International Journal of Advanced Research in Physical Science (IJARPS)
Volume 8, Issue 4, 2021, PP 1-15
ISSN No. (Online) 2349-7882
www.arcjournals.org

Analytical Qualitative and Quantitative Model of the Transport of Photons and Accelerated Particles through Layers of Materials in the Generalized Diffusion Approximation. Mean Range, Backscattering and Transmission Coefficients, Energy of Backscattered Particles, Particle and Energy Distributions along the Coordinate, Angular Dependencies

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Abstract: *An analytical qualitative and quantitative model of the transport of photons and accelerated particles through the layers of materials in the generalized diffusion approximation is formulated consistently. It is based on the limiting cases of straightforward and diffusion transport, and also their stitching together. Mean ranges of the particles along the coordinate are calculated and analyzed. Analytical formulas are derived for the particles backscattering coefficient in straightforward and diffusion approximations, and their dependence on the angle of incidence of the particles on the surface. Analytical formulas are derived for the particles mean energy loss in layers and mean energy of the particles backscattered from the layer of material, as well as their dependence on the particles angle of incidence on the surface. An analytical formula is derived for the reflection coefficient of the beam energy from the surface of the layer in the diffusion approximation for a wide range of materials, as well as its dependence on the particles angle of incidence on the surface. Analytical formulas are derived for the transmission coefficient of particles through a layer of material in the straightforward and diffusion approximations, and their dependence on the particles angle of incidence on the surface. The distributions of particles and energy deposition over the depth of the layer are obtained. The possibility of a spatial maximum of energy input of a particle beam is analytically justified, the depth of this maximum location is calculated, as well as its dependence on the particles angle of incidence on the surface. The applicability and error origin the of the analytical model of the transport of photons and accelerated particles through the layers of materials in the approximation of generalized diffusion are estimated.*

Keywords: *accelerated particles, photons, generalized diffusion, straightforward transport, diffusion transport, mean range of the particles along the coordinate, the particles backscattering coefficient, the mean energy of the particles backscattered from the layer of material, the reflection coefficient of the beam energy from the surface of layer, the transmission coefficient of particles through the layer of material, particle and energy deposition distributions over the depth of the layer.*

1. INTRODUCTION

The general problem of photons and accelerated particles transport through layers of materials has been considered for a long time (and is still considered by many researchers) to be difficult for analytical solutions, and was solved mainly by the Monte Carlo method [1]. However, in many cases analytical models and solutions, even approximate ones, are required. Firstly, they give a general visual picture of what is happening. Secondly, they are ideal for optimization problems. Thirdly, they work more reliably as an element of a more general and complex problems. And already G. Bethe and J. Jacob [2] in their age theory considered the semi-analytical spatial problem of accelerated electrons transport in the diffusion approximation. Moreover, the created approach proposed an analytical solution to the problem for materials with atomic charge Z> 7. Essential in the approach was the selection of the initial stage of transport and the creation of the concept of isotropization length. This stage provides the transformation of monodirectional beam electrons transport to diffusion transport and gives the possibility to describe

the further problem by diffusion theory. Nevertheless, it was not possible to get the analytical solution of the problem and to estimate the electron ranges along the coordinate and reflection coefficients in this work. One of the reasons for this was the limitations of diffusion approximation, since in many important problems the transport is not completely diffusive, and in some cases, it is almost straightforward.

However, in the works performed at the Kurchatov Institute [3,4], it was possible to formulate the spatial-energy theory of the degradation-diffusion cascade and the model of generalized diffusion, which provide analytical solutions for a wide range of problems. In general, it gave the possibility to obtain solutions for the generalized diffusion of charged particles, atoms, and molecules in a wide range of initial energies. The transport problems of relativistic and nonrelativistic electron beams [3–8], physics of the upper atmosphere [4.8], and kinetics of the gamma laser [8,9] were considered. Later [10], it was possible to generalize the approach and to describe the transport of photons in transparent and nontransparent materials, typical for the problems of medical physics and optics, and also to calculate the volume reflection coefficient of particles from the materials in a straightforward approximation. Subsequently [11], a unified model of generalized diffusion for electrons and photons was formulated, including the concept of an imaginary particle source, which is located inside the layer and generates an isotropic particle flow in all directions.

In this paper, a substantial qualitative and quantitative development of the generalized diffusion model is carried out in relation to the more general problem of the photons and accelerated particles transport through layers of materials. For the first time, more than a dozen formulas were derived to describe the backscattering and transmission of particles through layers of materials, as well as the reflection coefficient of the beam energy from a layer, and the distribution of particles and energy deposition over the depth of a layer. The dependences of the main transport parameters on the particles angle of incidence on the surface of the layer are obtained.

2. Transport of Photons and Accelerated Particles in the Generalized Diffusion Approximation

We assume that in a layer of active material, fast particles usually undergo scattering and gradual deceleration, and photons undergo scattering and instant absorption. The transport of particles (photons and accelerated particles) in a layer of material in the generalized diffusion approximation is described by the ratio of the absorption length L_a and the transport mean free path L_s. The absorption length for accelerated particles is the mean path that a particle travels until its complete deceleration (absorption) due to inelastic collisions with atoms of the material.

$$L_a = -\int_0^{E_0} \frac{dE}{dE/ds}, \tag{1}$$

where $dE/ds = N\int_0^E \sigma(\Delta E)\Delta E d(\Delta E)$ is the mean energy loss of a particle per unit path; E is the current value of kinetic energy; E_0 is the initial energy of the particle; s is the current path; $\sigma(\Delta E)$ is the total differential cross-section for energy loss of all channels of energy loss. The sign minus is introduced to take into account the fact that the particle energy decreases with an increase of the path: $dE/ds < 0$. In some cases, there is no need to calculate accurately the complex integral and we can use its estimation:

$$L_a = -\frac{E_0}{dE/ds}. \tag{2}$$

To describe the photons transport, the absorption length can be associated with the linear absorption coefficient μ_a, so in the simplest case [11]:

$$L_a = 1/\mu_a\,. \tag{3}$$

The transport mean free path (scattering length) is characterized by the distance at which the direction of motion of the particle changes significantly:

$$L_s = \left(2\pi N\int_{-1}^{1}\sigma(\cos\Theta)(1-\cos\Theta)d(\cos\Theta)\right)^{-1}, \tag{4}$$

where $\sigma(\cos\theta)$ is the differential cross-section of all scattering channels.

