UDC 53.088.22:539.1.074.6:006.915+621.397.46 DOI:

Estimating the influence of various factors on the uncertainty of light collection simulation in scintillators

V. Tarasov, B. Grynyov, N. Gurdzhian, O. Zelenskaya, L. Mitcay,
L. Vaschenko

Institute of Scintillation Materials, National Academy of Sciences of Ukraine, Nauki Ave., 60, 61072, Kharkiv, Ukraine
nana.mneyan@gmail.com

Abstract

The paper is dedicated to the evaluation of statistical uncertainty of simulating the process of light transfer in NaI (Tl) and BGO scintillators by Monte Carlo method. The DETECT2000 program with a unified surface model was used. The process of light transfer (“fate”) by light photons was traced from the moment of appearance in the scintillator to the moment of passing through its exit window. The light collection coefficient was determined as the ratio of the number of photons that passed through the exit window to a given number of emitted photons. Different values of the number of emitted photons, optical transparency coefficients and fractions of the surface diffuse reflection were set. Multiple repetitions of the simulation process for a different set of properties made it possible to evaluate the precision and type A uncertainty of simulating the light collection coefficient for all possible options. It is shown that the uncertainty decreases when the statistics of the emitted photons is increased, and increases when the transparency and diffuse reflection fraction are decreased.

Keywords: scintillator; light collection; Monte Carlo simulation method; DETECT2000 program; unified surface model; precision; type A uncertainty.

Received: 26.01.2022 Edited: 23.06.2022 Approved for publication: 29.06.2022

1. Introduction

Evaluation of light collection in scintillators is an important final step when characterizing scintillators in terms of absolute light yield. An attempt was made to experimentally determine the value of a light collection coefficient using a light-measuring ball [1]. However, the laboriousness, the uncertainty in the magnitude of the scintillator transparency coefficient included in the calculations and the need to take into account a number of photometric quantities, make its application problematic. Subsequently, the evaluation of light collection was carried out by calculation. Initially, analytical methods were used taking into account various influencing factors [2]. Then, computational numerical methods for simulating various processes, including light collection, became widespread. Most often, to solve the problems of radiation transfer, both ionizing and light, a probabilistic numerical method, which is Monte Carlo method (MCM), was used [3, 4].

Institute of Scintillation Materials of the National Academy of Sciences of Ukraine also performs work on simulating the process of light collection in scintillators using MCM [5, 6]. However, the uncertainty of light collection simulation by MCM has not yet been evaluated and has not yet been described in the literature. Therefore, it was of great interest to evaluate statistical uncertainty of simulating the light collection coefficient by MCM. In this paper, these estimates were made for cylindrical single crystals based on NaI(Tl) and BGO. To implement the MCM, the DETECT2000 program was used [7].

The purpose of the paper: evaluation of statistical components of uncertainty – precision and type A uncertainty – when simulating a light collection coefficient by MCM in NaI(Tl) and BGO scintillators taking into account various influencing factors.

2. Description of the DETECT2000 program

DETECT2000 is based on its original version DETECT [8].

In these programs, when simulating the passage of light in scintillators, individual scintillation photons are generated in a given quantity in a certain place. A random direction of each photon is set and its “fate” is played (absorption, exit from the medium or registration by a photodetector) when it moves through different components of the optical system. Any element of the system can be specified as a volume bounded by flat, cylindrical or other surfaces.

Each optical element is characterized by a refractive index, volumetric absorption and light scattering, which are played out using the length of a free path of the photon in a given medium.

