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Accounting for effective specularity in the DETECT2000 program when determining light collection coefficients using NaI(Tl) and BGO scintillators as an example

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The paper compares the light collection coefficients obtained for cylindrical NaI(Tl) and BGO scintillators in the DETECT2000 program and in the program characterizing the surface by its effective specularity. The results of the latter agree well with experiment. The best approximation of the results was obtained in the DETECT2000 program model of the UNIFIED optical surface, in which the roughness is specified by the "fraction of specularly reflected rays" parameter. Using this description of the surface in the DETECT2000 program, the dependence of the light collection coefficients on the contribution of specular reflection, optical absorption, reflection coefficient of the external reflector and scintillator size were studied. It is shown that the light collection coefficient of scintillators decreases with increasing effective specularity above 40 %, namely, by 4–8 % for NaI(Tl) and by 12–14 % for BGO, with different model parameters. This is due to an increase in the fraction of trapped light in the scintillator. It is also shown that the deterioration of the light collection coefficient is largely due to a decrease in optical absorption and, to a lesser extent, by a decrease in the reflectance of the external reflector and an increase in the scintillator size.

Keywords: scintillator, Monte Carlo method, DETECT2000 program, surface model UNIFIED, effective specularity, light collection coefficient.

Облік ефективної дзеркальності в програмі DETECT2000 при визначенні коефіцієнтів збору світла на прикладі сцинтиляторів NaI(Tl) і BGO. *В.А.Тарасов, Л.І.Міцай, О.В.Зеленська, Б.В.Гриньов, Н.Р.Гурджян, Л.Л.Ващенко*

У роботі проведено порівняння коефіцієнтів світлозбирання, отриманих для циліндричних сцинтиляторів NaI(Tl) та BGO у програмі DETECT2000 та у програмі, що характеризує поверхню її ефективною дзеркальністю. Результати останньої добре узгоджуються з експериментом. Найкраще наближення результатів отримано при використанні в програмі DETECT2000 оптичної поверхні зі змінною шорсткістю (тип UNIFIED). З використанням даного опису поверхні у програмі DETECT2000 досліджувалась залежність коефіцієнтів світлозбирання від вкладу дзеркального відбивання, оптичного поглинання, коефіцієнта відбивання зовнішнього відбивача та розміру сцинтилятора. Показано, що коефіцієнт світлозбирання сцинтиляторів зменшується при зростанні ефективної дзеркальності вище 40 %, а саме на 4–8 % для NaI(Tl) та на 12–14 % для BGO, за різних параметрів моделі. Це пов'язано зі збільшенням частки захопленого світла в сцинтиляторі. Також показано, що погіршенню коефіцієнта світлозбирання більшою мірою сприяє збільшення коефіцієнта оптичного поглинання і, меншою мірою, зменшення коефіцієнта відбивання зовнішнього відбивача та збільшення розмірів сцинтилятора.

1. Introduction

The light collection coefficient is an important parameter of scintillators for characterizing their absolute light output, when choosing options for processing and packaging of scintillators and for optimizing detector designs. The experimental determination of the light collection coefficient is laborious and introduces a large uncertainty into the result [1]. Computational methods for estimating light collection are more common. Along with analytical methods [2], various numerical methods are used, including the Monte Carlo method (MCM) [3, 4].

The Institute for Scintillation Materials National Academy of Sciences of Ukraine also carries out work on modeling the light collection process in scintillators [5–7]. At one time, a significant amount of data on the light collection coefficients for scintillators on a base of NaI(Tl), CsI(Tl), BGO, CWO a wide range of sizes was obtained by M.E.Globus using the concept of effective specularity (ES) of the rough surface [8, 9]. These data were confirmed by a large number of measurements of parameters such as intrinsic resolution and relative light output of scintillation detectors. The data on light collection coefficients have been successfully used to solve problems in scintillation technology [10, 11].