An analog of the transport mean free path for photons is determined by the linear scattering coefficient of photons μ_s, as well as by the scattering anisotropy factor g (the average cosine of the angle of the elementary scattering event) [11], so that:

$$L_s = \frac{1}{\mu_s(1-g)} = \frac{1}{\mu_s'}. \quad (5)$$

Here $\mu_s' = \mu_s(1-g)$ is the transport scattering coefficient.

The key parameter of the model is the diffusion ratio

$$R = \frac{L_a}{L_s} = \frac{\mu_s(1-g)}{\mu_a}. \quad (6)$$

The form of the trajectory of particles motion is determined by the ratio of the absorption length and the scattering length. Indeed, in the case of $R << 1$, the particle will pass the absorption length and be absorbed by the material without noticeable curvature of its straightforward trajectory. Therefore, the mean range L along coordinate in this case is obviously equal to the absorption length:

$$L = L_a. \quad (7)$$

In the opposite limiting case $R >> 1$, the particle many times changes its direction of movement until the complete deceleration (absorption), and the transport is diffusive. It is significant that in the intermediate case the transport can be analyzed in a following manner [2]. At the first stage, an initially monodirectional particle beam at a length L_s acquires a random directional motion. Finally, in the second stage, the transport becomes diffusive.

In the case of $R >> 1$, the mean range L along the coordinate x corresponding to the direction of the initial velocity of the particle beam is calculated in the diffusion approximation [4]:

$$L = \sqrt{2Dt} = \sqrt{\frac{2}{3}L_s L_a}, \quad (8)$$

where $D = 1/3\, L_s v$ is the diffusion coefficient; $t = L_a / v$ is the diffusion time; v is the particle velocity. The mean range in this case is close to the geometric mean value from the absorption length and the scattering length.

However, even if the diffusion ratio is large, transport in the layer is not always described by the diffusion approximation. If the layer is thin (in the approximation of thin films) and its thickness is $H < L_s$, then, when passing through such a layer, the particle trajectory is almost straightforward.

It is not difficult to estimate by dispersion the distributions of particles absorption length and energy deposition, etc. However, it must be emphasized that caution must be taken in estimating distributions. In particular, in some cases, estimates of diffusion distributions are not applicable for $x<L_s$, since at first the particles cannot move diffusely. In addition, in some cases, the model requires a more rigorous consideration of the role of boundary conditions in the system. In this sense, the most accurate are not differential, but integral parameters of the diffusion theory, such as the mean range L along coordinate. In general, the mean range L along coordinate can be calculated by stitching together the limiting cases:

$$L = L_a \text{ for } R \leq 2/3; \quad (9)$$

$$L = \sqrt{(2/3)L_a L_s} \text{ for } R > 2/3. \quad (10)$$

The resulting stitching is consistent within 10-30% over the entire range of diffusion ratios with the results of Monte Carlo calculations for the main cases.

3. MEAN RANGE L ALONG COORDINATE AND DOSE CHARACTERISTICS OF NONRELATIVISTIC AND RELATIVISTIC ELECTRON BEAMS

For consideration of an example of transport of accelerated electrons, the well-known formulas were used [8]. In the nonrelativistic case, the scattering length can be calculated by the formula

$$L_s = \frac{2E^2}{\pi K^2 e^4 \sum_i N_i Z_i (Z_i+1)(ln(1+1/\eta_i)-1/(1+\eta_i))}, \quad (11)$$

where each of the members of the sum correspond to a certain type of atoms of the material; $K = 1/(4\pi\varepsilon_0)$; ε_0 is the electric constant; e is the electron charge; N_i and Z_i are, respectively, the concentration and charge in units of e of atoms of type i; $\eta_i = \frac{1}{2}(\frac{h}{2\pi mv}\frac{1{,}12Z_i^{1/3}}{0{,}855a_0})^2$ - screening angle; h is Planck's constant; m is the mass of the electron; a_0 is the Bohr radius. In this case, an elastic collision corresponds to a set of collisions, leading to a significant change in the direction of motion of a fast electron.

The absorption length $L_a(E)$ is calculated using the Bethe formula:

$$L_a = -\int_{E_{min}}^{E_0} \frac{dE}{\frac{dE}{ds}} \approx \frac{E_0^2}{4\pi K^2 e^4 \sum_i N_i Z_i (ln(4E_0/(I_0 Z_i))}, \quad (12)$$

where s is the path of electron; $I_0 \approx 10$ eV. Here, during integration, the logarithmic dependence on the integration parameter was neglected, as well as the contribution to the absorption length of the trajectory fragment corresponding to low energy values.

Fig. 1 presents the nonrelativistic range L along coordinate calculated by using the model of generalized diffusion of electrons with an energy of 3-100 keV for characteristic materials with different charge numbers (Z = 2.7 - polyethylene, Z = 10 - quartz, Z = 33 - arsenic, Z = 82 - lead). At an energy less than 3 keV, an error appears in the formulas due to the fact that they were derived for high energies exceeding I_0 Z. At an energy greater than 100 keV, an error appears in the formulas due to the fact that the electron becomes relativistic.

