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Study on Electron/Positron Scattering in Solid Targets Using Accurate Transport Cross-sections: Comment on Z. Rouabah et al Papers

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Abstract We should be very careful, when we applied a combination between two models, especially if the first one is stochastic (probabilistic) and analytic (deterministic) for the second , which is the case of the papers of Rouabah et al[Appl. Surf. Sci. 255 (2009) 6217 and Appl. Surf. Sci. 256 (2010) 3448]. In fact, this work has an aim to show the valuable approaches to study the transport of electron/positron in solid target. Our work is presented as a comment on the papers of Rouabah et al. Indeed, after mentioned some weak points of Rouabah et al works we have discussed different points: the screened Born transport cross-section (TCS) and the true model of Jablonski[Phys. Rev. B 58 (1998) 16470], the large deviation between Rouabah et al TCSs and the accurate values, the combination between Monte Carlo simulation and Vicanek and Urbassek theory[Phys. Rev. B 44 (1991) 234] and the normalization condition as well. Besides, we have given some recommendations on the range calculation using Monte Carlo method.

Keywords Electron Scattering, Positron Scattering, Transport Cross-Sections, Electron Range, Monte Carlo Simulation, Deterministic Model, Range of Penetration

1. Introduction

The electron and positron material interaction has a great importance in several domains of the analytical techniques of the material such as electron probe microanalysis, electron energy-loss spectroscopy, Auger electron spectroscopy, positron annihilation spectroscopy, etc. Electron-transport calculations are usually performed by means of either analytical theory or Monte Carlo simulation. It is important to know that the latter (Monte Carlo method) has become a powerful tool in the calculation and prediction of radiation effects in the solids. Both methods require an accurate knowledge of the cross-section for elastic scattering of electrons as functions of the projectile kinetic energy E. For that reason, Rouabah et al[1-3] have been interested to propose a simplified expression of the transport cross-section of electron and positron by basing on analytical expression reported by Jablonski[4]. The direct calculation of the deviation between their interpolated results and the accurate values shows that there are drastic deviations. In addition, Rouabah et al have combined between the Vicanek and Urbassek theory[5] (deterministic model) and the Monte Carlo simulation (probabilistic model) to investigate the transport of 0.5–4keV electrons in solid targets[1, 6]. However, when we applied a combination between two different methods we should be very careful especially if the first model is stochastic (probabilistic) and the second is analytic (deterministic). After a careful analysis of Refs.[1-3, 6-8] we notice that there is an abnormal problem in number of questions: the expression of the electron TCS[1-3], the combination between Monte Carlo and analytic model[1, 6], the backscattering coefficient results[1,6-8], the range of penetration[1, 6-8] and the large deviation of their results[1-3, 6-8]. Moreover, some errors are repeated in all Rouabah's papers[1-3, 6-8] (see below). We note that we have focused our attention on Rouabah's paper "[1]" which was the base of number of their other works.

So, the present work shows necessary considerations to study the transport of the slow electrons and positrons in solid targets.

This paper is organized as follows. In Section 2 we describe our comments on the methods used in the calculations: the transport cross-sections, the normalized combination between the Monte-Carlo simulation and the Vicanek and Urbassek theory, the electron range, the mean

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number of wide angle collisions and the analytical backscattering coefficient. Finally, Section 3 contains the conclusion.

2. Methods and Comments

Our comment on the Rouabah et al works could be summarized on three subjects: their transport cross-section (TCS), their combination between analytic and stochastic models and their calculated range using Monte Carlo method.

2.1. Comment on Rouabah et al TCSs

Rouabah et al suggested a simplified expression of the electron transport cross section using a simple fit. However, actually, they have attributed in their work[1-3, 6-8], an old screened TCS (denoted σ_{tr}^{B}) to Jablonski[4]. Indeed, firstly, we will present the demonstration that σ_{tr}^{B} is more than 60 years old; then we present the true Jablonski TCS.

2.1.1. The Screened Cross Sections and the Wentzel Model (1927)

According to Fernandez-Varea et al[9]: "*The Wentzel[10] approach for describing elastic scattering of particles with charge Z'e (Z ' =- 1 and + 1 for electrons and positrons, respectively) by atoms of atomic number Z is based on the simplified scattering potential*

$$V(r) = \frac{ZZ'e^2}{r}\exp(-r/R) \tag{1}$$

where the exponential factor tries to reproduce the effect of screening. The screening radius R may be estimated from the Thomas-Fermi model of the atom, which yields"

$$R \approx C_F a_0 Z^{-1/3} \tag{2}$$

where a_0 *is the Bohr radius (* $a_0 = \frac{\hbar^2}{me^2}$ *) and* $C_F = 0.8853414$.

"However, it is more expedient to determine R so as to obtain agreement with more accurate elastic scattering cross sections"[9].

Generally, R has been taken using the next form (see Nigam[11] (**1959**)):

$$R \approx R_0 / \mu \tag{3}$$

where $R_0 \approx C_F a_0 Z^{-1/3}$ and μ is a constant (generally μ>1 which signifies that R<R_0).

It could be noted that, at high incident electron energies we take μ = μ^{∞}[12]. Moreover, the first order Born approximation is valid only at that case (see below). Thus:

$$R \approx R_0 / \mu^{\infty} \tag{4}$$

The agreeable value of μ^{∞} depends on the used screened potential and the energy[12]. For example, some authors take $\mu^{\infty} = 1.12$ as value corresponding to the Thomas Fermi potential (i.e. $R \approx a_0 Z^{-1/3} = R_0 / C_F$ see[11-14]).