This fruitful approach can be applied in determining light collection coefficients for other scintillation materials. Unfortunately, the software implementation of modeling using the ES concept has not been preserved. Debugging a simulation built on these principles requires redevelopment of programs or the use of already known programs built on similar principles.

The concept of ES refers only to the description of a rough surface. The modeling itself is based on the construction of the trajectories of the rays emitted inside the scintillator. The construction of trajectories consists of the following stages: radiation of rays, crossing of possible boundaries, absorption in the bulk, processes at the boundaries of media (reflection, refraction). The initial directions of the rays are set uniformly. Only one ray is emitted in each direction with a fictitious intensity decreasing along the path of the ray in the bulk and upon reflection from the scintillator surfaces. The construction of the ray trajectory with the initially specified direction ends when it hits the photomultiplication detector (PM) or when the minimum intensity of the beam is reached.

This is reminiscent of MCM, where the simulation of the passage of light in volumes and at the boundaries of environments also occurs as the construction of ray trajectories and consists of the above stages. But this is not MCM, in which the selection of certain events during simulation is carried out from some distributions corresponding to the probabilities of real physical processes. Another difference lies in the fact, that the fate of each emitted beam is monitored in the MCM until it is absorbed in the volume or on the surface of the scintillator, or until it hits the PM. However, in both cases, the approaches are very close and it is advisable to apply a fruitful approach using the concept of ES in existing programs based on MCM.

Simplicity, visibility and the possibility of constructing beam trajectories for objects with complex geometry ensured the implementation of MCM modeling of the light passage in a number of programs. For example, the well-known high-energy physics toolkit Geant4 (CERN) [12, 13] includes a block of programs that allows modeling the transfer of optical photons, taking into account absorption and reflection coefficients, refractive indices and surface properties of various materials. CERN also developed a separate package of Litrani programs for simulating the light passage. Litrani programs [14–16] have the ability to take into account the optical anisotropy of media and simulate the detection of light by different types of PM. The Zemax package [17] also allows you to simulate the light passage in optical systems. During modeling, it is possible to create sets of surfaces with certain parameters.

The DETECT2000 program [18] is very popular. We chose this program precisely because it (with a certain selection of the rough surface model) makes it possible to characterize the rough surface by the fraction of specularly reflected rays — a parameter similar to ES in [9]. The description of the DETECT2000 program operation principle is also given in the previous work of the authors [19].

In this article, using the known NaI(Tl) and BGO scintillators as an example, an attempt was made to show the possibility of approximating the simulation results using the MCM-based program (DETECT2000) to the results described for these objects in [9]; for this, the DETECT2000 parameter "part of specular-reflected rays" was used. Additionally, the article considers in more detail than in [9] the effect of a parameter similar to ES on light collection coefficient under various modeling conditions.

Purpose of the work: Using examples of comparative modeling of light collection coefficient for known scintillators, to connect the MCM DETECT2000 programs with the ES factor and investigate in more detail the effect of this factor on light collection coefficient when the simulation conditions in DETECT2000 are changed.

2. Surface models and their correspondence in programs with effective specularity (ES) and DETECT2000

The ES model is based on the description of the rough surface as a collection of microsites randomly oriented relative to the base surface [9]. P.Bouger gave this idea about a rough surface in the 18th century [20]. At large angles of light observation relative to the normal to the surface, a rough surface gives a mirror shine. It comes from microsites, which are oriented in such a way that the angle of incidence of the rays on them is equal to the angle of the reflected rays, which are directed to the observer or the photodetector (PM). At various angles of incidence, the intensity of specularly reflected light from a rough surface is different. From the intensity of light registered by the PM at different angles of light incidence, it is possible to detect the relative number of microsites with different inclinations to the base surface, that is, to estimate the surface relief [1, 21]. Based on this, angular distributions of both specularly reflected light intensities and orientations of microsites can be constructed. According to the type of these distributions, it is possible to characterize a rough surface. The values of these distributions averaged for all angles also characterize a rough surface. In the ES model, such an averaged characteristic is given either by the degree of surface diffusivity or by the average effective specularity p [9]. Thus, the relative intensity of the light specularly reflected from the rough surface and the relative number of microsites with different inclinations to the base surface are related to each other.

