MONTE CARLO SIMULATING THE ELECTRON EMISSION FROM SURFACES OF OBJECTS BEING UNDER RADIATION

Mikhail ZHUKOVSKIY[(1)], Mikhail SKACHKOV[(2)], Gerd-Ruediger JAENISCH[(3)], Carsten BELLON[(3)], Andreas DERESCH[(3)]

[(1)]KELDYSH INSTITUTE FOR APPLIED MATHEMATICS OF RAS, Moscow, Russia

[(2)]MOSCOW ENGINEERING PHYSICS INSTITUTE (STATE UNIVERSITY), Moscow, Russia

[(3)] FEDERAL INSTITUTE FOR MATERIALS RESEARCH AND TESTING, Berlin, Germany

INTRODUCTION

Investigating the process of transformation of X-ray radiation into electron flux is important in radiography because most of the registration equipment is based on measuring the electron characteristics. In addition the distribution of electrons leaving the surfaces of objects are of interest when creating amplifier screens or developing new X-ray equipment. A statistical algorithm of modeling the flux of electrons leaving the boundary surfaces of objects illuminated by ionizing radiation is developed in the presented work.

Evolution of the electron flux begins with the interaction between photons and objects of complex geometry and materials of nontrivial physical properties. The flux of incoherent and photo electrons is forming in these materials and a portion of it leaves the object surface and spreads into the environment. The first stage of modeling the electron flux therefore is to analyze the processes of interaction between photons and complex objects. The second stage is to determine an initial spectral distribution and a spatial one for the charged particle flux generated on the object surface.

To solve the problem of the first stage it is necessary to construct an efficient technique for simulating the processes of radiation transformation in multicomponent objects of a complex form. The choice of the object description method, including the discretization of spatial structures, and the Monte Carlo method modification is developed taking into account the main goal – the efficient calculation of the spatial and spectral distributions of electron flux produced due to the interaction between ionizing radiation and object materials [1].

The technique of statistically modeling the transport of free electrons generated in matter under radiation is considered in the report. The model of thickened trajectories (MTT) is the central part of this technique. The advantage of MTT is to retain thelies in achieving calculation efficiency without using the rough distributions of multiple scattering theory. The electron characteristics distributions for MTT are obtained beforehand using the so called model of individual collisions

(MIC). The two models have approximately the same accuracy, but MTT is considerably more efficient than MIC. The electron path in matter is modeled in MTT by making use of the so called "embedded trajectory". In contrast to the real trajectory, where the nodes are the collision points, the transition from one embedded trajectory node to another is the result of multiple scattering.

PHYSICAL MODEL

Models of interaction between photons and matter are constructed based on a general idea of the physics of absorption and scattering of penetrating radiation in materials [2, 3]. For photons of energies less than 1 MeV the relevant processes are photo absorption, incoherent scattering, and coherent scattering. Modeling the electron transfer in matter is carried out taking into account the ionization of atoms by the electrons and multiple elastic scattering of the electrons [4]. The cross sections of incoherent and coherent scattering of photons were taken from the ENDF database provided by the National Nuclear Data Center of Brookhaven National Laboratory.

The production of high energy electrons in the objects' materials is caused by the photo-absorption and incoherent scattering processes. The main types of interaction between electrons and those materials are elastic and ionizing collisions. The electron energy loss caused by all processes is described by the stopping power $\kappa(\varepsilon)$ with ε being the energy of the electron. This value is interpreted as force acting upon the electron: $\boldsymbol{f}(\boldsymbol{p}) \equiv -\kappa(\varepsilon)\,\boldsymbol{p}/p$ ($\boldsymbol{p}$ – momentum vector, p – momentum magnitude). The equation $\mathrm{d}\varepsilon/\mathrm{d}s = f$ with initial condition $\varepsilon(s=0) = \varepsilon_0$ (s – electron path length) is solved along the electron trajectory for calculating its total energy loss.