The transport cross section corresponds to the screened Differential Cross Section (DCS) (which is obtained from the first order Born approximation), which gives[9]

$$\sigma_{tr}^{B} = \frac{(ZZ'e^2)^2}{(p\beta c)^2} 2\pi \left[\ln\left(\frac{1+A}{A}\right) - \frac{1}{A+1} \right] \tag{5}$$

The screening parameter A is given by[7]:

$$A \equiv \frac{1}{4}(\hbar / p)^2 R^{-2} \tag{6}$$

where p is *the* momentum and β is the velocity of the scattered particle in units of the speed of light *c*.

At no relativistic domain (v<<c), the equation (6) can be rewritten as follows:

$$A = \frac{1}{4}\frac{\hbar^2}{2mE}\left(R_0 / \mu^{\infty}\right)^{-2} = \frac{e^2}{8C_F^2 a_0}\frac{\mu^{\infty 2} Z^{2/3}}{E} \tag{7}$$

Or

$$\frac{1}{A} = \frac{8C_F^2 a_0}{e^2}\frac{E}{\mu^{\infty 2} Z^{2/3}} = 0.23044\frac{E}{\mu^{\infty 2} Z^{2/3}} \tag{8}$$

Let's put $\varepsilon_0 = \frac{1}{A}$,

$$\varepsilon_0 = \frac{1}{A} = \frac{8C_F^2 a_0}{e^2}\frac{E}{\mu^{\infty 2} Z^{2/3}} = 0.23044\frac{E}{\mu^{\infty 2} Z^{2/3}} \tag{9}$$

Consequently, the equation (5) can be rewritten as follows:

$$\sigma_{tr}^{B} = \frac{(ZZ'e^2)^2}{(p\beta c)^2} 2\pi \left[\ln(1+\varepsilon_0) - \frac{\varepsilon_0}{1+\varepsilon_0} \right] \tag{10}$$

At no relativistic domain, σ_{tr}^{B} can be rewritten as follows:

$$\sigma_{tr}^{B} = \frac{(Ze^2)^2}{4E^2} 2\pi \left[\ln(1+\varepsilon_0) - \frac{\varepsilon_0}{1+\varepsilon_0} \right] \tag{11}$$

From equation (9) the energy E is given by:

$$E = \frac{e^2 \mu^{\infty 2} Z^{2/3} \varepsilon_0}{8C_F^2 a_0} \tag{12}$$

Consequently, the equation (11) can be rewritten as follows:

$$\sigma_{tr}^{B}=\frac{(ZZ'e^2)^2}{4\left(\frac{e^2\mu^{\infty 2}Z^{2/3}\varepsilon_0}{8C_F^2a_0}\right)^2}2\pi\left[\ln(1+\varepsilon_0)-\frac{\varepsilon_0}{1+\varepsilon_0}\right]=\frac{(ZZ'e^2)^2\left(8C_F^2a_0\right)^2}{4\left(e^2\mu^{\infty 2}\varepsilon_0Z^{2/3}\right)^2}2\pi\left[\ln(1+\varepsilon_0)-\frac{\varepsilon_0}{1+\varepsilon_0}\right]$$

$$\Rightarrow\sigma_{tr}^{B}=\frac{32\pi Z^{2/3}C_F^4a_0^2}{\mu^{\infty 4}\varepsilon_0}\left[\ln(1+\varepsilon_0)-\frac{\varepsilon_0}{1+\varepsilon_0}\right] \quad (13)$$

We have shown that the first order Born approximation applied on the screened potential gives the same transport cross section σ_{tr}^{B} attributed by Rouabah et al to Jablonski[4]. Consequently the age of σ_{tr}^{B} is more than 60 years old (since the works of *Wentzel (**1927**) and* Nigam **1959**). *We note that Rouabah et al have repeated this error (the attribution of σ_{tr}^{B} to Jablonski[4]) in all their works[1-3, 6-8]*. Consequently, all these works must be **reviewed**.

2.1.2. The Demonstration that the TCS Derived by Jablonski[4] is not σ_{tr}^{B}

We recall that Jablonski said in his abstract[4]: "*Analytical description of photoelectron and Auger-electron transport in solids requires values of the transport cross sections σ_{tr} for electron energies between **50** and **2000** eV. An analytical formula is proposed to provide needed values of σ_{tr} for energies in this range and for all elements*."

To proof that σ_{tr} derived by Jablonski[4] is not σ_{tr}^{B} we can base on Jablonski "himself"[4] as follows:

1. The great proof is the above calculations (see above "section I").

2. *The symbolization differences between σ_{tr}^{B} and σ_{tr}:* Jablonski[4] used the symbolization σ_{tr} in the Abstract, equations: (2[definition], 21,24a, 25, 27, 32 ..) however he used the separate symbolization σ_{tr}^{B} (i.e. without multiplying it by $G(\varepsilon_0)$) only in equations (8 and 15) and **he don't use it** in his **results section**.

3. *The index B in σ_{tr}^{B}*: Jablonski (himself) said[4]:"the index B denotes the first-order Born approximation."

4. The index "∞" in μ^{∞} which signifies "At *sufficiently high incident electron energies*[12]", which is not the case of Jablonski study[4] {50-2000 eV}. Knowing that Jablonski himself said[4]: " The constant μ in the screening parameter γ depends on energy, especially at energies below 1 keV. The use of the asymptotic value μ^{∞} is justified only at energies exceeding 5 keV".

