INFLUENCE OF ELECTRON MOTION IN TARGET ATOM ON STOPPING POWER FOR LOW-ENERGETIC IONS

by

Nenad STEVANOVIĆ *, ***Vladimir M. MARKOVIĆ, Momir ARSENIJEVIĆ, and Dragoslav NIKEZIĆ***

Faculty of Science, University of Kragujevac, Kragujevac, Serbia

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In this paper the stopping power was calculated, representing the electrons of the target atom as an assembly of quantum oscillators. It was considered that the electrons in the atoms have some velocity before interaction with the projectile, which is the main contribution of this paper. The influence of electron velocity on stopping power for different projectiles and targets was investigated. It was found that the velocity of the electron stopping power has the greatest influence at low energies of the projectile.

Key words: stopping power, energy loss, quantum harmonic oscillators

INTRODUCTION

The interaction of ions with matter is the subject of investigation in many areas of physics such as: atomic and nuclear physics, plasma physics, solid state physics, radiation physics, astrophysics, and other [1]. There are open problems for investigation of interactions of low energy ions with target atoms [2, 3] as well as passing of low-energy photons through the matter [4].

The study of the mechanisms where an ion (in further text projectile) losses its energy while interacting with matter has great significance. The stopping power, S, is one of the most important variables in that field and it is defined as the ratio of energy, dE, lost on some distance, dx, and that distance is: $S = -\mathrm{d}E/\mathrm{d}x$.

By using the quantum-mechanical treatment in the first Born approximation, Bethe has obtained the following expression for stopping power [5]

$$S \quad \frac{z_1^2 e^4}{4\pi\varepsilon_0^2 m_e v^2} N z_2 \ln \frac{2 m_e v^2}{I} \tag{1}$$

where N is the number of atoms , v – the projectile velocity, z_1 and z_2 are atomic numbers of the projectile and the target, and I – the mean ionisation potential of the target atom.

For calculation of stopping power, the states of the projectile and electrons in target atom before and after interaction must be known. The states of the projectile were presented as plane waves, but for states of electrons in the target atom some approximations were used in literature. Bohr [6] has modelled electrons in target atom as a set of classical harmonic oscillators. Similar approach was applied by Sigmund and Haagerup [7], who modelled target electrons as assemble of quantum harmonic oscillators. Stevanovic and Nikezic [8, 9] extended the model presented in [7] and applied for the projectile that contains bounded electrons and must be treated as partially stripped ion. It was shown that the projectile excitation contributes up to 20% to the total energy loss in the lower energy region.

Cabrera-Trujillo [10] also treated electrons in target atom as quantum oscillators, where total stopping power was presented as a sum of orbital stopping powers. It was shown that orbital ionizing potential I_j is equal to energy of the oscillator, $I_j = \hbar\omega_j$ [10].

These models were developed for fast projectiles, where the velocity of electron in the target atom can be neglected. But, for low-energetic projectiles (ions) this assumption is not justified.

In this paper stopping power was calculated by modelling electrons in the target atoms as assemble of quantum oscillators where the velocity of target electrons was taken into account. Influence of the electron velocity on stopping power was considered in this paper.

METHODOLOGY

According to quantum-mechanical model, the stopping power can be calculated as [5-10]

$$S \quad N \underset{m\ m_0}{} (E_m \quad E_{m_0}) \overset{Q_{\max}}{\underset{Q_{\min}}{}} \mathrm{d}\sigma(Q)_m \tag{2}$$

* Corresponding author; e-mail: nstevanovic@kg.ac.rs

where E_m and E_{m_0}, are eigenvalues of electron energy in the target atom energy for excited and ground states, respectively; $d\sigma_m$ is differential cross-section of interaction projectile and target electrons. Q_{min} and Q_{max} are minimal and maximal transferred energies of the projectile. The summation goes over all energetic states, m_j, of the target atom. In developed form the stopping power can be expressed as

$$S = \frac{z_1^2 e^4}{8\pi\varepsilon_0^2 m_e v^2}\frac{N_0}{M_a}\sum_{j=1}^{z_2}\sum_{m_j \neq m_{0j}}(E_{m_j}-E_{m_{0j}})\int_{Q_{min}}^{Q_{max}}\left|M_{m_j m_{0j}}\right|^2\frac{dQ}{Q^2} \tag{3}$$

where M_a is the molar mass of target atom, m_e – the mass of electron, v – the projectile velocity, N_0 – the Avogadro number, z_1 and z_2 are the atomic numbers of projectile and target atoms, respectively; j denotes the electrons in target atom. Matrix element $M_{m_j m_{0j}}$ for harmonic oscillator is equal to [7-10]

