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Calculation of stopping power for partially stripped ions using an oscillator model

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Abstract. Collision of swift ions with atoms was considered in this paper. The projectile and target atoms were modeled as assemblies of quantum oscillators and it was assumed that both, target and projectile could be excited or ionized, without charge exchange. The model presented here is an extension of the one given by Sigmund and Haagerup [Phys. Rev. A **34**, 892 (1986)]. The number of electrons bound to the projectile, as a function of the projectile velocity, was used from Cabrera-Trujillo et al. [Phys. Rev. A **55**, 2864 (1997)]. Contributions to energy loss from excitation of the projectile and targets were separately considered. It has been found that projectile excitation contributes up to 20% to the total energy loss in the lower energy region. Comparisons with other authors, including SRIM 2003, are also given and good agreement was found.

PACS. 34.50.Bw Energy loss and stopping power – 95.30.Ky Atomic and molecular data, spectra, and spectral parameters (opacities, rotation constants, line identification, oscillator strengths, gf values, transition probabilities, etc.)

1 Introduction

Motion of swift charged particles and their penetration in a medium has been the subject of research in various areas of physics and other branches of science, such as atomic and nuclear physics, astrophysics, medical radiology, materials science and engineering, micro and nano-science, technology, etc. The stopping power, S, is one of the most important variables in this field of physics. It is defined as the ratio of energy, dE, lost on some distance, dx, and that distance, ($S = -dE/dx$).

According to the first Born approximation the stopping power of a swift bare projectile with velocity v was described by Bethe theory [1,2]

$$S = \frac{4\pi z_1^2 e^4}{m_e v^2} N z_2 L \tag{1}$$

where: N is the number of medium atoms in an unit volume, z_2 is the atomic number of the target; $z_1 e$ is the charge of the projectile; m_e is the rest mass of the electron and the symbol L is the stopping number.

The target atom could be considered and modeled as an assembly of classical linear harmonic oscillators with frequency, ω. This model was firstly introduced and used in the stopping power calculation performed by Bohr [3–5], where the projectile was considered as a point like charged particle.

The model of oscillators was used for determination of a higher order correction in the expression for stopping power [6]. Sigmund and Haagerup [7] modeled the target atom as an assembly of quantum oscillators. They calculated the stopping number $L^{osc}(v, \hbar\omega)$ as a function of the projectile velocity v and the excitation energy of the target oscillators, $\hbar\omega$. The stopping number, $L^{at}(v)$ of an atom, was obtained as a sum of the stopping numbers of quantum harmonic oscillators, weighted by the dipole oscillator strengths, f_{nn0}, of that atom,

$$L^{at}\left(v\right) = \sum_n f_{nn0} L^{osc}\left(v, E_n - E_{n0}\right). \tag{2}$$

Summation has to be performed along all states of the discrete and continual spectrum.

This approach was employed by Jansen and Mikkelsen [8] to calculate the energy loss of H_2^+ in amorphous carbon and for a number of other materials [9,10].

A common characteristic of these papers is that the projectile was considered as a point like charged particle. However, when the projectile interacts with target atoms, some target electrons could be captured causing reduction of the projectile charge [11]. It has been described that the projectile is not fully stripped, even at larger energies up to 10 MeV/nucl, [12].

When both, the projectile and the target carry orbital electrons, collision energy loss occurs through three mechanisms: excitation of target atoms only; excitation of the projectile atom only; and finally excitation of both, projectile and target.

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Just the first mechanism occurs for a fully stripped projectile, and all energy loss results in energy transfer to the target. If the partially stripped ion is excited in a collision, the projectile would be slowed down, but no energy deposition in the target would occur.

The situation becomes more complicated if the projectile is in a metastable state. In such a case, the target could be excited without projectile slowing down. It is even possible that the ion can accelerates after a collision (partially for a light projectile on a heavy target) by converting internal energy to kinetic energy (super elastic collision).

Many attempts have been made to determine stopping of partially stripped ions using Bethe theory. Kim and Cheng [13] suggested replacement of the projectile nuclear charge, z_1, and the target mean ionizing energy, I_2, with their effective values, z_{eff} and I_{eff}, which depend on the projectile properties. Moneta and Czerbniak [14] used the first Born approximation and semi-classical impact parameter description allowing projectile excitation and ionization without electron exchange to calculate the stopping power for a partially stripped projectile. Tsuchida and Kaneko [15,16] derived an analytical formula for the electronic stopping power for swift frozen-charge-state projectiles with two electrons in metastable states. Recently, Glazov [17] calculated the stopping power of a frozen charge projectile taking into account: elastic collisions; excitation or/and ionization of the target accompanied by projectile excitation. Cabrera-Trujillo et al. [18] calculated the energy loss of partially stripped projectiles using Bethe's theory. Excitations and ionizations of both, projectile and target were taken into account, but without charge exchange. The number of electrons bound to the projectile was calculated using the adiabatic Bohr criterion in conjunction with the Thomas-Fermi model of an atom.

By modeling target atoms as an assembly of quantum oscillators, Sigmund and Haagerup [7] derived an expression for the stopping power for a fully stripped ion. They suggested that the stopping number could be calculated as a sum of stopping numbers of oscillators weighted by dipole oscillator strengths of a given target.

Recently, the stopping power was calculated using the first Born approximation, and modeling the target and the projectile as quantum oscillators [19]. The assumption was made that the projectile could be excited and ionized, not only the target. The stopping power was given as a function of the excitation energy of the projectile and the target. The influence of projectile excitation on stopping power was investigated and it was most significant in the Bragg peak region.

Kaneko [20] derived the energy loss of hydrogen-like and helium-like projectiles in a frozen charge state during the passage, without consideration of projectile excitation.

In the low energy region it is necessary to take into account some corrections [21] listed below. The shell correction becomes significant when the projectile velocity is not much higher than $z_2^{2/3}v_0$ (v_0 is Bohr velocity and $v_0 = 2.18 \times 10^6$ m/s). Barkas's correction has the largest contribution when $v \sim (z_1 z_2)^{1/3} v_0$. In addition, Bloch's correction is significant when $v \sim 2z_1 v_0$ [21]. In the present paper the projectile velocity, v, is larger than both the average orbital velocity of target electrons $v > z_2^{2/3}v_0$, and the 1s orbital velocity $v > z_1 v_0$.

An analytical expression for the energy loss of a projectile with bounded electrons was derived in the presented paper. Excitation and ionization of both, projectile and target, without a charge exchange between them, was considered here. A partially stripped ion and a target were modeled as assemblies of quantum harmonic oscillators.

In Section 2 of the presented paper, the stopping power will be given in terms of partial stopping numbers as a function of excitation energy of the projectile and the target. The given expression is written in a form convenient for weighting according to the dipole strength of a given combination of the projectile and the target, as suggested in [7,8]. Contributions to the stopping power from projectile and target excitation will be presented separately. Shell, Barkas and Bloch corrections are included in the expression for total stopping power at the end of Section 2. The results and a conclusion are presented in Sections 3 and 4.

