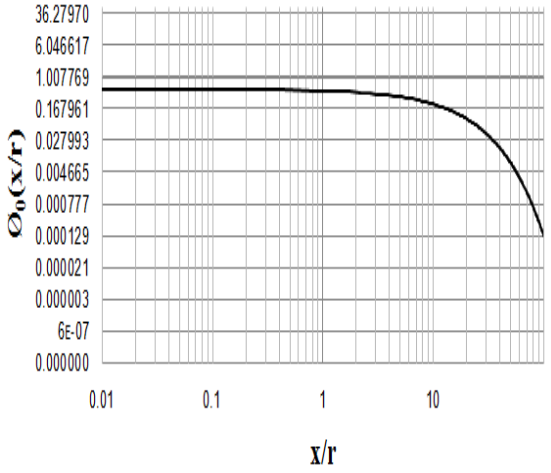

FIGURE 2. Screening Function of Aluminum in respect to Thomas-Fermi model.

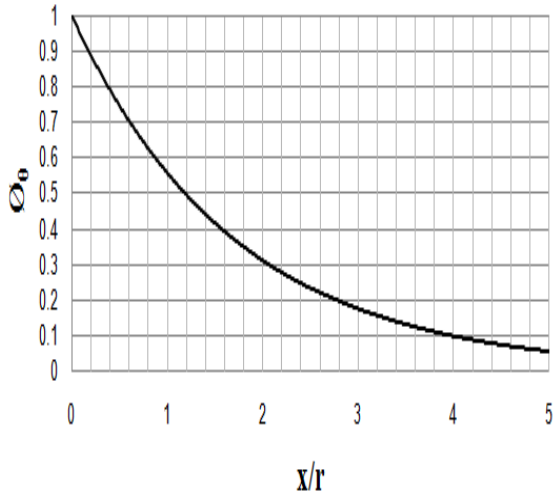

FIGURE 3. Screening Function of Aluminum.

Figure 2 represent the relationship between x/r on the x-axis and the value of $\emptyset_0$ at the y-axis. When the $\emptyset_0$ value increase; the $\frac{x}{r}$ value decrease and the fixed value of $\emptyset_0$ still constant then drops continuing with increase $\frac{x}{r}$ value.

Figure 3 represent the relationship between $\frac{x}{r}$ on the x-axis and the value of $\emptyset_0$ at the y-axis. It represent an exponential behavior, the maximum value of $\emptyset_0 = 1$ correspond to zero value of $\frac{x}{r}$. Figure 4 showed the function of Aluminum due to equation (27) by using Somerfield.

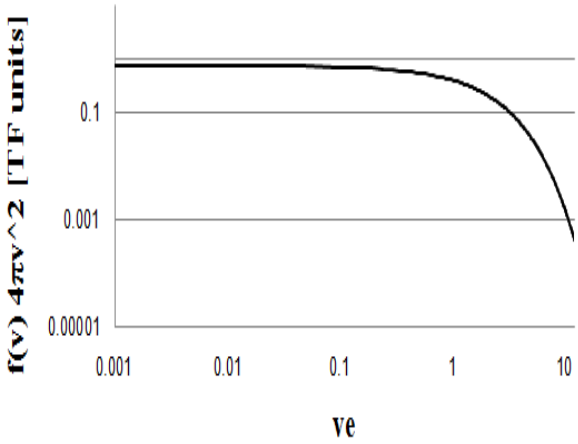

FIGURE 4. The distribution of velocity estimated according to Thomas Fermi.

It represents the relationship between V_e at x-axis and $\mathbf{f_V}$ on y-axis. From this figure we can note the value of $\mathbf{f_V}$ will decrees gradually when V_e increases. While, on the left side we note increase in V_e with increase of $\mathbf{f_V}$ then reach the peak point. But on the right side the relationship is invisible between $\mathbf{f_V}$ and V_e.

IV. CONCLUSION

The Thomas Fermi model highlights the behavior of parameters of atoms which depend mainly on the atomic number. The properties of scaling has great roles for majoring the stopping forces. On theoretical

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basis the Aluminum atom velocity behaviors is met mainly in large distance $\phi_r(x) = 144/x^3$. For the small distance ϕ_r will expressed as exponential.

REFERENCES

1. VAgnello M., Belli G., Bendiscioli G., Bertin A., Botta E., Bressani T., Bruschi M., Bussa M. P., Busso L., Calvo D. et al. (1995): "Antiproton Slowing Down in H2 and He and Evidence of Nuclear Stopping Power", Phys Rev Lett 74, 371–374.
2. Bloch F., (1933): "Bremsverm¨Ogen Von AtomenMitMehrerenElektronen", Z Physik 81, 363–376.
3. Møller S. P., Uggerhøj E., Bluhme H., Knudsen H., Mikkelsen U., Paludan K. and Morenzoni E., (1997): "Direct Measurement of the Stopping Power for Antiprotons of Light and Heavy Targets", Phys Rev A 56, 2930–2939.
4. Arista N. R., (2002): "Energy Loss of Heavy Ions in Solids: Non-Linear Calculations for Slow and Swift Ions", NuclInstrum Methods", B195, 91–105.
5. Lindhard J. and Scharff M. (1953): "Energy Loss in Matter By Fast Particles of Low Charge", Mat FysMedd Dan Vid Selsk 27 no. 15, 1–31.
6. Rahi, S.K., Nasser, Z.S., Shakir, I.A. "The effect of gamma rays in some optical and physical properties" Journal of Global Pharma Technology, 2019
7. Ashley J. C., Ritchie R. H. and Brandt W. (1972): "Z3 1 Effect in the Stopping Power of Matter for Charged Particles", Phys Rev B 5, 2393–2397.
8. Bush V. and Caldwell S. H. (1931): "Thomas-Fermi Equation Solution By the Differential Analyzer", Phys Rev 38, 1898–1902.
9. Gombas P. (1956): "StatistischeBehandlung Des Atoms", In S. Fl¨ugge, editor, Handbuch der Physik, vol. 36, 109–231. Springer, Berlin.
10. Sommerfeld A. (1932): "Asymptotische Integration Der Differentialgleichung Des Thomas-Fermischen Atoms", Z Physik 78, 283–308.
11. Sigmund P., Sharma A., Schinner A. and Fettouhi A. (2005): "Valence Structure Effects in the Stopping of Swift Ions".
12. Sigmund P. and Schinner A. (2006): "Shell Correction in Stopping Theory", NuclInstrum Methods B 243, 457–460.