5. The calculated deviation mentioned in Jablonski abstract[4] correspond to $\sigma_{Tr}=\sigma_{Tr}^{B}G(\varepsilon_0)$ (see equation (27) in Jablonski paper[4])

6. We note that the index B of σ_{tr}^{B} denotes first order Born approximation. However, the first order Born approximation is not valid at lower energies (see[4]; E must verify $E\geq 69.4Z^{2/3}$; thus, the electron energy should exceed 229.2 eV for carbon or 1277.7 eV for gold) which is not the case, too, of 50-2000 eV especially for heavy atoms. In addition Jablonski himself said[4]:"Thus, *the accuracy of the first-order Born approximation for σ_{tr} is generally rather **poor**. To obtain a more accurate analytical expression for σ_{tr}, we need an additional analytical function G(ε0) correcting the cross section σ_{tr}^{B}* ".

7. We recall also that Jablonski (himself) said[4]:"*An improved analytical expression **is derived** here to provide **reasonably accurate values** of σ_{tr} in the energy range of interest for surface-sensitive electron spectroscopies, i.e.,50–2000 eV.*" We note that the deviation of σ_{tr}^{B} by comparison to that obtained by quantum methods reached drastic values. In Table 1 we presented σ_{tr}^{B}, σ_{tr}^{M-S} (tabulated by Mayol and Salvat[15] who used the Relativitic Partial Waves Expansion Method (RPWEM)) and the percentage deviation between them. For example, we remark that at E=250 eV the percentage deviation of σ_{tr}^{B} reaches ≈1500 % for Au (Z=79). Has Jablonski proposed such approximation and said "…**reasonably accurate values of σ_{tr} .."**?

8. In the abstract of[4], Jablonski said: "*For atomic numbers up to 30, the mean deviation between accurate values of σ_{tr} and values from the analytical formula reaches 0.5%. For several elements with larger atomic numbers, this deviation increases to **5%,** although it is much lower for the majority of cases*" . However, from Table 1, we can remark that the deviation of σ_{tr}^{B} is always greater than 2%. Moreover, we found that the deviations reached drastic values: 30%, 50%, 200 %, 1500%,.. Consequently, and certainly, σ_{tr}^{B} is not the TCS mentioned in the abstract of Jablonski paper[4].

Actually the TCS derived by Jablonski lies in his paper[4]: "Thus, the accuracy of the first-order Born approximation for σ_{tr} is generally rather poor. To obtain a more accurate analytical expression for σ_{Tr} , we need an additional analytical function $G(\varepsilon_0)$ which correcting σ_{Tr}^{B}

$$\sigma_{Tr} = \sigma_{Tr}^{B} G(\varepsilon_0) \tag{14}$$

With

$$G(\varepsilon_0) = \varepsilon_0 \exp\left\{ \sum_{i=1}^{4} A_i \left[\ln(10\varepsilon_0)^{i/2} \right] \right\} \tag{15}$$

where A_0 , A_1 , A_2 , A_3 , and A_4 are fitted constants for each element."

2.1.3. Rouabah et al TCS[1]

Before quoting our point of view of this section, we recall that Rouabah et al used the same transport cross section expressed by equation (13) where the only difference is that μ^{∞} has been taken as a free parameter. Thus, to determine μ^{∞} , they have adjusted σ_{Tr}^{B} to Mayol et al TCS[15]. After a fitting process, they suggested the next interpolation form of μ^{∞} given by:

$$\mu^{\infty} = 2.17\times10^{-7}Z^3 - 1.54\times10^{-4}Z^2 + 0.03Z + 0.89 \tag{16}$$

Since Rouabah et al[1] adjusted σ_{Tr}^{B} to σ_{Tr}^{M-S} [15]; by basing on the equation (13), it is easily to conclude that "μ^{∞}" is given by:

$$\mu^{\infty} = \left(\frac{32\pi Z^{2/3} C_F^4 a_0^2 \mu^{\infty 2} Z^{2/3}}{0.23044 \times E \times \sigma_{Tr}^{M-S}} \right)^{1/4} \times \left[\ln(1+\varepsilon_0) - \frac{\varepsilon_0}{1+\varepsilon_0} \right]^{1/4} \tag{17}$$

The equation (17) clearly shows that μ^{∞} (*as adjusted parameter*) is a function of Z and E, but Rouabah et al[1] expressed it using equation (16) which depends only on Z. May be the authors of[1] or any one said that "*Rouabah et al. expression depends implicitly on E. In fact what was done μ^{∞} is calculating for each element as a function of energy. Then finding an optimal value for μ^{∞} for each element (i.e. for each z). Finally, one fitted μ^{∞} as a function of z for all the elements of interest. So, μ^{∞} depends explicitly on z but* ***implicitly*** *on E*". Our response will be presented as follows:

- To said that an arbitrary function $f(x,y,..)$ depends implicitly on the energy (as example), we should find a relation between at least one parameter (x or y ..) depends explicitly on the energy otherwise $f(x,y,..)$ is independent explicitly and implicitly on the energy.

For example, if $f(x,y) = \sqrt{x+y}$ and $x = E^2$ we can said that *f(x,y,..)* depends explicitly on x and implicitly on E. Indeed, the equation (16) does not any relation with the energy; neither explicit nor implicit.