2 Calculation of the stopping power

Stopping power, S, can be calculated through the following equation [13,17]

$$S = N\left\{\sum_{m>m0}(E_m - E_{m0})\int d\sigma_{0m} + \sum_{n>n0}(E_n - E_{n0})\int d\sigma_{n0} + \sum_{m>m0;\, n>n0}\left((E_m - E_{m0}) + (E_n - E_{n0})\right)\int d\sigma_{nm}\right\}. \tag{3}$$

The first sum on the right side of equation (3) represents contributions to the stopping power due to excitation of target atoms while the projectile remains unexcited; the second term represents a process of projectile excitation while the target atoms remain unexcited, and the third term represents the contribution to the stopping power due to excitation of both, projectile and target atoms. E_n and E_{n0} are eigen energies of the projectile and E_m and E_{m0} are eigen energies of the target atom. The differential cross section, $d\sigma_{nm}$, for the interaction between the projectile and the target atom with transferred energy dQ, in equation (3) is given as

$$d\sigma_{nm} = \frac{2\pi e^4}{m_e v^2}\left|F^p_{nn0}(-\vec{q})\right|^2\left|F^t_{mm0}(\vec{q})\right|^2\frac{dQ}{Q^2}. \tag{4}$$

Inelastic scattering amplitudes of the projectile and the target are defined as

$$F^p_{nn0}(-\vec{q}) = \langle n|\, z_1 - \sum_i e^{-i\vec{q}\cdot\vec{r}_i}\, |n_0\rangle \tag{5a}$$

$$F^t_{mm0}(\vec{q}) = \langle m|\, z_2 - \sum_j e^{i\vec{q}\cdot\vec{r}_j}\, |m_0\rangle \tag{5b}$$

where $Q = \hbar^2 q^2/2m_e$ is the energy transferred, and $\hbar\vec{q} = \hbar(\vec{k} - \vec{k}_0)$ represents the momentum transfer. $\hbar\vec{k}_0$ and $\hbar\vec{k}$ are linear momentums of the projectile before and after collision. The law of energy conservation has the following form for the process considered

$$\frac{\hbar^2 k_0^2}{2M_1} - \frac{\hbar^2 k^2}{2M_1} = (E_n - E_{n0}) + (E_m - E_{m0})\,. \tag{6}$$

The minimum kinetic energy, which a projectile losses to excite itself and the target, can be derived from equation (6) and expression $\vec{q} = \hbar(\vec{k} - \vec{k}_0)$. By this approach the following expression is obtained

$$\left((E_n - E_{n0}) + (E_m - E_{m0}) + \frac{m_e}{M_1}Q\right)^2 = 2m_e v^2 Q \tag{7}$$

where, M_1 is the projectile mass and m_e is the electron mass. Using equation (7) the lower limit of integrals in equation (3) for transferred energy is given as

$$Q_{min} = \frac{\left((E_n - E_{n0}) + (E_m - E_{m0})\right)^2}{2m_e v^2}. \tag{8a}$$

In calculations presented in [17,18], the maximum momentum transfer was assumed to be equal to that between a heavy particle and an electron

$$Q_{max} = 2m_e v^2. \tag{8b}$$

According to equations (4–8), the expression for stopping power for a partially stripped ion, given by equation (3), becomes

$$S = \frac{4\pi e^4}{m_e v^2} N \left\{ \frac{1}{2} N_2 \sum_{m>m0} \int_{\frac{(E_m - E_{m0})^2}{2m_e v^2}}^{2m_e v^2} |F^p_{n0n0}|^2 f^t_{mm0}(Q) \frac{dQ}{Q} \right.$$
$$+ \frac{1}{2} N_1 \sum_{n>n0} \int_{\frac{(E_n - E_{n0})^2}{2m_e v^2}}^{2m_e v^2} f^p_{nn0}(Q) \left|F^t_{m0m0}\right|^2 \frac{dQ}{Q}$$
$$+ \frac{1}{2} N_1 N_2 \sum_{m>m0;\, n>n0} \frac{(E_m - E_{m0}) + (E_n - E_{n0})}{(E_m - E_{m0})(E_n - E_{n0})}$$
$$\left. \times \int_{\frac{((E_n - E_{n0}) + (E_m - E_{m0}))^2}{2m_e v^2}}^{2m_e v^2} f^p_{nn0}(Q) f^t_{mm0}(Q)\, dQ \right\} \tag{9}$$

where

$$f^i_{kk0}(Q) = \frac{E_k - E_{k0}}{N_i Q} \left|F^i_{kk0}\right|^2$$

are generalized oscillator strengths, N_i is the number of bound electrons ($i = p$ for a projectile and $i = t$ for a target).

The expression for the stopping power, given in equation (9), could be written as a sum of partial stopping numbers

$$S = \frac{4\pi e^4}{m_e v^2} N \left\{ N_2 L_t^{at} + N_1 L_p^{at} + N_1 N_2 L_{t,p}^{at} \right\} \tag{10}$$

where the partial stopping numbers for the target atom and the projectile ion are defined over the partial stopping numbers of oscillators as [7,8]

$$L_t^{at} = \sum_{m>m0} f^t_{mm0} L_t^{osc}\left(\frac{2m_e v^2}{E_m - E_{m0}}\right),$$
$$L_p^{at} = \sum_{n>n0} f^p_{nn0} L_p^{osc}\left(\frac{2m_e v^2}{E_n - E_{n0}}\right),$$
$$L_{t,p}^{at} = \sum_{m>m0,\, n>n0} f^t_{mm0} f^p_{nn0} \times L_{t,p}^{osc}\left(\frac{2m_e v^2}{E_m - E_{m0}}, \frac{2m_e v^2}{E_n - E_{n0}}\right). \tag{11}$$

The partial stopping numbers for oscillators, L^{osc}, have forms

$$L_t^{osc} = \frac{1}{2} \sum_{m>m0} \int_{\frac{(E_m - E_{m0})^2}{2m_e v^2}}^{2m_e v^2} \left|F^p_{n0n0}\right|^2 f^t_{mm0}(Q) \frac{dQ}{Q},$$
$$L_p^{osc} = \frac{1}{2} \sum_{n>n0} \int_{\frac{(E_n - E_{n0})^2}{2m_e v^2}}^{2m_e v^2} f^p_{nn0}(Q) \left|F^t_{m0m0}\right|^2 \frac{dQ}{Q}$$
$$L_{t,p}^{osc} = \frac{1}{2} \sum_{m>m0;\, n>n0} \frac{(E_m - E_{m0}) + (E_n - E_{n0})}{(E_m - E_{m0})(E_n - E_{n0})} \times \int_{\frac{((E_n - E_{n0}) + (E_m - E_{m0}))^2}{2m_e v^2}}^{2m_e v^2} f^p_{nn0}(Q) f^t_{mm0}(Q)\, dQ. \tag{12}$$

