Vacuum 85 (2010) 245–252

Contents lists available at ScienceDirect

Vacuum

journal homepage: www.elsevier.com/locate/vacuum

Practical calculations of stopping powers for intermediate energy electrons in some elemental solids

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ARTICLE INFO

Article history:
Received 12 July 2009
Received in revised form
11 June 2010
Accepted 13 June 2010

Keywords:
Bohr adiabatic criterion
Effective charge
Electron stopping power
Tietz screening function

ABSTRACT

This study presents calculation results of the stopping power (SP) of electrons of kinetic energy from 10 eV to 100 keV for some elemental solids. The method is based on utilization of the modified Bethe–Bloch SP expression and analytical expression for effective atomic electron number and effective mean excitation energies of target atoms, and for effective charge of incoming electrons, Sugiyama's semi-empirical formula is embedded in the formula. An analytical expression for the practical SP calculations using Bethe approximation and Thomas–Fermi model of atom is taken from an pervious study and the calculated results of the SPs from this formula for electrons in some elemental solids, such as Al, Si, Cr, Ni, Cu, Ge, Pd, Ag, Pt, and Au, are calculated and rigorously compared with experimental data, Penelope code results and with results of other calculations such as the non-relativistic Bethe SP equation and the empirical modification of the Bethe equation by Joy and Luo. The results are found to be in good agreement for some targets but some limited agreement for some energies and targets is also observed.

1. Introduction

The electron stopping powers (SPs) of solids are important in a wide field of applications and fundamental research, for example quantitative calculation of the dosage in radiation therapy, Monte Carlo (MC) simulation study in electron microscopy, quantitative surface analysis and the design of particle detectors. In these fields and in medicine, radiation physics, chemistry and biology, it is often important to have simple but accurate information about the SP of various media for the energetic electrons. In literature, a variety of SP formulas can be found for different energy regions, but the stopping power formulas give varying results for different energy regions and targets [1–11]. The electron SPs at energies above 10 keV (high energy regions) for elemental solids are theoretically well described and can be found in tables given in ESTAR (NIST database) [12], ICRU 37 Report [7], Berger and Seltzer [8] and Pages et al. [11], but practical calculation models of the SP below 10 keV are rare.[1,5,6] Sugiyama [6] and Gümüş [5] obtained SP values for intermediate electrons energies using a modified Rohrlich and Carlson [13] model. Sugiyama [6] and Gümüş [5], applied the Bohr stripping criterion to target atoms for effective charge and effective mean excitation energy. In applying this, Sugiyama [6] used the Thomas–Fermi atomic model and also evaluated the integrals numerically related to effective charge and effective mean excitation energy. This method produced some uncertainties since in the model the upper limit of the integral has to be determined. The reason for this deviation originated from the effective electron number and effective mean excitation energy calculation methods in which the upper limit of the integral has to be determined. Therefore, uncertainties arise both due to choice of screening function of the Thomas–Fermi atom and also to numerical calculations of integrals of Z^* and I^* (Sugiyama [6], Eqs. (4) and (5)).

In recent years, a universal fitting expression for the electron SPs for energies between 200 eV and 30 keV reported by Jablonski et al. [14]. The experimental stopping power values (Joy et al., [15]; Kalil et al. [16]; Garber et al. [17]; Fitting [18]; Ishigure et al. [19] Al-Ahmad and Watt [20]; Luo et al. [21], Luo [22]) for low energies, even below 100 eV, are available in the extensive compilation of Joy's database of electron–solid interactions (Joy [23]). The published material refers to numerous elemental solids and compounds (Tanuma et al. [4]; Joy [23]; Akkerman and Chernov [24]). It is shown that starting from the Rohrlich and Carlson model and employing the Tietz screening function the stopping power can

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doi:10.1016/j.vacuum.2010.06.004

be calculated successfully in a more practical manner than ever with a fairly good agreement. A practical expression for the Monte Carlo (MC) simulation of electron transport is required for quantification of Auger-electron spectroscopy (AES) [25], X-ray photoelectron spectroscopy (XPS), and electron-probe microanalysis (EPMA) (Gauvin [26]; Ritchie [27–29]; Llovet et al. [30]).

In this work it is aimed to apply a practical expression for electron SP calculation and thus make a comprehensive comparison with the experimental data and other theoretical models. For this purpose, the semi-empirical effective charge expression for incoming electrons is employed to fit the Peterson and Green [31] method by Sugiyama [6], and in order to obtain analytical expression for the number of active electrons and effective mean excitation energy of target atom, we used the Tietz screening function [32]. Finally, these analytical expressions by embedding in to an SP formula, a practical SP calculation formula is applied to elemental solid targets.

