

RESEARCHING THE SPECTRUM OF BREMSSTRAHLUNG GENERATED BY THE RIUS-5 ELECTRON ACCELERATOR

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Annotation. The generation of bremsstrahlung produced by interaction between RIUS-5 electron beam and tantalum target is considered. The model of individual collisions is used to describe the radiation transport. This model is convenient for the efficient calculations parallelization on supercomputers having the heterogeneous architecture. Weight modifications of Monte-Carlo method are built. The modifications are worked out for hybrid parallelization. Parallel code is designed for modeling of electron and photon transport by usage of graphical processors as arithmetical coprocessors and using the NVIDIA[®] CUDA technology. The algorithm is tested by comparing the results of calculations using the MCNP package. Satisfactory agreement for results is shown. The comparison between the numerical simulation and the experimental data is carried out. It shows qualitative coincidence and quantitative satisfactory agreement between the calculated and experimental data.

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1 INTRODUCTION

The results of a numerical study of the bremsstrahlung spectrum generated by a relativistic electron beam of linear accelerator RIUS-5 (http://ckp-rf.ru/ckp/equipped/?SECTION_ID=476&ELEMENT_ID=421947) are considered. Mathematical modeling on high-performance computing system of hybrid architecture is used. The research is actual for the efficient analysis of modern and advanced bremsstrahlung sources and for studying the interaction between gamma-radiation and matter. The mathematical modeling is an effective way to evaluate the parameters of the bremsstrahlung because the physical experiments are rather expensive. Moreover, they are often impossible.

It is impossible to evaluate the results of interaction between radiation and matter using the integral parameters like absorbed radiation dose and dose rate in some practically important cases. One of them is the radiation impact on microelectronics investigating. There is required the detailed analysis of the radiation field based on direct individual particle collisions consideration. The model of the bremsstrahlung and secondary electrons transport in a complex environment is developed¹. Sizes of the environment heterogeneities may be comparable to the particle path length within the bound of this consideration. Hybrid supercomputers and modern technologies of parallel computing using the stream processors accelerator (NVIDIA © CUDA) allow simulating the charged particles transport without using approximate theories.

The bremsstrahlung modeling algorithms based on weight modifications of Monte Carlo method are considered in the paper. These algorithms give a possibility of the effective parallelization on hybrid computing systems². The results of comparative calculations using MCNP package show satisfactory agreement with the calculations carried out using the elaborated method. The comparison of the bremsstrahlung energy spectra obtained by an experiment using the accelerator RIUS-5 and computed photon energy distribution are demonstrated.

2 MODEL OF INTERACTION BETWEEN RADIATION AND MATTER

The model of photons and electrons interaction with matter is constructed in compliance with the peculiarities of the hybrid parallelization technology. This model is described in the work¹. The time of the radiation flux duration is proposed to exceed significantly the particle lifetime in matter. The quasi-stationary integral-differential equations of photons and electrons transport are valid in this case.

One assigns a functional on the space of transport equation solutions to every measured in experiment value. The random particle trajectories are simulated to evaluate the functional. The contributions of these trajectories in the detector are summarized. Trajectory modeling is carried out within the developed physical model of radiation interaction with matter^{1,2}. The interaction modeling uses the sampling the random variables - probability distributions of the particle characteristics (momentum, energy, scattering angle, the way to the point of collision, etc.). The distributions are built by collision's cross sections (full and differential) treating.

2.1 Electron interaction with matter

Following processes of electron interaction are considered:

- elastic scattering on the atoms leading to deflection of the electron from the initial motion direction;

- excitation of atoms results in low electron energy loss;
- impact ionization accompanied with arising the secondary electron of continuous spectrum;
- radiation deceleration in atomic Coulomb field resulting in bremsstrahlung photon generation.

The model¹ of the electron's interaction with matter based on handling the cross sections of processes in question is worked out by the authors of the paper. The main source of the cross section tabulated data is the database of the National Center for Nuclear Data (<http://www.nndc.bnl.gov/sigma/>).

Modelling of radiation interaction processes is carried out using probability distributions $F_x(\xi)$, $\xi \in (0,1)$, where x is the characteristic of radiation particle (momentum, energy, scattering angle, etc.), and ξ is a uniformly distributed random variable.