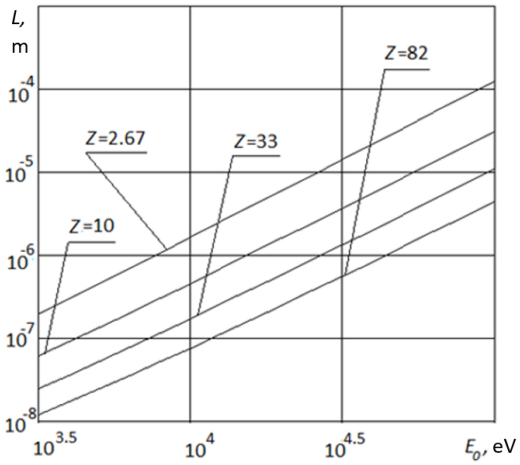

Fig. 1

The analysis shows that, in the considered range of electron energies, the stitching of the straightforward and diffusion approximations of the generalized diffusion model takes place in the Z range from 2.6 (at high energies) to 3.6 (at low energies). Since the transition from one approximation to another is smooth, for most cases we can approximately assume that the transition from one approximation to another occurs at $Z \approx 3$. The straightforward approximation works for smaller Z, and the diffusion approximation works for large Z.

It is significant that, in accordance with the formulas, the mean range L along coordinate in the straightforward approximation is proportional to

$$L \sim Z^{-1}, \quad (13)$$

while in the diffusion approximation

$$L \sim Z^{-1,5}. \quad (14)$$

Note that the obtained data on the mean range L along coordinate on average within 10-30% are consistent with the experiments and calculations by the Monte Carlo method. Analysis shows that the function

$$f(Z, E_0) = \frac{L_a}{L_s(Z+1)} \quad (15)$$

weakly depends on the charge number Z = 1-82 (within ± 5%) and electron energy (within ± 20%), since this dependence is determined mainly by logarithms. Therefore, in the considered range of the charge number and energy with an accuracy of 20%, the diffusion ratio is given by the formula:

$$R=f(Z+1), \quad (16)$$

where $f \approx 0.16$.

The radiation dose D is determined by the radiation energy absorbed by a unit mass of a material, and can be related to the beam intensity I (measured in J/cm^2), the mean range L along coordinate, and the material density ρ by the formula:

$$D = \frac{I}{L\rho}. \quad (17)$$

The product $L\rho$ in accordance with (13, 14) weakly depends on the material, so that in the diffusion approximation (qualitatively valid for almost the entire Mendeleev periodic table) proportionality is observed:

$$D \sim Z^{0,5}. \quad (18)$$

This dependence becomes even weaker when you consider that in heavy nuclei the proportion of neutrons in the nucleus increases, and the mass of the nucleus increases faster than the charge.

Let us consider a typical example [12,13], when an electron stream with an energy of 30 keV can appear during separation of an adhesive tape, and 10^{10} electrons enter per cm^2 of surface. The stitching of the straightforward and diffusion approximations at this energy takes place for the charge number of the nucleus of atoms Z = 2.8, which is close to the average charge number of the nucleus of atoms of polyethylene (Z = 2.7). The model of generalized diffusion in this case gives the mean range of the electron (in the straightforward approximation) L = 12.9 μm. The material receives energy $4{,}8 \cdot 10^{-5}$ J/cm^2 per volume of $1{,}29 \cdot 10^9$ m^3. For polyethylene with a density of 920 kg/m^3 this gives a considerable radiation dose of 40 Gray.

On the whole, the dependence of the dose for characteristic material s on the electron energy (for a fixed flux of 10^{10} electrons per cm^2) is shown in Fig. 2.

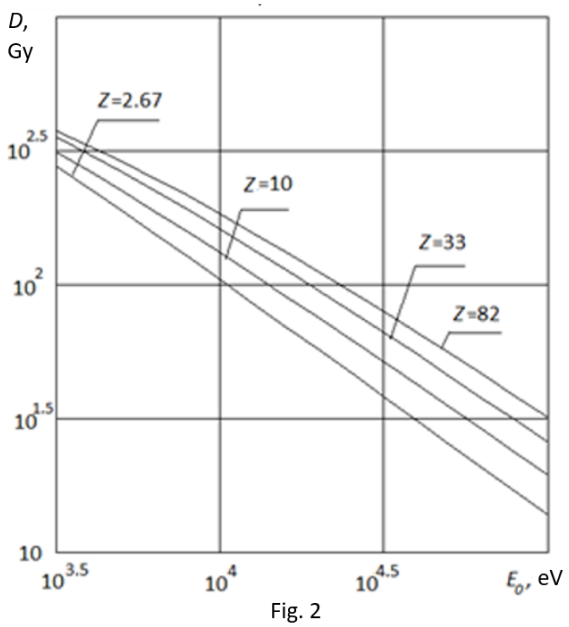

Fig. 2

It follows from this that the radiation dose when separation off adhesive tapes from various materials (and, possibly, when breaking and tearing of other materials) can exceed the natural radiation dose per

year by up to 4 or more orders of magnitude. Such powerful doses can lead to chemical destruction of the micro- and nanolayer of the material and provide, for example, damage to an electronic device or biological object.

In the relativistic electrons case, we have:

$$L_s = \frac{m^2c^4\beta^4\gamma^2}{2\pi K^2e^4\sum_i N_iZ_i(Z_i+1)(ln(1+1/\eta_i)-1/(1+\eta_i))}, \quad (19)$$

$$L_a = \frac{m^2c^4\beta^2(\gamma-1)}{4\pi K^2e^4\sum_i N_iZ_i(ln(2mv^2\gamma^2/(I_0Z_i))-\beta^2)}. \quad (20)$$

In these formulas, $\beta = v/c$, where c is the speed of light, $\gamma = 1 / (1 - \beta^2)^{1/2}$, $\eta_i = \frac{1}{2}(\frac{h}{2\pi mc\beta\gamma}\frac{1,12Z_i^{1/3}}{0,855a_0})^2$.