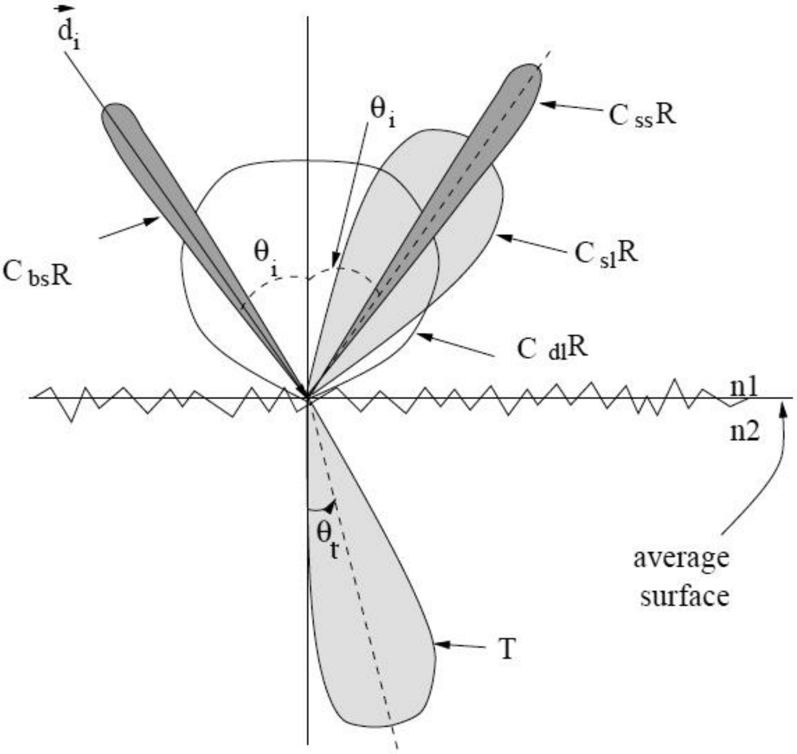

Fig. 1. Intensity of the reflected and refracted rays in the unified model

Reflection or refraction is played out on the surfaces of optical elements for a photon using the refractive indices for the adjacent media, as well as well-known Snell's laws and Fresnel's formulas [9].

For each case of reflection, refraction or scattering of a photon, the program determines a new direction of movement, identifies the component, in which it is moving, and calculates the next intersection with the surface.

The photon moves in the optical system until it is absorbed or registered, or leaves the system.

In addition to optical characteristics of the medium, the type of surface and the presence of an external reflector strongly influence the “fate” of a photon. The DETECT2000 software provides various options for surface models: polished, rough, painted, metal (mirror). The program also uses a unified surface model [10], which gives a better approximation to real surfaces. It represents the surface in the form of microfaces and makes it possible to set different ratios of the reflected light components using appropriate weighting factors.

Fig. 1 shows the reflected and refracted components of the surface radiation in the unified model and the weighting factors that determine their probability.

Fig. 1 shows the following symbols:

d_i is the direction of an incident ray;

θ_i is the angle of an incident ray with respect to the average surface normal;

θ_t is the angle of refraction with respect to the average normal;

T is the distribution of refracted rays;

n1 is the refractive index of the medium from which the beam falls;

n2 is the refractive index of the medium into which the beam penetrates;

C_{bs} is the coefficient that determines the probability of back reflection;

C_{ss} is the coefficient that determines the probability of specular reflection relative to the average surface normal;

C_{sl} is the coefficient that determines the probability of specular reflection relative to the microface normal;

C_{dl} is the coefficient that determines the probability of Lambert diffuse reflection.

The sum of the four coefficients must remain equal to 1.

In this paper, we used a unified model, in which back scattering and specular reflection from microfaces were not taken into account, i.e. the weighting coefficients C_{bs} and C_{sl} were set equal to zero. Only the fractions of specular and diffuse reflection from the surface, C_{ss} and C_{dl} respectively, varied. This approach is close to the “effective specularity” model, which was used to calculate the light collection coefficients for various versions of scintillators [11]. Preliminary calculations of the light collection coefficients carried out for such objects using the DETECT2000 program with a unified model showed good agreement with the results [11].

3. Simulation of Light Collection Coefficients

During the simulation, a different number of emitted light photons N_{emit} was sequentially set for each

Table 1

Specified influence coefficients

Scintillator	D, mm	nD	N_{emit}, photons	n	k, cm^{-1}	k_{ref}	Effective surface specularity, %
NaI(Tl)	40	1.85	1000–100000	7	0.005, 0.01	0.95, 0.9	40
BGO	40	2.15	1000–100000	7	0.02, 0.2	0.95, 0.9	40

scintillator. Further, influencing factors were added, such as the refractive index nD, the transparency coefficient k (in cm^{-1}) and the external reflection coefficient k_{ref}. The "fate" of the photon was traced until it passed through the exit window of the scintillator. For each dataset, the simulation process was repeated n times. The range of specified values for N_{emit} and influence coefficients is shown in Table 1.