Developed model is represented mostly in the work¹.

The bremsstrahlung generation process in the target node of RIUS-5 accelerator is considered below. The experimental data are obtained for incident beam of electrons with energy 2.5 MeV and *Ta* target of 1 mm thickness (see section 6).

The stopping path of an electron of 2.5 MeV energy in *Ta* is about 1.2 mm (<http://physics.nist.gov>). Therefore, the most part of photons is generated in *Ta* target of 1 mm thickness (see fig. 11). The impact ionization and bremsstrahlung in *Ta* are the main collision processes.

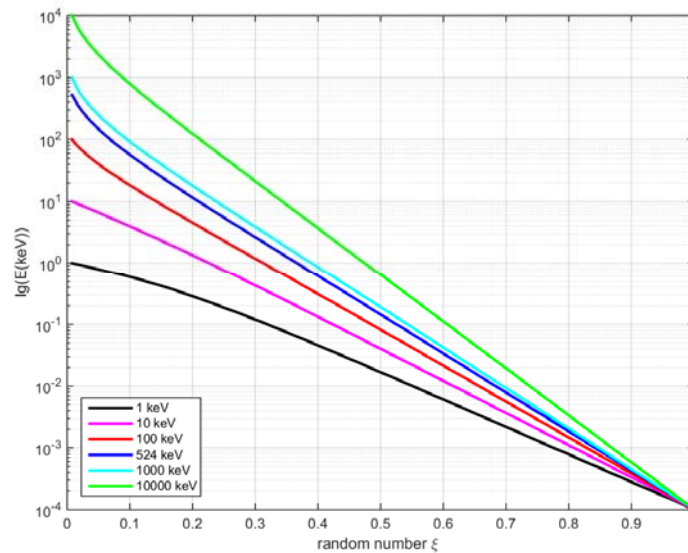


Fig. 1: Bremsstrahlung photon energy probability distribution in tantalum, the incident electron energies are shown at down left.

The differential cross section of bremsstrahlung $\partial\sigma/\partial E_{ph}$ is inversely proportional to the photons energy E_{ph} . After transformations we get: $\lg(E_{ph}) \sim \xi$. Therefore, the logarithm of the

bremsstrahlung photons energy behaves like almost line function. Bremsstrahlung simulation is carried out using the function $F_{br} = \lg(E_{ph})$. Fig. 1 represents the graphs of function $F_{br}(\xi)$ for tantalum at different energies of incident electrons.

The formula for the probability density function of the polar angle between photon and incident electron momentums was obtained from works^{3,4}:

$$p(u) = C \left[u \exp\{-au\} + du \exp\{-3au\} \right], \quad u \in (0, u_{\max}). \quad (1)$$

Here: $a = 5/8$, $d = 27$, $u = \theta E_{ph} / m_e c^2$, $u_{\max} = \pi E_{ph} / m_e c^2$; E_{ph} is the energy of bremsstrahlung photon. Azimuthal angle is distributed isotropic: $\varphi = 2\pi \cdot \xi$, $\xi \in (0, 1)$.

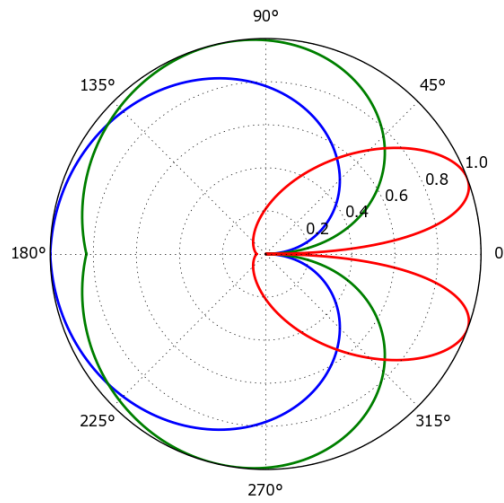


Fig. 2: The indicatrix of photon emission angle (energy of photon: red line – 500 keV; green line – 100 keV; blue line – 50 keV).