TECHNIQUE OF SIMULATING THE IONIZING RADIATION TRANSFORMATION

It is necessary to use some discrete model for the description of the spatial distribution of physical characteristics of the object materials when modeling the interaction between radiation and matter in a 3D statement of the problem. In practice the mathematical modeling for the considered problems often consists of the investigation of the radiation transformation processes in objects described by parts of constant physical properties (for example sandwich structures constructed of different materials). The corresponding piecewise constant medium can be adequately described by the explicit definition of dividing surfaces between its homogeneous parts. Such kind of surface-oriented description of objects results in the possibility to determine the appropriate structures by using closed envelopes [5].

The computing technique based on the surface-oriented description of multicomponent objects of complicated shape includes:

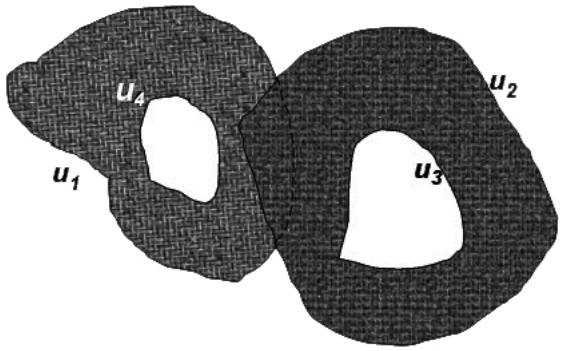
- The object's description based on the precise definition of boundaries of homogeneous inner structure parts of the object and on setting the corresponding dividing closed envelopes;

- The efficient ray-tracer algorithm for calculating the operator of tracing the investigated object for determination of the materials' optical thickness along the photon motion direction. This algorithm is based on finding points of intersection between the ray "source-detector" and the surfaces dividing the homogeneous parts of the object;
- The calculation method for simulating the transformation of penetrating radiation in the objects, accounting for incoherent and coherent scattering, and photo absorption. The technique is constructed by using the weighted Monte Carlo method in accordance with the principle of the information value maximum. The developed algorithm allows for efficient parallel calculations on multiprocessor computers.

The surface oriented models describe objects by means of definition of their boundaries determined explicitly or implicitly by closed envelopes. The description of a heterogeneous medium of piecewise homogeneous structure is carried out by using the pair (μ, U), where $\mu = \{\mu_p\}$ is a set of parameters defining material characteristics. In particular, μ_p $(p = 1,..., P)$ can be a vector specifying the coefficients of attenuation for the photons of given energy in the p^{th} homogeneous part of the object. $U = \{u_q\}$ $(q = 1,..., Q)$ is a set of dividing envelopes defining the boundary between homogeneous parts of the object.

Let $F = \{f_k\}$ $(k = 1,..., K)$ be the data set characterizing the object image (distribution of optical thickness) on the detector surface (registration surface). Then a connection between the inner structure of the object and its image for the given configuration of dividing envelopes $\{u_q\}$ and set $\{\mu_p\}$ is written by using the operator equation $A(\mu, U) = F$, where A is a connection operator. The result of application of the operator A is a distribution of optical thickness on the registration surface and the effect of A is called an object tracing.

The triangulation model is usually used for sampling surfaces of closed envelopes (Figure 1). It is to be taken into account that the object tracing requires multiple transitions from one coordinate system to another. Therefore the description of the envelopes is constructed to be as invariant with regard to rotating and shifting frame of axes as possible. Within the bounds of such a description all vertices of triangles are written as the set of points $\{P_m\}$, $m = 1,..., M$, and the corresponding set of triangles is specified as the set of connections $T_n\left(P_{i_n}, P_{j_n}, P_{k_n}\right)$, $n = 1,..., N$, $i_n, j_n, k_n = 1,..., M$. The mentioned set of connections is invariant with regard to linear transformations of coordinates, allowing minimization of the computation amount required when tracing an object.



$$U=\{u_q\},\quad q=1,\ldots,Q$$

$$\mu=\{\mu_p\},\quad p=1,\ldots,P$$

$$\{T_n\},\quad n=1,\ldots,N$$

$$\{P_m\},\quad m=1,\ldots,M$$

$$\{i_n,j_n,k_n\},\quad i,j,k\in\{1,\ldots,M\}$$

Figure 1. Description of object by envelopes.

The equality $A(\mu,U)=F(x,y)$ can be written as $F(x,y)=\sum_{p=1}^{P}\mu_p V_p(x,y)$ for a multicomponent structure of P different materials. Here $V_p(x,y)$ is the full optical thickness of the material of index p along the line $L(x,y)$ connecting the source S with the point (x,y) on the detector surface.