Based on the simulation results, the number of photons passing through the scintillator exit window N_{out} was recorded and the values of the coefficients of light collection τ were calculated using the formula:

$$\tau = \frac{N_{out}}{N_{emit}}. \quad (1)$$

Then, for each set of repeatedly obtained n values of τ, statistical characteristics of the simulation uncertainty τ by MCM were estimated: the precision $S_r(\tau)$ [12] and type A uncertainty $u_A(\overline{\tau})$ [13].

4. Results and Discussion

The scattering of the values of the light collection coefficient τ in NaI(Tl) and BGO scintillators obtained with repeated variants of simulation with specified values of the influence coefficients is shown in Fig. 2.

From Fig. 2 one can see that when N_{emit} statistically increases from 1000 to 100000, the repeatability of the simulation results τ for both NaI(Tl) and BGO significantly improves. This is due to a decrease in the scattering of mean paths and photon loss probabilities from simulation to simulation with an increase in the statistics of given emitted photons.

The results of evaluating the precision indicators $S_r(\tau)$ of simulating the coefficient τ by MCM under given conditions are shown in Fig. 3.

As follows from Fig. 3, the simulation precision τ dramatically improves (the value of $S_r(\tau)$ decreases) as the specified value of N_{emit} increases from 1000 to 10000 and improves more smoothly when N_{emit} > 10000 (or is proportional to $1/\sqrt{n}$). This is associated with the improved repeatability of results (see Fig. 2).

Simulation precision decreases with degradation of the scintillator transparency and the diffuse reflection of its surface. In this case, the average value of the simulated coefficient τ decreases, which leads to an increase of the calculated value of $S_r(\tau)$. For a scintillator based on NaI(Tl), a twofold degradation in the specified transparency leads to a 10% decrease of the simulated coefficient value and decreases its precision by 1.5–2 times when