The probability distributions of the photon angle cosine are obtained by integrating the formula (1). Fig. 2 shows the indicatrix of photon emission angle.

The atom ionization process results in knocking out an electron from some atomic shell. The incident electron loses part of its kinetic energy. The “ionization” energy loss distribution density $f_n(E|E_0)$ is equal to

$$f_n(E|E_0) = \delta(E - E_n) \sigma_n(E_0) / \sum_{n=1}^{N_{sh}} \sigma_n(E_0).$$

Here: $\sigma_n(E_0)$ - cross section of ionization of n^{th} atomic shell; E_n - binding energy of atomic electron; E - incident electron energy loss. Two electrons are produced by ionization of atomic shell. Primary electron has larger energy and secondary one (recoil electron) has smaller energy. The distribution density of energy transfer from primary electron to secondary one is

$$f_n^{\text{sec}}(E|E_0) = \frac{d\sigma_n}{dE} \sigma_n \eta(E_0 - E_n) / \sum_{n=1}^{N_{sh}} \sigma_n.$$

Summing these formulas and integrating the sum on transferred energy we obtain the distribution of the transferred energy:

$$F_{ion}(E | E_0) = \sum_{n=1}^M \eta(E_0 - E_n) \frac{\sigma_n(E_0)}{S(M)} \left\{ \eta\left(\frac{E_0 - E_n}{2} - E\right) \int_0^E \frac{d\sigma_n}{dt} dt + 1 \right\}.$$

Here: $S = \sum_{n=1}^M \sigma_n(E_0)$, and $M = \sum_{n=1}^{N_{sh}} \eta(E_0 - E_n)$, $\eta(x) = \{1, x > 0; 0, x < 0\}$ - Heaviside's function. The corresponding probability distribution density is represented in the fig. 3.

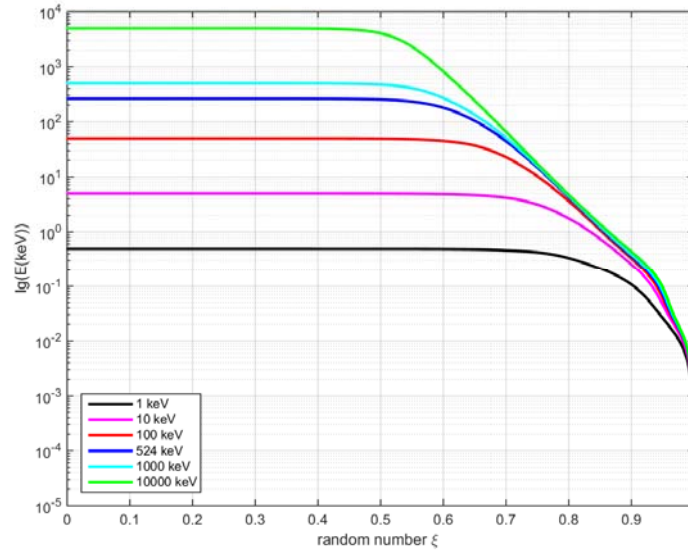


Fig. 3: Energy probability distribution of recoil electron in tantalum, the incident electron energies are shown at down left.

Simulation of the bremsstrahlung transport is carried out taking into account all the processes of interaction between photons and matter.

2.2 Interaction between photon and matter.

The following types of collisional processes are considered:

- coherent scattering;
- Compton scattering;
- photo absorption;
- pair production.

The Compton and coherent photon scattering are considered below in more details. These processes are predominant for bremsstrahlung generated in the RIUS-5 accelerator. Most of the photons arises in tantalum target but they interact mainly with the atoms of aluminum.

The Klein-Nishina differential cross section describes Compton scattering on a free electron. Binding of an electron in an atom is taken into account by introducing the scattering functions⁵ $I(q, Z)$:

$$\frac{d\sigma_C}{d\theta} = \frac{d\sigma_{KN}}{d\theta} I(q, Z). \quad (2)$$

Probability distribution of $\cos\theta(\xi)$ (θ is the scattering angle) calculated by integrating the formula (2) is shown in the fig. 4.