- Rouabah et al[1] have adjusted σ_{Tr}^{C} to σ_{Tr}^{M-S} [15]. So, the large deviation between them (see below) is the proof of the weak point of this choice.
- Elsewhere, we note that the TCS results of[1] (denoted by σ_{Tr}^{c} in their tables (1-4)[1]) don't correspond to their fit given by equation (16). After a number of tests we think that they have used the next expression:

$\mu^{\infty} = 2.17\times10^{-7}Z^3 - 1.54\times10^{-4}Z^2 + 0.03367Z + 0.89$

2.1.4. The Invalidity of Rouabah et al TCS[1]

To show that Rouabah et al *TCS* fit[1] is **not accurate**, we can based on their data results themselves. In fact, Table (2) represents their TCS[1], Mayol and Salvat TCS[15] and the percentage deviation between them. We think that, these deviations are clearly ***invalidates*** their proposal fit (*for Al: 21% and 12 % at E=250 and 500 eV... respectively, for Cu: 41%, 20% and 10.2 % at E=250, 500 and 1000 eV respectively, for Au:* ***96****% and* ***30.3*** *% at E=250 and 500 eV respectively* ....). Unfortunately, this Rouabah et al TCS[1] has been used in other Rouabahah's papers[1, 6-8]. Consequently all their works[**1, 6-8**] must be reviewed and revised.

2.1.5. The Invalidity of Rouabah et al TCS[2]

Rouabah et al[1], in order to show that their model[1] is valid, have presented three tables carrying out a comparative study: their TCS (σ_{Tr}^{C})[1], TCS of their previous work (σ_{Tr}^{R})[2], σ_{Tr}^{B} given by equation (13) and the TCS tabulated by Mayol and Salvat (σ_{Tr}^{M-S})[15] where it is clear that σ_{Tr}^{C} is in better agreement with σ_{Tr}^{M-S} than both σ_{Tr}^{R} and σ_{Tr}^{B} . By contrast, this latter is not the proof of the validity of their fit[1], but it is the proof of the invalidity of σ_{Tr}^{R} [2] and σ_{Tr}^{B} . Concerning the invalidity of σ_{Tr}^{B} at lower energies; it has been discussed above. However, the invalidity of their σ_{Tr}^{R} "[2]" can be proved as follows:

Rouabah et al carried out an erratum[16] on their results of[2] in which they precise[16]:

"(i) in all the text, the statement percentage deviation has to be replaced by relative deviation.

(ii) In table (4) and fig.1, the deviations D and D' are expressed in absolute units and not as percentages.".

We think that it will be better that if the table (4) and Fig. 1 of[2], expressed as percentage commonly used in literature (i.e. more appropriate than absolute units).

So, to prove that the TCS of[2] is **inaccurate**, we can combine between their results published in[2] and their erratum[16]. Take for example their table (4) of their work[2], the colon D (which corresponds to the deviation of their results) of Au (Z=79) we find the next results: 4.62, 1.61, 0.49, 0.29, 0.16, .. According to their erratum[16] "*the*

deviations D are expressed in absolute units and not as percentages" so, these values (4.62, 1.61,…) are in absolute units; by consequence these **deviations become in percentage** as follows: 462%, 161%, 49%, 29%, 16% .. These deviations are totally unacceptable for the fitting process. Indeed, we should multiply their published deviations by 100 (on other word the error factor is $\mathbf{10^4\%}$). Consequently, we note and we reconfirm that their erratum[16] also **invalidates** their work[2].

2.1.6. The Invalidity of Rouabah et al TCS[3]

Rouabah et al[3] repeated approximately the same above mistake of[1] in the case of positron. After an adjustment process to Dapor results[17], they are suggested two interpolation forms of μ^{∞} given by:

$$\mu^{\infty} = 5.07 - 4.3\exp\left(-\frac{z}{39.17}\right) \quad (18)$$

$$\mu^{\infty} = 50.785 + 0.106z - 1.14\times10^{-3}z^2 + 4.93\times10^{-6}z^3 \quad (19)$$

To show that Rouabah et al interpolated TCS[3] is not accurate; we can base only on their data results. In fact, Table (3) represents their TCSs[3], Dapor TCS[17] and the percentage deviation between them. These deviations are clearly ***invalidates*** their proposal.

2.2. The Combination between Monte Carlo Simulation and Vicanek and Urbassek Formula

Before giving our point of view; we recall that Rouabah et al[1] have used Monte Carlo simulation (MC) to calculate the range and Vicanek and Urbassek formula to calculate the backscattering coefficient (BSC).
In their MC simulation they used the screened Rutherford cross section, given by:[18]

$$\frac{d\sigma_{el}}{d\Omega} = \frac{e^4 z^2}{4E^2(1-\cos\theta+2\beta_N)^2} \quad (20)$$

where z, θ,e and E are the atomic number, the scattering angle, the electron charge, and the electron energy in eV, respectively. The parameter β represents an atomic screening parameter which is given by, $\beta_N = \mu Z^{2/3}/E$, where:

$$\mu(E) = 19.10\times10^{-11}E^3 - 9.97\times10^{-7}E^2 + 26.27\times10^{-4}E + 7.25 \quad \text{for (Al)} \quad (21)$$

$$\mu(E) = 45.38\times10^{-11}E^3 - 26.32\times10^{-7}E^2 + 54.31\times10^{-4}E + 16.6 \quad \text{for (Cu)} \quad (22)$$

The Transport cross section (*denoted σ_{Tr}^{M} in the following)* obtained by integrating $\frac{d\sigma_{el}}{d\Omega}$ is given by:

$$\sigma_{Tr}^{M} = \int(1-\cos\theta)\frac{d\sigma_{el}}{d\Omega}d\Omega \quad (23)$$

In Vicanek and Urbassek formula, the BSC (η) is expressed as[5],

$$\eta = \left(1 + a_1\frac{1}{\nu^{\frac{1}{2}}} + a_2\frac{1}{\nu} + a_3\frac{1}{\nu^{\frac{3}{2}}} + a_4\frac{1}{\nu^2}\right)^{\frac{-1}{2}} \quad (24)$$

with : $a_1 = \frac{6}{\sqrt{\pi}}$, $a_2 = \frac{27}{\pi}$, $a_3 = \frac{27}{\sqrt{\pi}}\left(\frac{4}{\pi}-1\right)$ and $a_4 = \left(\frac{3}{2}-\sqrt{2}\right)^{-2}$.