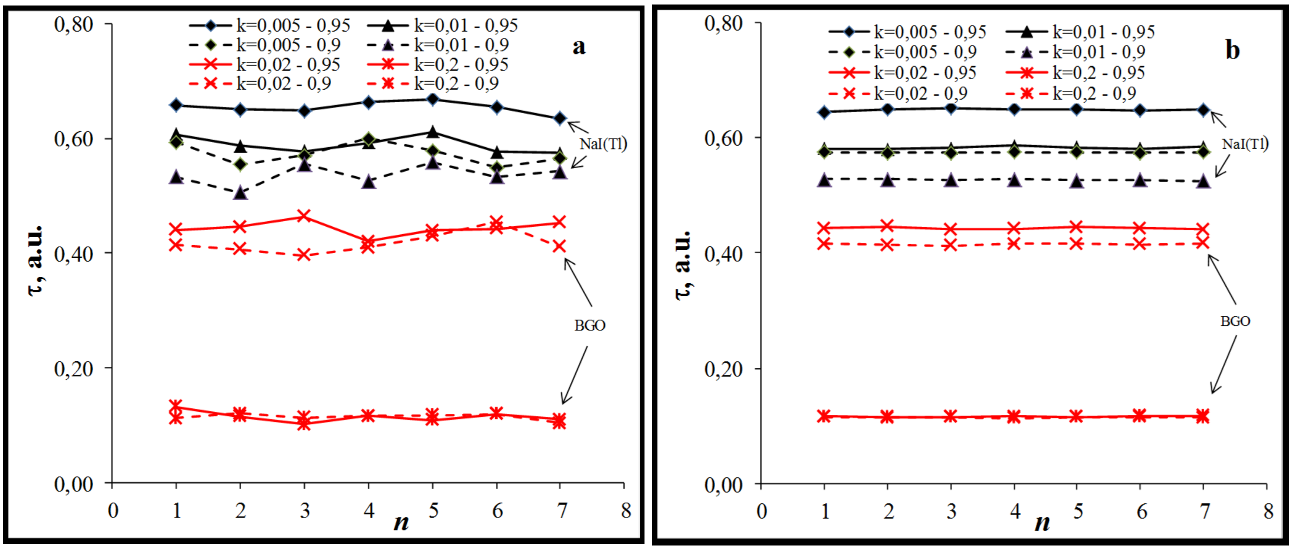

Fig. 2. Light collection coefficient τ simulated by MCM under given conditions and with different numbers of emitted photons: a) N_{emit} = 1000, b) N_{emit} = 100000

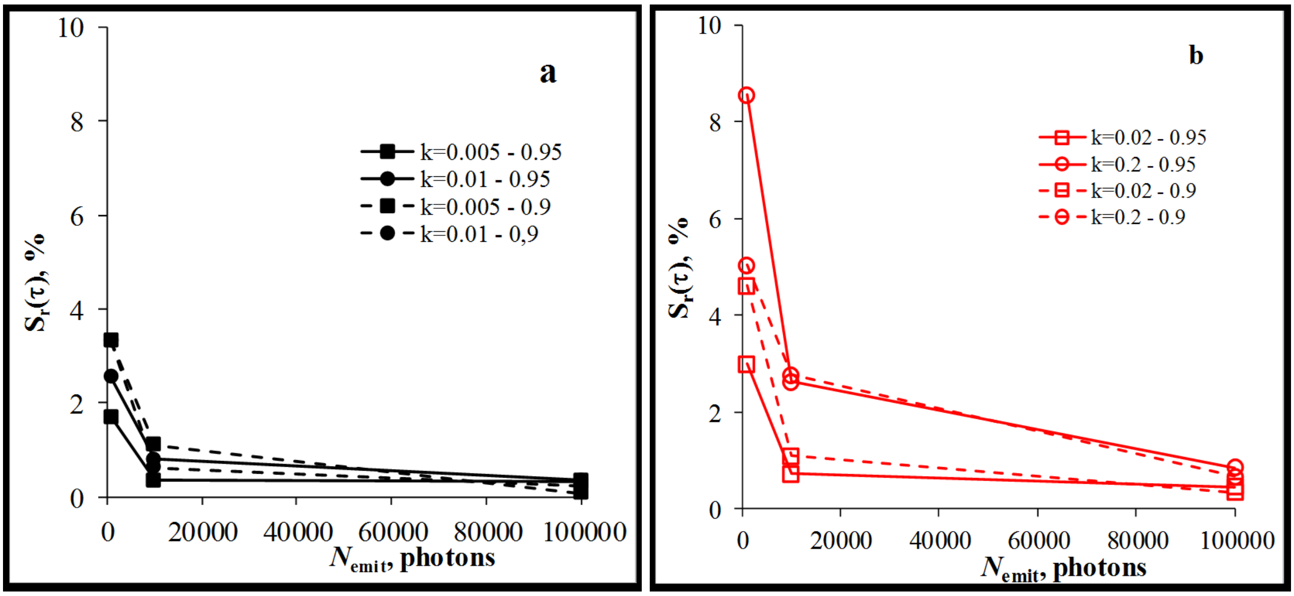

Fig. 3. Precision indicators Sr(τ) of simulating the coefficient τ by MCM in scintillators: a) NaI(Tl), b) BGO

$1000 < N_{emit} < 10000$. With a further increase of N_{emit}, the precision changes only slightly. For a scintillator based on BGO, the simulation of light collection, with the transparency reduced by 10 times, leads to a decrease of the simulated coefficient value τ by almost 4 times, which degradates its precision by 2.8–3.6 times, when $1000 < N_{emit} < 10000$, and by 2 times when $N_{emit} > 10000$. At simultaneous setting of degraded values of the transparency coefficients and surface diffuse reflection, the value of the simulation precision τ changes additionally. The nature of the change is also shown in Fig. 3.