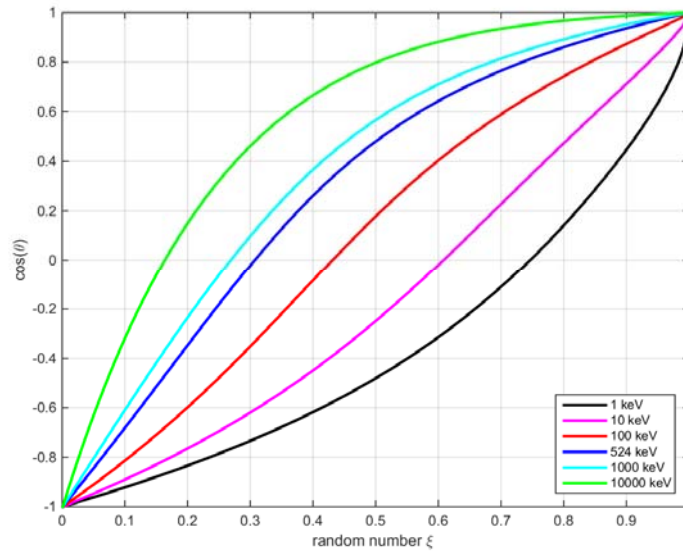


Fig. 4: Probability distributions of the angle cosine for Compton scattering in aluminum.

Probability distributions of $\cos\theta(\xi)$ for the coherent scattering are obtained analogously.

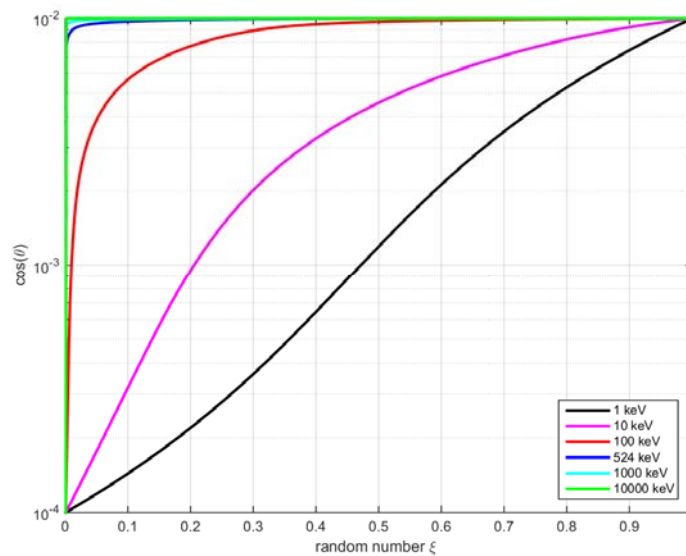


Fig. 5: Probability distributions of the angle cosine for coherent scattering in aluminum.

They are shown in the fig. 5.

3 ALGORITHMS OF BREMSSTRAHLUNG GENERATION MODELING

The algorithms of radiation transport statistical modeling are based on the probabilistic interpretation of the integral transport equation kernel. The kernel of integral operator is considered as the density of moving probability from one trajectory point to another. Random trajectories of particles are computing using probability density. Contribution of every particle trajectory is calculated for evaluating the desired value⁶. This value is represented as functional on the space of transport equation solution.

3.1 Evaluating the functional by Monte Carlo method

The trajectory $T = \{x_0, x_1, \dots, x_N\}$ of the particle (where x is a point of the phase space) ends because of absorption or departure from the considered region of object. The goal of the radiation transport simulation is to compute values being measured in the experiment. This values are functional:

$$J_h = (f, h) = \int f(x)h(x)dx. \quad (3)$$

Here $f(x)$ is a solution of transport equation and $h(x)$ is defined by type of measured value.

Monte Carlo method is used to evaluate the functional (3). Used modifications of the Monte Carlo method are based on representing the integral equation solutions by Neumann's series⁶.

