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Maurizio Dapor
Istituto Trentino di Cultura, dapor@itc.it

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PENETRATION OF POSITRONS IN SOLID TARGETS

Maurizio Dapor

Istituto Trentino di Cultura (I.T.C.), I-38050 Povo, Trento, Italy

Telephone number: 39 461 314572 / FAX number: 39 461 314591 / E.Mail: dapor@itc.it

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Abstract

The study of the interaction of positron beams with solid targets has been approached by several investigators, also due to its importance for positron annihilation spectroscopy. This technique allows non-destructive investigations of the structural defects of surfaces and interfaces: in particular information is provided about the nature and distribution of point defects in solid materials. The solution of the diffusion equation, necessary to obtain the fractions of incident positrons annihilated at different depths inside the target, requires the knowledge of the positron stopping profile, i.e., the initial depth distribution of the thermalized positrons. Also transmission of positrons is of great interest because, according to the present model, it allows one, once backscattering is known, to calculate the total fraction of particles absorbed by the target as a function of depth and primary energy. A theoretical model is proposed to compute both stopping profiles and transmission of positrons: the theory is compared with the Mills and Wilson experimental data concerning low energy positrons ($<$ 6 keV).

Key Words: Positron, positron annihilation spectroscopy, positron stopping profile, transmission of positrons.

Introduction

The subject of positron-solid interaction has been investigated by a number of researchers. Excellent reviews about the subject have been given by Dupasquier and Zecca [28], Schultz and Lynn [68], and in the context of characterization of defects in Si and SiO_2 using positron-beams, by Asoka-Kumar *et al.* [9].

The problem, which is not new [70], has received recent attention because of its importance in positron annihilation spectroscopy, Monte Carlo simulation of positron penetration in the matter and also in purely theoretical approaches [1, 2, 10, 14, 36, 39, 40, 48, 49, 50, 51, 52, 64, 69, 74, 75].

This paper studies monoenergetic beams of positrons striking solid targets. In particular, the implantation profile of positrons, i.e., the depth distribution of the positrons that have reached thermal energies, is explored. When slow positrons strike a solid target, the particles penetrate the material and, in a time much shorter than the positrons' lifetime, reach thermal equilibrium with the lattice. After the positrons have been implanted they propagate through the sample before annihilation. The quantitative understanding of defects distribution is obtained by the study of diffusion of thermalized positrons. To solve the corresponding diffusion equation an analytical expression to describe the implantation profile is of fundamental importance.

An accurate knowledge of elastic and inelastic scattering processes is essential for modelling particle beam behavior inside solid targets both when the particle history is simulated by Monte Carlo method and also when transport theoretical descriptions are undertaken. Inelastic scattering and stopping power of slow particles penetrating solid targets have been extensively studied. Both numerical and analytical approaches to the calculations of inelastic mean free path and energy loss in different energy ranges can be found in literature [5, 6, 7, 8, 11, 27, 29, 30, 41, 55, 57, 58, 59, 60, 61, 62, 67, 71, 73]. Also the problem of an accurate calculation of elastic scattering cross section of low-medium energy electrons and positrons by complex atoms has been approached by

Symbol Table

x	film thickness [Å]
E_o	particle primary kinetic energy [eV]
E	particle kinetic energy [eV]
θ	scattering angle [rad]
$d\sigma/d\Omega$	differential elastic scattering cross section [$Å_2$/ster]
σ_{tr}	transport cross section [$Å^2$]
$-dE/dx$	stopping power [eV/Å]
R	range [Å]
r	backscattering coefficient
ν	$\{(1-r^2) / 2r\}$
μ	$\{(1+r^2) / 2r\}$
N	number of atoms per unit of volume in the target [$Å^{-3}$]
ξ	$N\sigma_{tr}$ x
n	$N\sigma_{tr}$ R mean number of wide angle collisions suffered by the particle before slowing down to rest
$f_A(x)$	fraction of particles absorbed by an unsupported thin film of thickness x
$f_B(x)$	fraction of particles backscattered by an unsupported thin film of thickness x
$f_T(x)$	fraction of particles transmitted through an unsupported thin film of thickness x
$h_A(x)$	fraction of particles absorbed in a surface layer of thickness x
h_B	backscattering coefficient
$h_T(x)$	fraction of particles transmitted through an imaginary boundary at depth x below the surface of a bulk
$\rho(x)$	implantation profile [$Å^{-1}$]
τ	derivative of f_B at the origin

a number of investigators [3, 12, 13, 17, 25, 26, 32, 33, 34, 35, 37, 38, 42, 46, 47, 53, 54, 61, 63, 65, 72, 78].