The tracing algorithm consists of two stages:

- The set of triangles intersected by the given ray is determined. This “qualitative” stage is carried out by using the framework (edges and vertices) of triangles, in that the intersection between the ray and the triangles is determined by use of a special inequality system;
- The coordinates of intersection points between the ray and every triangle found in the first stage are calculated (“quantitative” stage).

Realization of such an algorithm permits the calculation of the connection operator and to find the distribution of the optical thickness $V(x,y)$ without taking into account connections between different triangles on the surface. Only the list of surface points $\{P_m\}$ and the corresponding list of triangles $T_n\left(P_{i_n},P_{j_n},P_{k_n}\right)$ are used. This approach yields a simple tracing algorithm based on analyzing the separate surface triangles.

Main features of the problem are the relationships between spatial parameters of the discussed processes. Namely, the thickness of the material envelope and photon path lengths are typically much larger than the electron stopping power. Therefore only a small part of the electrons can reach a boundary surface of the object. This fact considerably decreases the efficiency of directly using the Monte Carlo method.

The developed technique allows constructing an efficient approach to calculation of electron flux leaving the object based on the principle of maximum information value of photon trajectories (the scheme of the technique is presented in Figure 2).

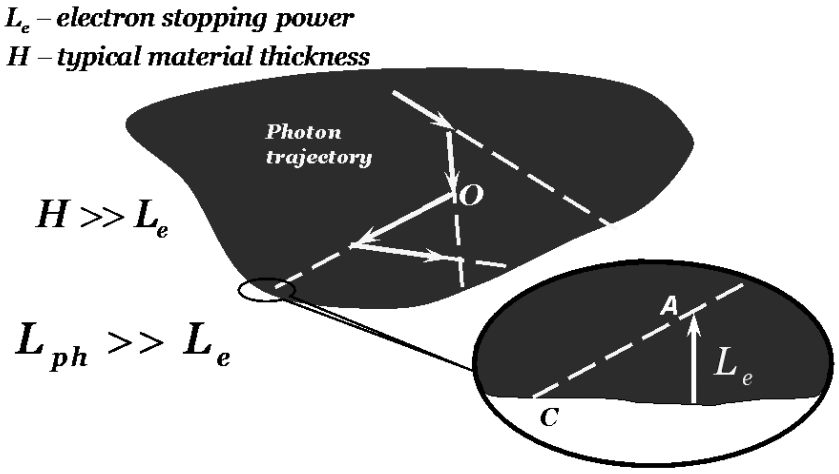


Figure 2. Scheme of determination of electron contribution section of photon ray.

A contribution from every segment of the photon trajectory is computed by determining the "useful" section of the segment prolongation (OC) up to the intersection with the boundary surface of the object, from which generated electrons are capable of leaving the object (AC on the Figure 2).

Then a point of electron creation is sampled using a constructed conditional probability distribution. The generated electron is assigned some statistical weight calculated according to the probability of interaction between the photon and matter in section AC and the probability of the corresponding process (photo absorption or incoherent scattering).

Transport of the generated electron up to its leaving the object is modeled in a thin layer near the boundary surface by use of the next stage of the developed method.

MODELING OF ELECTRON TRANSPORT

Statistically modeling the transport of electrons or other charged particles is of great difficulty compared to photon transport modeling. The interaction of neutral particles with matter is characterized by a relatively small number of collisions and the line segments of particle motion between the collisions. One of the possible processes of interaction between a photon and matter (absorption, coherent or incoherent scattering) takes place. In contrast the transport of electrons occurs under the continuous influence of Coulomb forces. As a result a huge number of elementary interactions happen. For instance, a 500 keV photon loses its energy after approximately ten collisions, while an electron loses the same energy over the course of about 10^5 interactions.

A technique of statistically modeling the electron transport in matter is developed. The "model of thickened trajectories" (MTT) described below is the central part of this technique. The advantage of MTT is the retention of the calculation efficiency without using the rough distributions of

multiple scattering theory. The electron characteristics distributions for MTT are obtained beforehand by using the so called model of individual collisions (MIC). MTT and MIC have approximately the same accuracy, but MTT is considerably more efficient.