Let us consider the radiation transport in a restricted environment. Assume that the cross sections $\sigma(x) = \sigma_a(x) + \sigma_s(x)$ of the interaction between radiation and matter and corresponding macroscopic cross-sections $\mu_j = \rho\sigma_j$, $j = a, s$, where σ_a and σ_s are the absorption and scattering cross section correspondingly, are known. The probability distributions of $\cos\theta = F_\theta(\xi)$ (scattering angle) and $\Delta E = F_{\Delta E}(\xi)$ (photon energy loss in the inelastic collision) are known too.

The particle trajectory from the phase space point x' to the point x is built as follows. Absorption or scattering is sampled in accordance with probabilities $p_a = \frac{\mu_a}{\mu}$, $p_s = \frac{\mu_s}{\mu}$,

$\mu = \mu_a + \mu_s$. If scattering occurs, then:

1. a new direction of particle motion $\mathbf{\Omega}$ and the new energy E are played by use of distributions $F_\theta(\xi)$ and $F_{\Delta E}(\xi)$;
2. the path l in the direction $\mathbf{\Omega}$ is played according to probability distribution density $p_l = \mu(\mathbf{r}' + \mathbf{\Omega}l) \exp(-\tau(\mathbf{r}'; \mathbf{\Omega}l))$;
3. new point of interaction $\mathbf{r} = \mathbf{r}' + \mathbf{\Omega}l$ is calculated;
4. if the particle is absorbed or leaves the object, current trajectory ends.

Let n to be a link number of the particle trajectory, and t is a number of constructed trajectory. Then the desired functional assessment can be carried out (3) as follows:

$$J_h = M \left[\sum_n h(x_n) \right] \approx \frac{1}{T} \sum_{t=1}^T \left[\sum_n h_t(x_n) \right], \text{ where } T \text{ is a count of built trajectories.}$$

Here M is the mathematical expectation and h_t is value of function h (see (3)) on the trajectory number t . This algorithm is called the method of direct test or analog Monte Carlo method.

3.2 Weight functions of Monte Carlo method

The required functional (experimentally measured value) evaluation using the analog Monte Carlo method may not be effective when a small part of trajectories gives information about the task solution. It may happen that a small fraction of the particles reaches the detector, for example, in strongly absorbing media.

We can construct trajectories in a different way using other transition density $q(x', x)$ and other initial density $\varphi(x)$. The functions $q(x', x)$ and $\varphi(x)$ have to be selected so that $q(x', x) \neq 0$, $\varphi(x) \neq 0$ where $k(x', x) \neq 0$, $f_0(x) \neq 0$. Under these conditions of "unbiased" estimation⁶ the "weights" are introduced by the formulas:

$$W_0(x_0) = \frac{f_0(x_0)}{\varphi(x_0)}, \quad W_n(x_n) = W_{n-1}(x_{n-1}) \frac{k(x_{n-1}, x_n)}{q(x_{n-1}, x_n)}.$$

Evaluation of J_h is determined in this case as:

$$J_h = M \left[\sum_n W_n h(x_n) \right]. \quad (4)$$

The following weight modifications of Monte Carlo method are implemented in developed algorithm.

Weights replacing the sampling of absorption. The act of particles absorption or scattering is not determined by means of playing the random value in this modification. The particle is supposed never to disappear. It is scattered and its statistical weight after interaction is equal to p_s – the probability of particle's "survival". This weight makes sense to the average portion of photons being not absorbed in this act of interaction.

Accordingly, the weight (4) is calculated by the formula

$$W_n(x_n) = W_{n-1}(x_{n-1}) p_s(x_n), \quad W_0 = 1.$$

The formal increase of particles' sources is occurred in this modification. The fact reduces the dispersion of result.

Another modification is constructed using the *weights replacing the particle emission*. A particle can leave an object when the radiation transport is simulated. It means the particle trajectory is finished. It is possible to increase informational value of the trajectories. We suppose the particle never to leave environment instead of sampling a random event of this leaving. Particles "weight" is reduced multiplicatively by the probability of "non-leaving" in this case. It is necessary to change the sampling of particle free path because of changing the distribution of particle free path between two consequent points of collision.

An important feature of the considered weight modifications is the reducing of the conditional branches number in the algorithm. This is significant for developing the code for mathematical modeling by using the hybrid computing systems.