2.1 Calculation of partial stopping numbers, L^{osc}, of oscillators

In this section the partial stopping numbers for oscillators are calculated. The first partial stopping number defined in equation (12) represents an interaction between the projectile and target where the projectile remains in a ground state while the target is excited

$$L_t^{osc} = \frac{1}{2} \sum_{m>m0} (E_m - E_{m0}) \times \int_{\frac{(E_m - E_{m0})^2}{2m_e v^2}}^{2m_e v^2} \left|F^p_{n0n0}(-\vec{q})\right|^2 \left|F^t_{mm0}(\vec{q})\right|^2 \frac{dQ}{Q^2}. \tag{13}$$

A harmonic-oscillator model is used for calculation of the inelastic target scattering amplitude, F_{mm0}, as in [7]

$$\left|F^{t}_{mm0}\right|^2 = \frac{1}{m!}\left(\frac{Q}{\hbar\omega}\right)^m e^{-\frac{Q}{\hbar\omega}}, \quad \text{and} \quad E_m - E_0 = m\hbar\omega_t. \tag{14}$$

Then equation (13) becomes

$$L^{osc}_t = \frac{1}{2}\sum_{m>m0}\frac{\hbar\omega_t}{(m-1)!}\int\limits_{\frac{(m\hbar\omega_t)^2}{2m_e v^2}}^{2m_e v^2}\left|F^p_{n0n0}(-\vec{q})\right|^2\left(\frac{Q}{\hbar\omega_t}\right)^m \times e^{-\frac{Q}{\hbar\omega_t}}\frac{dQ}{Q^2}$$
$$= \frac{1}{2}\sum_{m>m0}\frac{1}{(m-1)!}\int\limits_{\frac{m^2\hbar\omega_t}{2m_e v^2}}^{\frac{2m_e v^2}{\hbar\omega_t}}\left|F^p_{n0n0}\right|^2 t^{m-2}e^{-t}dt. \tag{15}$$

In the rightmost part of equation (15) the variable Q is substituted in $t = Q/\hbar\omega_t$. The integration in equation (15) could be split into two parts [15]: the first part is integration from $t_{min} = m^2\hbar\omega_t/2m_e v^2$ to t_0, and the second part is integration from t_0 to t_{max}. t_0 represents the value of integration limits and it is sufficiently small to justify application of the dipole approximation to the inelastic scattering amplitude as $|F^t_{mm0}|^2 = |\langle m|\sum_j e^{i\vec{q}\cdot\vec{r}_j}|m_0\rangle|^2 \approx q^2|d_{mm0}|^2$, where $\mathbf{d}_{mm0}$ is the dipole matrix element. Hence, equation (15) becomes

$$L^{osc}_t = \frac{1}{2}\sum_{m>0}\frac{1}{(m-1)!}\int\limits_{\frac{m^2\hbar\omega_t}{2m_e v^2}}^{t_0}\left|F^p_{n0n0}\right|^2 t^{m-2}e^{-t}dt + \frac{1}{2}\sum_{m>0}\frac{1}{(m-1)!}\int\limits_{t_0}^{\frac{2m_e v^2}{\hbar\omega_t}}\left|F^p_{n0n0}\right|^2 t^{m-2}e^{-t}dt. \tag{16}$$

Taylor's expansion, $e^{-t} \approx 1$, could be used in the first term on the right side of equation (16); the first term ($m = 1$) of the expansion sum gives the largest contribution. The order of summation and integration could be exchanged in the second term of equation (16). Using $\sum\limits_m t^{m-1}/(m-1)! = e^t$, equation (16) becomes

$$L^{osc}_t = \frac{1}{2}\int\limits_{\frac{\hbar\omega_t}{2m_e v^2}}^{t_0}\left|F^p_{n0n0}\right|^2\frac{dt}{t} + \frac{1}{2}\int\limits_{t_0}^{\frac{2m_e v^2}{\hbar\omega_t}}\left|F^p_{n0n0}\right|^2\frac{dt}{t} = \frac{1}{2}\int\limits_{\frac{\hbar\omega_t}{2m_e v^2}}^{\frac{2m_e v^2}{\hbar\omega_t}}\left|F^p_{n0n0}\right|^2\frac{dt}{t} \tag{17}$$

and

$$L^{osc}_t = \frac{1}{2}\int\limits_{\frac{(\hbar\omega_t)^2}{2m_e v^2}}^{2m_e v^2}\left|F^p_{n0n0}(Q)\right|^2\frac{dQ}{Q}. \tag{18a}$$

In a similar way the partial stopping number for a projectile oscillator, L^{osc}_p, could be obtained as

$$L^{osc}_p = \frac{1}{2}\int\limits_{\frac{(\hbar\omega_p)^2}{2m_e v^2}}^{2m_e v^2}\left|F^t_{m0m0}(Q)\right|^2\frac{dQ}{Q}. \tag{18b}$$

The atomic form factors F^i_{00} are equal to $F^i_{00} = z_i - {}_iM_{00}$; M_{00} are matrix elements ${}_iM_{00} = \langle 0|\sum_j e^{-i\vec{q}\cdot\vec{r}_j}|0\rangle$, calculated from Cabrera-Trujillo et al. [18] as

$${}_iM_{00} = N_i\left[1 - A_iQ\left(\frac{0.37}{A_iQ + 13.88} + \frac{0.63}{A_iQ + 0.96}\right)\right] \tag{19}$$

where $A_i(v) = (2m_e/\hbar^2)\Lambda^2_i(v)b^2$ are functions of the projectile velocity v, defined by Cabrera-Trujillo et al. [18] and this expression is valid within the Thomas-Fermi model of an atom.