The developed method consists of three main parts:

1. Handling of the required data (angle and energy distributions, cross sections, etc.) and preparing probability distribution tables for sampling all essential values (type of process, energy losses, angle of elastic scattering);
2. Monte Carlo (MC) computation of the multidimensional distributions of electron characteristics using MIC. The distributions are then used when modeling the electron transport.
3. MC modeling the electron transport in matter within the framework of MTT using the distributions calculated in step 2.

The first stage is carried out on a standard PC, while the 2nd and 3rd tasks require the use of multiprocessor computers and need some hours of computation time to reach enough accuracy on hundred processors. It should be noted that the 2nd problem is solved once for a given material and energy range and the results can then be used in various physical applications.

MTT [6] is used for the description of electron motion in solids. It belongs to the class of models based on enclosed trajectories. However, in contrast to known algorithms, MTT does not use approximate distributions from multiple collisions theory. All distributions needed for sampling the electron trajectories' parameters are computed by using MIC. For this purpose an auxiliary task on scattering electrons moving in some tube is solved (see Figure 3).

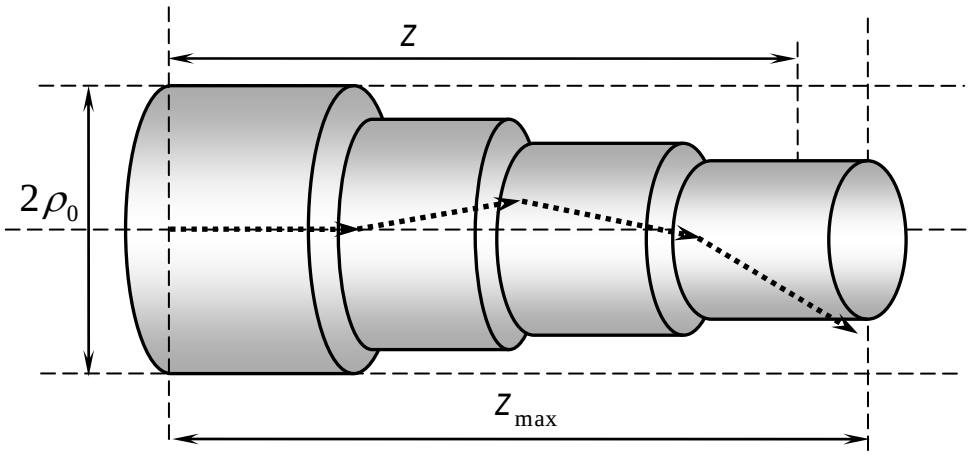


Figure 3. Problem of electron motion in tube.

The diameter 2ρ of the tube is changed along the electron trajectory and depends on its current energy: $2\rho = n\lambda$, $\lambda = \left(\sigma_{el} \cdot N\right)^{-1}$, with N - atom concentration, σ_{el} - elastic scattering cross-section, n - some parameter depending on material and initial electron energy (usually about 10, n is chosen according to the requirement of approximately uniform distribution of electrons by length of the tube; too large a value of ρ leads to a decrease in accuracy of the model, too small a value leads to a decrease in efficiency). The length of the tube L (used for constructing the grid on *z* for registration of electrons) is given by the condition of an electron energy loss of 10% of the initial electron energy. An estimation of $L = z_{\max}$ can be determined using the continuous slow-down approximation.

Thus, the following distributions are obtained:

- Density of displacement distribution $f_1(z \mid E_0)$;
- Density of electron energy distribution $f_2(E \mid z, E_0)$;
- Density of scattering angle distribution $f_3(\cos\theta_e \mid E, z, E_0)$.

These distributions are used for sampling all needed values when modeling the electron transport. The scheme of Monte Carlo simulation of electron transport is described below.

- Sampling the electron displacement z (along tube axis) using the distribution $z\left(\gamma \mid E_0\right)$;
- Calculation of coordinates of the next trajectory node;
- Sampling of the new motion direction according to the distribution $\cos\theta\left(\gamma \mid z, E_0\right)$;
- Sampling of the new electron energy from the distribution $E\left(\gamma \mid \cos\theta, z, E_0\right)$.

