Position –Dependent of Relative Energy Straggling

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Abstract.

Collisional electronic energy-loss straggling has been studied theoretically on the basis of the distant-collision contribution to straggling. The present work is to estimate the energy straggling of sub-shell for target atoms using impact parameter representation of swift charged particle under grazing incidence of solid targets. The effect of excited core electrons which has frequently been neglected is shown to be significant .The numerical formulas, found in the research ,were solved by using computer program in (Fortran-90).

1-Introduction.

In 1915 ,N.Bohr [1] predicted that fluctuation of the energy loss ΔE of a beam of charged particles penetrating matter is characterized by the variance ,

$$\langle(\Delta E - \langle\Delta E\rangle)^2\rangle = NR\Omega^2 \qquad \text{........ (1)}$$

with the straggling parameter Ω^2 given by:

$$\Omega^2 = \Omega_B^2 = 4\pi z_1^2 z_2 e^4 \qquad \text{.......(2)}$$

where <ΔE> is the mean energy loss over a traveled path length R, N the number of atoms per volume in the stopping material , and z_1, z_2 the atomic number of beam and material atoms , respectively .

Equation (1) assumes the stopping medium to be random and the path length R sufficiently small so that the variation with beam energy of the cross sections responsible for energy loss can be ignored [2,3] .

Equation (2) assumes free-Coulomb scattering between beam particles and the electrons of the stopping medium .Bohr showed that unlike the mean energy loss , straggling is rather insensitive to the binding of target electrons .The underlying reason is the fact that the integral

$$\Omega^2 = \int T^2 d\sigma(T) \quad \text{........(3)}$$

is dominated by large values of the energy transfer T per collision event even though the differential cross section dσ (T) is heavily peaked toward small T .

Equation(2), in conjunction with equation (1) ,seems to constitute one of the most lasting and universally-valid results of the theory of particle penetration .Its range of validity reaches far beyond the initial application area .Nevertheless there are limitations which , according to common knowledge , may roughly be classified into three groups ,

1-At low projectile speed , comparable to electron velocities in the target, Ω^2 tends to slightly increase above the Bohr value with decreasing velocity before dropping toward zero [4].

2- At high speed , relativistic corrections beyond those mentioned already by Bohr [1] become necessary [5] and ,

3-Charge exchange may not be neglected in general as a source of energy-loss straggling [6].

2-Theoretical Scheme .

The basics of binary stopping theory have been described in references [7,8], and an extensive documentation on the computation of stopping forces including several add-ons has appeared recently[9]. The purpose of the present research is to add specific features pertinent to straggling.

On the other word ,we can say that the energy-loss straggling originates in intrinsic quantum at fixed impact parameter and in positional fluctuation . The variance of energy-loss distribution with respect to thickness is given by[10].

……..(4) $$\frac{d\Omega^2}{dx} = \int d^2 p N(p) \langle T^2(p) \rangle$$

Where

N (p) is the density of target atoms at distance (p) from the trajectory ,

$\langle T^2 \rangle = \Sigma_i(\hbar\ \omega_i)^2 P_i\,(p)$,

$\hbar\,\omega_i$ is the excitation energy for level i ,

$P_i\,(p)$ is the probability for excitation.

At fixed impact-parameter (p) we have $\langle T^2 \rangle = (\langle T \rangle)^2$ where $\langle T \rangle$ is given it's free-Coulomb value and equation (4) reduces to known Bohr's value .

…….(5) $$\frac{d\Omega^2}{dx} = 4\pi N z_1^2 z_2 e^4$$

The Bethe's theory (1930) has been applied to bulk straggling in Livingston and Bethe(1937) and Fano (1963) [11,12].The result may be written in the form,

…..(6) $$\frac{d\Omega^2}{dx} = 4Nz_1^2 z_2 e^4 \left[1 + \left(\frac{1}{mv^2} \right) \sum_i f_i \hbar\omega_i \ln\left(\frac{2mv^2}{\hbar\omega_i} \right) \right]$$

Where f_i is dipole oscillator strength obeying the sum rule $\Sigma_i f_i = 1$.