To describe implantation profiles some general aspects of particle-solid interaction should be summarized [16, 19, 20, 22, 23, 43, 44, 45, 66]. When a particle beam is directed against a solid film, some particles, after a number of elastic and inelastic collisions with the atoms of the target, come back and emerge from the surface, while some other particles are transmitted and emerge from the back of the sample. The particles that completely lose their energy before reaching one of the two surfaces are absorbed by the target. The sum of the fractions of absorbed, backscattered and transmitted particles is equal to 1 and each of them lies in the range 0-1. Their value depends on the thickness x of the target. There exists, in particular, a thickness R so that, for each $x > R$, the fraction of transmitted particles is 0, while that of backscattered ones reaches its maximum value, generally known as the backscattering coefficient r. In this context, then, a target will be considered as a thin film if its thickness is lower than R and a bulk for thickness greater than R. Of course, if a thin film is deposited on a bulk, due to backscattering from the substrate, the fractions of particles absorbed, backscattered and transmitted are different from the corresponding fractions in the absence of the substrate.

As a consequence the depth distribution of absorbed positrons in a bulk must be computed by taking into account these effects of backscattering. This is the aim of this paper.

Depth Distribution

Mills and Wilson [52] assume that the implantation profile $\rho(x)$ in a thick target is computable by

$$\rho(x) = -(df_T/dx) \tag{1}$$

where f_T is the fraction of particles of primary energy E_0 transmitted through an unsupported thin film of thickness x.

By using this equation, as recognized by Mills and Wilson [52], the backscattering from the substrate is neglected. The effect of backscattering from the substrate was discussed extensively in previous papers [16, 19, 20, 22] and shown to produce the following effects: the number of particles absorbed in a surface layer of a bulk of a given material is greater than the number of particles absorbed in a film of equal thickness, while that of particles permanently transmitted across an imaginary boundary below the surface of a bulk of a given material is less than the number of particles transmitted through a film of equal thickness.

It is then necessary to find an expression of the transmitted fraction through an imaginary boundary at depth x below the surface of a bulk, say h_T, which takes into account backscattering from the substrate. This can be done by observing that [16, 19, 20]

$$\begin{aligned} h_T &= f_T - f_T r + f_T r f_B - f_T r f_B r + f_T r f_B r f_B - f_T r f_B r f_B r + \ldots \\ &= f_T \{(1-r)/(1 - r f_B)\} \end{aligned} \tag{2}$$

where f_B is the fraction of backscattered particles for an unsupported thin film of thickness x.

For a bulk the backscattered fraction h_B is simply given by the backscattering coefficient r, while, for the conservation of the total number of particles, the fraction h_A of particles absorbed in a surface layer of thickness x is given by

$$h_A = (1 - r - h_T) \tag{3}$$

If f_A is the fraction of particles absorbed by an unsupported thin film of thickness x, then (see ref. [19, 20, 22, 23, 66])

$$f_A = (1 - f_B - f_T) \tag{4}$$

$$f_B = r\,\{(1 - \exp(-2\nu\tau\xi)) / (1 - r^2\exp(-2\nu\tau\xi))\} \tag{5}$$

and

$$f_T = \{((1-r^2)\exp(-\nu\tau\xi)) / (1-r^2\exp(-2\nu\tau\xi))\} \tag{6}$$

where

$$\tau = df_B/d\xi\,|_{\xi=0} \tag{7}$$

$$\nu = \{(1-r^2) / 2r\} \tag{8}$$

$$\xi = N\sigma_{tr}\,x \tag{9}$$

Here N is the number of atoms per unit of volume in the target, and σ_{tr} the transport cross section.

