# ON THE OPTIMUM GEOMETRIC SHAPES OF ZnSe-BASED SCINTILLATION ELEMENTS

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We have carried out Monte-Carlo calculations of the light collection coefficient τ for different shapes of ZnSe-based scintillators Applying a theoretical model, it has been shown, that the light collection optimization can be reached in scintillators with a geometry where the chaotic light collection is realized. Experimentally it was supported that for detectors of rectangular and cylindrical types with rounded vertexes or edges, the light output increase of up to 20% has been observed, provided the regular light beam dynamics was changed to chaotic. This work has been carried out with support under CRDF Project UE2-2484-KK-02.

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One of the main parameters characterizing quality of detectors of "scintillator-silicon photodiode" type (SD) is their sensitivity to β- and γ-radiation [1,2]. Parameters of the existing SD can be improved by increasing the scintillator (S) volume and the photodiode (PD) sensitive surface. However, because of various technological and physical factors, it is not always possible [3].

A promising way to improve the SD sensitivity is finding optimum shapes of S, which would ensure maximum values of light collection coefficient τ and, consequently, of the light output.

We have carried out calculations of τ for different S shapes, taking ZnSe(Te) crystals as an example. The values of τ (fraction of light coming from the output window of S) were determined by the Monte-Carlo method (MC). The calculation algorithm accounted for the sample geometry, absorption in the S material ($\alpha$ =0,1...0,2 cm$^{-1}$), refraction index ($n$=2,58), light scattering indicatrix at the "crystal-reflecting covering" interface, as well as several other parameters. Different shapes of ZnSe(Te) scintillators were considered, including polyhedrons (parallelepiped, parallelepiped with rounded upper edge, tetrahedral truncated pyramid, tri- and hexahedral prism, as well as hemisphere. The obtained values of τ for scintillators with output windows corresponding to the PD sensitive area ($S$=1cm$^2$) are presented in Table 1.

Table 1

| Scintillator shape | Light collection coefficient, τ | |
|---|---|---|
| | Scintillations uniformly distributed over the volume | Scintillations located in the surface-adjacent layer |
| Pyramid, sides at 60° | 0.60 | 0.668 |
| Pyramid, sides at $45^0$ | 0,49 | 0,51 |
| Hemisphere | 0.457 | 0.652 |
| Trihedral prism (variant 1) | 0.357 | 0.378 |
| Hexahedral prism (variant 1) | 0.202 | 0.221 |
| Trihedral prism (variant 2) | 0.147 | 0.146 |
| Hexahedral prism (variant 2) | 0.145 | 0.147 |
| Cube with edge rounding | 0.339 | 0.371 |
| Cube | 0.144 | 0.145 |

It can be seen from Table 1 that variation of the scintillator shape can lead to substantial (up to 3 times) changes in τ. The lowest τ values are observed for scintillators of regular shapes (parallelepiped, cylinder, prism). From the other side, the shapes of tetrahedral pyramid with the sides inclined at $60^0$ and of hemisphere favor the light coming out of the crystal. For the shape of pyramid, low τ is observed when the sides are inclined at $45^0$, which corresponds to the vertex angle of 90°, i.e., the scintillator is an angular reflector. Light collection processes for this case are analyzed in the Appendix. This analysis shows that in this case large fraction of light is captured by total internal reflection, thus lowering the values of τ. This seems to be a common picture for all scintillators of regular shapes (parallelepipeds, cylinders, prisms).

To find out the optimum shape of a scintillator, i.e., to obtain the maximum τ, we have proposed to use a theoretical approach where an adequate model of physical detectors is mathematical billiard [4,5]. In this approach, the beam picture is considered in a special phase space of the dynamic system that corresponds to the detector (billiard). Then on the phase portrait of light collection one can see changes and peculiar features of the beam picture that cannot be observed in the conventional geometrical space. This, in particular, allows us to establish more profound physical reasons of light capture in the crystal volume and to propose new ways of excluding it. The light capture is directly related to the presence of a regular component (RC) of the beam propagation in detectors of regular shape (spherical, cylindrical, rectangular). Each specified RC beam occupies its once and forever fixed region in the phase space. Location of the regularity zone can be such that RC beams belonging to it will never reach the output window of the detector or will not get into the output aperture (under condition of full internal reflection) and became captured inside the crystal volume. As distinct from this, all beams of the chaotic component (CC) will, in due course of time, fill one and the same region of the phase space, i.e., chaotic trajectories are undistinguishable from one another. In addition, CC

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always has intersections with the light output zone (in the phase space). Independently on the output window location and the presence of internal total reflection, chaotic beams always come out of the detector. Therefore, all CC beams make their contributions to the light output. As chaotic trajectories are undistinguishable, this contribution is approximately the same for each of such beams. Therefore, the larger is CC, the higher is the light output of a detector. Relationship between RC and CC contributions, or, in other words, dynamic structure of mixed phase space of a detector strongly depends upon its shape. Thus, to improve the detector light output, one can efficiently use chaotization of light beams in the detector (billiard). Transition to stochasticity is obtained by appropriate changes in the detector shape.