The first term is Bohr's classical result and the second term ,being proportional to Plank's constant does not have a classical analog. It produces a small shoulder , which is frequently neglected in bulk straggling . Since the significance of close collision is reduced in surface stopping this term gain significance . The distant-collision contribution to straggling differs from the corresponding contribution to the stopping power by a factor $\hbar\,\omega_i$ under the sum . This implies that the distant part of the position-dependent straggling can be constructed *from the corresponding expression for the stopping power [10] by insertion of the factor . This yield :*

….(7) $$\left(\frac{d\Omega^2}{dx} \right)_{dis.} = \left(\frac{2Nz_1^2 z_2 e^4}{mv^2} \right) \sum \left(\frac{\omega_i}{z_i} \right) f_i(\hbar\omega_i) \int_{\frac{2\omega_i z}{v}}^{\infty} dt k_1\left(\sqrt{t^2 + \alpha_i^2} \right)$$

Where,

$\alpha_i = (C\hbar\,\omega_i/mv^2)^2$; $C = 2e^{-\gamma} = 1.1229$.

γ=0.5772 is Euler's constant.

K_1 is modified Bessel functions .

We can rewrite equation (7) in the following form :

$$\left(\frac{d\Omega^2}{dx}\right)_{dis.} = \left(\frac{2Nz_1^2 z_2 e^4}{mv^2}\right)\sum\left(\frac{\omega_i}{z_i}\right) f_i(\hbar\omega_i)\left[\int_{\frac{2\omega z_i}{v}}^{0} dtk_1\left(\sqrt{t^2+\alpha_i^2}\right)+\int_0^{\infty} dtk_1\left(\sqrt{t^2+\alpha_i^2}\right)\right]$$

(8)

The quantum contribution to straggling parameter relative to Boher straggling according to equation (5) can takes the following form rewriting equation (8),

$$\frac{\Omega^2}{\Omega_B^2} = \sum_i\left(\frac{\omega_i}{z_i}\right) f_i(\hbar\omega_i)\left(\frac{\omega_i z_0}{2v}\right) k_0\left(\frac{\omega_i z_0}{2v}\right) k_1\left(\frac{\omega_i z_0}{2v}\right) + \sum_i\left(\frac{\omega_i}{z_i}\right) f_i(\hbar\omega_i)\int_{\frac{2\omega z_i}{v}}^{0} dt\left(\sqrt{t^2+\alpha_i^2}\right)$$

(9)

A computer program was written in Fortran -90 language , which consists of a subroutines calculated the modify Bessel functions k_0 and k_1 together with Gaussian quadratic method for solving the numerical integration .

Results and Discussion .

The energy straggling relative to Bohr energy straggling (Ω^2/Ω^2_B) of individual atomic shells can be calculated from equation (9) . Another example illustrated the relative significance of inner and outer electrons for the relative energy straggling , using a computer program and the information from reference [11]. Fig.(1) illustrated the energy straggling relative to Bohr energy straggling (Ω^2/Ω^2_B) in each atomic shell of Aluminum (Al) at different velocities ($v=10v_0$,$v=5v_0$, $v=2.5v_0$ and $v=v_0$) . Fig.(1-a) illustrated the transition bulk behavior at around z=0 ,where the relative energy straggling is dominated by 2p electrons , toward large distance where the valence excitation dominate . The influence of 2p electrons is still visible at $v=5v_0$ and $v=2.5v_0$, Figs.((1-b) and (1-c)) but they do not dominate at any distance , and at $v=v_0$ only valence electrons contribute to straggling Fig.(1-d) . Fig.(2) illustrate the energy straggling relative to Bohr energy straggling (Ω^2/Ω^2_B) in atomic sub-shell 1s ,2s+2p ,3s+3p and total straggling of Aluminum (Al) at four velocities ($v=10v_0$, $v=5v_0$, $v=2.5v_0$, $v=v_0$). At velocity $v=10v_0$ the inner shell-1s for (Al) is visible and drop off rapidly in the region

(z>0)of the bulk material . At proton velocities $v=5v_0$ for (Al) is still visible and decreases off rapidly at (z>0) but at $v=2.5v_0$ and $v=v_0$ there is no contribution of this sub-shell . The sub-shell 2s+2p for (Al) at velocities $v=10v_0$, $v=5v_0$ and $v=2.5v_0$ is dominant and decreases exponentially toward large distances while at low velocity $v=v_0$ there is no contribution to the sub-shell 2s+2p for (Al) . The sub-shell 3s+3p is visible but contribute poorly for (Al) at velocities ($v=10v_0$, $v=5v_0$ and $v=2.5v_0$) but it is dominate at velocity $v=v_0$. This feature entered the analysis of reference [12] but was found to be less prominent there .

Figs.(2-a , 2-b ,2-c and 2-d) illustrate total position-dependent energy straggling relative to Bohr energy straggling (Ω^2/Ω^2_B) for (Al) at different velocities ($v=10v_0$, $v=5v_0$, $v=2.5v_0$ and $v=v_0$) . A nearly exponential decrease is seen in all four cases , consistent with theoretical results reported in references [13,14] . The slope decreases with increasing (z) because of an increasing adiabatic radius . This is in good qualities is in agreement with the exponential observations reported in[12] .