Transport cross section describes the effects of angular deflections due to elastic scattering processes.

Equations (5) and (6) have been firstly deduced by H.W. Schmidt in 1907 [66] by using the so called multiple reflection model. Such a model, subsequentely used by various authors [16, 19, 20, 22, 23, 43, 44, 45], assumes fixed probabilities of absorption, backscattering, and transmission. Actually absorption, backscattering, and transmission depend both on the angular distribution and the energy changes of the particles penetrating in the solid target. For a discussion about this subject see references [43, 44, 45]. The present author, in a recent paper [23], deduced more general equations that take into account the energy dependence of the backscattering coefficient. Nevertheless, the very good agreement between eqs. (5), (6), (7), (8) and (9) and experiment [19, 20, 22] indicates that the underlying approximation is a good one and that generalized equations are, for practical purposes, not strictly necessary.

To model particle beam behaviour, an accurate knowledge of inelastic scattering processes is also essential. These inelastic processes will be introduced, in the present theory, through the stopping power -dE/dx, E = E(x) being the mean particle energy at depth x.

Using eqs. (2), (5) and (6), one gets

$$h_T = (1-r)\exp(-\nu\tau\xi) \tag{10}$$

Then, the depth distribution corrected for the substrate effects on the transmission is

$$\rho(x) = (-dh_T/dx) = \nu\tau\,(1-r)\exp(-\nu\tau\xi)\,(d\xi/dx) \tag{11}$$

From eqs. (9) and (11) one obtains:

$$\rho(x) = N\nu\tau\,(1-r)\exp(-\nu\tau\xi)\,\{\sigma_{tr} + x\,(dE/dx)\,(d\sigma_{tr}/dE)\} \tag{12}$$

Equation (12) should be used for the computation of the implantation profiles (rather than the derivative of $-f_T$) because these equation takes into account the influence of the substrate [19, 20].

It follows from eq. (12) that the computation of the depth distribution can be performed if τ, the backscattering coefficient r, the energy dependence of the transport cross section σ_{tr} and of the stopping power dE/dx are known.

Evaluation of τ

Using eq. (12), one gets:

$$\tau = \{\rho(0) / (N\nu(1-r)\sigma_{tr}(E_0))\} \tag{13}$$

Such an expression is not very useful because the value of $\rho(0)$ is typically not known. Let us consider $f_T(x)$. Its derivative calculated at x = 0 can be experimentally determined more easily than $\rho(0)$ and, as a consequence, it is more useful to find a relationship between τ and $f_T^{\cdot}(0)$.

Using eqs. (5) and (6), one gets:

$$(df_T/d\xi) = \tau f_T\,(f_B - \mu) \tag{14}$$

where

$$\mu = \{(1 + r^2)/2r\} \tag{15}$$

In conclusion, since $f_T(0) = 1$ and $f_B(0) = 0$,

$$\tau = -\,\{f_T^{\cdot}(0) / N\sigma_{tr}\,(E_0)\,\mu\} \tag{16}$$

where

$$f_T^{\cdot}(0) = df_T/dx\,|_{x=0} \tag{17}$$

It can be useful to compare eq. (13) with eq. (16) to evaluate the ratio κ between $\rho(0)$ and $-f_T^{\cdot}(0)$:

$$\kappa = \{\rho(0)/-f_T^{\cdot}(0)\} = \{(\nu/\mu)\,(1-r)\} \tag{18}$$

For a backscattering coefficient r = 0.2, for example, κ = 0.74.