In programs, based on the concept of effective specularity (ES) [9], three types of scintillator surfaces were used (regardless of the scintillator shape): D denotes the rough surface with effective specularity $p = 0.58$; d denotes the rough surface with $p = 0.75$; S denotes the polished surface with $p = 1.00$. These models also used external reflectors: diffuse with reflectance $k = 0.95$ (DR) and specular with $k = 0.8$ (SR), both without optical contact with the surface.

In [9], five combinations of external reflectors and scintillator surface treatment were used for modeling:

1) DD (the first letter is the processing of the end remote from the photodetector, the second is the processing of the side surface) — rough end $p = 0.58$ with DR, rough side surface $p = 0.58$ with DR;

2) dd-rough end $p = 0.75$ with DR, rough side surface $p = 0.75$ with DR;

3) DS-rough end $p = 0.58$ with DR, polished side surface $p = 1.0$ with SR;

4) dS-rough end $p = 0.75$ with DR, polished side surface $p = 1.0$ with SR;

5) SS-polished end $p = 1.0$ with DR, polished side surface without reflector.

The following variants of scintillator surface models are provided in the DETECT2000 program:

1) optically smooth surface (POLISH);

2) rough surface (GROUND);

3) surface covered with an opaque diffuse reflector (PAINT);

4) surface with an opaque specular reflector (METAL);

5) surface with variable roughness (UNIFIED).

For PAINT and METAL surfaces, optical contact of the reflector with the surface is assumed. For POLISH, GROUND and UNIFIED surfaces, you can specify the reflection coefficient (assuming a diffuse reflector without optical contact with the surface). The UNIFIED model of the DETECT2000 program allows you to set the fraction of specularly reflected light for a rough surface, which in meaning corresponds to the p parameter in the program with ES. This allows direct comparison of the simulation results of both programs. The difference is that in the UNIFIED model, the specularly reflected light fraction can be set in the range from 0 to 1, while in the model with ES, the parameter p is limited from below by the value of 0.58.

2.1 Objects and modeling conditions

The simulation was carried out in the DETECT2000 program with the determination of light collection coefficients for cylindrical scintillators based on NaI(Tl) single crystals with dimensions ∅40×40 mm, ∅40×160 mm and ∅100×100 mm, as well as for cylindrical scintillators based on bismuth germanate single crystals BGO with

Table 1. Light collection coefficients obtained by modeling in the DETECT2000 program and published data [9] for a number of detector configurations based on NaI(Tl) and BGO* single crystals

Surface model according to [9]				DD	*dd*	DS	dS	SS
Model parameters		End	Crystal	ES 0.58	ES 0.75	ES 0.58	ES 0.75	ES 1.00
			ExtRefl	DR 0.95	DR 0.95	DR 0.95	DR 0.95	DR 0.95
		External surface	Crystal	ES 0.58	ES 0.75	ES 0.58	ES 1.00	ES 1.00
			ExtRefl	DR 0.95	DR 0.95	SR 0.80	SR 0.80	not
Light collection coefficients	NaI(Tl)	∅40×40 mm	DET2000	0.655	0.625	0.567	0.537	0.392
			Ref [9]	0.662	0.624	0.529	0.492	0.394
		∅40×160 mm	DET2000	0.349	0.386	0.446	0.425	0.365
			Ref [9]	0.407	0.411	0.406	0.391	0.363
		∅100×100 mm	DET2000	0.564	0.541	0.424	0.414	0.382
			Ref [9]	0.550	0.520	0.425	0.412	0.387
	BGO	∅40×40 mm	DET2000	0.442	0.409	0.390	0.347	0.250
			Ref [9]	0.433	0.393	0.345	0.315	0.250
		∅40×160 mm	DET2000	0.194	0.205	0.218	0.207	0.187
			Ref [9]	0.219	0.217	0.200	0.196	0.189
		∅60×60 mm	DET2000	0.372	0.345	0.329	0.300	0.229
			Ref [9]	0.381	0.348	0.302	0.280	0.238