In relation (24), ν is the mean number of wide angle collisions defined as,

$$\nu = NR\sigma_{tr} \quad (25)$$

where σ_{tr} is the transport cross-section, R is the range of penetration and N is the number of atoms per unit of volume in the solid target given by:

$$N = \frac{N_{Av}\rho}{A} \quad (26)$$

where N_{Av} , ρ and A are the Avogadro number, the density and the atomic mass of the target respectively.

So, to calculate ν , Rouabah et al[1] used MC simulation to calculate the range and for this raison, they think that they have carried out a combination between MC simulation and Vicanek and Urbassek formula. We think that the word "combination" is not appropriate because, we think that to do a combination between MC and the analytic model; the authors of"[1]" should be used the same elastic and inelastic models (i.e. the same input data). To show that the authors of[1] have not carried out a normalized combination, we have presented in Table (4) σ_{Tr}^{C} and σ_{Tr}^{M} where we remarked a big difference between them (i.e. the TCS used by[1] in Vicanek and Urbassek expression do not correspond to that obtained by integrating $\frac{d\sigma_{el}}{d\Omega}$ used by them in their MC code).

Besides, is this combination between Monte Carlo method and Vicanek and Urbassek theory evident and realistic? Most part of the response is mentioned in our paper[19]. Indeed, we have showed that: firstly, the Monte Carlo method is more recommended, generally, to be used in the calculation of the backscattering coefficient than Vicanek and Urbassek theory (with a condition to use the same input data)[19].

Consequently, we did not need to use this combination. Secondly, the use of this combination should be done by taking into account the normalization condition[19].

To make clear the normalization problem, we can give the following example:

Let's note by N_0, N_a and N_b: the incident particles number, the absorbed particles number and the backscattered particles number. We suppose that N_0=10 (to facilitate calculations)

We suppose also that Monte Carlo method gives backscattering coefficient BSC1=0.3 (so we conclude that in this case N_b=3 and Na=7), and their model (combination between Monte Carlo and Vicanek and Urbassek model) gives BSC2=0.2 (so we conclude that in this case N_b=2 and N_a=8). Now, if we take BSC2 as a reference for calculations (accurate results), the absorbed particles number is 8, but when we use Monte Carlo, N_a is 7. Consequently, this is a contradiction: which is the correct 7 or 8? The problem of the normalization becomes very difficult when the target is a thin film[19] which is the case of their paper[6].

Consequently, both their works[1, 6] must be reviewed.

Moreover, we note that Rouabah et al[6] have used the Vicanek and Urbassek formula to calculate the backscattering coefficient in function of the film thickness. Let's ask a question: who showed that the mathematical expression of the backscattering coefficient developed by Vicanek and Urbassek (equation (24)) is applicable for thin films? Knowing that this formula is valid only for semi-infinite solid case or for thin film with a thickness for which we can consider it as a semi-infinite solid. We note that Vicanek and Urbassek said -as example- the next clear expression "***The present scheme has to be completed by semi-infinite medium boundary condition***[5]". This latter is the second proof of the no evidence of their BSC results in function of the film thickness, in one hand, and the equation (24) is not applicable for thin films, in another hand.

2.3. The Electron Range, the Mean Number of Wide Angle Collisions and the Backscattering Coefficient Results

Rouabah et al[1] used Monte Carlo simulating individual electron scattering events where the elastic model is that given by equations (20-22) and the inelastic processes are handled in terms of Gryzinski`s excitation function[20]. The Gryzinski`s differential cross section is given by,

$$\frac{d\sigma(\Delta E)}{d\Delta E}=\frac{\pi e^4}{(\Delta E)^3}\frac{E_B}{E}\left(\frac{E}{E+E_B}\right)^{\frac{3}{2}}\left(1-\frac{\Delta E}{E}\right)^{\frac{E_B}{(E_B+\Delta E)}}\times \left\{\frac{\Delta E}{E_B}\left(1-\frac{E_B}{E}\right)+\frac{4}{3}\ln\left[2.7+\left(\frac{E-\Delta E}{E_B}\right)^{\frac{1}{2}}\right]\right\} \quad (27)$$

where ΔE, E_B, and E are the energy loss, the mean electron binding energy, and the primary projectile energy, respectively.

The electron range (R) calculated by Rouabah et al[1] can be deduced by using their data tables[1]. So, from th e equations (25-26) we conclude that R can be written a s follows:

$$R=\frac{A}{N_{Av}\rho}\frac{\nu}{\sigma_{tr}} \quad (28)$$

Consequently:

$$R_{Al}=16.5931\frac{\nu}{\sigma_{Tr}^{C}}(A°) \quad (29)$$

$$R_{Cu}=11.7908\frac{\nu}{\sigma_{Tr}^{C}}(A°) \quad (30)$$

So their electron range R_{Al} and R_{Cu} can be calculated by combining between the equations (29, 30) and their data (Tables 1, 2 and 4 of[1]).