The integrals in equations (18a) and (18b) can be written as

$$I_i(Q) = \int\left|F^i_{00}\right|^2\frac{dQ}{Q} = \int\left(z_i - {}_iM_{00}\right)^2\frac{dQ}{Q} = \left(z_i - N_i\right)^2\ln(Q) + Y_i(Q) \tag{20a}$$

where $Y_i(Q)$ are calculated as

$$Y_i(Q) = N_i\left(\frac{1.9N_i}{13.88 + A_iQ} + \frac{0.38N_i}{0.97 + A_iQ} - (0.9N_i - 1.3z_i)\ln(A_iQ + 0.97) - (0.1N_i - 0.74z_i)\ln(A_iQ + 13.88)\right). \tag{20b}$$

By applying the lower integration limit in equation (20a) and using Taylor's expansion of function $Y_i(Q)$ one can obtain

$$I_i(Q_{min}) = (z_i - N_i)^2\ln(Q_{min}) + N_i(0.3N_i + 1.9z_i). \tag{21a}$$

For the upper integration limit one can obtain

$$I_i(Q_{max}) = (z_i - N_i)^2\ln(Q_{max}) + N_i(2z_i - N_i)\ln(AQ_{max}). \tag{21b}$$

By inserting equations (21a, 21b) in equations (18a, 18b) the following was obtained

$$L^{osc}_t = \left\{(z_1 - N_1)^2\ln\left(\frac{2m_e v^2}{\hbar\omega_t}\right) - \frac{1}{2}N_1\left((0.29N_1 + 1.9z_1) + (N_1 - 2z_1)\ln\left(\frac{4m_e^2\Lambda_1^2 b^2 v^2}{\hbar^2}\right)\right)\right\}, \tag{22a}$$

$$L_p^{osc} = \left\{ (z_2 - N_2)^2 \ln\left(\frac{2m_e v^2}{\hbar\omega_p}\right) - \frac{1}{2} N_2 \left((0.29N_2 + 1.9z_2) \right.\right.$$
$$\left.\left. + (N_2 - 2z_2) \ln\left(\frac{4m_e^2 \Lambda_2^2 b^2 v^2}{\hbar^2}\right)\right)\right\}. \quad (22b)$$

The third partial stopping number of an oscillator, given by equation (12) could be written as

$$L_{t,p}^{osc} = \frac{1}{2} \sum_{m>n0;\, n>n0} \left((E_m - E_{m0}) + (E_n - E_{n0})\right) \times \int_{\frac{((E_m-E_{m0})+(E_n-E_{n0}))^2}{2m_e v^2}}^{2m_e v^2} \left|F_{nn0}^p\right|^2 \left|F_{mm0}^t\right|^2 \frac{dQ}{Q^2}. \quad (23)$$

According to equation (16) the last expression could be transformed into

$$L_{t,p}^{osc} = \frac{1}{2} \sum_{m>0;\, n>0} (m\hbar\omega_t + n\hbar\omega_p) \frac{1}{m!n!} \times \int_{\frac{(m\hbar\omega_t+n\hbar\omega_p)^2}{2m_e v^2}}^{2m_e v^2} \left(\frac{Q}{\hbar\omega_t}\right)^m \left(\frac{Q}{\hbar\omega_p}\right)^n e^{-\left(\frac{1}{\hbar\omega_t}+\frac{1}{\hbar\omega_p}\right)Q} \frac{dQ}{Q^2}. \quad (24)$$

After substitution of $t = (1/\hbar\omega_t + 1/\hbar\omega_p)Q$, equation (24) becomes

$$L_{t,p}^{osc} = \frac{1}{2} \sum_{m>m0;\, n>n0} \frac{1}{m!n!} \frac{m\varepsilon_t^n \varepsilon_p^{m-1} + n\varepsilon_t^{n-1}\varepsilon_p^m}{(\varepsilon_t + \varepsilon_p)^{m+n-1}} \times \Gamma\left(m+n-1, \frac{(m\varepsilon_t + n\varepsilon_p)^2}{\varepsilon_t + \varepsilon_p}\right) \quad (25)$$

where $\varepsilon_t = \hbar\omega_t/2m_e v^2$ and $\varepsilon_p = \hbar\omega_p/2m_e v^2$ and $\Gamma(n,x) = \int_x^\infty \xi^{n-1} e^{-\xi} d\xi$ is the Gamma function.

The partial stopping number $L_{t,p}^{osc}$ given in equation (25) was calculated numerically and fitted as a function of $\varepsilon_t^{-1} = y$ and $\varepsilon_p^{-1} = x$. The following was obtained

$$L_{t,p}^{osc}(y,x) = 0.1 - 0.001y - 2.5 \times 10^{-7} y^2 - 0.001x - 2.5 \times 10^{-7} x^2 + 0.51 \ln(y) + 0.51 \ln(x). \quad (26)$$

2.2 Calculation of partial stopping numbers, L^{at}, for the target and the projectile

The partial stopping numbers of the target and the projectile, defined in equation (11), could be calculated as a sum of oscillator stopping numbers, defined in equations (22a, 22b, 26) [7]. Summation is over all states of the discrete and continual spectrum, weighted by dipole oscillator strengths, f_{ii0}, of given atoms. One must replace excitation/ionization energies of atoms, $E_i - E_{i0}$ with excitation energies of quantum harmonic oscillators, $\hbar\omega$.

All terms in L_t^{osc} equation (11), are independent of excitation/ionization energies, except for the first logarithmic term. The final expression for the partial stopping number, L_t^{at}, has the form

$$L_t^{at} = (z_1 - N_1)^2 \ln\left(\frac{2m_e v^2}{I_2}\right) - \frac{1}{2} N_1 \left((0.29N_1 + 1.9z_1) + (N_1 - 2z_1) \ln\left(\frac{4m_e^2 \Lambda_1^2 b^2 v^2}{\hbar^2}\right)\right). \quad (27)$$

Here $\ln I = \sum_m f_{mm0} \ln(E_m - E_{m0})$ and $\sum_m f_{mm0} = 1$ as given in reference [7].

Cabrera-Trujillo [22] treated target electrons as harmonically bounded and obtained the total stopping cross section as a sum of orbital electronic cross sections. Taking into account the property of dipole oscillator strength of the quantum harmonic oscillator in the ith orbit, $f_{m_i m_0}^{(i)} = \delta_{m_i m_0}$, they concluded that the orbital ionization potential I_i is equal to $I_i = \hbar\omega_{i0}$ [22]. In this paper the approach used is a little bit different. The dipole oscillator strengths in equation (11) are not for oscillators, but for atoms, and summation was performed over discrete and continual atomic energy spectra. This way excitation and ionization of atoms were taken into account.

Similarly, the partial stopping number, L_p, becomes

$$L_p^{at} = (z_2 - N_2)^2 \ln\left(\frac{2m_e v^2}{I_1}\right) - \frac{1}{2} N_2 \left((0.29N_2 + 1.9z_2) + (N_2 - 2z_2) \ln\left(\frac{4m_e^2 \Lambda_2^2 b^2 v^2}{\hbar^2}\right)\right). \quad (28)$$

Calculation of the partial stopping number, $L_{t,p}$, given in equation (11) was performed by summation over projectile and target states.