ES — effective specularity;
DR 0.95 — diffuse reflector with a reflection coefficient of 0.95;
SR 0.80 — specular reflector with a reflection coefficient of 0.80.
*) See above for more detailed description of models and designations.

dimensions ∅40×40 mm, ∅40×160 mm and ∅60×60 mm. The results were compared with the ES data published in [9] for the corresponding cylindrical scintillators.

The UNIFIED type surface model allows you to set the proportions of specular and diffusely reflected light. The values of the model parameters were chosen in accordance with the combinations of external reflectors and scintillator surface treatment given in [9] for the model with ES. During the simulation, the refractive indices n averaged over scintillator luminescence spectra were set equal to 1.85 for NaI(Tl) and 2.15 for BGO.

When comparing the programs DETECT2000 and [9], the following values of optical absorption coefficients k (cm^{-1}) of the scintillator were set: for NaI(Tl) $k_1 = 0.005$, for BGO $k_1 = 0.02$. Other values of the optical absorption coefficients were also used: for NaI(Tl) $k_2 = 0.01$; for BGO $k_2 = 0.2$. When comparing the programs, the coefficients of the effective specularity of the surface p used in [9] were set: $p = 0.58$ and $p = 0.75$. Other values of the effective specularity were also set, in percent: for NaI(Tl) and BGO: $p = 40$, 60, 80, 100. The reflection coefficients of the external reflector k_{ref} were set as in [9]: $k_{ref} = 0.95$ for DR and $k_{ref} = 0.8$ for SR when comparing the programs. Other values of k_{ref} were also set.

The light collection coefficients were determined for various numbers Nemit of emitted rays (from 10^3 to 10^5 rays). The points and directions of the emission of rays were drawn from uniform spatial distributions, both for NaI(Tl) and BGO. The average values of the light collection coefficients were based on the simulation results for 7 runs for each set of specified parameters. There is a certain scatter between the results of individual simulation runs [19] (it is noticeable for a small number of emitted rays $N_{emit} = 1000$). However, due to a fairly large number of launches, the average light collection coefficients remain approximately the same with different numbers of emitted rays for the same set of conditions. Here, the results for the case of $N_{emit} = 100000$ are presented.

