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Electron impact stopping powers for elemental and compound media

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ABSTRACT

A semi-analytical model is proposed for evaluating the electron stopping powers (ESPs) of material media including both elements and compounds in the energy range 1.0 eV–100 MeV. This paper reports details of our calculations using the effective atomic electron number, effective mean excitation energies of target atoms and realistic electron density distribution of the target atoms. This simple formula is capable of generating accurate cross-section for diverse systems. We present here only few simple cases. In comparison with other theoretical predictions, our calculated ESPs for elemental [C, Al, Cu, Pt, Au and Pb] and compound [H_2O, $C_5H_5N_5O$, GaAs, $Bi_2Sr_2CaCu_2O_8$, SiO_2 and ZnTe] media agree reasonably well with the experimental findings.

1. Introduction

Electron stopping powers (ESPs) of material media, usually defined as the average energy loss per unit distance along the electron path (in the units of energy/length), are needed in diversified areas of researches and applications, involving energy loss, including quantitative calculations of the dosages in radiation therapy for living tissues, Monte Carlo simulation study in electron microscopy for manipulating materials in both nuclear and space applications, quantitative surface analysis, the design of particle detectors [1], etc. It demands a simple-to-use formula capable of furnishing reasonably accurate ESPs of different media over a wide range of projectile energies. To date there are considerable attempts to calculate on ESPs using various formulas, methods and models [2–15]. Some of them are heavily dependent on fitting species dependent parameters, some are relied on accurate oscillator strength evaluation, some are involved in evaluating the complex dielectric response function, etc. However, for different energy regime, many of them are intuitively divided into slots to represent ESPs. Moreover, their application to molecular targets still poses considerable challenges. The search for a formula, with validity over a wide range of incident energies and for a large domain of species, motivated the present work.

Rohrlich and Carlson [2] have reported a formula for the average rate of energy loss of positrons and electrons in passing through matter. Sugiyama [13] has reported two approaches to derive ESP formulas: (a) the Bethe-Bloch formulas [8], referred to here as Bethe formula, and (b) the Lindhard-Scharff-Schiott theory [3,14]. We follow closely the Rohrlich and Carlson [2] based on the earlier work of Bethe formula [16]. This model without the shell- and density-corrections [4,9,14] shows reasonable results for the incident electron energies ranging 50 keV to a few MeV.

Sugiyama [7,13,15] introduced the effective charges [6], z^* of the projectile and Z^* of the target atom, and effective mean excitation energy (EMEE) I^* to modify the formula of Rohrlich and Carlson [2]. Gümüs group [11,12] further modified the formulas of Rohrlich and Carlson [2] and Sugiyama [7,15] to obtain analytic expressions for Z^* and I^* of the target atom using the Tietz screening function [17]. For the incident energies 10 eV $\leq E \leq$ 100 keV, this model yields fairly accurate ESPs. For 200 eV $\leq E \leq$ 30 keV, Jablonski et al. [9] have

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reported an empirical formula with species dependent parameters that rely heavily on the available experimental data. At $E \geq 1$ keV, the ESPs for elemental solids are calculated successfully and are available in Pages et al. [5] and ESTAR database [18].

From all these theoretical works, it is apparent that none of the above-mentioned formulas is able to describe the experimental ESP data at the energies $E < 10$ eV. Moreover, no single formula, available in the literature, goes smoothly from $E = 1$ eV to ultrahigh energies to reproduce simultaneously the available experimental data up to about 10 MeV and the ESTAR-generated ESP data beyond. In particular, the formula of Gümüs group [11,12], which can describe the experimental data beyond 10 eV, is not applicable to the energy region dominated by Bremsstrahlung. On the other hand, ESTAR, claimed to be reliable in the high and ultra-high energies, where no experimental data are available, is found to reproduce the experimental ESP data in the light elemental targets beyond 10 keV. It is, therefore, desirable to find a simple-to-use formula capable of reproducing successfully the experimental ESPs at lower energies and the ESTAR-evaluated ESPs from the Bremsstrahlung data.

The purpose of this study is to present a formula after proper modifications of the earlier formulas in Refs. [2,7,11,12] incorporating the effective charges, z^* and Z^* as well as the target EMEE I^*. The numerical density distributions (DDs) of the target electrons are evaluated numerically using the multi-configuration code of Desclaux [19], which uses the Dirac-Hartree-Fock electron wave functions. These realistic DDs are then employed to calculate both the effective charges and mean excitation energies of the target elements and molecules considered herein. The numerical DDs are represented by the piecewise cubic spline functions to evaluate the integrals [see Eqs. (3) and (4), shown below] for the effective charge Z^* and EMEE I^*.