$$\left|M_{mjm_0j}\right|^2 = \frac{1}{m_j!}\left(\frac{Q}{\hbar\omega_j}\right)^{m_j} e^{-\frac{Q}{\hbar\omega_j}} \tag{4}$$

where $E_{m_j} - E_{m_{0j}} = m_j\hbar\omega_j$

By using energy conservation for collision projectile with electron in target atom, the maximal transferred energy of the projectile is

$$Q_{max} = 2m_e v^2 - 2m_e\vec{v}\vec{v}_j \tag{5}$$

where $\vec{v}$ and $\vec{v}_j$ are velocities of the projectile and target electron before collision. Lower boundary of integration Q_{min} has a form [5-10]

$$Q_{min} = \frac{(E_{m_j}-E_{m_{0j}})^2}{2m_e v^2} = \frac{(m_j\hbar\omega_j)^2}{2m_e v^2} \tag{6}$$

Upper boundary for summation over energetic states in eq. (3) can be determined from the condition that maximal transferred energy is transformed for transition to state m_{max} as

$$\frac{(m_{max}\hbar\omega_j)^2}{2m_e v^2} = 2m_e v^2 - 2m_e\vec{v}\vec{v}_j \tag{7}$$

From eq. (7) it can be obtained

$$m_{max} = \frac{2m_e v\sqrt{v^2 - \vec{v}\vec{v}_j}}{\hbar\omega_j}$$

This must be an integer because quantum number m denotes energy levels from 1 to m_{max}.

Using eqs. (4)-(7), the solution of eq. (3) can be presented by gamma function

$$S = \frac{z_1^2 e^4}{4\pi\varepsilon_0^2 m_e v^2}\frac{N_0}{M_a}\frac{1}{2}\sum_{j=1}^{z_2}\sum_{m_j=1}^{\frac{2m_e v\sqrt{v^2-\vec{v}\vec{v}_j}}{\hbar\omega_j}}\frac{1}{(m_j-1)!}\left[G\left(m_j-1,\frac{m_j^2\hbar\omega_j}{2m_e v^2}\right) - G\left(m_j-1,\frac{2m_e(v^2-\vec{v}\vec{v}_j)}{\hbar\omega_j}\right)\right] \tag{8}$$

The expression for stopping power, eq. (8), obtained in this paper is different in respect to stopping power calculated in [5-10] because the velocity of target electron $\vec{v}_j$ is introduced here.

The electron's velocity in a given orbital can be evaluated using virial theorem [10]. The virial theorem formulates a general relation between mean value of the kinetic energy $\langle|\hat{T}|\rangle$ and potential $\hat{V}$. In the case of stationary states and spherically symmetric potential $V(r) \propto r^n$, above mentioned relation takes simple form $2\langle|\hat{T}|\rangle = n\langle|\hat{V}|\rangle$. For harmonic potential, $n = 2$, electron's kinetic energy is equal to its potential energy, *i. e.* ionisation energy of a given electron's orbital is

$$\hbar\omega_j = I_j = \frac{m_e v_j^2}{2} \tag{9}$$

The projection of electron velocity $\vec{v}_j$ to projectile velocity $\vec{v}$ is p_z, then the following expression is valid $\vec{v}\vec{v}_j\cos(\theta) = vv_j p_z$.

According to these considerations, eq. (8) becomes

$$S = \frac{z_1^2 e^4}{4\pi\varepsilon_0^2 m_e v^2}\frac{N_0}{M_a}\frac{1}{2}\sum_{j=1}^{z_2}\sum_{m_j=1}^{\frac{2m_e v\sqrt{(v^2-vv_j p_z)}}{I_j}}\frac{1}{(m_j-1)!}\left[G\left(m_j-1,\frac{m_j^2 I_j}{2m_e v^2}\right) - G\left(m_j-1,\frac{2m_e(v^2-vv_j p_z)}{I_j}\right)\right] \tag{10}$$

The projection $p_z = \cos\theta$ can take values between $p_{zl} = -1$ (the projectile and the electron have opposite velocity directions before interaction) and $p_{zu} = +1$ (the projectile and the electron have the same velocity directions before interaction). The condition for interaction is that projection of electron's velocity is smaller than velocity of the projectile, $v_j p_{zu} > v$. In the opposite case, the projectile can not reach electron and interaction will not occur. Hence, for a given projectile and electron velocity, the upper values of projection must be equal to

$$p_{zu} = \begin{cases} 1, & \text{if } v \geq v_j \\ \dfrac{v}{v_j}, & \text{if } v < v_j \end{cases}$$