We note that we have used the same code used by the authors of[1] but, unfortunately, we have not found the same results. So, in Table (5) we have presented their R_{Al} and R_{Cu} by substituting their data in the equations (29, 30)[1] and that obtained by using the same Monte Carlo code (denoted R^{MC} in the following).

The problem is the following: *how to show that their results (denoted R^R) do not correspond to the true results*? We assume that there are three methods (or we propose three methods) as follows:

The first method: is to use the Monte Carlo simulation using the same scheme explained by[18] and calculating the range (this way is the typical method for verification).

The second method: is to find a published work calculated the range for Al and Cu using the same Monte Carlo scheme. For this point, we note that we have not found any previous works calculating this one using the same procedures except the work of Bentabet[19] but the elastics models are not the same.

The third method: this latter is possible and practice. So, this method has been raised by Jablonski et al[21-22] «who used two types of algorithms one simulating individual electron scattering events and the other implementing CSDA. They found that both algorithms were in satisfactory agreement for primary energies exceeding 1 keV. At lower energies there were deviations up to 10% occurred due to numerical approximations[21]». We note that our work[19] confirm the later "notification of Jablonski et al". On other words, since the authors of[1] have used the Monte Carlo simulating individual electron scattering events to calculate the range then their range should be near to that obtained by using CSDA (the deviation must be less than 10% particularly for E>1keV) otherwise there is a problem in their accuracy results.

The range calculated using the CSDA is given by $R=\int_{E_0}^{0}\frac{dE}{S(E)}$ where E_0 and S(E) are the primary energy and the stopping power of primary particle respectively. The integration was performed, generally, from the primary energy E_0 to the cutoff energy instead of 0 eV.

Indeed, we note that in our work[19] we have calculated the range using CSDA for Al. So, Table (6) represents their range (R^R), the range by using the same code (R^{MC}), the range using CSDA (R^{CSDA}) and the deviation between them. We note that Rouabah et al[1] have taken 20 eV as a cutoff energy however the R^{CSDA} calculated by[19] has been done for the cutoff energy equal to 100 eV. Consequently, when

we added the range between 20 eV to 100 eV the deviation becomes greater (reaches ≈13 % for E=2keV). Therefore, on the basis of Jablonski et al notification, while the deviation is more than 10% (particularly for E>1 keV) then the results of[1] are ***incorrect***. Consequently, all their results concerning the mean number of wide angle collisions and the backscattering coefficients are incorrect. We note that this error has been repeated by Rouabah et al in their work[6]. By consequence, both their works[1, 6] must be reviewed.

Important remarks:

■ We are recognized that the notification "to say that the algorithm range is true it must be no deviations between the ranges obtained analytically and that obtained by using CSDA in Monte Carlo scheme otherwise the used Monte Carlo code is wrong (except a statistical fluctuation, due to the use of the Monte Carlo simulation)" was the notice of the reviewer chosen by the Journal Nucl. Instrum. Methods Phys. Res. B to review the paper[19]. We think that this notification is the key to confirm the validity of the Monte Carlo Algorithm range.

■ In the case of the Monte Carlo method the statistical fluctuation error is calculated as $1/\sqrt{N}$, where N is the number of initial particles[22]. Since 104 particle histories were used by the authors of[1], this statistical error is found to be about 1%. On other words, the deviation of their ranges[1, 6] is not due to the statistical fluctuation but there is an error calculation.

3. Conclusions

In summary, in this comment we have showed that Rouabah et al transport cross sections are *inaccurate and* in reality were *not based* on *Jablonski's*[4], as well. Moreover, their combination between Monte Carlo and Vicanek and Urbassek theory is not normalized and all their results concerning the mean number of wide angle collisions and the backscattering coefficients must be reviewed and revised. In other words, our work about Rouabah et al papers[1-3, 6-8, 16] can be summarized by point as follows:

1. σ_{Tr}^{B} (Transport cross section) attributed in[1-3, 6-8] to Jablonski[4] is not true, but it is an old cross-section.
2. Actually the transport cross section of Jablonski[4] is that given by $\sigma_{Tr}=\sigma_{Tr}^{B}G(\varepsilon_0)$
3. The tabulated results of σ_{Tr}^{C} (their tables 1-3 of[1]) do not correspond to their fit by using:

$$\mu^{\infty}=2.17\times10^{-7}Z^{3}-1.54\times10^{-4}Z^{2}+0.03Z+0.89$$

4. μ^{∞} Depends on Z and E but not only on Z.
5. The passage from μ^{∞} depends on Z and E to μ^{∞} depends only on Z is not justifiable, if is not impossible.
6. The deviation of (15 %.., 20%,.., 25%, ..30%,...40%, …) shows clearly the invalidity of their fit[1-3].
7. The combination between Monte Carlo and Vicanek and Urbassek theory has been used without a normalized manner[1, 6].
8. The ranges calculated by Rouabah et al[1, 6] are not correct.
9. The mean number of wide angle collisions of Rouabah et al are not correct[1].
10. Some (if it is not all) their backscattering coefficients [1, 6-8] are not correct.
11. We recall that Rouabah et al have calculated the range by using Monte Carlo simulation where they used the screened Rutherford cross section and the Gryzinski model to describe the elastic and inelastic collisions respectively. We confirm that either by using CSDA or scattering by event of Monte Carlo schemes, the range calculated by Rouabah et al[1, 6, 8] do not correspond to the true values (of Gryzinski range).
12. Their erratum[16] itself invalidates their work[2].