Evaluation of the backscattering coefficient r

The backscattering coefficient r represents that fraction of the impinging particles reflected by a solid target, namely the value assumed by f_B when x becomes larger than the maximum penetration range R. For beams of

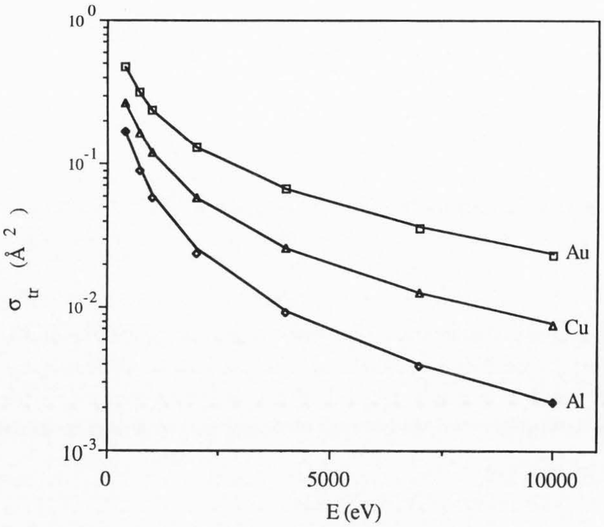

Figure 1. Energy dependence of the transport cross section in positron-atom elastic scattering collisions. Diamonds, triangles and squares represent numerical results for Al, Cu and Au, respectively, as reported by Liljequist *et al.* [46]. Solid lines were obtained by using eq. (21) with the following values for the parameters:

Al: $A_0 = 0.0722$; $A_1 = 0.368$; $A_2 = -0.1131$;

Cu: $A_0 = -0.321$; $A_1 = 0.4342$; $A_2 = -0.1007$;

Au: $A_0 = 0.4898$; $A_1 = 0.2605$; $A_2 = -0.078$.

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positrons, Aers [2] gave the following function of the primary energy:

$$r(E_0) = b_1 - b_2 \exp(-b_3 E_0) \tag{19}$$

where the coefficients b_1, b_2 and b_3 depend on the atomic number of the target and were determined by fitting Aers' Monte Carlo results. They can be found, for various elements, in reference [2]. As shown by Aers [2], experimental data of Mäkinen *et al.* [49] and Coleman *et al.* [14] are in good agreement with eq. (19). In this work, we used the Aers' expression for the computation of the backscattering coefficient because it is specific for positrons. Of course, the backscattering fraction for electrons, positrons and light ions, can be evaluated by other analytical expressions proposed in the literature (see, for example, ref. [4, 18, 31, 56, 76, 77], by Monte Carlo simulations (see, for example, ref. [2, 14, 21, 24, 36, 50, 51], and also by experiment. Recent experimental data for positron backscattering coefficient can be found in ref. [10, 14, 49, 50, 51].

Transport cross section σ_{tr}

Transport positron-atom elastic scattering cross section describes the effects of angular deflections due to elastic scattering processes. It is defined by

$$\sigma_{tr} = 2\pi \int_0^\pi d\sigma/d\Omega\,(1-\cos\theta)\sin\theta\,d\theta \tag{20}$$

where $d\sigma/d\Omega$ is the differential elastic scattering cross section and θ the scattering angle. Accurate descriptions of the differential elastic scattering cross section calculation methods can be found, for example, in ref. [13, 17, 25, 32, 33, 34, 35, 37, 38, 42, 47, 53, 54, 63, 65, 78]. In a recent paper [26], the present author showed that, in the energy range $400 \leq E \leq 10{,}000$ eV, a suitable functional form for the energy dependence of transport cross section in the positron-atom elastic scattering processes is given by

$$\ln \sigma_{tr} = A_0 + A_1 \ln E + A_2 \ln^2 E \tag{21}$$

The values of the best fit parameters A_0, A_1, and A_2 depend on the atomic number of the target. They have been reported in ref. [26] for all the elements of the periodic table in the atomic number range $1 \leq Z \leq 92$. Figure 1 presents a comparison between the numerical results of Liljequist *et al.* [46] and eq. (21).