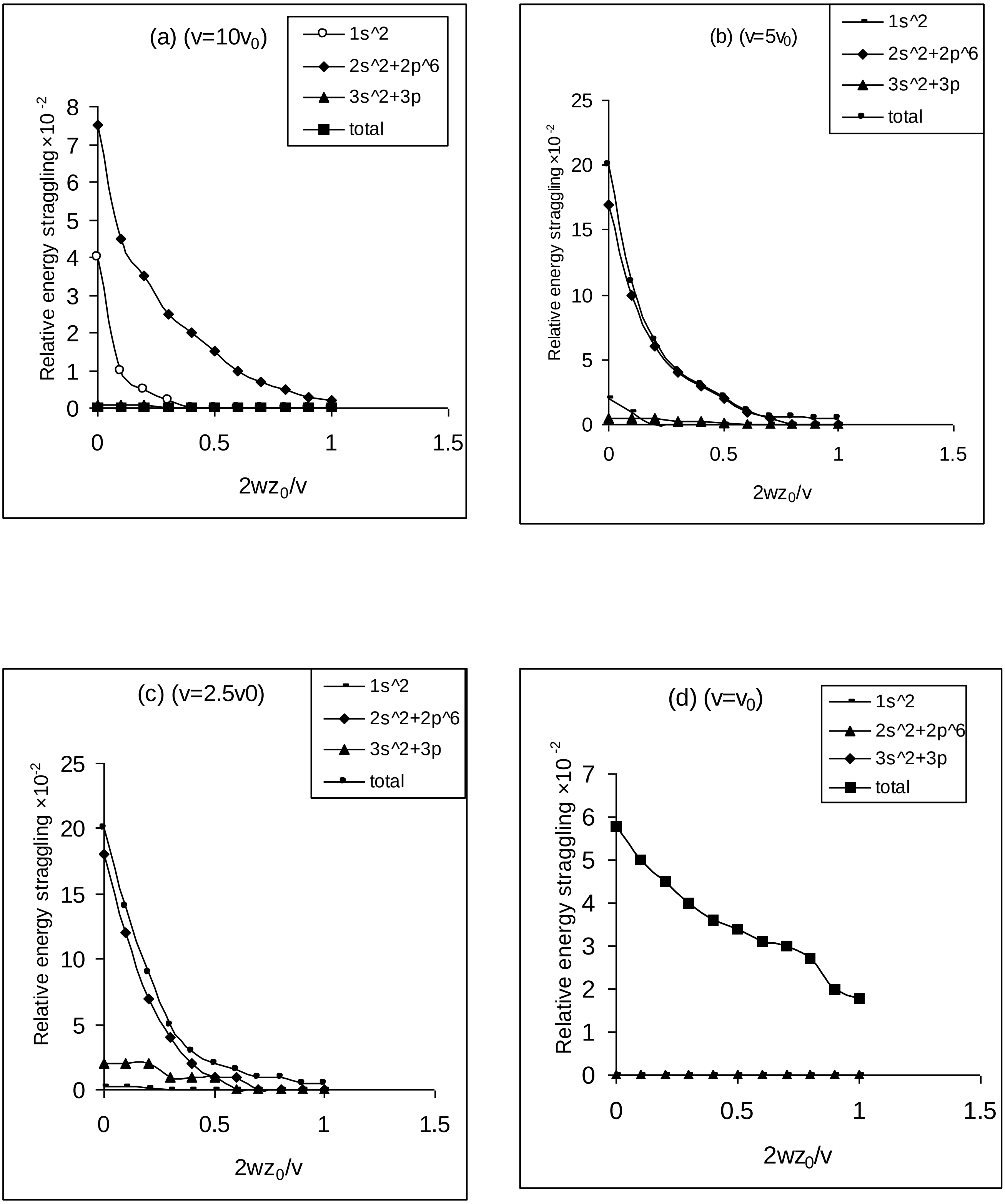

Fig.(1): Position – dependent of relative energy straggling for sub shells of atomic Al.
(a) $v=10v_0$, (b) $v=5\ v_0$, (c) $v=2.5v_0$, and (d) $v=v_0$