Table (1). Transport Cross Section (in A°^{2}) and the deviation of σ_{Tr}^{B} to σ_{Tr}^{M-S}. D: is the deviation. $D=\left|\left(\sigma_{Tr}^{M-S}-\sigma_{Tr}^{B}\right)/\sigma_{Tr}^{M-S}\right|$.

σ_{Tr}^{M-S}: The electron transport cross section tabulated by Mayol and Salvat[15]. σ_{Tr}^{B}: TCS of Born approximation given by (13) with μ^{∞}=1.22

	Al			Cu			Ag			Au		
E(eV)	σ_{Tr}^{B}	σ_{Tr}^{M-S}	D(%)	σ_{Tr}^{B}	σ_{Tr}^{M-S}	D(%)	σ_{Tr}^{B}	σ_{Tr}^{M-S}	D(%)	σ_{Tr}^{B}	σ_{Tr}^{M-S}	D(%)
250	1.06	0.8048	31.7	3.616	1.351	167.7	7.261	1.661	337.1	14.78	0.95	1455.8
500	0.391	0.3265	19.8	1.4548	0.7411	96.3	3.112	1.056	194.7	6.84	0.99	590.9
1000	0.132	0.1205	9.5	0.5241	0.3258	60.9	1.175	0.5262	123.3	2.74	0.69	297.1
1250	0.09196	0.08593	7.0	0.3706	0.2428	52.6	0.841	0.4057	107.3	1.98	0.58	241.4
1500	0.0681	0.06483	5.0	0.2777	0.1895	46.5	0.636	0.3247	95.9	1.52	0.49	210.2
1750	0.0527	0.05089	3.6	0.217	0.1528	42.0	0.4997	0.2673	86.9	1.21	0.42	188.1
2000	0.0421	0.04115	2.3	0.1746	0.1265	38.0	0.405	0.2249	80.1	0.98	0.36	172.2

Table (2). Energy dependence of the transport cross-sections and the deviation of σ_{Tr}^{C} to σ_{Tr}^{M-S} in function of Z expressed in A° 2. σ_{Tr}^{M-S} : The electron transport cross section tabulated by Mayol and Salvat[15]. σ_{Tr}^{C} : The electron transport cross section tabulated by[1].

$$D' = \left| \left(\sigma_{Tr}^{M-S} - \sigma_{Tr}^{C} \right) / \sigma_{Tr}^{M-S} \right|$$

	Z=1			Z=13			Z=29		
E(eV)	σ_{Tr}^{C} [1]	σ_{Tr}^{M-S} [15]	D' (%)	σ_{Tr}^{C} [1]	σ_{Tr}^{M-S} [15]	D' (%)	σ_{Tr}^{C} [1]	σ_{Tr}^{M-S} [15]	D' (%)
250	0.0169	0.01767	4.36	0.974	0.8048	21.02	1.904	1.351	40.93
500	0.005	0.00517	3.29	0.366	0.3265	12.10	0.891	0.7411	20.23
1000	0.0015	0.00149	0.67	0.1255	0.1205	4.15	0.359	0.3258	10.19
1250	0.001	0.001	0.00	0.0876	0.08593	1.94	0.262	0.2428	7.91
1500	0.00072	0.00072	0.00	0.0651	0.06483	0.42	0.2	0.1895	5.54
1750	0.00055	0.00054	1.85	0.0504	0.05089	0.96	0.159	0.1528	4.06
2000	0.00043	0.00043	0.00	0.0404	0.04115	1.82	0.13	0.1265	2.77
	Z=47			Z=60			Z=79		
E(eV)	σ_{Tr}^{C} [1]	σ_{Tr}^{M-S} [15]	D' (%)	σ_{Tr}^{C} [1]	σ_{Tr}^{M-S} [15]	D' (%)	σ_{Tr}^{C} [1]	σ_{Tr}^{M-S} [15]	D' (%)
250	2.088	1.661	25.71	2.01	1.77	13.56	1.86	0.95	95.79
500	1.182	1.056	11.93	1.26	1.25	0.80	1.29	0.99	30.30
1000	0.56	0.5262	6.42	0.656	0.663	1.06	0.75	0.69	8.70
1250	0.426	0.4057	5.00	0.51	0.52	1.92	0.61	0.58	5.17
1500	0.3368	0.3247	3.73	0.41	0.42	2.38	0.5	0.49	2.04
1750	0.2743	0.2673	2.62	0.34	0.35	2.86	0.42	0.42	0.00
2000	0.2285	0.2249	1.60	0.289	0.29	0.34	0.36	0.36	0.00

Table (3). Transport cross –section (in $A^{\circ 2}$). σ_{Tr}^{R1} : Rouabah et al TCS given by (13, 18)[3]. σ_{Tr}^{R2} : Rouabah et al TCS given by (13, 19)[3]. σ_{Tr}^{D} Dapor TSC[17]. D_1: percentage deviation between σ_{Tr}^{R1} and σ_{Tr}^{D}. D_2: percentage deviation between σ_{Tr}^{R2} and σ_{Tr}^{D}.