Stopping power dE/dx

The stopping power, namely the mean energy loss per unit path-length, is given, in atomic units, by Ashley [6] as:

$$-dE/dx = \int \omega p(E,\omega)\,d\omega \tag{22}$$

over the allowed values of the energy transfer ω. Here $p(E,\omega)$ is the probability of an energy loss ω per unit distance travelled by a positron of energy E. If q is the momentum transfer and $\epsilon(q,\omega)$ is the complex dieletric function describing the response of the medium, assumed homogeneous and isotropic, then p is given by

$$p(E,\omega) = (1/\pi E) \int_{q1}^{q2} (dq/q)\,\Im\{-1/\epsilon(q,\omega)\} \tag{23}$$

where

$$q_1 = \sqrt{2}\,(\sqrt{E} - \sqrt{E-\omega}) \tag{24}$$

and

$$q_2 = \sqrt{2}\,(\sqrt{E} + \sqrt{E-\omega}) \tag{25}$$

In the present work, the author used the numerical results of Ashley [6].

Results and Discussion

Starting from data of transmission through unsupported thin films (f_T), one can obtain the value of τ {eq. (16)} and use eq. (12) to provide an accurate description of the depth distribution.

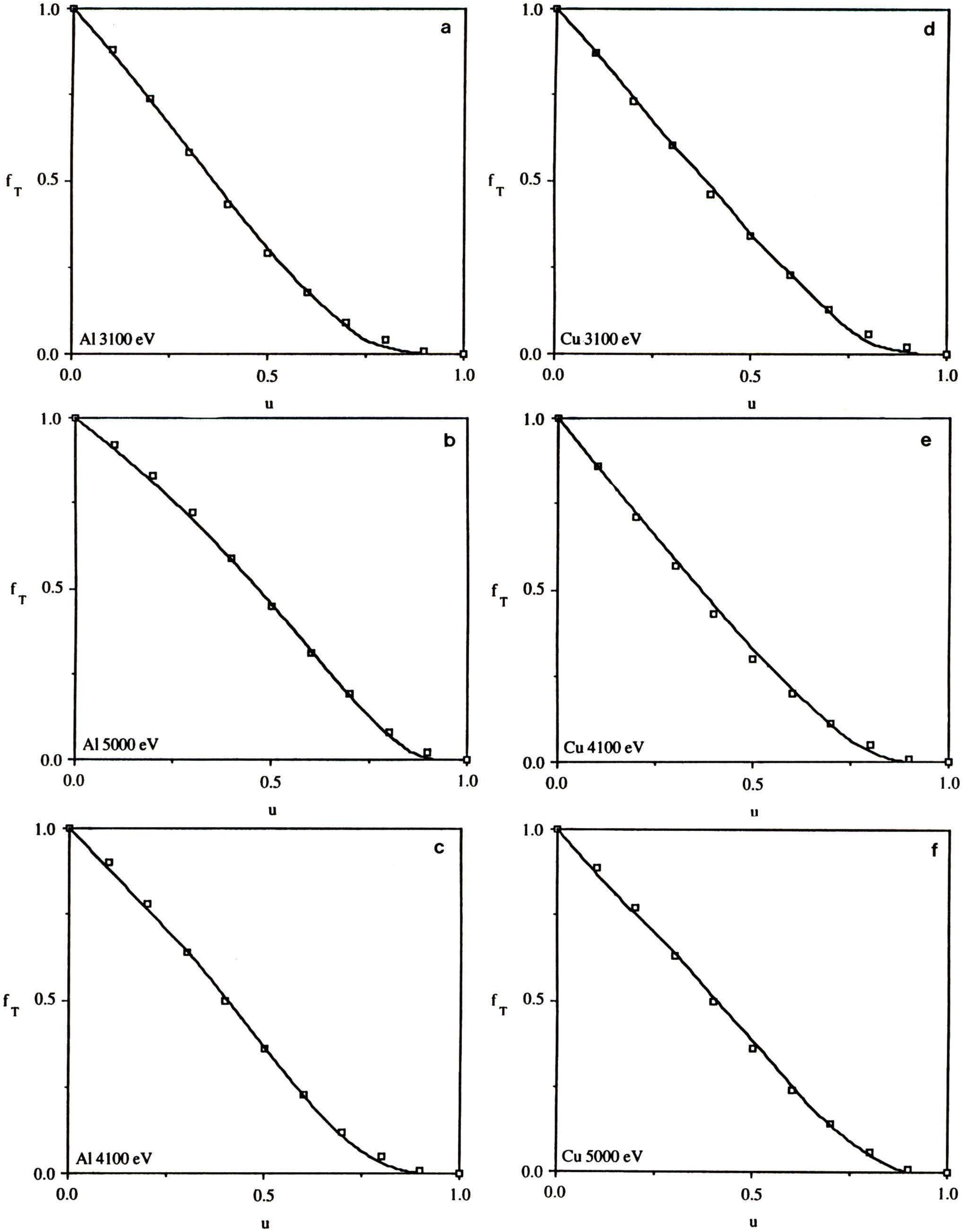

Figure 2. Fraction of positrons transmitted through Al (**a**, **b**, and **c**) and Cu (**d**, **e**, and **f**) in films as a function of the reduced film thickness u = x/R (x = film thickness, R = maximum penetration range) and positron energy. Squares represent experimental data of Mills and Wilson [52]. Solid lines were obtained by using eq. (6).