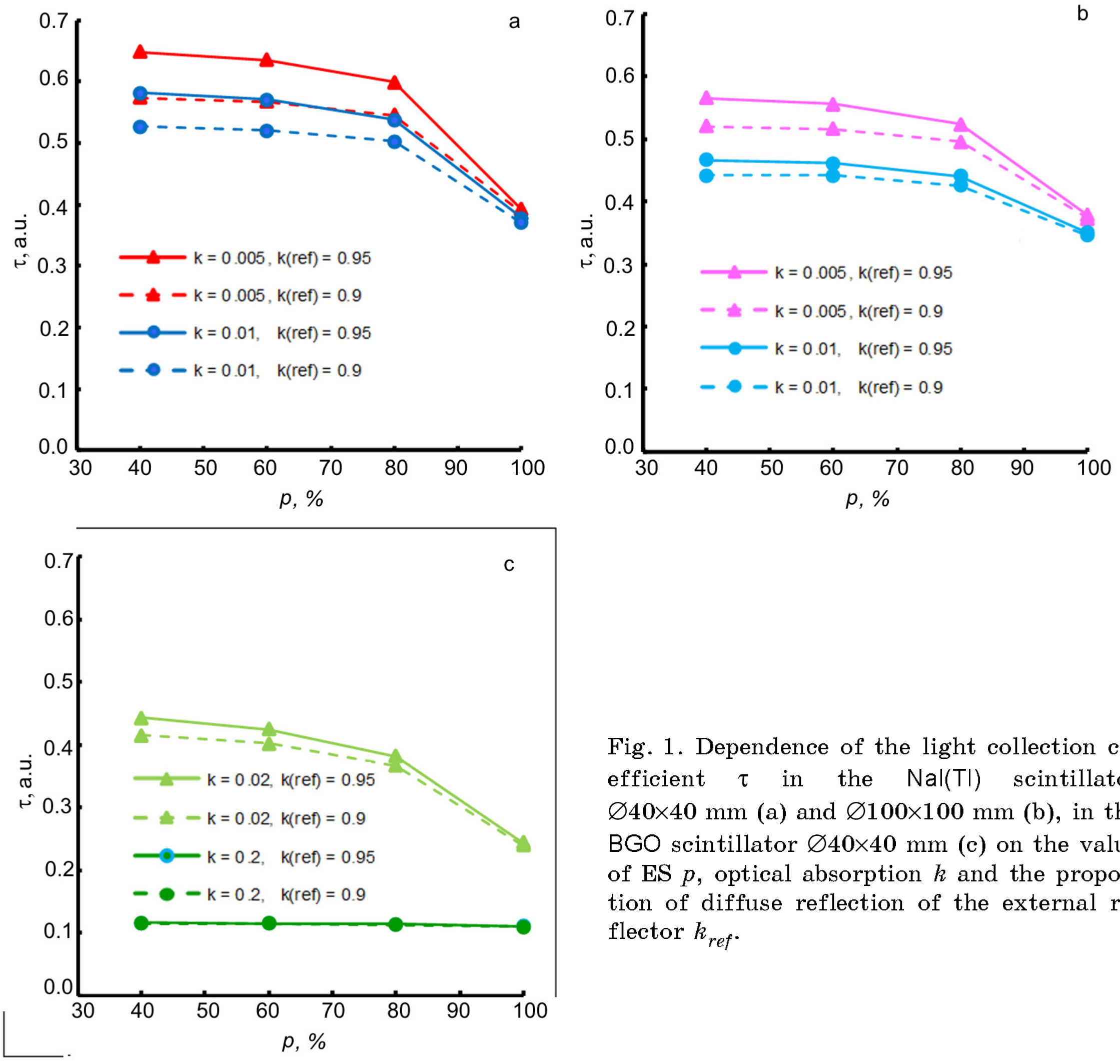

Fig. 1. Dependence of the light collection coefficient τ in the NaI(Tl) scintillator ∅40×40 mm (a) and ∅100×100 mm (b), in the BGO scintillator ∅40×40 mm (c) on the value of ES p, optical absorption k and the proportion of diffuse reflection of the external reflector k_{ref}.

3. Results and discussion

Comparison of program results

The results of simulation in the DETECT2000 program and the ES program data obtained in [9] are presented in Table 1.

The case of all polished crystal surfaces (*SS*) for all sizes NaI(Tl) and BGO gives the best approximations of the two programs results. The difference in light collection coefficients is mainly 0.5–1.2 %, and for BGO, ∅60×60 mm, — less than 4 %.

For equal-sized NaI(Tl) crystals of ∅40×40 mm and ∅100×100 mm, as well as for BGO of ∅40×40 mm and ∅60×60 mm with rough surfaces (*DD* and *dd*), there is also a good agreement between the results: differences are from 0.15 % to 3.5 %. Results of options *DD* and *dd* for long-sized NaI(Tl) ∅40×160 mm and BGO ∅40×160 mm crystals differ more — from 5.5 % to 14.2 %. For all crystal variants with combined surfaces (*DS* and *dS*), the differences are 5–13 %, and only for NaI(Tl) O100×100 mm, they are minimal — 0.2–0.3 %. Even such a result for combined surfaces can only be obtained by complicating the detector description in DETECT2000. The use of single surfaces of any options (POLISH, GROUND, PAINT, METAL, UNIFIED) leads to a 1.5–2-fold difference between the simulation results and the literary ones. This is due to the fact that the *DS* and *dS* versions use a mirror reflector as a reflector with a polished cylindrical surface without optical contact with the surface. DETECT2000 does not have this option. The closest variant of METAL uses a specular reflector in contact with the surface. Only the introduction of an additional cylindrical reflecting surface forming a gap made it possible to bring the