For electrons in the energy range from units of keV to units of MeV

$$R = const\frac{Z+1}{\gamma}, \quad (21)$$

where the constant is half an order of magnitude less than unity, γ is the relativistic factor, Z is the charge number of the nucleus of the atoms of the material. Estimates show that the straightforward approximation takes place for materials with Z = 1-3, the diffusion one for $Z > 10 \div 20$. (This statement is valid in a wide range of electron beam energies, starting from a few keV. And only for relativistic electrons at $E > m\,c^2$, when the mean range L is proportional to the first and not the second power of energy, the trajectory of the electrons is somewhat straightened.)

It follows from the formulas that the mean range L of nonrelativistic fast electrons is proportional to the square of their initial energy.

In the relativistic case, if the material consists of light atoms, the mean range L is proportional to the first power of energy. If the material consists of heavy atoms, due to the influence of elastic collisions, the mean range L is proportional to the initial energy to the power of 3/2.

The formulas confirm that for light atoms the range L is proportional to Z^{-1}, and for heavy ones it decreases even faster and is proportional to $Z^{-3/2}$.

4. Transport of Particles in a Layer of Material in a Straightforward Approximation

The generalized diffusion model allows one to make estimates of the particles backscattering coefficient from various materials. Thus, in the model of diffusion transport, dominant scattering leads to large backscattering coefficients close to unity. On the contrary, in the model of straightforward transport, a small probability of scattering leads to backscattering coefficients much less than unity.

We start with the calculation of the particles backscattering coefficient from a thick layer of material in a straightforward approximation.

We first make an estimate for the beam normally incident on the layer. In the case of straightforward transport of particles, when $R << 1$, the probability of particle scattering is small compared with the probability of absorption and is determined by $R = \frac{L_a}{L_s}$. It must be taken into account that a particle can only return back to the layer boundary from a depth of $L_a/2$, so that the probability of scattering at this length is $\frac{L_a}{2L_s}$.. Moreover, taking into account the approximately equal (50 percent) probability of particle scattering back and forth, we obtain a somewhat overestimated estimate for the particles backscattering coefficient:

$$K_r \approx 0,25R. \quad (22)$$

The overestimation of the estimate is due to the fact that far from all particles from such a depth are able to reach the layer boundary.

The method of diagrams allows to obtain more accurately the particles backscattering coefficient in a straightforward approximation. We generalize the problem, assuming that in the general case the beam

falls at an arbitrary angle to the boundary of the surface of the layer.

The model for calculating the particles backscattering coefficient is illustrated by the diagram in Fig. 3. The particle passes the boundary of the layer *FE* at the point *D* (chosen as the origin) in the direction *DO* (direction *x*) at an angle α to the boundary of the layer *FE* and is capable of linearly passing the absorption length L_a. In this case, there is a small probability that at some point *O* on the interval of the path *dx* there will be an isotropic scattering of the particle, so that the particle will eventually slow down on the surface of the sphere $FMEM_1$.. The relative probability of isotropic scattering of a particle along the absorption length L_a. is determined by the diffusion ratio R = L_a/L_s, so that on the interval of the path, the probability of a particle returning to the boundary is equal to:

$$dp = \frac{dx}{L_a}\frac{S_{\text{FME}}}{S_{FMEM_1}}R = \frac{dx}{L_s}\frac{S_{\text{FME}}}{S_{FMEM_1}}. \quad (23)$$

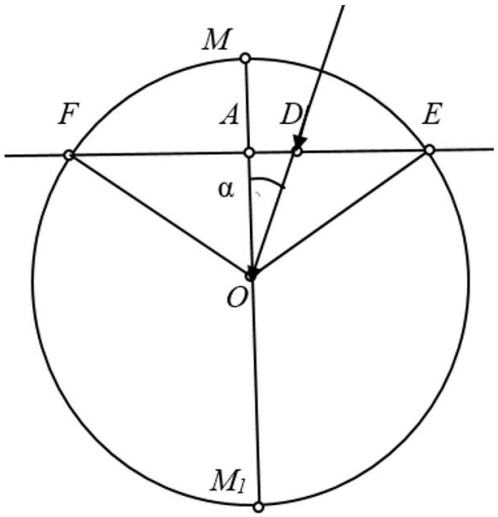

Fig. 3

(The ratio of the area of the *FME* segment to the surface area of the sphere $FMEM_1$ characterizes the relative probability of particle reflection.) Let us find the maximum mean free path of the particle *DO* in material, determined by the ability of the reflected particle to reach the boundary of the layer at point *A*:

$$DO+OA=DO(1+\cos\alpha)= L_a, \quad (24)$$

Where the maximum is

$$DO=L_a/(1+\cos\alpha). \quad (25)$$

Integration of the obtained probability within the permissible range from zero to *DO* gives for the total probability of the particle returning from the layer the particles backscattering coefficient (the notations of the radius of the sphere *OE* = *r* and the segment height *MA* = *h* are introduced):

$$k_r = \frac{1}{L_s}\int_0^{L_a/(1+\cos\alpha)}\frac{S_{\text{FME}}}{S_{FMEM_1}}dx = \frac{1}{L_s}\int_0^{L_a/(1+\cos\alpha)}\frac{2\pi rh}{4\pi r^2}dx = \frac{1}{L_s}\int_0^{L_a/(1+\cos\alpha)}\frac{h}{2r}dx =$$
$$\frac{1}{2L_s}\int_0^{L_a/(1+\cos\alpha)}\frac{L_a-x(1+\cos\alpha)}{L_a-x}dx = \frac{1}{2L_s}\int_0^{L_a/(1+\cos\alpha)}dx - \frac{1}{2L_s}\int_0^{\frac{L_a}{1+\cos\alpha}}\frac{x\cos\alpha}{L_a-x}dx = \frac{R}{2(1+\cos\alpha)} + \frac{\cos\alpha}{2L_s}\int_0^{\frac{L_a}{1+\cos\alpha}}dx -$$
$$\frac{\cos\alpha}{2L_s}\int_0^{\frac{L_a}{1+\cos\alpha}}\frac{L_a}{L_a-x}dx = \frac{R}{2} + \frac{R\cos\alpha}{2}\int_0^{\frac{L_a}{1+\cos\alpha}}\frac{1}{L_a-x}dx = \frac{R}{2} - \frac{R\cos\alpha}{2}ln\frac{1+\cos\alpha}{\cos\alpha} = \frac{(1-\cos\alpha\, ln\frac{1+\cos\alpha}{\cos\alpha})R}{2}. \quad (26)$$