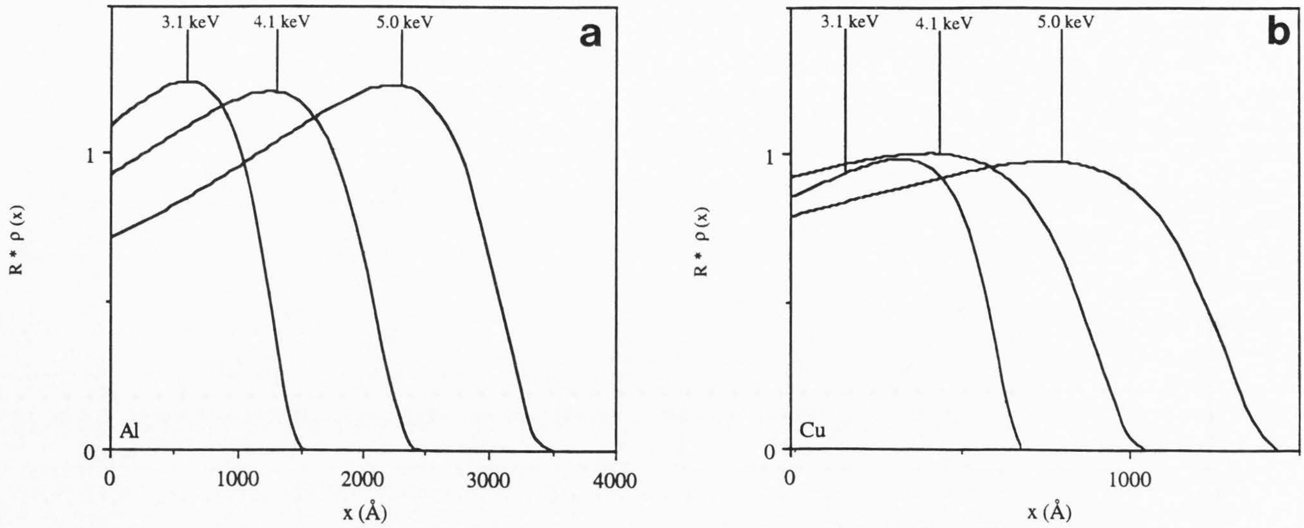

Figure 3. Implantation profiles of positron beams striking solid Al and Cu at various primary energies obtained by using eq. (12).

Mills and Wilson [52] reported measurements of the transmission of low energy positrons through thin films of Al and Cu. The comparison with the theory {eq. (6)} is shown in Figure 2 where transmitted fractions are reported as functions of the reduced thickness $u = x/R$ (R is the maximum penetration range as computed by Ashley data of stopping power [6].

Figures 3a and 3b represent implantation profiles computed by using eq. (12).

The usual assumption made until now is that the depth distribution has the form of a Makhov function. As remarked by several investigators, on the other hand, although this approximation has been used extensively to describe the implantation profiles, Monte Carlo calculations should be used to accurately determine the distribution [1, 2, 9, 36]. Unfortunately, such calculations are very time-consuming and, as a consequence, best fit functions of Monte Carlo data have been recently proposed (2, 36).