Table 2. Relative light collection coefficients for NaI(Tl) and BGO under various specified conditions

p, %	k_{ref}, arb.un.	NaI(Tl)					BGO		
		k, cm^{-1}	Ø40×40 mm		Ø100×100 mm		k, cm^{-1}	Ø40×40 mm	
			τ_{rel}	Δ, %	τ_{rel}	Δ, %		τ_{rel}	Δ, %
40	0.95	0.005	1	–	1	–	0.02	1	–
80			0.92	-8	0.93	-7		0.86	-14
100			0.60	-40	0.67	-33		0.55	-45
40	0.9		1	–	1	–		1	–
80			0.95	-5	0.95	-5		0.88	-12
100			0.67	-33	0.72	-28		0.58	-42
40	0.95	0.01	1	–	1	–	0.2	1	–
80			0.92	-8	0.94	-6		0.98	-2
100			0.65	-35	0.75	-25		0.96	-4
40	0.9		1	–	1	–		1	–
80			0.95	-5	0.96	-4		0.98	-2
100			0.70	-30	0.78	-22		0.95	-5
	0.95	0.01/0.005	0.90	-10	0.83	-17	0.2/0.02	0.26	-74
	0.9		0.92	-8	0.85	-15		0.28	-72
	0.9/0.95	0.005	0.88	-12	0.92	-8	0.02	0.94	-6
	0.9/0.95	0.01	0.91	-9	0.95	-5	0.2	0.99	-1

simulation results in DETECT2000 closer to the literature data [9].

In general, the comparison shows a fairly good approximation of the simulation results obtained in the two programs. Considering also the correspondence between the data [9] and the results of experimental measurements, one can hope to obtain sufficiently reliable data on the light collection coefficients for various objects using DETECT2000.

Simulation of light collection coefficients of scintillators with variation of model parameters

A significant role in the models is played by the ES parameter of the rough surface (in the UNIFED DETECT2000 surface model, these are the fractions of light reflected specularly and diffusely). In the future, this parameter for both programs will be denoted as ES or p. In [9], it is indicated that at a value of less than 0.58, the ES loses its meaning (does not exist). At the same time, in DETECT2000 there are no restrictions on the proportion of specular reflection in the parameters of the UNIFIED surface model with variable roughness. It can change from 0 to 1. At the same time, as modeling in DETECT2000 showed, the light collection coefficients for both NaI(Tl) and BGO remain almost constant when p varies from 0 % to 40 %. In this regard, further studies were carried out at p values from 40 % to 100 %.

The results of simulation of light collection in NaI(Tl) and BGO at different values of ES, p, optical absorption coefficients k and reflectance of the external reflector k_{ref} are shown in Fig. 1.

Comparison of Fig. 1a and Fig. 1b shows that with an increase in the ES from 40 % to 80 % the light collection coefficient in NaI(Tl) gradually decreases. The nature of the dependences has the same form for both scintillators and for different specified conditions. At ES exceeding 80 %, a significant deterioration in the light collection coefficient occurs, which, as indicated in [2], is associated with a large increase in the fraction of captured light in the scintillator. Fig. 1c shows that for BGO with a low optical absorption coefficient, as well as for NaI(Tl) scintillators, when the ES increases from 40 % to 80 %, the light collection coefficient decreases smoothly; and when the ES exceeds 80 %, it decreases sharply. With a high coefficient of optical absorption of the BGO scintillator, light losses at all ES values are large and the light collection coefficient is also low.