According to these considerations, upper boundary of sum in the eq. (10), as integer number, has values between

$$N_{lj} = N_j(p_z = p_{zu}) = \frac{2m_e v\sqrt{v^2 - vv_j p_{zu}}}{I_j}$$

and

$$N_{uj} = N(p_z = -1) = \frac{2m_e v\sqrt{v^2 + vv_j}}{I_j}$$

Therefore, there are $N_{sj} = N_{uj} - N_{lj} + 1$ values of the upper boundary of the sum, *i. e.*, N_{sj} groups of electrons which interact with projectile. Because the directions of electrons' velocities are equally possible, the probability that the projectile interacts with some subgroups of electrons is $1/N_{sj}$. The eq. (10) becomes

$$S = \frac{z_1^2 e^4}{4\pi\varepsilon_0^2 m_e v^2} \frac{N_0}{M_a} \frac{1}{2} \sum_{j=1}^{z_2} \frac{1}{N_{sj}} \sum_{m_j=1}^{N_{ij}} \sum_{m_j=1}^{N_{lj}} \cdots$$

$$\cdots \sum_{m_j=1}^{N_{uj}} \frac{1}{(m_j-1)!} \left[G\left(m_j+1, \frac{m_j^2 I_j}{2m_e v^2}\right) - G\left(m_j+1, \frac{2m_e(v^2 - v v_j p_z')}{I_j}\right) \right] \quad (11)$$

The projection p_z, in the second term of eq. (11), is changed from the p_{zl} to p_{zu} with the step of

$$\Delta p_z = \frac{p_{zu} - p_{zl}}{N_{sj} - 1} = \frac{p_{zu} - 1}{N_{sj} - 1}$$

It can be written

$$p_z = p_{zu} - (k-1)\frac{p_{zu} - (-1)}{N_{sj} - 1}$$

for $k = 1, .., N_{sj}$.

Finally, the eq. (11) can be written in the form

$$S = \frac{z_1^2 e^4}{4\pi\varepsilon_0^2 m_e v^2} \frac{N_0}{M_a} \frac{1}{2} \sum_{j=1}^{z_2} \frac{1}{N_{sj}} \sum_{k=1}^{N_{ij}} \sum_{m_j=1}^{N_{ij}} \frac{1}{(m_j-1)!} \left[G\left(m_j+1, \frac{m_j^2 I_j}{2m_e v^2}\right) - G\left(m_j+1, \frac{2m_e\left[v^2 - v v_j \left(p_{zu} - (k-1)\frac{p_{zu} - (-1)}{N_{sj} - 1}\right)\right]}{I_j}\right) \right] \quad (12)$$

RESULTS

In this paper, the stopping power was derived, where motion of target electrons before interaction with the projectile was taken into account, and the obtained expression was presented by eq. (12). The stopping power given by eq. (12) is a function of projectile energy (or velocity v). The stopping power for the following projectile-target pairs was calculated: H-H, He-C, and He-O. To apply eq. (12) it is needed to determine ionizing potentials for all the target atom orbitals, I_j and velocities of electrons v_j in given orbitals. The ionizing potentials I_j were determined in [10] and their values for H, He, and C atoms are: for H, $I_{H1} = 15$ eV; for He atom, $I_{He1,2} = 38.83$ eV; and for O atom, $I_{O1} = = 729.41$ eV, $I_{O2} = 56.86$ eV, and $I_{O3} = = 46.64$ eV. The electron velocity v_j in a given orbital j is calculated by eq. (9). The expression for the stopping power, given by eq. (12), can be applied for point-like projectile with velocity $v > z_1^{2/3} v_0$ [9, 10] ($v_0 = 2.16 \cdot 10^6$ m/s is Bohr velocity) where electron capture is neglected.

The stopping power of hydrogen target for hydrogen ion as a function of the projectile energy (eq. 12) is given in fig. 1 and presented by solid line. Dash-dot line presents the stopping power calculated according to the formula given in [7], while dashed line presents stopping power calculated in [10]. Scatter circle presents data obtained from SRIM2006 [11].

A good agreement has been found between all groups of data for the larger projectile energy. The results were presented for the projectile energy larger than 25 keV where electron capture is neglected and projectile can be treated as point like particle. It can be seen that influence of the electron velocity is larger for slower projectile, where projectile velocity has similar value as target electron. The stopping power calculated in this paper, eq. (12), is lower than that in [7, 10] because target electron has some energy before interaction, and projectile can loose a smaller amount of energy than in the case of interaction with electron at rest. Due to electron motion in the target before interaction with projectile, the stopping power is lower for about 25% for H-H interaction.