Comparative results of evaluating the precision $S_r(\tau)$ and type A uncertainty $u_A(\overline{\tau})$ of simulating the coefficient τ by MCM in scintillators at different transparency values for $N_{emit} = 1000$ and $k_{ref} = 0.95$ are shown in Fig. 4.

The results of the estimation of statistical uncertainty of simulating the coefficient τ by MCM in scintillators for all considered options are given in Table 2.

5. Conclusion

The use of the DETECT2000 program with a unified surface model makes it possible to obtain the values of the light collection coefficients close to the values available in the literature for similar scintillators and light collection conditions. This allowed to apply this variant of light collection simulation to evaluate the indicators of statistical uncertainty for light collection simulation by MCM in NaI(Tl) and BGO scintillators with various options for light collection conditions.

It is shown that the precision and type A uncertainty of light collection simulation by MCM

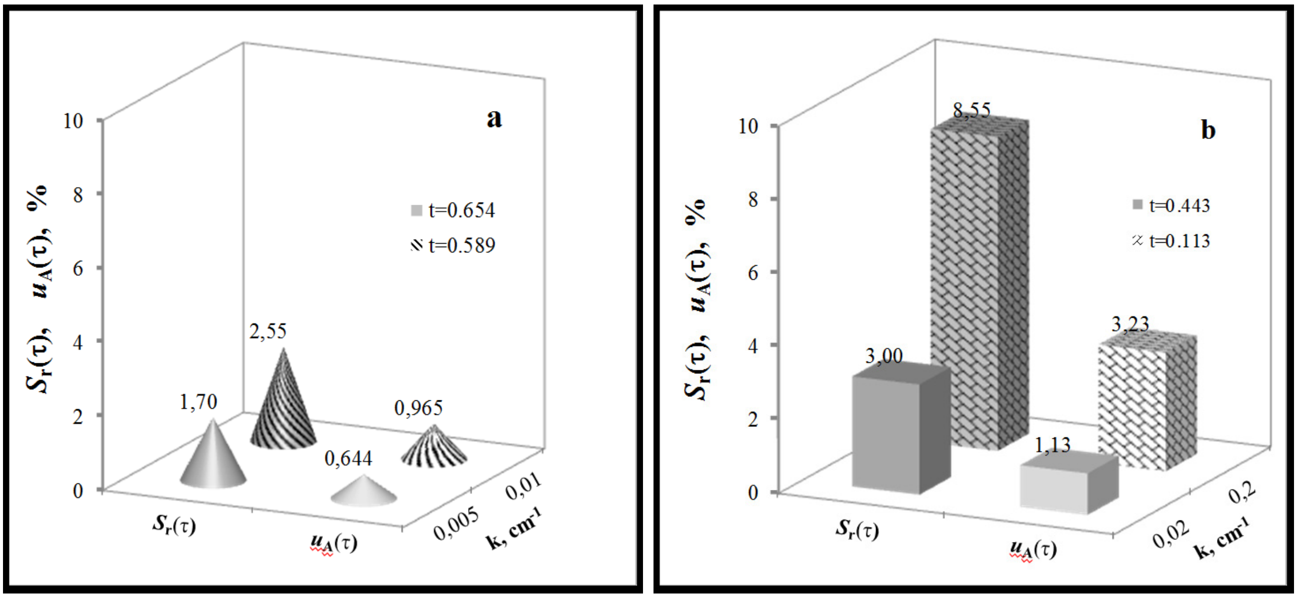

Fig. 4. Comparison of estimates of statistical uncertainty of simulating the coefficient τ by MCM in scintillators: a) NaI(Tl), b) BGO

Table 2

Indicators of statistical uncertainty of simulating the coefficient by MCM in scintillators