Considerable increasing of the efficiency can be obtained by working out weighted versions of the Monte Carlo method for radiation registration simulating. These modifications can be used to compute the desired functional (4) on the space of the transport equation solutions.

The main purpose of using the weight modifications is to increase the informational value of the particle trajectories, i.e. to enlarge the number of trajectories giving the contribution to the desired value. The approaches to developing the modifications depend on the physical content of the evaluated functional.

4 MODELING OF BREMSSTRAHLUNG USING THE HYBRID COMPUTING

Statistical evaluating of the mathematical expectation of the desired functional corresponding to measured value involves serial independent modeling of a large number of random trajectories. The additive contribution of each trajectory to the cumulative result is computing. Computational modeling scheme of every trajectory link is the same.

The algorithms having the large number of independent computing branches (trajectories of particles) could be simply parallelized and scaled. Parallelizing can be implemented on any computing architectures. The CUDA technology is destined to carrying out the high performance parallel calculations on graphical processors (GPU)^{7,8}. This technology is implemented on the hardware designed for computing of the huge number of independent similar operations.

Using the GPU as arithmetical co-processor (GPGPU technology) has some peculiarities.

First. There is no concurrent access to data in the frame of the CUDA technology. The available opportunities for programming the sync points is often not sufficient to ensure full control over access to shared resources. Consequently, one needs to make data decomposition. The simplest version of this decomposition is to provide a unique computing memory region for each computing thread to record the output data.

Second. Conditional transition is the hardest operation when graphical processor is used. Moreover, the graphics processor doesn't execute conditional transitions in principle. Both branches of the algorithm are running at the same time and then one of two results is canceled. This feature makes designer to create the most linear algorithms or to "straight" the existing ones. For example, it is often easier to calculate the values of all having elements in opposite to check the necessity of an element.

Third. GPUs have several types of memory. Each type has its advantages and disadvantages. Approaches to work with different types of memory differ markedly. These differences should be taken into account when developing the algorithm. It should use right part of memory which would be most effective in a given part of the algorithm.

Effective scheme of algorithm constructing for hybrid supercomputers is developed by analysis of hardware (video adapter capabilities) and software tools provided by CUDA technology.

The following components of the computing algorithm and its software implementation can be mentioned in this scheme.

- Weight modification of the Monte Carlo method when a random particle trajectory

simulation is carried out “by the collisions”. It is assumed that the particle is “survived” at every point of interaction with a weight being equal to the probability of no absorption (for photon). This variant of the algorithm allows reducing the result dispersion and minimizing the number of conditional jumps in a software implementation.

- “Multicore” version of the code. Every stage of a single particle trajectory simulation (tracing object, physics simulation, data acquisition) is calculated by a separate computing GPU core. This makes it possible to achieve a high degree of homogeneity of computational threads and to simplify noticeable the handling of data within a single core. This approach is optimal because the data loading and unloading of computing core require no additional resources.

- Work with system memory. Exchange operations are the most difficult when the code programming uses CUDA technology. Analysis of algorithm, software and hardware allows optimizing the usage of different types of graphical card memory. Using the results of the analysis gives more than tenfold increase of the parallel program efficiency.

Cascade of the particles simulation requires the implementation of different parts of the general algorithm on CPU and on GPU. Parts having the high calculation density are performed on GPU, and the others are carried out on CPU. This separation is not a trivial task and requires careful analysis of computing density at all stages of the algorithm performance.

Analysis of elaborated method shows that the simultaneous modeling of the photons and electrons trajectories causes a high non-uniform density of computing at different stages of the algorithm performing. Parts of the algorithm have low-density computations (modeling of photon collisions, appearing the Compton and photo electrons etc.) Other parts have high-density computing (object ray-tracing, electron trajectories simulating).

The algorithm in question is upgraded to simulate the cascade processes using the GPU. The improved algorithm is effective computing method for particle transport simulation on hybrid supercomputers⁹. Calculations of low calculation density are carried out using the central processors, and computing of high calculation density is performed on graphical processors.

5 ALGORITHMS TESTING

The developed algorithms are implemented as the parallel software module for performing the calculations on supercomputer of the heterogeneous architecture. Parallel computing on the nodes of the hybrid computing system is carried out using the MPI interface. The calculations on graphical accelerators use NVidia© CUDA technology.

