Calculation of $\gamma$–quanta passage through substance with Monte-Carlo method at x-ray images simulation

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Abstract. Software, developed in RFNC–VNIIEF for x-ray images simulation using Monte-Carlo method is described. The software is a part of an x-ray method used for investigation of an equation of state (in this case hydrogen isotopes: protium and deuterium) in a megabar pressure range. Interaction of $\gamma$–quanta with a substance is considered. Effect of a scattered radiation on the x-ray images formation is estimated.

Introduction
During several last years RFNC–VNIIEF carries out the works on experimental investigation of the equation of states (EOS) of the hydrogen isotopes in the low temperatures and ultra-high pressures range. During these works we solved several tasks. A compression device, based on a magneto-cumulative generator [1] was designed and developed. “Cold” pressures of 5 and more megabars could be reached in this device. Its parameters were optimized in order to decrease as much as possible pressure gradients in the compression chamber in the moments, when the pressures, required for the experiments, [2] are reached. Pulsed radiography method of a density measurement of compressed substances, based on a betatron [3], was developed. The software for the x-ray images calculation with the Monte-Carlo method is a part of this method. There are several reasons to use the software of this type. The compression experiments are explosive. A high-explosive charge of about 16 kilograms is used in each experiment. So, it is necessary to protect the equipment with heavy protection elements. The protection elements and a research object are the sources of a scattered x-ray radiation that worsens the x-ray image of the research object. This leads to increase of measurement errors. That is why the task of the radiation yield channel optimization in order to decrease the value of the scattered radiation is urgent now. The x-ray images calculation with the Monte-Carlo method helps to reveal the elements of the radiation output channels that make the highest contribution to the scattered radiation.

1. Software capabilities
1.1. General characteristic of the software. Using the Monte-Carlo method the software solves the equation of the $\gamma$–quanta transfer for the one-dimensional systems, simple two-dimensional and three-dimensional systems and their combinations. Presentation of interaction cross section has a tabular form with several types of interpolations in order to obtain continuous energy dependence on the cross section. A database for the cross sections of the $\gamma$–quanta interactions with the substance was formed on basis of
Storm-Israel data [4]. The database for the $\gamma$–quanta formation cross sections was formed on basis of several sources - from libraries ENDL-82 and ENDF/B-6, JENDL-32 [5, 6].

Possibilities of the systems geometry setup are limited by simple spherical, elliptical, cylindrical, plane and conical blocks and their 3D combinations. This makes it possible to solve complicated and substantial 3D tasks. Simplicity of the initial data setup and general high productivity of the software operation are provided. The database for the $\gamma$–quanta interaction cross sections includes the data of the works [4, 7]. Functions of a non-coherent scattering are taken from the works [8]. Form-factors of a coherent scattering are taken from the work [9].

The software calculates the following values: fluxes and currents of the particles on the system surface, numbers of reactions in the areas, heating of an area and other characteristics as a function of energy, time, spatial coordinates, angular data and other parameters.

Points in space, areas and surfaces of the considered system could be the sources of the $\gamma$–quanta. There are several types of selection of the initial direction and energy of the $\gamma$–quanta. The source of the $\gamma$–quanta could be taken from an earlier created file.

Two schemes of a calculation efficiency increase are realized in the software: (1) multiplication and a reel on the surfaces of the system geometry; (2) one of the methods of a local evaluation – a “method of trial particles” to estimate the particles fluxes, coming to the setup goal (point).

1.2. Realization of the processes of the $\gamma$–quanta interaction with the substance

1.2.1. Non-coherent scattering. A differential cross section of the non-coherent scattering of the $\gamma$–quanta on an electron is described with a formula:

$$
\frac{d\sigma_{inc}}{d\Omega} = \frac{1}{2} \sqrt{\frac{1 + \cos^2 \theta}{(1 + \varepsilon(1 - \cos \theta))^2}} \left\{ 1 + \left( \frac{\varepsilon^2(1 + \cos \theta)^2}{(1 + \cos^2 \theta)(1 + \varepsilon(1 - \cos \theta))} \right) S(\vec{q}, Z) \right\}^{2}
$$  