Scintil-lator	Size, mm	nD	k, cm^{-1}	k_{ref1}	N_{emit}, photons	$\bar{\tau}$	$S_r(\tau)$, %	$u_A(\bar{\tau})$, %	k_{ref2}	$\bar{\tau}$	$S_r(\tau)$, %	$u_A(\bar{\tau})$, %
NaI(Tl)	∅40×40	1.85	0.005	0.95	1000	0.654	1.70	0.644	0.9	0.573	3.316	1.253
					10000	0.650	0.35	0.132		0.573	1.105	0.418
					100000	0.649	0.33	0.124		0.574	0.078	0.029
			0.01	0.95	1000	0.589	2.55	0.965	0.9	0.536	3.318	1.254
					10000	0.583	0.79	0.300		0.526	0.619	0.234
					100000	0.582	0.35	0.133		0.527	0.233	0.088
BGO	∅40×40	2.15	0.020	0.95	1000	0.443	3.00	1.133	0.9	0.417	4.61	1.744
					10000	0.442	0.72	0.271		0.418	1.10	0.417
					100000	0.443	0.45	0.171		0.415	0.34	0.129
			0.2	0.95	1000	0.114	8.55	3.230	0.9	0.114	5.04	1.907
					10000	0.115	2.62	0.989		0.114	2.77	1.049
					100000	0.116	0.85	0.321		0.115	0.67	0.253

improve by 5–10 times when the statistics of given emitted photons is increased by 100 times, which is associated with a decrease in the scattering of mean paths and photon loss probabilities from simulation to simulation.

It was found that the estimation of statistical characteristics of simulation uncertainty depends on the given optical and surface properties of the scintillator – the transparency and fraction of the surface diffuse reflection. Degradation of these characteristics leads to a decrease of the average value of the simulated light collection coefficient and increase of the calculated values of the estimated characteristics.

Оцінювання впливу різних факторів на невизначеність моделювання світлозбирання у сцинтиляторах

В.О. Тарасов, Б.В. Гриньов, Н.Р. Гурджян, О.В. Зеленська, Л.Й. Міцай, Л.Л. Ващенко

Інститут сцинтиляційних матеріалів НАН України, пр. Науки, 60, 61072, Харків, Україна
nana.mneyan@gmail.com

Анотація

Роботу присвячено оцінюванню статистичної невизначеності моделювання за методом Монте-Карло процесу перенесення світла у сцинтиляторах NaI(Tl) та BGO з урахуванням впливу заданих властивостей. Застосовувалася програма DETECT2000 з використанням уніфікованої моделі поверхні "unified", яка дає найкраще наближення до реальних поверхонь. Вона представляє поверхню у вигляді мікрограней та створює можливість задавати різні співвідношення компонентів відбитого світла за допомогою відповідних вагових коефіцієнтів. Модель дозволяє задавати ефективну дзеркальність поверхні та дає гарний збіг розрахункових значень коефіцієнтів світлозбирання з літературними даними. Під час моделювання процесу перенесення світла для кожного світлового фотона із заданої кількості простежувалася їхня "доля" від моменту появи у сцинтиляторі до моменту проходження через його вихідне вікно. Коефіцієнт світлозбирання визначався як відношення числа фотонів, що пройшли через вихідне вікно, до заданого числа фотонів, що випромінюються. Задавалися різні значення: числа фотонів, що випромінюються, коефіцієнтів оптичної прозорості та частки дифузного відбиття поверхні. Багаторазове повторення процесу моделювання для різноманітного набору заданих властивостей дозволило оцінити прецизійність та невизначеність, що розрахована за типом А, для моделювання коефіцієнта світлозбирання різних можливих варіантів. Знайдено, що показники прецизійності та невизначеності за типом А моделювання зменшуються зі збільшенням статистики фотонів, що випромінюються, та збільшуються при зменшенні прозорості та частки дифузного відбиття.

Ключові слова: сцинтилятор; світлозбирання; моделювання за методом Монте-Карло; програма DETECT2000; уніфікована модель поверхні "unified"; прецизійність; невизначеність за типом А.