The trajectory of the electron is terminated when it leaves the object or loses its energy.

EXAMPLES

The following computational results show the efficiency application of the presented technique. An aluminum tube is irradiated by a gamma flux from a source based on the isotope Se-75. The scheme of the experiment is represented in Figure 4.

The flux densities of electrons leaving the outer and inner boundaries of the tube are given in Figure 5. This figure shows, in particular, that the electron flux has two maxima on the outer surface of the object, while only one maximum exists on the inner surface. This fact can severely influence the interpretation of an image of the tube's inner structure.

Spectra of leaving electrons are presented in Figure 6. It is interesting that the electron spectrum possesses the same structure as the flux.

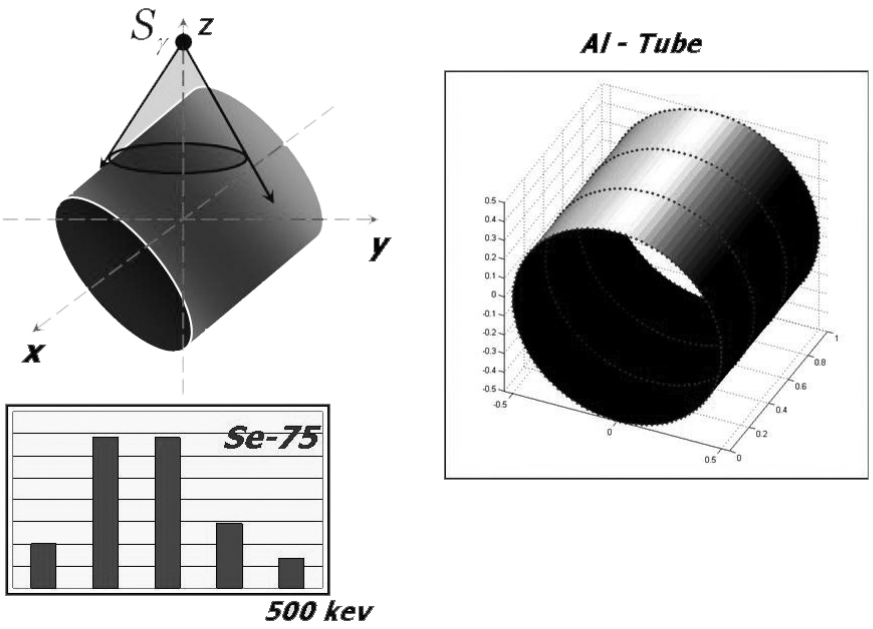


Figure 4. Scheme of computing experiment.

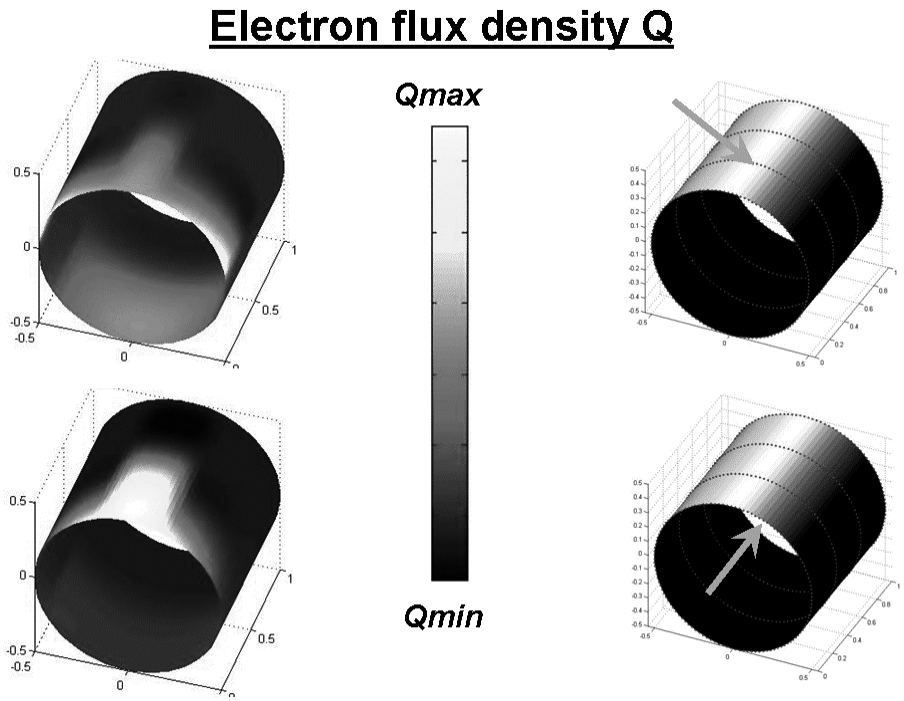


Figure 5. Electron flux.