In order to simplify derivation of the expression for stopping power, corrections were neglected in this section. They will be added and discussed in the following section. Hence, the quadratic terms in equation (26) (x and y are proportional to $\sim 1/2m_e v^2$; x^2 and y^2 to $\sim(1/2m_e v^2)^2$) that are responsible for shell correction are not taken into account here (see Ref. [20]). Then, the partial stopping number $L_{t,p}$ becomes

$$L_{t,p}^{at} = 0.1 + 0.51 \ln\left(\frac{2m_e v^2}{I_2}\right) + 0.51 \ln\left(\frac{2m_e v^2}{I_1}\right). \quad (29)$$

Finally, the expression for the total stopping power given by equation (10), becomes

$$S = \frac{4\pi e^4}{m_e v^2} N \Bigg\{ N_2 (z_1 - N_1)^2 \ln\left(\frac{2m_e v^2}{I_2}\right) - \frac{1}{2} N_1 N_2 \Bigg((0.29 N_1 + 1.9 z_1) + (N_1 - 2z_1) \ln\left(\frac{4m_e^2 \Lambda_1^2 b^2 v^2}{\hbar^2}\right)\Bigg) + N_1 (z_2 - N_2)^2 \ln\left(\frac{2m_e v^2}{I_1}\right) - \frac{1}{2} N_1 N_2 \Bigg((0.29 N_2 + 1.9 z_2) + (N_2 - 2z_2) \ln\left(\frac{4m_e^2 \Lambda_2^2 b^2 v^2}{\hbar^2}\right)\Bigg) + N_1 N_2 \left(0.1 + 0.51 \ln\left(\frac{2m_e v^2}{I_2}\right) + 0.51 \ln\left(\frac{2m_e v^2}{I_1}\right)\right)\Bigg\}. \quad (30)$$

This expression may be split into two parts: the first one represents the contribution due to excitation of the target, S_t,

$$S_t = \frac{4\pi e^4}{m_e v^2} N N_2 \Bigg\{ (z_1 - N_1)^2 \ln\left(\frac{2m_e v^2}{I_2}\right) - \frac{1}{2} N_1 \left((0.29 N_1 + 1.9 z_1) + (N_1 - 2z_1) \ln\left(\frac{4m_e^2 \Lambda_1^2 b^2 v^2}{\hbar^2}\right)\right) + N_1 \left(0.05 + 0.51 \ln\left(\frac{2m_e v^2}{I_2}\right)\right)\Bigg\} \quad (31)$$

and the second one, S_p, represents the contribution due to projectile excitation

$$S_p = \frac{4\pi e^4}{m_e v^2} N N_1 \Bigg\{ (z_2 - N_2)^2 \ln\left(\frac{2m_e v^2}{I_1}\right) - \frac{1}{2} N_2 \left((0.29 N_2 + 1.9 z_2) + (N_2 - 2z_2) \ln\left(\frac{4m_e^2 \Lambda_2^2 b^2 v^2}{\hbar^2}\right)\right) + N_2 \left(0.05 + 0.51 \ln\left(\frac{2m_e v^2}{I_1}\right)\right)\Bigg\}. \quad (32)$$

2.3 Calculation of the stopping power with shell, Barkas and Bloch corrections

The oscillator stopping number defined by equation (13) with the shell correction has the form (see Appendix A)

$$L_{tc}^{osc} = z_1^2 \left(\ln\left(\frac{2m_e v^2}{\hbar\omega}\right) - \frac{C}{N_2}\right) + \frac{1}{2} N_1 (2z_1 - N_1) \left(\ln\left(A_1 2 m_e v^2\right) - 2\ln\left(\frac{2m_e v^2}{\hbar\omega}\right)\right) - \frac{1}{2} N_1 (0.29 N_1 + 1.9 z_1) \quad (33)$$

where the shell correction is obtained as [7]

$$\frac{C}{N_2} = 3 \frac{\hbar\omega}{2m_e v^2}. \quad (34)$$

Two terms were used in reference [7] to describe the shell correction. Since the projectile velocities considered in this paper are larger than $z_2^{2/3} v_0$ only the first term of the shell correction was taken into account. The subscript "c" in the stopping number L_{tc}^{osc} (see Eq. (33)) means a *corrected* stopping number.

According to equation (11), the corrected stopping number of the target atom has the form

$$L_{tc}^{at} = z_1^2 \left(\ln\left(\frac{2m_e v^2}{I_2}\right) - \frac{N_2^{1.4} v_0^2}{v^2}\right) + \frac{1}{2} N_1 (2z_1 - N_1) \left(\ln\left(A_1 2 m_e v^2\right) - 2\ln\left(\frac{2m_e v^2}{I_2}\right)\right) - \frac{1}{2} N_1 (0.29 N_1 + 1.9 z_1) \quad (35)$$

where the shell correction

$$\frac{C}{N_2} = 2 \frac{K_1}{2m_e v^2} = \frac{N_2^{1.4} v_0^2}{v^2}$$

is taken from [2].

Similarly, the partial stopping number, L_p, becomes

$$L_{pc}^{at} = z_2^2 \ln\left(\frac{2m_e v^2}{I_1}\right) + \frac{1}{2} N_2 (2z_2 - N_2) \left(\ln\left(A_2 2 m_e v^2\right) - 2\ln\left(\frac{2m_e v^2}{I_1}\right)\right) - \frac{1}{2} N_2 (0.29 N_2 + 1.9 z_2). \quad (36)$$

In this case, the shell correction for the projectile in equation (36) equal to $N_1^{1.4} v_0^2 / v^2$ was not taken into account as its value is less than 3% in comparison to the shell correction for the target given in equation (35). Equation (29) was used for the partial stopping number, L_{tp}^{osc}. The quadratic terms were neglected because the shell correction is taken into account in equation (35).

The Bloch correction was derived by Bloch [23] in an investigation of similarities and differences between classical and quantum-mechanical calculations of stopping power. This correction can be found in [24] and has the form

$$z_1^2 L_{Bloch} = -y^2 \sum_{n=1}^{\infty} \frac{1}{n\left(n^2 + y^2\right)} \tag{37}$$

where $y = z_1\alpha/\beta$, $\alpha = 1/137$ is a constant of the fine structure and $\beta = v/c$.

The Barkas correction is proportional to odd power of the projectile charge and makes stopping power of a negative charge somewhat smaller than that for a positive charge, with the same mass and velocity. The first theory using the Barkas effect was developed in [6,25]. Their results were presented in the following form

$$L_{Barkas} = \frac{\gamma F_{ARB}\left(b/x^{1/2}\right)}{z_2^{1/2} x^{3/2}} \tag{38}$$

where $\gamma = 1.41$ and $x = (\beta/\alpha)^2/z_2$. Tabulation of function F_{ARB} can be found in [6] and the values of constant b are given in [26]. According to equation (10), the final expression for stopping power with necessary corrections has the form

$$S_c = \frac{4\pi e^4}{m_e v^2} N \Big\{ N_2 L_{tc}^{at} + N_1 L_{pc}^{at} + N_1 N_2 L_{t,p}^{at} + \left(z_1 - N_1\right)^3 N_2 L_{Barkas} + \left(z_1 - N_1\right)^2 N_2 L_{Bloch} \Big\}. \tag{39}$$

3 Results

Passing through matter, the projectile nucleus could carry some bounded electrons, even when its velocity is larger than the orbital velocity of electrons [13,20]. The projectile charge is variable along the trajectory and the effective charge z_{eff} was introduced as a function of the projectile velocity. z_{eff} is smaller than z_1 even on larger velocities [11]. In this work, the number of electrons bounded to the projectile at a certain velocity was adopted from Cabrera-Trujillo et al. [18]. The relative number of electrons, N_1/z_1, bounded in a projectile, is presented in Figure 1 as a function of the projectile energy.

