The study of the straggling energy loss

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Abstract

Straggling is the broadening of energy distribution of a beam charge particle penetrating through a material medium. The calculations represent a problem of considerable complexity. The theoretical literature on straggling is rather limited compared to the one on stopping cross section. In the present work, the energy loss of straggling has been studied theoretically for interaction of C, O, Ne, Cl and Al ions in Ni target.

The present work is a part of a thesis submitted for the PhD Degree in Physics, in 2012 [1]. A program SanarVrns.for has been written in FORTRAN-90 using Compaq Visual FORTRAN V6.6 for compiling, linking and executing. A copy of the program is available in [1].

Introduction

Energy-loss straggling denotes the development of the width and shape of the energy spectrum of an initially monochromatic beam as a function of time or path length [2]. Straggling is an inherent feature of stopping measurements which cannot be reduced indefinitely by making more measurements. In many applications, information on the scatter of data is just as important as mean values [3]. Assuming that all the target electrons contribute to the energy loss, Bohr (1915) provided a simple expression for the value of the energy-loss straggling in the case of an elemental target [4]. Bohr straggling equation and its frequently used to estimate the corresponding energy-loss straggling value for the case of high projectile velocities [5]. Quantum mechanics causes the energy loss to fluctuate from one collision event to another, even at one and the same impact parameter. For composite projectiles such as heavy ions carrying electrons, the charge and the excitation state may vary over a trajectory, and since the energy loss typically depends on the projectile state, additional fluctuations arise [6]. Energy-loss straggling has atomistic and statistical aspects which will be discussed at present work.
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The dielectric formalism provides simple expressions for describing the energy loss and energy loss straggling of a fast projectile moving through matter with certain kinetic energy. The dependence on target properties account through its energy loss function [7].

**Basic Theory**

Bohr showed that unlike the mean energy loss, straggling is rather insensitive to the binding of target electrons. He predicted that the fluctuation of the energy loss $\Delta E$ of a beam of charged particles penetrating matter is characterized by the variance parameter $W$ given by[8]:

$$W = W_B = 4\pi Z_1^2 Z_2 e^4.$$ (1)

In classical theory, the energy loss at a given impact parameter is uniquely defined if the electron is at rest initially. In semi-classical theory, the energy loss is a fluctuating quantity even at a given impact parameter.

A fundamental aspect of the Bohr theory is the splitting into two regimes for small and large impact parameter: close interaction is taking to follow Rutherford’s law [9].

$$T_{close}(p, v) = \left(\frac{Z_1^2 e^4}{p^2 m v^2}\right)f_{close}(p)$$ (2)

Where $b = \frac{2Z_1 e^2}{m v^2}$ is the collision diameter.

$$f_{close}(p) = \frac{1}{1 + \left(\frac{b}{2p}\right)^2}$$ (3)

For distant interaction the energy transfer versus impact parameter $p$ is described as excitation of harmonic oscillators by a time varying electric field in the dipole approximation [10,11].

$$T_{dis}(p, v) = \frac{2Z_1^2 e^4}{m^2 v^2 p^2} f_{dis}(p)$$ (4)

With,

$$f_{dis}(p) = \left\{ \left(\frac{\omega p}{v}\right)K_1\left(\frac{\omega p}{v}\right)\right\}^2 + \left\{\left(\frac{\omega p}{v}\right)K_0\left(\frac{\omega p}{v}\right)\right\}^2$$ (5)

Where $\omega$ is the oscillator frequency and $K_0$ and $K_1$ are modified Bessel function in standard notion [12].

According to close and distant, collision energy transfer given in
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\[ S = \int_0^\infty 2\pi p dp T(p) \]
\[ = \int_0^{p_0} 2\pi p dp T_{\text{close}}(p) + \int_{p_0}^\infty 2\pi p dp T_{\text{dis}}(p) \]

(6)

Where \( p_0 \) is critical distance where close and distant, collision are equal.

and the definition of relative variance in energy [2],

\[ W = \int 2\pi p dp T^2 \]

(7)

Where \( T \) is the energy transfer for close and distant collision,

\[ T = \frac{2Z_i^2 e^4}{mv^2 p^2} f(\alpha p / v) \]

(8)

Using a dimension parameters,

\[ x = \frac{\alpha p}{v} ; \quad p = \frac{v}{\omega} x , \quad \text{then} \quad dp = \frac{v}{\omega} dx \]

Therefore Eqs. (2-5) become,

\[ T = \frac{2Z_i^2 e^4}{mv^2 (\frac{v}{\omega} x)^2} f(x) \]
\[ = \left( \frac{2Z_i^2 e^4}{\xi^2} \right) \left( \frac{\omega}{v} \right) \frac{f(x)}{x^2} \]

(9)

With \( \xi = \frac{mv^3}{Z_i e^2 \omega} \).