It is taken into account that the maximum mean free path of a particle in a material is L_a and

$$DO+OF=x+r=L_a,$$

where from

$$r=L_a-x. \quad (27)$$

In addition, it is taken into account that

$MA+AO=h+x\cos\alpha=r=L_a-x$,

where from

$h=L_a-x(1+\cos\alpha)$. (28)

If the particle beam falls on the layer normally and α = 0, the formula for the particles backscattering coefficient equal to the ratio of the number of reflected particles I_2 to the number of particles I_0 falling on the layer is simplified and looks as follows:

$$k_r = \frac{I_2}{I_0} = \frac{(1-ln2)R}{2} = 0{,}153R. \quad (29)$$

For nonrelativistic electrons with an energy of 3-100 keV in materials with a charge number Z in accordance with (16), the particles backscattering coefficient is equal to:

$$k_r = 0{,}024(Z+1). \quad (30)$$

To verify the obtained formula (29), the particles backscattering coefficient was calculated by the Monte Carlo method. A comparison of the dependence of the particles backscattering coefficient from materials with different diffusion ratios is shown in Fig. 4 and 5 (on a more detailed scale). From a comparison of the graphs, it can be seen that the dependences are of the same qualitative nature up to a 100% coefficient. The best match occurs for R << 1, which is not surprising, since the zeroth approximation of the calculation is based on the straightforward approximation. However, for example, even at R = 1, the difference does not exceed 15%.

In some cases, it is important to know which part of the particles passes through a given of thickness x in a straightforward approximation - to find the particle transmission coefficient k_t. For photons, such an estimate can be made using the Bouguer-Lambert law [14]:

$$k_t = \frac{I_1}{I_0} = exp(-\mu x). \quad (31)$$

Here I_1 is the number of particles passing through the layer, and it is assumed for simplicity that the particles normally fall onto the layer.

In the case of transport of accelerated particles, another model works, because, as noted above, the deceleration of particles in the material occurs gradually. Moreover, in the estimation, we can assume that for a layer of thickness $H<L_п\cos\alpha$, the main part of the particles passes through this layer, and for a layer of thickness $H>L_п\cos\alpha$ the main part of the particles is not able to overcome this layer.

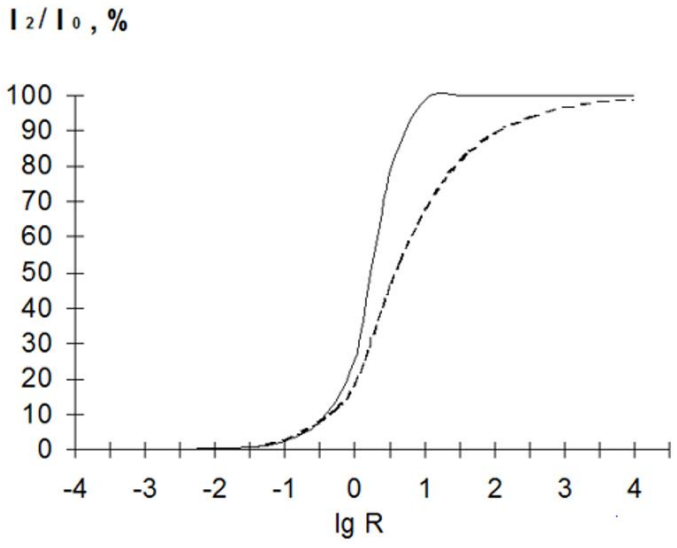

Fig. 4

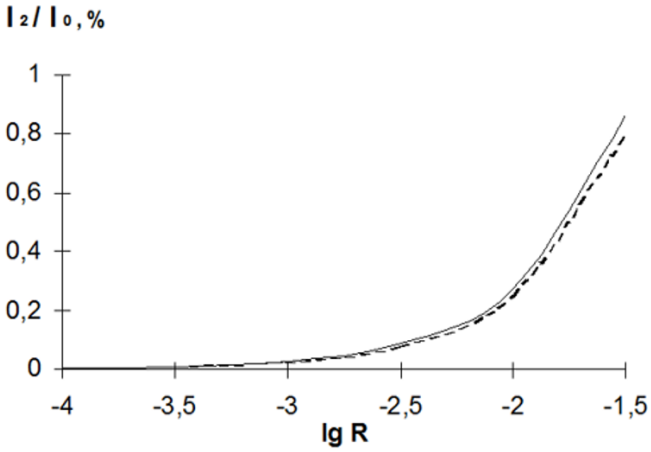

Fig. 5

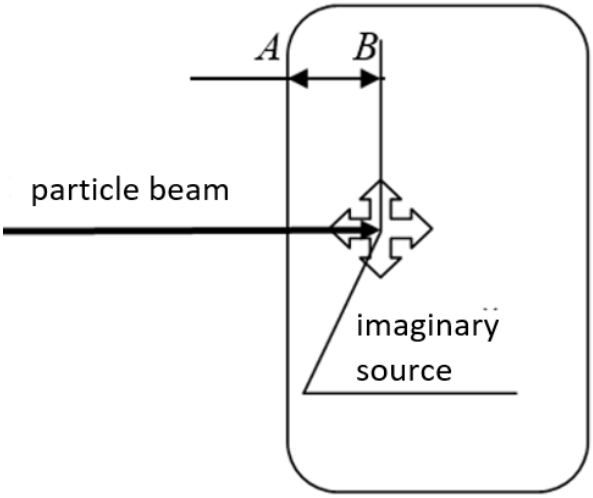

Fig. 6

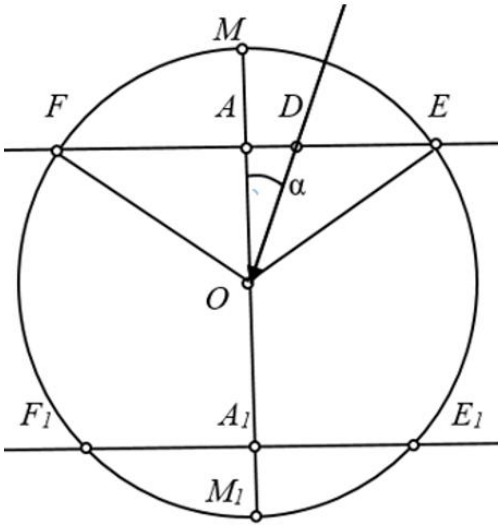

Fig. 7

5. An Imaginary Isotropic Source of Particles. Backscattering and Transmission of Particles in the Diffusion Approximation