Оценивание влияния различных факторов на неопределенность моделирования светособирания в сцинтилляторах

В.А. Тарасов, Б.В. Гринев, Н.Р. Гурджян, О.В. Зеленская, Л.И. Мицай, Л.Л. Ващенко

Институт сцинтилляционных материалов НАН Украины, пр. Науки, 60, 61072, Харьков, Украина
nana.mneyan@gmail.com

Аннотация

Работа посвящена оценке статистической неопределенности моделирования методом Монте-Карло процесса переноса света в сцинтилляторах NaI(Tl) и BGO. Использовалась программа DETECT2000 с применением унифицированной модели поверхности "unified". Прослеживался процесс переноса света ("судьба") световыми фотонами от момента возникновения в сцинтилляторе до момента прохождения через его выходное окно. Коэффициент светособирания определялся как отношение числа фотонов, прошедших через выходное окно, к заданному числу эмитируемых фотонов. Задавались различные значения числа эмитируемых фотонов, коэффициентов оптической прозрачности и доли диффузного отражения поверхности. Многократное повторение процесса моделирования позволило оценить прецизионность и неопределенность по типу А моделирования светособирания для различных наборов свойств. Показано уменьшение неопределенности при повышении статистики эмитируемых фотонов и увеличение – при понижении прозрачности и доли диффузного отражения.

Ключевые слова: сцинтиллятор; светособирание; моделирование методом Монте-Карло; программа DETECT2000; унифицированная модель поверхности "unified"; прецизионность; неопределенность по типу А.

References

1. Toporets A.S. Optika sherokhovatoy poverkhnosti [Rough surface optics]. Leningrad, Mashinostroyenie Publ., 1988. 191 p. (in Russian).
2. Tsirlin Yu.A. Svetosobiraniye v stsintillyatsionnykh schetchikakh [Light collection in scintillation counters]. Moscow, Atomizdat Publ., 1975. 264 p. (in Russian).
3. Derenso S.E., Rilers J.K. Monte Carlo calculations of the optical coupling between bismuth germanate crystals and photomultiplier tubes. *IEEE Trans. Nucl. Sci.*, 1982, NS-29, no. 1, pp. 191–194.
4. Carrier C., Lecomte R. Theoretical modeling of light transport in rectangular parallelepipedic scintillators. *Nucl. Instr. Meth.*, 1990, A292, no. 3, pp. 685–692.
5. Tarasov V. et al. Light collection simulation in the scintillation detectors of short-range radiation. *Functional materials*, 2010, vol. 17, no. 1, pp. 100–106.
6. Kilimchuk I.V., Tarasov V.A., Vlasova I.D. Study of light collection as a function of scintillator surface roughness. *Radiation Measurements*, 2010, vol. 45, issues 3–6, pp. 383–385.
7. Cayouette F., Moisan C., Zhang N., Thompson C.J. Monte Carlo modeling of scintillator crystal performance for stratified PET detectors with DETECT2000. *IEEE Trans. Nucl. Sci.*, 2002, vol. 49, no. 3, pp. 624–628. doi:10.1109/TNS.2002.1039539
8. Knoll G.F., Knoll T.F., Henderson T.M. Light collection in scintillation detector composites for neutron detection. *IEEE Trans. Nucl. Sci.*, 1988, vol. 35, no. 1, pp. 872–879.
9. Butikov Ye.I. Optika: Uchebnoye posobiye dlya vuzov [Optics: Textbook for universities]. N.I. Kaliteevsky (Ed.). Moscow, 1986. 512 p. (in Russian).
10. Levin A., Moisan C. A More Physical Approach to Model the Surface Treatment of Scintillation Counters and its Implementation into DETECT. TRI-PP-96-64, Oct 96. Presented to the 1996 IEEE Nuclear Science Symposium of Anaheim. Available at: https://inis.iaea.org/collection/NCLCollectionStore/_Public/29/030/29030591.pdf
11. Globus M.Ye., Grinov B.V. Neorganicheskiye stsintillyatory. Novyye i traditsionnyye materialy [Inorganic scintillators. New and traditional materials]. Kharkov, Akta Publ., 2001. 408 p. (in Russian).
12. State standard of Ukraine ISO 5725-2:2005. Accuracy (correctness and precision) of measurement methods and results. Part 2 (GOST ISO 5725-2-2003, IDT). Kyiv, 2006. 50 p. (in Ukrainian).
13. State standard of Ukraine RMG 43:2006. Metrology. Application of “Expression guide measurement uncertainty” (RMG 43-2001, IDT). Kyiv, 2006. 18 p. (in Ukrainian).