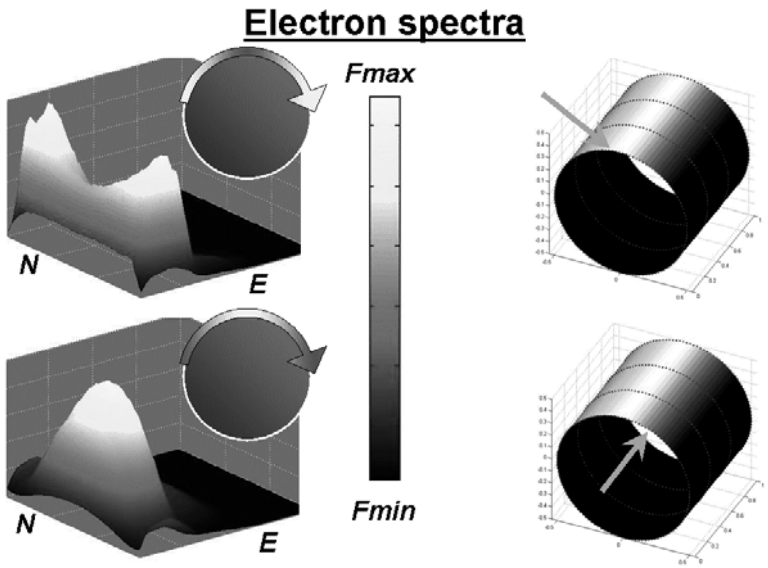


Figure 6. Electron spectra.

CONCLUSION

The efficient statistical method of modeling the electron emission from outer and inner boundary surfaces of objects being under X-ray radiation is developed. The modeling method is based on the principle of the maximum of the photon trajectory information value. Semi-analytical modifications of the Monte Carlo method are made relying on replacing the part of the random quantities by their probable values. The developed method gives the possibility to compute spatial and energy distributions of emitted electrons and different functionals of the distributions corresponding to measured values.

A new model of electron transport in dense material is constructed and included in the method. The model is based on the beforehand calculation of electron flux characteristics distributions and on the nested trajectories method.

Comparative analysis between the presented method and well known MCNP has shown advantages of the presented algorithms. In particular, the calculation time is typically at least 10 times less when using the developed technique.

REFERENCES

1. G.-R. Jaenisch, C. Bellon, U. Samadurau, M. Zhukovskiy, and S. Podoliako “Monte Carlo radiographic model with CAD-based geometry description.” Insight **48** 10 (2006) 618-623.
2. U. Fano, L. V. Spencer, and M. Berger, “Penetration and Diffusion of X Rays”, Encyclopedia of Physics, 38/2, Springer-Verlag, Berlin (1959).
3. L. V. Spencer, “Theory of Electron Penetration”, Phys. Rev. **98** (1955) 1597-1615

4. V. I. Boyko, V. A. Skvortsov, V. E. Phortov, I. V. Shamanin, “The interaction between the charged particles pulsed beams and matter.” (In Russian). Moscow, Physmatlit Press, 2003.
5. M. Zhukovskiy, S. Podoliako, G.-R. Tillack, and C. Bellon, “Monte Carlo Simulation of Photon Transport Coupled to CAD Object Description.” In: D. O. Thompson and D. Chimenti (Eds.): Review of Progress in Quantitative Nondestructive Evaluation, Vol. 23, AIP, Melville, 2004, pp. 515-521.
6. M. Zhukovskiy and M. Skachkov, “On the statistical methods of modeling the electron transport in matter.” (in Russian). Vestnik of MSTU, 1(32) 2009, 31-46