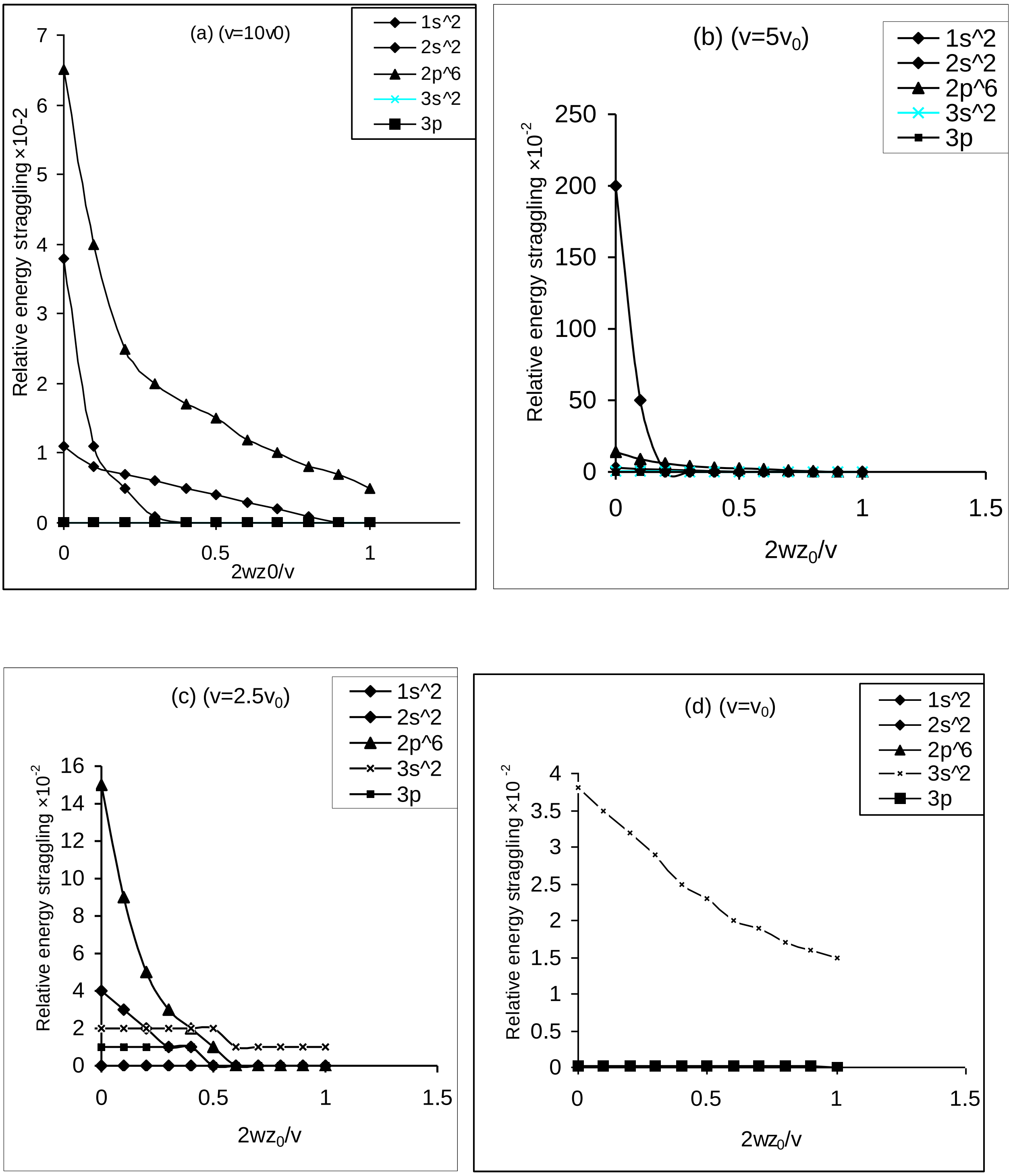

Fig. (2) : Straggling parameter relative to Bohr's straggling for Al (a) $v=10v_0$, (b) $v=5\ v_0$, (c) $v= 2.5v_0$, and (d) $v=v_0$.

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أعتماد الموقع على تطوح الطاقة النسبي

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الخلاصة.

تم دراسة تطوح فقدان الطاقة الالكتروني التصادمي نظريا على مبدأ إسهامات التصادمات البعيدة للتطوح . العمل المنجز يكون لحساب تطوح الطاقة للغلاف الثانوي باستخدام بعد التصادم (impact-parameter) للجسيمات المشحونة السريعة التي تمس (تكشط) (Grazing incidence) الأهداف الصلبة. غالبا ما يهمل تأثير الالكترونات الداخلية المتهيجة في السابق ،بينما تبين خلال هذه الدراسة أن لها تأثير ذو قيمة في حدود معينة من السرع. تم حل الصيغ العددية التي استخدمت في البحث بواسطة برنامج حاسوبي يتضمن برامج فرعية بلغة (فورتران -90) .