Numerical experiment is performed for testing methodology. The scheme of the experiment is shown in the fig. 7. Tantalum plate of $h=4$ mm thickness is irradiated by the electron beam of 4 MeV energy. Photon fluxes through the top and bottom bound surface of the plate are evaluated. The same calculations are performed using MCNP software¹⁰.

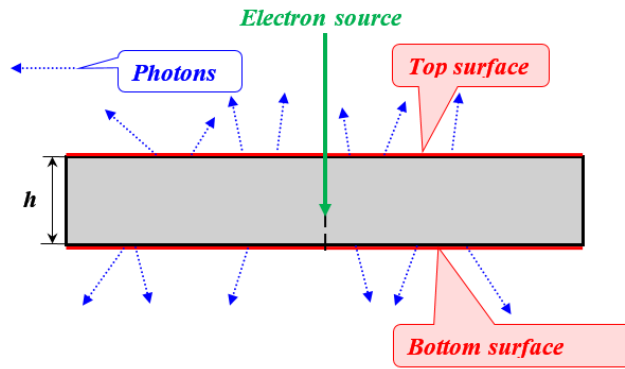


Fig. 7: Scheme of the numerical experiment.

Bremsstrahlung spectrum is represented on the fig. 8 and 9. Graphs of the energy distribution of the photons emitted from irradiated surface of the target (top surface) are shown in the fig. 8. Graphs of energy distribution of the photons emitted from the bottom surface of the plate are presented in the fig. 9. The blue line corresponds to the results obtained by developed method, red one corresponds to results obtained by MCNP package. The presented figures show satisfactory agreement of calculations results performed using the developed algorithms and MCNP package.

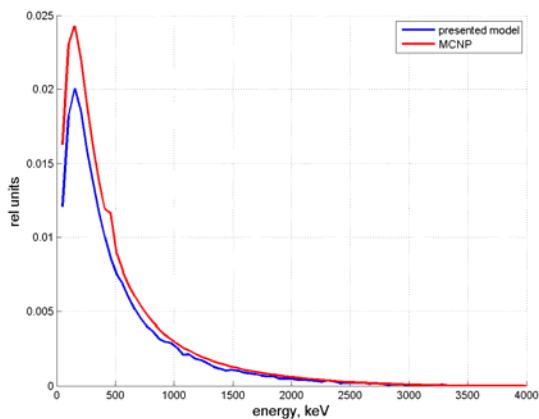


Fig. 8: Photon spectrum from the top surface (irradiated surface) of the plate.

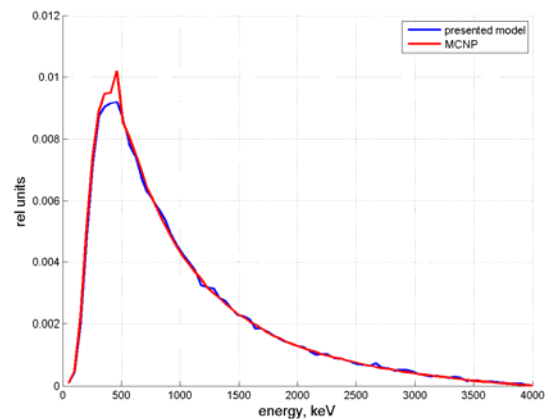


Fig. 9: Photon spectrum from the bottom surface of the plate.

6 MODELING OF EXPERIMENT USING THE RIUS-5 ACCELERATOR

The simulating the bremsstrahlung radiation experiment on the pulse electron accelerator RIUS-5 is considered below.

6.1 The X-ray pulse electron accelerator RIUS-5

Pulse accelerator RIUS-5 creates an electron current. The amplitude of the current is up to 10 kA. The pulse time is up to 20 ns and the average electron energy is about 2.5 MeV.



Fig. 10: RIUS-5 accelerator.

The appearance of RIUS-5 accelerator is shown in fig. 10.

Experiments on RIUS-5 were carried out in the Research Institute of Scientific Instruments (<http://www.niipriborov.ru>).