Although the present semi-analytical model is capable of calculating ESPs for elemental solid targets up to $Z = 92$, we consider here only few sample media for the energies 1 eV–100 MeV. Our results are compared with the available experimental and other theoretical findings including ESTAR [18]. To establish the suitability, the proposed formula has been tested systematically on 6 important compound media including 2 biological molecules, water (H_2O) and Guanine ($C_5H_5N_5O$) in nucleic acid, and 4 semiconductors, namely silica (SiO_2), Gallium arsenide (GaAs), Bi-High-T_C superconductor ($Bi_2Sr_2CaCu_2O_8$) and Zinc tellurium (ZnTe).

2. Basic theory

The formula of the stopping power for electron in a medium, modified by Refs. [11,12] from the formula of [2], is;

$$S = -\frac{dE}{dx} = 2\pi e^4 N_0 \frac{\rho}{AE} z^{*2} Z^* \left[\ln\frac{E}{I^*} + F(\tau)/2\right] eV/\text{Å} \quad (1)$$

with

$$F(\tau) = 1 - \beta^2 + \left[\left(\tau^2/8\right) - (2\tau+1)\ln 2\right]/\left(1+\tau^2\right). \quad (2)$$

Here, $\tau = E/mc^2$ is the kinetic energy in units of the electronic rest mass; e, N_0, ρ and A are, respectively, the electronic charge, Avogadro number, atomic density in gm/cm^3 and atomic mass in gm. E is the electron energy in eV and β is the velocity of incident electron in the unit of the velocity of light. In Eq. (1) the factor in front of the parenthesis can be written as $(\rho\alpha/AE)$ eV/Å, since $\alpha = 2\pi e^4 N_0 = 785$ [20].

The function $F(\tau)$ [7,11,12] has dependency not only on the projectile energy but also on its kind. However, it is independent of its atomic number Z. ESPs contain same relativistic components through τ and electron density in Eq. (1).

In order to determine Z^* and I^* of the target atoms, Gümüs and Kabadayi [12] used Thomas-Fermi theory [21] which describes an atom having Z bound electrons with radially symmetric electron density. Sugiyama [7] obtained Z^* and I^* from Bohr's stripping criterion for the effective charge of incident heavy ions and target atoms, and from the Lindhard and Schraff theory [22] concerning the quantities in EMEE I^*. These functions in Eq. (1) are given in Refs. [7,13] as;

$$Z^* = \int_{r_c}^{\infty} 4\pi r^2 n(r) dr \quad (3)$$

and

$$\ln I^* = \frac{1}{Z^*}\int_{r_c}^{\infty} \ln[\gamma\hbar\omega_p(r)] 4\pi r^2 n(r) dr. \quad (4)$$

here, r is the distance of the bound electron from the nucleus; $n(r)$, the electronic charge density in target, $\omega_p(r) = (4\pi e^2 n(r)/m)^{0.5}$, the local plasma frequency and $\gamma = 2^{0.5}$ [7,22]. The velocity of the incident electron v_i at its distance from the nucleus r_c satisfying Bohr's criterion is equal to that v_b of the bound electron. A bound electron for which $r > r_c$ moves with a velocity $v_b < v_i$ and can contribute to the stopping power. The inner electrons with $r < r_c$ and $v_b > v_i$ are rigidly bound leading to an insignificant energy loss of the incident electron. The quantity r_c is defined by the Bohr stripping criterion [23] $v_i = (b\hbar/m)(3\pi^2 n(r_c))^{1/3}$ with b as the proportionality constant of the order of 1.26 [7]. The quantity r_c is obtained from the potential-energy condition of Yarlagadda et al. [6]

$$\frac{1}{2}mv_i^2 + U(r_c) = 0, \quad (5)$$

as pointed out earlier with $v_i = v_b$. Here, $U(r)$ is the potential experienced by the incident electron. Sugiyama [7] employed the semi-empirical effective charge of the incident electron z^* as given by

$$z^* = 1 - \exp\left(-2200\beta^{1.78}\right). \quad (6)$$

This conforms to the reason that z^* increases with the incident energy as all processes contributing to the stopping power are enhanced with increasing velocity of the projectile electron.

Our proposed formula reported in this study embodies the following modifications in addition to the use of relativistic treatment for the incident and bound electrons and the realistic DDs:

1. The first term within the square brackets in the right-hand side of Eq. (1) has to be modified from $\ln\left(\frac{E}{I}\right)$ to $\ln\left(\frac{3.75E}{I}\right)$ to represent both the peak location and the magnitude of relative ESPs. This is linked to the fact that the energy loss in the low energy limit is proportional to the square of the effective velocity v_{eff} of the incident electron (see Fig. 3 of [6]). As the projectile electron approaches the bound electron, v_{eff} gets enhanced to increase it's effective energy E_{eff}, which is substantially greater than E in the low energy region. To simulate E_{eff}, a number of grid searches on an appropriate factor with E are found essential to provide an overall best description of the experimental data near the peak region of the elemental targets. This procedure results in the factor of 3.75 with E, which is found good also for