The advantage of the present work over the Monte Carlo simulations is in its simplicity: simple closed formulas always represent an evident advantage over numerical approaches. In addition, with this model, it is sufficient to use transport cross section to describe elastic scattering: the use of the analytical expression recently proposed by the present author [26] for calculating the transport cross section allows one to describe the elastic scattering processes avoiding the great amount of computation required by Monte Carlo simulations.

Another advantage is that the eq. (12) is not a best fit of experimental or Monte Carlo data with the consequent necessity of adjustable parameters. The two parameters in eq. (12) are physical quantities in principle measurable and with clear significance in terms of modelling the scattering process. In particular r is the backscattering coefficient. The value of τ can be experimentally determined in different ways, the simplest one seems to be the measurement of the slope of f_T at the origin.

Concerning the mentioned approximations involved in the multiple reflection method, they are not so drastic: the comparison of the theoretical results to the valuable experimental data of Cosslett and Thomas [15, 16] for the electrons and of Mills and Wilson [52] for the positrons, reported in recent papers [19, 20, 22] and in the present work, demonstrate that there is an excellent agreement between theory and experiment. In addition, the model results concerning depth distribution are in quite good agreement with Monte Carlo calculations [2, 36, 74, 75].

Conclusion

A theoretical model was proposed to compute both stopping profiles and transmission of positrons: the theory was compared with experimental data of Mills and Wilson [52]. An analytical expression for the stopping profile was proposed that depends on its value at the origin, the backscattering coefficient, the transport cross section, and the stopping power. It is suggested that measurement of transmission of positrons through thin films can be used to evaluate the depth distribution at the origin. Backscattering coefficient can be computed by the expression given by Aers [2] by fitting his Monte Carlo calculations. For energies lower than 10 keV, the transport cross section can be computed by the best fit of the numerical calculations proposed by the present author [25, 26], while, for the stopping power, numerical data of Ashley [6] can be used.

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Discussion with Reviewers

H. Niedrig: Electron and positron backscattering yields as a function of the incident energy (E_0 = 5-35 keV) have been reported by Massoumi *et al.* [50]. They found the ratio between electron and positron backscattering coefficient ranging from 1.75 to 1.22 with increasing the atomic number, whereas Baker and Coleman [10] found that for Al, Cu, Ag, and W (E_0 = 0.5-30 keV) the positron backscattering coefficient are generally about 50% smaller than those for electrons. Can you comment on this difference relative to your transport model?

Author: It is quite reasonable to assume that the backscattering yields depend on the mean number n of wide angle collisions suffered by the particle before slowing down to rest. For a discussion about this point of view see, for example, the papers of Vukanić *et al.* [77] and of Vicanek and Urbassek [76].

n can be easily evaluated as

$$n = R\, N\, \sigma_{tr} \tag{26}$$

where R is the range, N the number of atoms per unit of volume in the target and σ_{tr} the transport cross section.

In the energy range (E < 5 keV) examined, I found that the mean number of wide angle collisions before rest, as defined above, is always smaller for positrons than for electrons. Since the electrons suffer more wide angle collisions than positrons before slowing down to rest it seems reasonable to conclude that electrons have a probability of backscattering larger than positrons.

V.J. Ghosh: Without using Aer's expressions for backscattered fraction, how would the author fit the Mills and Wilson data?

Author: Backscattered fraction can be evaluated by other analytical expressions proposed in the literature. Recently, for example, analytical dependence of the backscattering coefficient by eq. (26) has been given by Vicanek and Urbassek [76]. This is only one of the more recent analytical expressions; see also ref. [77].

V.J. Ghosh: When fitting the Mills and Wilson [52] data using eq. (6), how were the values of r and τ obtained? Was τ obtaind from eq. (7) or eq. (16)?

Author: For r, as stated in the text, I used the expression given by Aers. Concerning τ, in **Results and Discussion**, I state: "Starting from data of transmission through unsupported thin films one can obtain the value of τ and use eq. (12) to provide an accurate description of the depth distribution." Thus, I used eq. (16).