(1)

where $d\Omega$ - element of a solid angle, $\theta$ - scattering angle, $r_0$ - classical electron radius, $\varepsilon$ - quantum energy in $mc^2$ units. Without multiplication on a function $S(\vec{q}, Z)$ the formula (1) represents a differential cross section of the non-coherent scattering of the $\gamma$–quanta on a free electron. At small energy transfers we take into account the electrons connectedness in an atom by multiplication of Klein-Nishina cross section on the function $S(\vec{q}, Z)$, where $\vec{q}$ - transferable pulse, $Z$ – atomic number of the substance. The values of the function $S(\vec{q}, Z)$, calculated in a model of the Hartry-Fock atom, are taken from [8].

Initial grid of the function $S(\vec{q}, Z)$ argument is setup in a variable $x = \sin(\theta/2)/\lambda$, $\lambda$ - wavelength in units $cm$ (1 $cm = 1.00202 \times 10^{-8}$ cm, 1/$\lambda = E/12400$, $E$ - in electron-volts). Initial interpolation is linear on $x$, and linear for the function $1/[1 + S(x)/Z]$. On the stage of the cross sections files preparation for the reactions simulation a transition to the variable $\tilde{x} = E \cdot \sin(\theta/2)$ is carried out, and the nodes are recalculated on a formula $\tilde{x}_i = x_i \cdot 12400$, and from the values of the function $S(\vec{q}, Z)$ they are recalculated to the function $\sqrt{\frac{S(x)/Z}{1 - S(x)/Z}}$ with the linear interpolation between the nodes.

1.2.2. Coherent scattering. Differential cross section of the coherent scattering is setup with the formula

$$
\frac{d\sigma_{coh}}{d\Omega} = \frac{1}{2} r_0^2 (1 + \cos^2 \theta)|F(\vec{q}, Z)|^2 .
$$  

(2)

Here $F(\vec{q}, Z)$ is a form-factor that presents a probability of the fact that a pulse $\vec{q}$ will be transferred to $Z$ atoms electrons without any absorption of the energy. The values of the form-factor that are calculated in the Hartry-Fock model are taken from [9].
1.2.3. Photo absorption. Cross sections of the photo absorption are taken from the work by Veigele [7]. These sections were obtained with analysis of a large number of experimental data and they are the most reliable in the field of $\gamma -$quanta energies near the K-shell level and below it. Since Veigele work the cross sections are presented up to the energy of 1 MeV only, for higher energies we used the data of Storm-Israel [4].

1.2.4. Pairs formation. A process of an electron-positron pair formation takes place at the $\gamma -$quantum energy higher than $2 \cdot mc^2$, where $mc^2 = 0.5110034$ MeV. The cross sections of the pairs formation and also the cross sections of the energy absorption were taken from [4]. For the description of the pair absorption process the following model was accepted. Electron of pair is absorbed in a point of the $\gamma -$quantum collision and the positron annihilates forming two $\gamma -$quanta. The first $\gamma -$quantum isotropically emitted with the energy $E_{pair} = 0.5110034$ MeV and the second quantum – in opposite direction with the energy $E_{pair}$.

1.2.5. Total cross section. A total cross section of the $\gamma -$radiation interaction with the substance is determined as a sum of cross sections of the above mentioned reactions (see, for example, Figure 1 for $^{74}$W): $\sigma_{tot} = \sigma_{inc} + \sigma_{coh} + \sigma_{phot} + \sigma_{pair}$ [barn/atom].

1.3. Implementation
Nowadays the program package that allows calculating the x-ray images of the device for the isentropic compression of the hydrogen isotopes using the Monte-Carlo method consists of 17000 lines of the code. A calculation rate is $\sim 70000$ trajectories per second (CPU Pentium 4, 3.6 GHz). One needs 140 Mbytes of RAM to calculate the x-ray image of 1000*1000 pixels size.