Figure 2 presents the stopping power for He-C interaction. The notation is the same as in fig. 1. The eq. (12) is valid for the projectile with energy larger than 250 keV. The behaviour of stopping power curves is similar as in fig. 1 and for lower projectile energy stopping power by eq. (12) is smaller for 10%, especially in Bragg peak region.

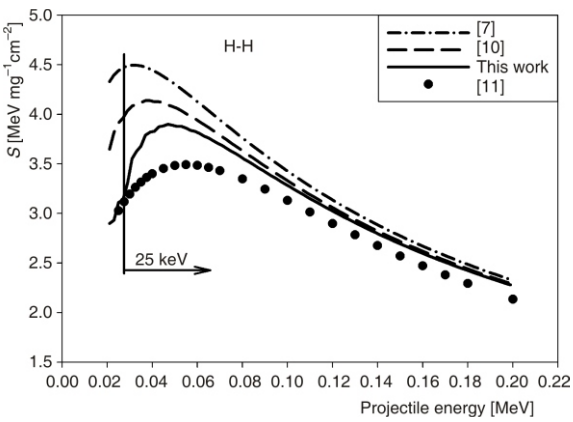

Figure 1. The stopping power of hydrogen for hydrogen projectile

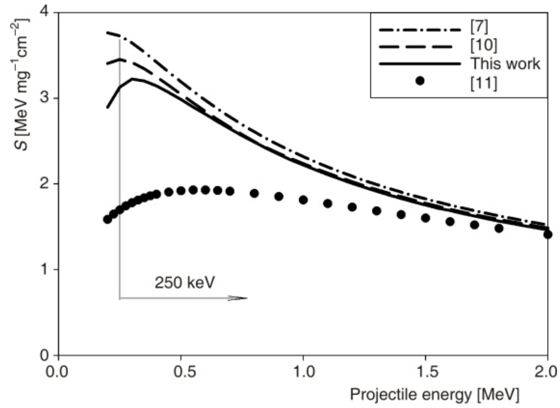

Figure 2. The stopping power of carbon for helium projectile

Figure 3 represents the stopping power of oxygen for helium projectile as a function of energy. The projectile energy is larger than 250 keV where electron capture is neglected. The influence of electron velocity is largest for the lower projectile energy, where the stopping power is smaller for 28%.

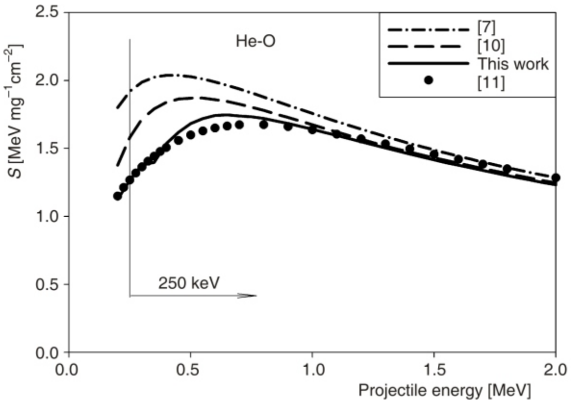

Figure 3. The stopping power of oxygen for helium projectile

For considered projectile-target interactions, it was shown that when electron velocity is taken into account, the calculated stopping power data (eq. 12) are close to data obtained by SRIM [11] and must be considered in further investigation.

CONCLUSIONS

In this work analytical expression for stopping power was obtained, where it was taken into account that target's electrons have non-negligible velocities before interaction with projectiles takes place. On the basis of (quantum) virial theorem, the velocity of each electron in a given atomic orbital is determined. Influence of the electron's velocities in the atoms of the target has been examined whereby the following results stands: (1) stopping power magnitude is lesser because of non-zero velocities of target electrons and (2) velocities of target electrons have the ultimate impact on stopping power at lower projectile's energies.

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**Ненад СТЕВАНОВИЋ, Владимир М. МАРКОВИЋ,
Момир АРСЕНИЈЕВИЋ, Драгослав НИКЕЗИЋ**

УТИЦАЈ КРЕТАЊА ЕЛЕКТРОНА У АТОМУ МЕТЕ НА ЗАУСТАВНУ МОЋ ЗА НИСКО ЕНЕРГЕТСКЕ ЈОНЕ

У овом раду је рачуната зауставна моћ, представљајући електроне у атомима мете ансамблом квантних осцилатора. При томе је разматрано да се електрони у атомима мете крећу одређеном брзином пре интеракције са пројектилом, што је главни допринос овога рада. Испитиван је утицај брзина тих електрона на вредност зауставне моћи за различите пројектиле и мете. Установљено је да брзине електрона на зауставну моћ имају највећи утицај при нижим енергијама пројектила.

Кључне речи: зауставна моћ, губитак енергије, квантни хармонијски осцилатор