(i) For close collision,

\[ f(x) = \frac{1}{1 + (\frac{1}{\xi x})^2} \]

(10)

and,

(ii) For distant collision,

\[ f(x) = x^2 [K_0^2(x) + K_1^2(x)] \]

(11)

Therefore, equation (7) becomes,

\[ W = \frac{W_B}{\xi^2} \int \frac{2dx}{x^3} \left| f(x) \right|^2 \]

(12)

Eq. (12) represents the variance in the energy loss of heavy ions taking in the consideration close and distant collisions,
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(i) For close collisions, substitute Eq. (10) into eq. (12) and integrate it, can get:

\[ W_{\text{close}} = \frac{W_B}{\xi^2} \int_{\xi_0}^{\xi} 2dx \frac{1}{x^3} \left[ 1 + \left( \frac{\xi}{x} \right)^2 \right] \]

\[ = 2W_B \xi \int_{\xi_0}^{\xi} dx \frac{\xi}{1 + (\xi x)^2} \]

\[ = W_B \frac{1}{1 + (\xi x_0)^2} \]  

(13a)

Therefore,

\[ \frac{W_{\text{close}}}{W_B} = \frac{1}{1 + (\xi x_0)^2} \]  

(13b)

Where \( x_0 = \frac{Q}{\nu} \), \( W_B = 4\pi Z_i e^4 \)

(ii) Distance collisions, substitute Eq. (11) into (12) and conveniently evaluated numerically,

\[ W_{\text{dis}} = \frac{W_B}{\xi^2} \int_{\xi_0}^{\xi} 2dx [K_0^2(x) + K_1^2(x)] \]  

(14)

And,

\[ \frac{W_{\text{dis}}}{W_B} = \frac{1}{\xi^2} \int_{\xi_0}^{\xi} 2dx [K_0^2(x) + K_1^2(x)] \]  

(14b)

Bethe’s quantum theory changed the form of Bohr’s stopping number \( L = \ln(C \omega / Z_i e^2 \nu) \):

1- Instead of one resonance frequency per individual electron, Bethe recovered the spectrum of resonance frequency \( \omega_\nu \) for the atom, weighted by dipole oscillator strengths \( f_\nu \) satisfying the sum rule

\[ \sum f_\nu = Z \]  

(15)

Just as in the quantum theory of optical dispersion and absorption.

2- Being based on lowest-order perturbation theory, Bethe’s theory approximates Thomson’s formula,

\[ T(p) = \frac{2mv^2}{1 + \left( \frac{pmv^2}{Z_i e^2} \right)^2} \]  

(16)

by \( T = 2(Z_i e^2 / p)^2 / mv^2 \), so that

\[ \frac{T_{\text{max}}}{T_{\text{min}}} = \left( \frac{P_{\text{max}}}{P_{\text{min}}} \right)^2 \]  

(17)

3- The effective minimum impact parameter becomes
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\[ P_{\text{min}} \approx \frac{\hbar}{2m\nu}, \]  

(18)
in Bethe theory. In other words, de Broglie’s wavelength replaces the classical collision radius \( b \). Bethe’s stopping number formula then reads [13],

\[ L = \sum \nu f_\nu \ln \left( \frac{2m\nu^2}{\hbar \omega_\nu} \right), \]

\[ \cdots \quad (19) \]

Results and Discussion

Newton–Raphson method [12] has been used in a program to evaluate \( p_0 \), which is the intercept point between close and distant collisions of energy transfer \( T \), and \( x_0 = \frac{\alpha p_0}{\nu} \). Figs. (1a-1e) show the variation of \( x_0 = \frac{\alpha p_0}{\nu} \) with \( \xi = m\nu^3 / Z_i e^2 \omega \) for interaction of C, O, Ne, Cl, Ar ions in Ni target. Figs. (1a-1e) have the same behavior and a minor difference in value for C, O, Ne, Cl, Ar ions in Ni target. The Maximum value of \( x_0 = \frac{\alpha p_0}{\nu} \) is around (4-2.5). Figs. (2) shows the variation of the relative variance to Bohr Formula for close and distant collisions given in Eqs. (13b, 14b) with dimensionless parameters \( \xi = m\nu^3 / Z_i e^2 \omega \) for Cl, Al, Ar, N ions in Al and C, Ni ions in C. The relative variance due close collisions is strongly dependent on energy parameter \( \xi \), while for distant collisions is approximately independent of \( \xi \) for present ions in C-target. The present method basically depends on extension limit for applying Bohr’s theory with stopping \( L = \ln(1.1223\xi) \), where \( L \leq 0 \) at low velocity (i.e. at low value of \( (1.1223\xi) \leq 1 \)). Taking in the consideration close and distant collisions one can extend limit of applying Bohr’s theory.

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![Graphs of C in Ni, O in Ni, Ne in Ni, Cl in Ni, and Ar ions in Ni](image)

Fig. (1) Shows the variety of wit, $\xi = \frac{mv^3}{Z_1 e^2 \omega}$ for C in Ni, O in Ni, Ne in Ni, Cl in Ni and Ar ions in Ni.
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Fig. (2) Shows the relative variance $W/W_0$ as a function of dimensionless parameters $\xi = m^2/Ze^2\omega$ for Cl, Al, Ar, N ions in Al.

$$\frac{BWW}{W_{\text{tot}}} = f_{\text{cl, e, inst}},$$

where $W_{\text{cl}}$, $W_{\text{dis}}$, and $W_{\text{tot}}$ represent the contribution of the relative variance due to different processes.
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 دراسة خسارة طاقة التطور

الخلاصة

التطور هو توزيع لأنشأ حزمة من الجسيمات المشحونة المارة خلال المادة . الحسابات تعتبر مشكلة كبيرة التعقيد . الدراسات النظرية للتطور كانت محددة مقارنة بتوفيق C, O,Ne, Cl المقاطع العرضي . العمل الحالي هو دراسة خسارة طاقة التطور لتفاعلات أيونات Ni بهدف . العمل الحالي هو جزء من أطروحة قدمت لنيل درجة الدكتوراه في عام 2012 Ar .

تم كتابة برنامج (Compaq Visual FORTRAN 90) وباستخدام sanarVrns for , واستخدام الربط المناسب بينهما ونسخه من البرنامج موجوده في المصدر [1] وتم الحصول على تطابق جيد مع الأعمال السابقة .