2. Calculation results of x-ray images
Use of calculation results of the “H$_2$” code [2] as the initial data and analysis of the results of the software for the x-ray images calculation caused some troubles. Formats of the input files of the x-ray images calculation program did not match the output files of the “H$_2$”, and the formats of the output files of the calculation section did not match the input of the visualization software. Besides, there were significant difference in internal presentation of the physical parameters of the studied object and recorder (geometry, sizes and composition of materials) in both programs. Also there were some limitations for names and location of the files of the task for the x-ray
images calculation. All these problems were solved by writing add-in programs. Firstly, we automated formation of the files set, that are the input files of the x-ray images calculation software, from the output data of the “H₂” code. Secondly, the files containing the calculation results on the x-ray images software calculation are converted for their further visualization.

The program has a feature of the x-ray radiation source parameters setup, and also features of visualization of the direct x-ray radiation, sum of direct and scattered radiation from different elements of the radiation output channel.

The geometry of the experiment is taken into account in the calculations of the x-ray images in the radiographic studies. After the experiment the alignment errors are also considered. Fig. 2 presents calculated x-ray diagram of the device at some displacement of the research object and the recorder relatively to the x-ray radiation beam. The calculated distribution of the scattered radiation is presented in Fig. 3.

The value of the scattered radiation does not exceed 6% of the value of the direct radiation. An element of the recorder protection (a combination of steel and aluminum plates) is the source of the main part of the scattered radiation.

For comparison Fig. 4 presents experimental x-ray image of the device obtained in the experiment on isentropic compression of solid D₂. In this moment the pressure in the compression chamber was \( \sim 3 \) Mbar.

One can see that the calculated and experimental x-ray images have qualitative similarity.

**Conclusion**

The paper presents the calculation results of the x-ray image that was obtained in one of the experiments on isentropic compression, using the software for x-ray images calculation, which solve the equations of the radiation transfer using the Monte-Carlo method. The calculated and experimental x-ray images are presented. The scattered radiation composes the small portion of the direct radiation (less than 6%). Nevertheless, to increase the contrast of the shot and measurement precision it is desirable to decrease the scattering. Use of the software for the x-ray images calculation makes it possible to reveal the elements of the radiation output channel that bring the most contribution into the scattered radiation.

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Figure 4. Experimental x-ray image.

References
[1] A.I. Pavlovskii et al. In book: Ultrahigh Magnetic Fields/Ed. V.M. Titov, G.A. Shvetsov. M. Nauka, 1984, p. 19.
[2] G.V. Boriskov et al. In book: VIII Hariton’s Readings on Problems of High Energy Physics. Sarov, 2006, p. 509 and p. 516.
[3] A.I. Bykov, N.I. Egorov, Yu.P. Kuropatkin, N.B. Lukianov, V.D. Mironenko, V.N. Pavlov, “Use of radiography to study EOS of condensed hydrogen isotopes within megabar pressure range”. Book of Abstracts, Nov. 5-10, 2006, Santa Fe, New Mexico, USA, p. 34
[4] E. Storm, H.I. Israel “Photon Cross Section from 1 kev to 100 mev for Elements Z = 1 to Z = 100”, Nucl. Data Tables, A7, 565-618, (1970).
[5] WINENDF, version from October 2002, IAEA. Release 8 library ENDF/B-6.
[6] ENDF-102 “Data Formats and Procedures for the Evaluated Nuclear data File ENDF/B-6”, V.McLane (BNL USA), September 1997.
[7] W.J. Veigele “Photon Cross Section from 0.1 kev to 1 mev for Elements Z=1 to Z=94”, Atomic Data Tables, 5, 51-111, (1973).
[8] D.T. Cromer, J.B. Mann “Compton Scattering Factors for Spherically Symmetric Free Atoms”, J.Chem.Phys., 47, 1892-1893, 1967;
Cromer D.T., Mann J.B. “Compton Scattering Factors for Aspherical Free Atoms”, J.Chem.Phys., 50, 4857-4859, (1969).
[9] H.P. Hanson, F. Herman, J.D. Lea, S. Skillman “HFS Atomic Scattering Factors”, Acta Cryst., 17, 1040-1044, (1964).