The numerical values of the simulation parameters and the obtained relative light collection coefficients for NaI(Tl) and BGO are given in Table 2.

As can be seen from the data in Table 2, for NaI(Tl) ∅40×40 mm, a 2-fold increase in the optical absorption coefficient k (from 0.005 cm^{-1} to 0.01 cm^{-1}) gives approximately the same contribution (~ 11 %) to the deterioration of light collection as a decrease by 5 % (from 0.95 to 0.9) of the diffuse reflection fraction of the external reflector k_{ref} (~ 13 %) while maintaining the optical absorption coefficient in the scintillator. A similar (for the same parameters) decrease in the optical absorption coefficient for NaI(Tl), ∅100×100 mm leads to a deterioration in light collection by ~ 20 %, which is 2 times higher than a 5 % decrease in the proportion diffuse reflection of the external reflector (~ 9 %). This may be due to a significant increase in the average path of light to the exit window in the case of a large scintillator and the exponential dependence of the light absorption probability on the absorption coefficient and path length.

From the data given in Table 2, it is also clear that the contribution of optical absorption to the deterioration of light collection in BGO significantly exceeds the contribution of diffuse reflection of the external reflector. When the optical absorption coefficient increases by 10 times (from 0.02 cm^{-1} to 0.2 cm^{-1}), the light collection coefficient decreases by 5 times. A 5 % decrease (from 0.95 to 0.9) in the fraction of diffuse reflection worsens the light collection by about 5 %.

4. Conclusions

The comparison of the MCM modeling of the light collection coefficient in NaI(Tl) and BGO scintillators with various surface treatment in the program with ES and the DETECT2000 program shows a good agreement between the results when using a UNIFIED-type surface model in DETEC2000, which actually takes into account the ES of a rough surface.

Differences in the results of determining the light collection coefficients for NaI(Tl) and BGO with various surface treatment options are the following:

for all sizes with (*SS*) surfaces — 0.5–1.2 % for NaI(Tl), less than 4 % for BGO;

for equal-sized crystals with surfaces (*DD*) and (*dd*) — from 0.15 % to 3.5 %;

for long crystals with surfaces (*DD*) and (*dd*) — from 5.5 % to 3.5 %;

for long crystals of NaI(Tl), ∅40×160 mm, and BGO, ∅40×160 mm, with (*DD*) and (*dd*) — from 5.5 % to 14.2 %;

for combined surfaces (*DS* and *dS*) of all types of crystals — 5–13 %, for NaI(Tl), ∅100×100 mm, — 0.2–0.3 %.

The results of the comparison show that, with the correct choice of the surface model, the programs based on DETECT2000 can actually operate with the same characteristics of a rough surface as the programs with ES, and they can be used to determine the light collection coefficient in scintillators.

When simulating the light collection coefficient in the DETEC2000 program (outside of the program comparison) using the UNIFIED type surface for equal-sized NaI(Tl) and BGO scintillators with changing in ES, the optical absorption coefficient and the reflection coefficient of the external reflector, the following results were obtained:

With an increase in ES from 40 % to 80 % the light collection coefficient drops from 4 % to 8 % for NaI(Tl) and from 12 % to 14 % for BGO (at $k = 0.02$ cm^{-1}), when various parameters of the scintillators are set. A 2-fold deterioration in optical absorption and a decrease in the diffuse reflection fraction by 5 % approximately equally (by 13–16 %) reduce the light collection coefficient for NaI(Tl), ∅40×40 mm. With an increase in the size of the NaI(Tl) crystal up to ∅100×100 mm, the effect of optical absorption is much higher than the fraction of diffuse reflection. For BGO, when the optical absorption deteriorates by a factor of 10, the effect of changing the diffuse reflectance fraction has practically no effect on the background of deterioration in the light collection coefficient by 75 %.

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