For a fully stripped ion ($N_1 = 0$), equation (30) is reduced to Bethe's formula

$$S = \frac{4\pi e^4}{m_e v^2} N z_1^2 N_2 \ln\left(\frac{2m_e v^2}{I_2}\right). \tag{40}$$

The stopping power of a hydrogen target for a hydrogen ion as a function of the projectile energy is given in Figure 2. Contributions to the stopping power from projectile excitation, S_p (Eq. (32) — triangle scatter) and target excitation, S_t, (Eq. (31) — short dashed line) were given in Figure 2. Their sum given by equation (30) is given in the same figure as a solid line. The dash-dot line presents the stopping power calculated according to the formula given by Cabrera-Trujillo et al. [18]. The scatter squares present data obtained from SRIM2003 [27], while the dash-dot-dot line is Bethe's formula. Good agreement was found between all groups of data if the energy was above 0.2 MeV. In the energy region right from the peak but below 0.2 MeV, the stopping power calculated according to Cabrera-Trujillo et al. [18] is slightly lower than the results obtained from SRIM2003 and equation (30). In the peak region and lower, a larger discrepancy between the expression from Cabrera-Trujillo et al. [18], equation (30) and SRIM2003 exists. In the low energy region, below 0.2 MeV, the contribution due to projectile excitation calculated from equation (32) is up to 20% in respect to the total stopping power.

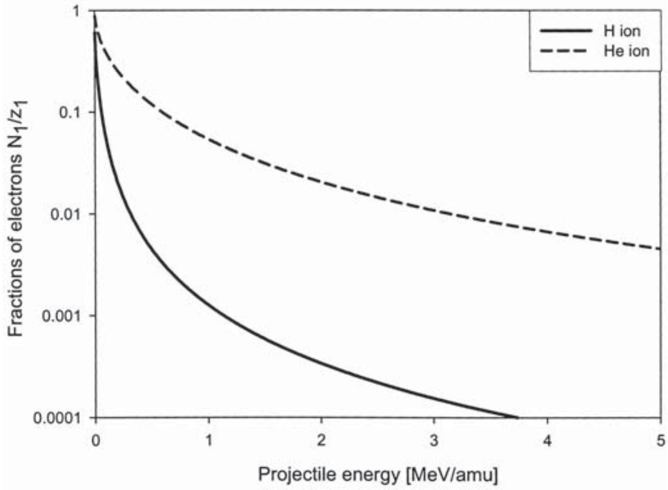

Fig. 1. Fraction of bounded electrons as a function of projectile energy for H and He ions [18].

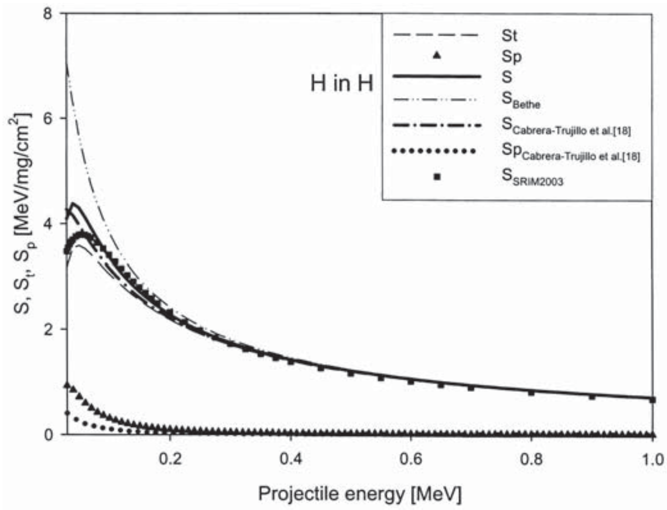

Fig. 2. Stopping power of hydrogen for hydrogen ions.

Figure 3 gives the stopping power of a He target for a hydrogen ion. The notation is the same as in Figure 2. The region of energy presented here is from 0.07 up to 1 MeV. The behavior of stopping power curves is similar as in Figure 2. Very good agreement exists between Cabrera-Trujillo et al. [18], SRIM2003 (Ref. [27]), and this work, (Eq. (30)). The contribution to the total stopping power

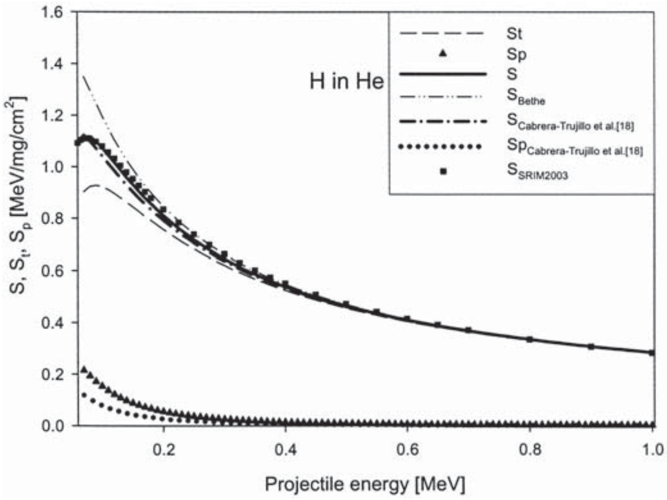

Fig. 3. Stopping power of helium for hydrogen ions.

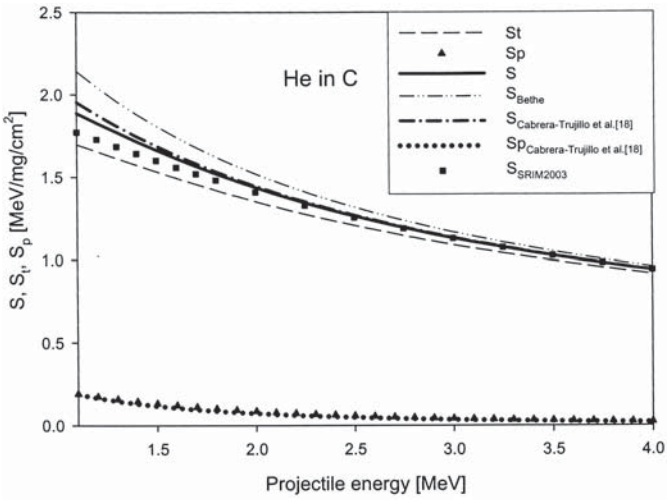

Fig. 4. Stopping power of carbon for helium ions.