A model with an imaginary isotropic source of particles, which is located at a depth of the scattering length, helps to describe transport in the case when the diffusion approximation works (Fig. 6). In this model, it is assumed that at the first stage of transport at the scattering length L_s, the initially unidirectional particle beam is isotropized, and at the second stage, the problem is reduced to considering particle transport from an imaginary isotropic particle source. In fig. 6, for simplicity, it is first assumed that the particles fall normally onto the layer.

Let us now analyze the process of backscattering (volume reflection) of particles from a layer of material in the diffusion approximation using the example of an electron beam. To describe this process, we use an illustration (Fig. 7) that looks similar to an illustration of a straightforward approximation, but essentially describes a completely different mechanism.

Consider the electrons incident on the boundary of the layer *FE* in the direction of *DO* at an angle α to the layer. By passing the scattering length (transport mean free path) $L_s = DO$, the electron beam becomes isotropic. Moreover, the depth of isotropization is equal to $L_i = AO = L_s \cos\alpha$. Point *O* can be considered as the source of an imaginary internal isotropic electron beam. Then, in the diffusion approximation, isotropic diffusion proceeds from point *O* at the mean range of electrons along the coordinate $FO = L = \sqrt{\frac{2}{3}L_sL_a}$ before the absorption of electrons on the surface of the sphere $FMEM_1$.

The exit of electrons to the boundary of the layer *FE* actually means their backscattering from the layer. Therefore, in the diffusion approximation, it is possible to estimate the backscattering coefficient of electrons (the fraction of reflected electrons) from the layer by the ratio of the segment *FME* area to the area of the entire sphere $FMEM_1$. With this in mind, the backscattering coefficient of electrons from the layer according to the proposed estimate is equal to

$$k_r = \frac{S_{FME}}{S_{FMEM1}} = \frac{2\pi\, FO\, MA}{4\pi\, FO^2} = \frac{\sqrt{\frac{2}{3}L_sL_a} - L_s\cos\alpha}{2\sqrt{\frac{2}{3}L_sL_a}} = \frac{1}{2} - \frac{\cos\alpha}{2\sqrt{\frac{2}{3}R}}. \quad (32)$$

Such an estimate will be somewhat underestimated, since the access of electrons onto a sphere segment *FME* in principle does not guarantee that they will not reach the boundary *FE* of the layer with exit from the layer. An error can also take place due to the limited number of diffusion collisions determined by the diffusion ratio $R = L_a/L_s$, which is about 10 for medium and heavy atoms.

Let us make an estimate for the electron flow normally incident on the layer boundary. For titanium ($R = 4.33$) k_r=0.21, which is almost 20% lower than the experimental one [15-16].

For

R=0.16(Z+*1*),

$$k_r = \frac{1}{2} - \frac{\cos\alpha}{0.653\sqrt{z+1}}. \quad (33)$$

In many real-life problems, it is apparently possible to use the analytical formulas given here to describe the impact of a beam with an uneven surface, having previously correctly estimated the average angle of incidence of electrons on a surface with correctly averaged coordinates.

A similar approach allows us to estimate the transmission coefficient of particles through the layer (the fraction of transmitted particles). After all, Fig. 6 is quite symmetrical with respect to the imaginary isotropic source of particles, the upper and lower boundaries of the layer from the point of view of diffusion transport have no special differences and the transmission coefficient of particles is calculated almost similar to the backscattering coefficient of particles. In this case, the exit of particles to the lower boundary F_1E_1 of the layer actually means their transmission through the layer. Therefore, in the

diffusion approximation, the transmission coefficient of particles through the layer can be estimated by the ratio of the area of the segment $F_1M_1E_1$ of the sphere to the area of the entire sphere $FMEM_1$:

$$k_t = \frac{S_{F_1M_1E_1}}{S_{FMEM_1}} = \frac{2\pi\, FO\, A_1M_1}{4\pi\, FO^2} = \frac{\sqrt{\frac{2}{3}L_sL_a} - H + L_s\cos\alpha}{2\sqrt{\frac{2}{3}L_sL_a}}. \quad (34)$$

Here, it is taken into account that the layer thickness $H=AA_1$ allows one to find

$$A_1M_1 = 2\sqrt{\frac{2}{3}L_sL_a} - H - MA = \sqrt{\frac{2}{3}L_sL_a} - H + L_s\cos\alpha. \quad (35)$$

6. THE MEAN ENERGY LOSS OF THE BACKSCATTERED PARTICLES AND THE REFLECTION COEFFICIENT OF THE BEAM ENERGY

As an example, consider the transport of accelerated nonrelativistic electrons. We make some preliminary remarks. The scattering length is inversely proportional to the square of the charge number of the atom of the material, and the absorption length is inversely proportional to the charge number. Therefore, as we move from lighter atoms to heavier ones, the imaginary source becomes closer to the surface of the layer, the electron energy of the imaginary source becomes closer to the initial energy of the beam electrons and the energy of the backscattered electrons also becomes closer to the initial energy.