V.J. Ghosh: What is the advantage of author's work over the Monte Carlo calculation? The Monte Carlo approach uses only elastic cross sections and the inelastic energy loss as input. The results give good agreement with measured backscattered fractions and the mean depth (see Ghosh and Aers [36], and references therein). This approach, in addition to the elastic cross sections and inelastic energy loss calcultions, requires experimental or theoretical input on the backscattered or transmitted fractions. The experimental data on backscattering or transmission is not available for all elements, for all energies.

Author: The advantage of the present work over the Monte Carlo simulation is in its simplicity: simple closed formulae always represent an evident advantage over numerical approaches. Concerning the necessity to give elastic scattering description both in theory and in Monte Carlo simulations, in my approach, it is sufficient to use transport cross section to describe elastic scattering; furthermore, I have given an accurate analytical expression to calculate low-medium energy positron transport cross section for all the atomic numbers from 1 to 92 in a recent paper [26]. On the other hand, in Monte Carlo simulation, the polar scattering angle θ, after an elastic collision, is calculated assuming that the probability:

$$P(\theta) = \left(\int_0^\theta d\sigma/d\Omega \sin\theta \, d\theta \right) / \left(\int_0^\pi d\sigma/d\Omega \sin\theta \, d\theta \right) \quad (27)$$

of elastic scattering into an angular range between 0 to θ is a random number uniformly distributed in the range 0-1.

For low energies electrons and positrons, no analytical expressions exist for the differential elastic scattering cross section and partial wave expansion method has to be used to obtain accurate results. This time consuming computation should be performed at each step of the particle trajectory. To obtain statistically significant results, the number of trajectories must be about 10^4-10^5. At each step, the particle kinetic energy is different and, as a consequence, differential elastic scattering cross section has to be recalculated. Even if Monte Carlo simulations use approximations (such as interpolation from available tabulations), it is evident that the use of the transport cross section in the present analytical model does not require the same amount of calculations.

V.J. Ghosh: Using the Monte Carlo value of r (from Aer's paper) undermines the author's assertion that the theory is a viable alternative to Monte Carlo calulations.

Authors: Monte Carlo is, in many cases, the best way to approach penetration of particles in solids. I have given above the advantages of the proposed model with respect to Monte Carlo data concerning the case of depth distribution of positrons in elemental solids. But I also used Monte Carlo simulations in my previous investigations. I have written, for example, Monte Carlo simulations in the past concerning high energy electrons (see, for example, ref. [21, 24]). Thus, my model is not in competition with Monte Carlo simulations but, as many other theories, is just a way to give quite accurate simple closed formulae when and where it is possible.

D. Liljequist: The multiple reflection method, although appealing in terms of simple, closed formulas, is a rather drastic transport theoretical approximation. It is, therefore, not evident to me that it will give sufficiently accurate results. Therefore, a more extensive comparison with experiment or with Monte Carlo data seems motivated. For example, I would be interested to see a comparison between the results in Figure 3 and a Monte Carlo simulation for the same cases. Could the author report on any such comparisons?

Author: I do not agree that multiple reflection method is a "drastic" transport approximation. The involved approximations have been sumarized in the paper but they do not seem so drastic, because the comparison between the valuable experimental data of Cosslett and Thomas [15, 16] and of Mills and Wilson [52] and theory show an excellent agreement (see, for example, ref. [19, 20, 21], and also, the present work). Concerning depth distribution, I do not know experimental data for a comparison, a part from the data reported in the Mills and Wilson paper [52], in that case, the authors present a manipulation of experimental transmission through thin films; the same data of transmission that I have compared to the model and found in very good agreement with it. The kind of manipulation of transmission data performed by Mill and Wilson to obtain the depth distribution ($-df_T/dx$) neglects backscattering from the substrate and it is, in my opinion, preferable to use the original experimental data of transmission for comparison. The agreement between my model and the Monte Carlo simulations (namely between theory and theory) is generally good: see for example depth distribution curves reported by Valkealahti and Nieminen [74, 75], by Aers [2], and by Ghosh and Aers [36].