The scheme of the anode-cathode zone of the accelerator is shown in fig. 11.

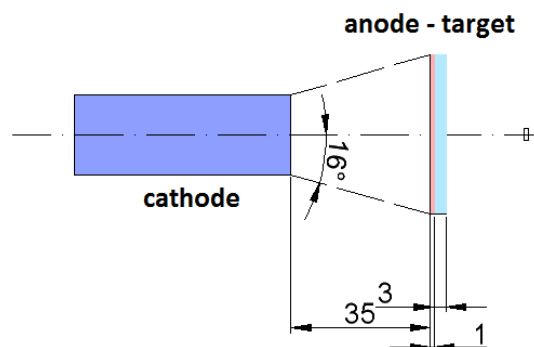


Fig. 11: Anod-cathode zone of the accelerator.

The cathode is a steel rod of 20 mm diameter. Distance from cathode to anode is 35 mm. Two-component target consists of tantalum (1 mm) and aluminum (3 mm). The maximum entry angle of the electrons at the target is 16 degrees.

6.2 Results of numerical experiment

Mathematical modeling of RIUS-5 bremsstrahlung is carried out on the heterogeneous computing system K-100 (<http://www.kiam.ru/MVS/resourses/k100.html>).

Bremsstrahlung is produced by interaction between the accelerated electrons and the double-layered target. Energy distribution of the bremsstrahlung photons is calculated (Fig. 12, black points).

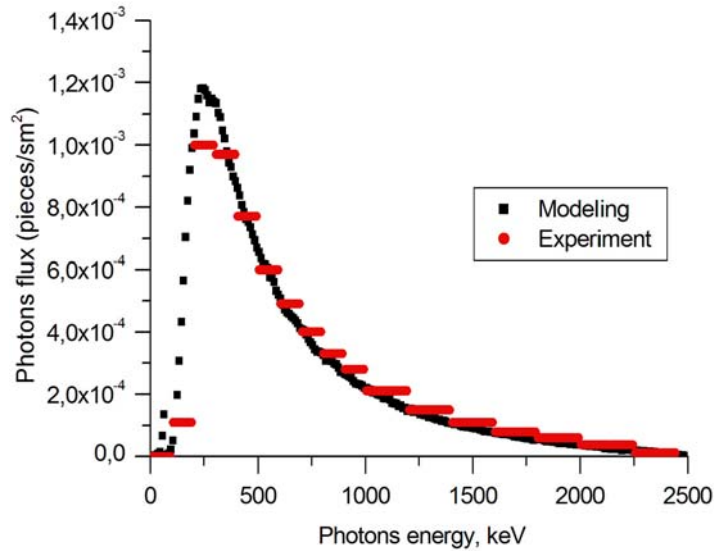


Fig. 12: Bremsstrahlung modeling results

A similar distribution was obtained using experimental-computing method, which was carried out in the Research Institute of Scientific Instruments (<http://niipriborov.ru/> RISI). This technique involves experimental determination of electrons spectrum and the calculating of the bremsstrahlung spectrum using software complex «BREMS» elaborated by RISI.

The results of comparison are presented in fig. 12. The energy distributions of the photons are shown in the figure. The x-axis represents the energy of photons. The ordinate represents the photon flux density ($1/\text{cm}^2$). The results are presented per one incident electron.

The results of the comparative analysis have shown satisfactory agreement between modeling and experimental data.

7 CONCLUSIONS

Experimental studies of the bremsstrahlung generated by the accelerator electron beam are extremely expensive. At the same time, the research of the radiation parameters is important for many practical applications. Mathematical modeling of the bremsstrahlung generation is an effective supplement and, in some cases, alternative to experimental studying.

A detailed analysis of the bremsstrahlung parameters is possible only with modern high-performance computing systems including heterogeneous (hybrid) supercomputers.

Presented paper continues investigations on simulating the experimental research of the electron accelerator bremsstrahlung². The paper presents the results of a numerical research of RIUS-5 bremsstrahlung. Comparison of energy distributions of photons produced by experiment and obtained by computing shows qualitative and quantitative agreement within the measurement error.

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