Let us estimate the mean energy loss of the backscattered electron by the transport time of the backscattered electron in the material (Fig. 7):

$$\Delta E = \frac{dE}{dt}t = \frac{dE}{dx}vt \approx \frac{E_0}{L_a}vt. \quad (36)$$

In the first part DO of motion of initially unidirectional beam electrons, we can estimate their motion as straightforward, so that here the mean energy loss is equal to

$$\Delta E_1 = \frac{E_0}{L_a}v\frac{L_s}{v} = \frac{E_0}{R}. \quad (37)$$

It is logical to assume that the bulk of the backscattered electrons is generated by an isotropic internal source electron in the upper hemisphere. In the simplest estimate, in a straightforward approximation, the time of electron return to the layer boundary is equal to $\frac{L_s\cos\alpha}{v}$, and the energy loss on the way back is equal to

$$\Delta E_2 = \frac{E_0}{L_a}v\frac{L_s\cos\alpha}{v} = \frac{E_0\cos\alpha}{R}. \quad (38)$$

The total energy loss is equal to

$$\Delta E = \frac{E_0(1+\cos\alpha)}{R}. \quad (39)$$

The fraction of energy loss is equal to

$$\delta = \frac{\Delta E}{E_0} = \frac{1+\cos\alpha}{R}. \quad (40)$$

For titanium and a beam with an initial electrons energy of 100 keV (R = 4.33) for $\cos\alpha = 1$, δ=46% (the empirical formula [16] gives δ=40% for silicon). For gold, δ = 13% (the empirical formula [16] gives δ = 20%).

The obtained formulas for the mean energy loss of the backscattered electron assumed the use of a diffusion model with an imaginary source of electrons, but considered the transport of electrons up and down as straightforward. Such an approximation gives a good qualitative and quantitative estimate for a wide range of materials with R >> 1.

Another variant for estimating the energy loss of a backscattered electron is based on a diffusive upward transport of the backscattered electrons, because (in contrast to the downward) this transport is provided by an isotropic electron source. Obviously, this model works for large R when the backscattered electron

has energy for diffusion transport. In the diffusion approximation, the time of electron return to the layer boundary is equal to

$$t_d = \frac{L_i^2}{\frac{1}{3}L_s v} = \frac{3L_s \cos^2\alpha}{v}, \quad (41)$$

and the energy loss on the way back is equal to

$$\Delta E_{2d} = \frac{E_0}{L_a} v \frac{3L_s \cos^2\alpha}{v} = \frac{3E_0 \cos^2\alpha}{R}. \quad (42)$$

Total energy loss is equal to

$$\Delta E_d = \frac{E_0(1+3\cos^2\alpha)}{R}. \quad (43)$$

Thus, for $\cos\alpha = 1$

$$\Delta E_d = 2\Delta E. \quad (44)$$

For titanium (R = 4.33) for $\cos\alpha = 1$, δ=92% (which differs markedly from the empirical 40%). The large error here can be explained by the fact that, as noted above, for small R the diffusion transport is not good, since during diffusion upward along the curved path, almost all the energy of the electrons is lost and they fail to exit the layer. Therefore, only that part of the electrons that moves almost straightforward is actually backscattered. For gold (R = 15), diffusion transport can take place and δ = 26% (which coincides well with the empirical 20%).

We conclude that the last formulas for the mean energy loss of the backscattered electron assumed the use of a diffusion model with an imaginary source of electrons, but considered the movement of electrons down as straightforward and up as diffusion. Such an approximation gives a good qualitative and quantitative estimate for the electron backscattering only for materials of heavy atoms.

Thus, the straightforward approximation for upward moving of electrons works in a wider range of materials. Therefore, the energy reflection coefficient of electrons (fraction of reflected energy) from the layer will be estimated by the formula:

$$k_E = k_r(1-\delta) = \left(\frac{1}{2} - \frac{\cos\alpha}{2\sqrt{\frac{2}{3}R}}\right)\left(\frac{R-1-\cos\alpha}{R}\right). \quad (45)$$

For titanium (R = 4.33) for $\cos\alpha = 1$, $k_E = 0.21 \times 0.54 = 0.113$, which is 30% lower than the empirical, but on the whole it can be considered as satisfactory agreement for such a complex process. Especially important is the qualitative agreement of the analytical formula with the real process.

7. THE DISTRIBUTIONЫ ALONG THE LAYER DEPTH OF THE PARTICLES AND OF THE BEAM ENERGY INPUT

The distribution of the particles along the layer depth x during diffusion as a random process is estimated by the Gaussian distribution. In the diffusion approximation, this distribution is determined mainly by the internal source of particles and has a maximum at $x = L_i$:

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) = \frac{1}{\sqrt{4/3\pi L_s L_a}}\exp\left(-\frac{3(x-L_s\cos\alpha)^2}{4L_s L_a}\right). \quad (46)$$

Here, the expectation $\mu = L_s \cos\alpha$, the dispersion $\sigma = \sqrt{\frac{2}{3}L_s L_a}$, $L_s = L_s(\frac{E_0}{\sqrt{2}})$, $L_a = L_a(E_0)$. Note that far from the maximum, this distribution gives an error, for example, because the particles are not able to penetrate the layer at a distance greater than the absorption length L_a.

The distributionы along the layer depth of the beam energy input near the maximum can be considered proportional to the distribution of particles. Far from the maximum, this estimation also gives an error/ However, this error due to small energy input in this place is usually insignificant.

The backscattering coefficient of particles from the layer can be calculated using (46) and is based on the fraction of particles backscattered from the layer:

$$k_{rd} = \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{0} exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)dx = \frac{1}{\sqrt{4/3\pi L_s L_a}}\int_{-\infty}^{0} exp\left(-\frac{3(x-L_s\cos\alpha)^2}{4L_s L_a}\right)dx. \quad (47)$$

This coefficient, calculated with the help of the differential distribution of particles, obviously behaves similarly to estimate (32), calculated with the help of the integral mean range of particles. In this case, the determination of the advantages and disadvantages of each of the estimates requires comparing them with experimental and numerical data.