Z	Ne (Z=10)					Al (Z=13)				
E(keV)	σ_{Tr}^{R1}	σ_{Tr}^{R2}	σ_{Tr}^{D}	D_1	D_2	σ_{Tr}^{R1}	σ_{Tr}^{R2}	σ_{Tr}^{D}	D_1	D_2
1	0.0624	0.0624	0.0458	36.24	36.24	0.0845	0.0847	0.0617	36.95	37.28
1.5	0.033	0.0331	0.0269	22.68	23.05	0.0461	0.0462	0.0374	23.26	23.53
2	0.0208	0.0208	0.018	15.56	15.56	0.0295	0.0295	0.0256	15.23	15.23
2.5	0.0144	0.0144	0.013	10.77	10.77	0.0207	0.0207	0.0188	10.11	10.11
3	0.0106	0.0106	0.00989	7.18	7.18	0.0154	0.0154	0.0145	6.21	6.21
3.5	0.0082	0.0082	0.00783	4.73	4.73	0.012	0.012	0.0116	3.45	3.45
4	0.0065	0.0066	0.00635	2.36	3.94	0.0096	0.0096	0.00949	1.16	1.16
	Cu (z = 29)					Ge (z = 32)				
1	0.1573	0.1571	0.119	32.18	32.02	0.1639	0.1571	0.128	28.05	22.73
1.5	0.0988	0.0988	0.0797	23.96	23.96	0.1054	0.0988	0.0855	23.27	15.56
2	0.0689	0.0689	0.0587	17.38	17.38	0.0745	0.0689	0.0631	18.07	9.19
2.5	0.0513	0.0513	0.0457	12.25	12.25	0.056	0.0513	0.0493	13.59	4.06
3	0.0399	0.0399	0.037	7.84	7.84	0.0439	0.0399	0.0401	9.48	0.50
3.5	0.0321	0.0321	0.0307	4.56	4.56	0.0355	0.0321	0.0334	6.29	3.89
4	0.0265	0.0265	0.0261	1.53	1.53	0.0294	0.0265	0.0284	3.52	6.69
	Au (z = 79)					U (z = 92)				
1	0.202	0.205	0.238	15.13	13.87	0.2116	0.2025	0.284	25.49	28.70
1.5	0.1582	0.1603	0.17	6.94	5.71	0.1699	0.1632	0.2	15.05	18.40
2	0.1281	0.1297	0.131	2.21	0.99	0.1402	0.1352	0.154	8.96	12.21
2.5	0.1065	0.1077	0.106	0.47	1.60	0.1183	0.1142	0.125	5.36	8.64
3	0.0902	0.0912	0.0889	1.46	2.59	0.1014	0.0982	0.105	3.43	6.48
3.5	0.0777	0.0785	0.0761	2.10	3.15	0.0882	0.0855	0.0897	1.67	4.68
4	0.0677	0.0684	0.0663	2.11	3.17	0.0776	0.0753	0.0782	0.77	3.71

Table (4). Energy dependence of the transport cross-sections in Al and Cu expressed in A°^{2}. σ_{Tr}^{M} : Present work by using the elastic model of[18].

$$D'' = \left|\sigma_{Tr}^{M} - \sigma_{Tr}^{C}\right| / \sigma_{Tr}^{M-S}$$

E (eV)	Al			Cu		
	σ_{Tr}^{C} [1]	σ_{Tr}^{M}	D'' (%)	σ_{Tr}^{C} [1]	σ_{Tr}^{M}	D'' (%)
50	5.501	5.528673	0.501	5.611	3.765532	49.009
250	0.974	0.93944	3.679	1.904	1.38317	37.655
500	0.366	0.3451	6.056	0.891	0.66652	33.679
750	0.1974	0.1838	7.399	0.532	0.40466	31.468
1000	0.1255	0.11582	8.358	0.359	0.27699	29.608
1250	0.0876	0.08039	8.969	0.262	0.20409	28.375
1500	0.0651	0.0594	9.596	0.200	0.15804	26.550
1750	0.0504	0.04586	9.900	0.159	0.12678	25.414
2000	0.0404	0.03656	10.503	0.130	0.10438	24.545

Table (5). the electron penetration range. $\mathbf{R^R}$: the electron range of Rouabah et al[1] by using equations (29-30). R^{MC} the electron range by using the same code used by Rouabah et al[1]

	Al				Cu			
E(keV)	σ_{Tr}^{C} [1]	v[1]	R^R[1]	R^{MC}	σ_{Tr}^{C} [1]	v[1]	R^R[1]	R^{MC}
1	0.1256	2.25	293,3	325	0.3595	4.96	162,9	198
2	0.0404	2.14	878,9	953	0.1299	4.60	417,2	503
3	0.0204	2.10	1712.2	1859	0.0689	4.57	782.04	932
4	0.0124	2.08	2780.2	2990	0.0433	4.51	1226.8	1462

Table (6). The electron penetration range in Al. R^R: the electron range of Rouabah et al by using equations (29-30). R^{MC} the electron range by using the same Monte Carlo code which has been used by Rouabah et al[1]. R^{MC2} the electron range by using Monte Carlo simulation calculated by[19]. R^{CSDA} the electron range obtained by using CSDA scheme calculated by[19]. $D^R = \left|\left(R^R - R^{CSDA}\right) / R^R\right|$

E(keV)	R^{MC2}[19]	R^{MC}	R^R[1]	R^{CSDA}[19]	D^R (%)
1	323	325	293,3	327	11,49
2	947	953	878,9	972	10,59
3	1841	1859	1712.2	1889	10,33
4	2960	2990	2780.2	3060	10,06

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