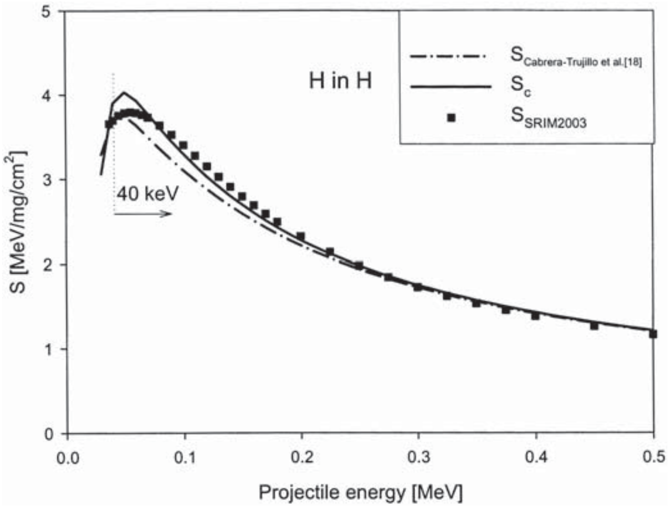

Fig. 5. Stopping power of hydrogen for hydrogen ions with corrections.

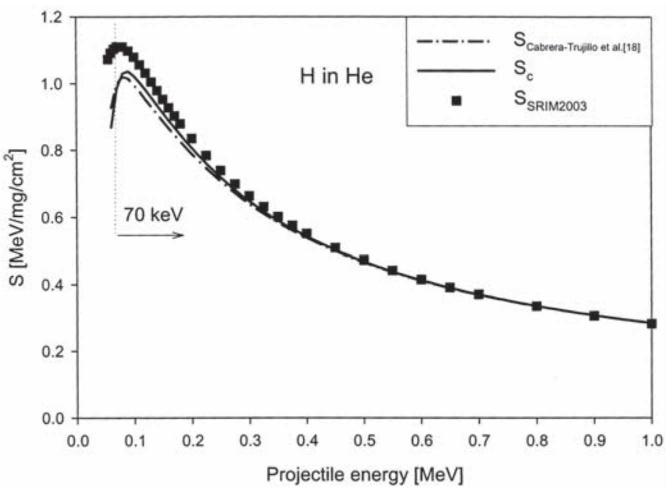

Fig. 6. Stopping power of helium for hydrogen ions with corrections.

due to projectile excitation, calculated by equation (32) is again up to about 18% and depends on the energy.

Figure 4 represents the stopping power of carbon for a helium projectile as a function of energy. The energy range is between 1.1 to 4 MeV. Agreement between the stopping power given by Cabrera-Trujillo et al. [18] and equation (30) is again very good, but both groups of results are larger than SRIM2003 in the energy region below 2 MeV. The contribution to the total stopping power due to projectile excitation is about 10% in respect to the total stopping power. It was previously shown that the stopping power is very dependent on the mean excitation energy [28]. In this paper the mean excitation energy of hydrogen, helium and carbon is 14.9 eV, 41 eV and 77.8 eV, respectively, taken from [24,26].

The results obtained using Bethe's formula are presented as dash-dot-dot curves in all graphs. The values are much larger than the ones obtained using all other considered methods in the low energy region.

The stopping powers calculated using the formulae given by Cabrera-Trujillo et al. [18] (line-dot-line) and equation (39) (solid line), with necessary corrections, are presented in Figures 5–7. The stopping power data from SRIM2003 [27] is also given in these figures.

Figure 5 represents the stopping power of hydrogen in hydrogen where the shell, Barkas and Bloch corrections were taken into account. The considered energy range of the projectile in this case is $E > 40$ keV, where the shell correction is not very significant. Due to the corrections introduced, both curves, given by Cabrera-Trujillo et al. [18] and equation (39), are lower in respect to those displayed in Figure 2, particularly in the area of the stopping maximum. The maximum is lower for about 10% and has shifted to the right. Better agreement with SRIM2003 data was obtained when the corrections were taken into account.

The stopping power of He atoms for a H ion, with corrections is represented in Figure 6. The energy range of the projectile is $E > 70$ keV, and it can be seen that both curves are slightly below the data from SRIM2003.

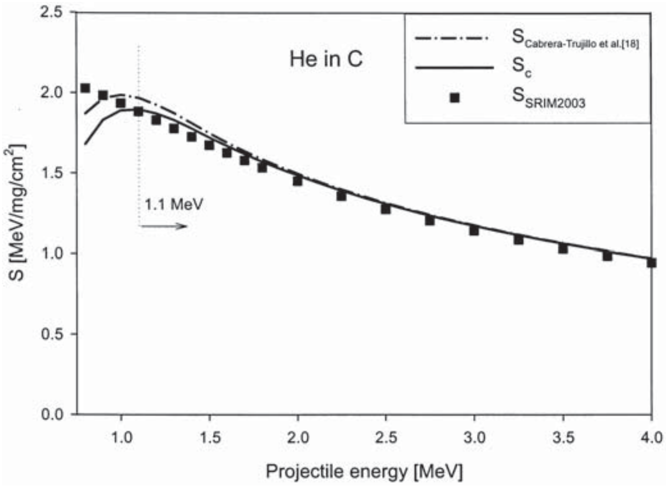

Fig. 7. Stopping power of carbon for helium ions with corrections.

Figure 7 represents the stopping power of C, for a He projectile. The energy range is the same as in Figure 4, i.e. $E > 1.1$ MeV. All data show very good agreement.

4 Conclusion

During slowing down, projectile ions may carry some bound electrons. Excitation of such a system is possible, and this is one of the possible mechanisms of energy loss. This process should be taken into account in stopping power calculations. Energy losses of hydrogen and helium ion projectiles were calculated considering both projectile and target atoms as assemblies of quantum harmonic oscillators.

Modeling of projectile and target as quantum harmonic oscillators represents calculation of partial stopping numbers over the states of quantum harmonic oscillators as in [7]. Then, weighting of partial stopping numbers according to the dipole oscillator strengths for a given projectile and target has to be done, as suggested in [7,8]. This model enables easier evaluation of generalized oscillator strengths. Thomas-Fermi theory which describes an ion with N_1 bound electrons with the radial symmetric electron density was accepted in this paper as in [18].

The stopping power obtained in this way behaved similarly to the one given by Cabrera-Trujillo et al. [18]. The process of projectile excitation is significant in the Bragg peak region where it enlarges the total stopping power. In this case, enlargement of the stopping power due to projectile excitation is from 10–20%.