The calculating procedure thus described, was applied to incoming electrons on Al, Si, Cr, Ni, Cu, Ge, Pd, Ag, Pt, and Au for electron energies between 10 eV and 100 keV. We have chosen targets where experimental SP data available for extensive comparison [13] of our results. Besides we have compared our results with calculated SPs from other estimates [3,4,24,33–38]

2. Calculation of electron stopping powers

The modified collision SP formula for incoming electrons can be written as [6,13]

$$S = -\frac{dE}{dx} = \frac{4\pi e^4 z^{*2}}{m v_1^2}\frac{\rho N_0}{A} Z_2^* \left\{ \ln\left(\frac{E}{I_2^*}\right) + F(\tau)/2 \right\} \qquad (1)$$

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

where m is the electron mass, v_1 is the incident electron velocity, E is the electron energy, $\tau = E/mc^2$is the kinetic energy in units of the rest mass, $N = N_0/A$ is the density of target atoms and * denotes an effective quantity, i.e. the effective charge of incident electron z^*, the effective number of target electrons Z_2^*, A is the atomic weight of the target element, N_0 Avogadro's number, and β is the ratio of v_1/c, with c the velocity of light and I_2^* the effective mean excitation energies (EMEE), ρ the mass density of the target. In Eq. (1) the factor in front of the parenthesis can be written as $(\rho k/A\beta^2)z^{*2}Z_2^*$, since $k = 4\pi e^4 N_0/mc^2 = 307075$ eV.cm^2 [39,40].

In order to determine of effective electron number, Z_2^* and EMME, I_2^* of target atom, it is necessary to know v_e as a function of r, where r is the distance from the nucleus. In this study, we use the Thomas–Fermi theory (TF) [41,42], which describes an atom with Z_2 bound electrons by the radially symmetric electron density,

$$n(r) = \frac{Z_2}{4\pi\Lambda r}\frac{d^2\Phi(x)}{dx^2} \qquad (2)$$

where $x = r/\Lambda$ and $\Phi(x)$ are the screening function obtained from solution of TF equation, and screening length respectively, and Λ is a variational parameter and obtained by minimizing the total energy as a function of the number of electron. According to Tietz [32], the screening function for the TF atom can be written as

$$\Phi(x) = \frac{b^2}{(x+b)^2} \qquad (3)$$

where b is chosen as $b = (8/\pi)^{2/3}$to normalize the electronic density [43]. By using Tietz screening function, Cabrera-Trujillo et al. [43] obtained the screening length as follows

$$\Lambda = 0.6064741719\, a_o Z^{-1/3} \qquad (4)$$

depending on atomic number.

In order to calculate critical length from adiabatic Bohr criteria, we used the electronic charge density

$$n_2(x) = \frac{Z_2}{4\pi\Lambda_2^3}\frac{F(x)}{x} \qquad (5)$$

where $F(x)$ is the second derivatives of screening function with respect to x, $(d^2\Phi(x)/dx^2)$. Cabrera-Trujillo et al. [43] obtained $x_c = r_c/\Lambda$ as,

$$x_c(v_1) = -2(b/3) + \frac{1}{\left[a/2 + (b/3)^3 + \sqrt{(a/2)^2 + a(b/3)^3}\right]^{1/3}}(b/3)^2 + \left[a/2 + (b/3)^3 + \sqrt{(a/2)^2 + a(b/3)^3}\right]^{1/3} \qquad (6)$$

where

$$a(v_1) = \frac{b^2}{0.60647}\frac{v_0^2 Z_2^{4/3}}{v_1^2} \qquad (7)$$

and v_0 is the Bohr velocity. The stripping length, in other word critical length, x_c, is directly determined from the Eq. (6).

Z_2^* and I^* can be obtained from Bohr's stripping criterion for the effective charge of heavy ions and target atoms, and from the Lindhard and Schraff theory [44], These functions in Eq. (1) is given by Sugiyama [6,39] as,

$$Z_2^* = \int_{r_c}^{\infty} 4\pi r^2 n(r) dr \qquad (8)$$

$$\ln I_2^* = \frac{1}{Z_2^*}\int_{r_c}^{\infty} \ell n\{\gamma\hbar\omega_p(r)\} 4\pi r^2 n(r) dr \qquad (9)$$

Z_2^* and I_2^* can be obtained analytically from these expressions by using Tietz [32] screening function of the TF atom. Where r is the distance from the nucleus and r_c is determined from adiabatic Bohr criterion [45,46]. Such a criterion can be written in the form of a potential-energy condition [47],

$$\frac{1}{2}mv^2 + U(r_c) = 0 \qquad (10)$$

where r_c is the distance from the nucleus of an electron bound to the target atoms for which its velocity is equal to the velocity of the incident electron ($v_1 = v_e$). An electron for which $r > r_c$ is moving with $v_e < v_1$ and therefore is contributed to the stopping power, but inner electrons in the target ($v_e > v_1$) are rigid bound and therefore are no energy transfer to these inner electrons.

Effective electron number charge of the target atom in the electron energy loss processes, $Z_2^*(v_1)$ can be expressed as

$$Z_2^*(v_1) = Z_2\frac{b^2(3x_c + b)}{(x_c + b)^3} \qquad (11)$$

from Eq. (8) [43]. For high incident energies (i.e. for $x_c \to 0$), Z_2^* will approach to Z_2 ($Z_2^* \to Z_2$).

In this study, the semi-empirical effective charge of incident electron z^* is used with z^* being given by