The energy coefficient of reflection of particles from the layer in the differential approximation will be estimated similarly to formula (45):

$$k_{Ed} = k_r(1-\delta) = \frac{1}{\sqrt{4/3\pi L_s L_a}}\int_{-\infty}^{0} exp\left(-\frac{3(x-L_s\cos\alpha)^2}{4L_s L_a}\right)dx\,(\frac{R-1-\cos\alpha}{R}). \quad (48)$$

The fraction of unreflected particles in the material is $k_{rd}$and is described by the function *f(x)* for *x*> 0. Each particle gave an energy input to the material E_0, so that the total energy input of this fraction is equal to $E_0(1-k_{rd})$.

The fraction of reflected particles is k_{rd}. Moreover, each particle gave an energy input to the material δE_0, so that the total energy input of this fraction is $\delta E_0 k_{rd}$..

As a result, due to the reflected particles, the energy input into the material is increased by K_r times, where

$$K_r = \frac{E_0(1-k_{rd})+\delta E_0 k_{rd}}{E_0(1-k_{rd})} = \frac{1-k_{rd}+\delta k_{rd}}{1-k_{rd}}. \quad (49)$$

Therefore, considering the contribution of reflected particles to the energy input to the material as a correction, we will estimate the distribution of the energy input over the depth of the layer per one particle of the beam according to the formula

$$f_{Ed}(x) = K_r E_0 f(x) = \frac{1-k_{rd}+\delta k_{rd}}{1-k_{rd}}\frac{E_0}{\sqrt{4/3\pi L_s L_a}}\exp\left(-\frac{3(x-L_s\cos\alpha)^2}{4L_s L_a}\right). \quad (50)$$

It is possible to calculate the above characteristics on the basis of derived above reflection coefficient of particles from the material $k_r = \frac{1}{2} - \frac{\cos\alpha}{2\sqrt{\frac{2}{3}R}}$..

In this case, the fraction of unreflected particles in the material is equal to 1-k_r and is described by the function *f(x)* for *x*> 0. In addition, each particle gave an energy input to the material E_0, so that the total energy input of this fraction is equal to $E_0(1-k_r)$.

The fraction of reflected particles is k_r. Each particle gave an energy input to the material δE_0, so that the total energy input of this fraction is $\delta E_0 k_r$

As a result, due to the reflected particles, the energy input to the material is increased by K_r times, where, by analogy with (49)

$$K_r = \frac{E_0(1-k_r)+\delta E_0 k_r}{E_0(1-k_r)} = \frac{1-k_r+\delta k_r}{1-k_r}. \quad (51)$$

Therefore, considering the contribution of reflected particles to the energy input to the material as a correction, we will estimate the distribution of the energy input of the beam over the depth per one particle of the beam by analogy with (50, 33) by the formula

$$f_E(x) = K_r E_0 f(x) = \frac{1-k_r+\delta k_r}{1-k_r}\frac{E_0}{\sqrt{4/3\pi L_s L_a}}\exp\left(-\frac{3(x-L_s\cos\alpha)^2}{4L_s L_a}\right). \quad (52)$$

The last formula is simpler and more analytical than the formula for $f_{Ed}(x)$, and therefore is better

suited for optimization problems. However, it is based on the integral characteristic k_r, and not the differential k_{rd}, and therefore, in some cases, may have less accuracy.

It is significant that the formulas for $f_{Ed}(x)$ and $f_E(x)$ are derived in the diffusion approximation when the loss of electron energy over the isotropization length is neglected under the assumption $L_s \ll L_a$. Taking this loss into account refines the formulas, in a first approximation it leads to a narrowing of the Gaussian bell and can be done by replacing $L = \sqrt{\frac{2}{3}L_s L_a}$ with $\sqrt{\frac{2}{3}L_s(L_a - L_s)}$. In this case, the final formulas for the distribution of energy input in the layer are as follows:

$$f_{Ed}(x) = \frac{1-k_{rd}+\delta k_{rd}}{1-k_{rd}} \frac{E_0}{\sqrt{4/3\pi L_s(L_a-L_s)}} \exp\left(-\frac{3(x-L_s\cos\alpha)^2}{4L_s(L_a-L_s)}\right), \quad (53)$$

$$f_E(x) = \frac{1-k_r+\delta k_r}{1-k_r} \frac{E_0}{\sqrt{4/3\pi L_s(L_a-L_s)}} \exp\left(-\frac{3(x-L_s\cos\alpha)^2}{4L_s(L_a-L_s)}\right). \quad (54)$$

8. CONCLUSION

Thus, an analytical model of generalized diffusion is consistently formulated in the work, based on the stitching of diffusion and straightforward approximations. The model allowed calculating, in a wide range of particle energies and parameters of the materials, the mean range along the coordinate of accelerated particles and photons, the backscattering coefficient of particles, the mean energy of particles backscattered from a layer of material, the reflection coefficient of the beam energy from the surface of the material, the transmission coefficient of particles through the layer of material, and also estimate the distribution of particles and energy deposition over the depth of the layer.

The obtained formulas allow a good understanding of the physical picture of the transport of photons and accelerated particles through the layers of materials. In addition, they are generally satisfactorily qualitatively and quantitatively consistent with the experiment and Monte Carlo calculations for such complex processes. Particularly important is the qualitative coordination of analytical formulas with the real picture of processes, which provides optimization opportunities for important modern problems in the field of new technologies, medical physics, electron microscopy, etc.

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Citation: *V.A.Nikerov (2021). Analytical Qualitative and Quantitative Model of the Transport of Photons and Accelerated Particles through Layers of Materials in the Generalized Diffusion Approximation. Mean Range, Backscattering and Transmission Coefficients, Energy of Backscattered Particles, Particle and Energy Distributions along the Coordinate, Angular Dependencies. International Journal of Advanced Research in Physical Science (IJARPS) 8(4), pp.1-15, 2021.*