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Appendix A

The oscillator stopping number for a target, given by equation (13), could be calculated in the following way. The atomic form factor for projectile F_{00}^p is equal to $F_{00}^p = z_1 - M_{00}$. Then the expression in equation (13) could be split into two terms, L_{t1}^{osc} and L_{t2}^{osc}

$$L_t^{osc} = L_{t1}^{osc} + L_{t2}^{osc} = \frac{1}{2} z_1^2 \sum_{m=1} (E_m - E_{m0}) \times \int \left| F_{mm0}^t \right|^2 \frac{dQ}{Q^2} + \frac{1}{2} \sum_{m=1} (E_m - E_{m0}) \times \int \left(-2z_1 M_{00} + M_{00}^2 \right) \left| F_{mm0}^t \right|^2 \frac{dQ}{Q^2}. \quad (A.1)$$

The first term of equation (A.1) represents the oscillator stopping number of the target for the point like projectile [7], while the second term are sources if the electronic structure of the projectile is taken into account.

According to [7,22] L_{1t}^{osc} has the form

$$L_{t1}^{osc} = z_1^2 \left(\ln \left(\frac{2m_e v^2}{\hbar\omega} \right) - \frac{C}{N_2} \right), \quad (A.2)$$

where C/N_2 is the shell correction and its first term is equal to [7]

$$\frac{C}{N_2} = 3 \frac{\hbar\omega}{2m_e v^2}. \quad (A.3)$$

By analogy to derivation of equation (18a), the second oscillator number given in equation (A.1) could be written as

$$L_{t2}^{osc} = \frac{1}{2} \int_{\frac{(\hbar\omega)^2}{2m_e v^2}}^{2m_e v^2} \left(-2z_1 M_{00} + M_{00}^2 \right) \frac{dQ}{Q}. \quad (A.4)$$

According to equation (19), equation (A.4) becomes

$$L_{t2}^{osc} = \frac{1}{2} N_1 \left\{ -(2z_1 - N_1) \ln(Q) + \frac{0.38N_1}{0.96 + AQ} + \frac{1.9N_1}{13.88 + AQ} + (1.3z_1 - 0.9N_1) \ln(0.96 + AQ) + (0.74z_1 - 0.1N_1) \ln(13.88 + AQ) \right\}_{Q_{min}}^{Q_{max}}. \quad (A.5)$$

For maximum and minimum values of transferred energy Q, the stopping number L_{t2}^{osc} has values

$$L_{t2}^{osc}(Q_{max}) = \frac{1}{2} N_1 (2z_1 - N_1) \ln(A_1)$$

$$L_{t2}^{osc}(Q_{min}) = \frac{1}{2} N_1 \big(0.29N_1 + 1.9z_1 - (2z_1 - N_1) \ln(Q_{min}) \big). \quad (A.6)$$

Using equations (A.2) and (A.6), after some transformations, the final form of the target oscillator stopping number becomes

$$L_t^{osc} = z_1^2\left(\ln\left(\frac{2m_e v^2}{\hbar\omega}\right) - \frac{C}{N_2}\right) + \frac{1}{2}N_1\,(2z_1 - N_1)\left(\ln(A_1 2m_e v^2) - 2\ln\left(\frac{2m_e v^2}{\hbar\omega}\right)\right) - \frac{1}{2}N_1\,(0.29N_1 + 1.9z_1)\,. \quad \text{(A.7)}$$

Analogously to the previous expression, the projectile oscillator number has the form

$$L_p^{osc} = z_2^2\left(\ln\left(\frac{2m_e v^2}{\hbar\omega}\right) - \frac{C}{N_1}\right) + \frac{1}{2}N_2\,(2z_2 - N_2)\left(\ln(A_2 2m_e v^2) - 2\ln\left(\frac{2m_e v^2}{\hbar\omega}\right)\right) - \frac{1}{2}N_2\,(0.29N_2 + 1.9z_2)\,. \quad \text{(A.8)}$$

References

1. H. Bethe, Ann. Phys. **5**, 325 (1930)
2. U. Fano, Ann. Rev. Nucl Sci. **13**, 1 (1963)
3. N. Bohr, Phil. Mag. **25**, 10 (1913)
4. N. Bohr, Phil. Mag. **30**, 581 (1915)
5. N. Bohr, Z. Phys. **34**, 142 (1925)
6. J.C. Ashley, R.H. Ritchie, W. Brandt, Phys. Rev. B **5**, 2393 (1972)
7. P. Sigmund, U. Haagerup, Phys. Rev. A **34**, 892 (1986)
8. J. Jansen, H.H. Mikkelsen, Nucl. Instr. Meth. B **115**, 39 (1996)
9. H.H. Mikkelsen, E. Mortensen, Nucl. Instr. Meth. B **48**, 39 (1990)
10. Y. Xia, C. Tan, W.N. Lennard, Nucl. Instr. Meth. B **90**, 88 (1994)
11. L.C. Northcliffe, Ann. Rev. Nucl. Sci. **13**, 67 (1963)
12. P. Sigmund, A. Schinner, Nucl. Inst. Meth. B **174**, 535 (2001)
13. Y.K. Kim, K.T. Cheng, Phys. Rev. A **22**, 61 (1980)
14. M. Moneta, J. Czerbniak, Nucl. Inst. Meth. B **90**, 67 (1994)
15. H. Tsuchida, T. Kaneko, J. Phys. B: At. Mol. Opt. Phys. **30**, 1747 (1997)
16. T. Kaneko, H. Tsuchida, J. Phys. B: At. Mol. Opt. Phys. **27**, 97 (1994)
17. L.G. Glazov, Nucl. Meth. B **195**, 118 (2002)
18. R. Cabrera-Trujillo, S.A. Cruz, J. Oddershede, J.R. Sabin, Phys. Rev. A **55**, 2864 (1997)
19. N. Stevanović, D. Nikezić, Phy. Lett. A **340**, 290 (2005)
20. T. Kaneko, Phys. Rev. A **43**, 4780 (1991)
21. P. Sigmund, *Particle Penetration and Radiation Effects* (Springer-Verlag, Berlin, Heidelberg, Germany, 2006)
22. R. Cabrera-Trujillo, Phys. Rev. A **60**, 3044 (1999)
23. F. Bloch, Ann. Phys. **16**, 285 (1933)
24. S.P. Ahlen, Rev. Mod. Phys. **52**, 121 (1980)
25. J.C. Ashley, R.H. Ritchie, W. Brandt, Phys. Rev. A **8**, 2402 (1973)
26. ICRU 49, Stopping powers and ranges for protons and alpha particles, International Commission of Radiation Units and Measurement, Bethesda, Maryland (1993)
27. J.F. Ziegler, J.P. Biersack, U. Littmark, "The Stopping and Range of Ion in Matter", Pergamon Press (1985) Calculations were performed with SRIM-2003 (see http://www.SRIM.org)
28. J.R. Sabin, J. Oddershede, Phys. Rev. A **26**, 3209 (1982)