We have carried out an experiment to prove viability of the stochastic approach in choosing the optimum shapes, taking ZnSe(Te) and CsI(Tl) scintillators as examples.

We compared light output values for cubic samples with two characteristic types of rounding: a) rounding of edges, b) cylindrical segment, c) rounding of angles (Fig.1) with light output values of a regularly shaped cubic sample (reference). The degree of rounding (centers and values of radii) were chosen in accordance with considerations of the statistical approach.

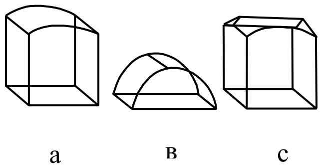

*Fig.1. Shapes of scintillation samples: a) cube with rounded edges; b) truncated cylinder; c) cube with rounded vertices*

All the samples studied, as well as the reference sample of 1×1×1cm$^3$ size, were made of one and the same crystalline ingot. The output window area for all scintillators was 1x1cм$^2$. All sides of the samples were polished.

The X-ray luminescence light output $L$ of the scintillators was recorded by an instrument for measurement of optical radiation power (KVARC – 01). An X-ray source REIS (effective energy 70 keV) was used for excitation. The signal obtained from the reference under the same conditions was taken as 100%. For the same shapes, Monte Carlo calculations of τ were carried out.

In Table 2, calculated values of $\tau$, $\tau/\tau_{cube}$ are given, as well as experimental data on light output with respect to the reference, $L/L_{cube}$.

Experimental data on $L$, obtained for scintillators of cubic shape with different types of roundings from the input window side, have shown that $L$ is increased by 16-20% as compared with cubic scintillator of the regular shape. This result is qualitatively confirmed by Monte-Carlo calculations of τ.

## CONCLUSIONS

Our theoretical and experimental studies have shown that the use of “chaotic billiard” forms if crystalline detectors lead to increased light output values. As the problem of light collection is largely a geometrical one, this conclusion can be also applied to scintillators of other types.

Table 2

| Scintillator shape from Fig.1 | Material | Volume $V$, cм$^3$ | $\tau$ | $\tau/\tau_{cube}$ | $L/L_{cube}$ |
|---|---|---|---|---|---|
| a | ZnSe(Te) | 0,92 | 0,1929 | 1,524 | 1,17 |
| | CsI(Tl) | 0,92 | 0,243 | 1,504 | 1,18 |
| c | ZnSe(Te) | 0,96 | 0,1787 | 1,41 | 1,11 |
| | CsI(Tl) | 0,96 | 0,2157 | 1,336 | 1,12 |
| в | ZnSe(Te) | 0,392 | 0,3292 | 2,6 | 1,22 |
| | CsI(Tl) | 0,392 | 0,3751 | 2,32 | 1,20 |
| reference | ZnSe(Te) | 1 | 0,1265 | 1 | 1 |
| | CsI(Tl) | 1 | 0,1615 | 1 | 1 |

## APPENDIX

### Light collection processes in the pyramid with vertex angle 90$^0$ (angular reflector)

In the pyramid with its sides at 45° to the base, i.e., when the vertex angle is 90°, the light collection coefficient is anomalously decreased. This can be explained in the following way.

Let us use the mirror reflections method [6]. We construct a two-dimensional image of the pyramid Ω and its reflection in the side faces (Fig.2). The trajectory of beam ABCD, subject to several reflections from the pyramid sides, is imaged as straight line A`B`CD. The largest beam trajectories that do not intersect with the pyramid base, are of length $a\sqrt{2}$, where $a$ is the pyramid base side. It is assumed that height $h$=const.

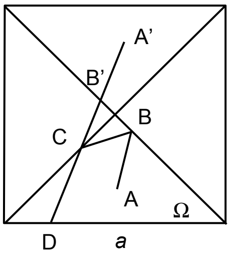

*Fig.2. Beam trajectories in the angular reflector (vertex angle 90$^0$)*

Conditions for the beam not coming out from the side face and going through the output window require that the incidence angle θ onto the base should be:

$$\theta < \theta_{ITR}^{b}; \frac{\pi}{4} + \theta > \theta_{ITR}^{s}; \frac{\pi}{4} - \theta > \theta_{ITR}^{s}, (1)$$

where $\theta_{ITR}^{b}, \theta_{ITR}^{s}$ are angles of internal total reflection on the base and the side surface.

A beam subsequently reflected from 2 or 3 faces comes back to the base at the same incidence angle. Neglecting non-zero reflection coefficients at normal incidence, we obtain the maximum beam path in such pyramid:

$$l_{\max} = \frac{a}{\cos\left(\frac{\pi}{4} - \theta^{s}_{ITR}\right)} = 0.43\ sm \qquad (2)$$

Fig.3 shows the distribution of beams coming to the photoreceiver over path lengths in the crystal. Different curves correspond to pyramids with different inclination of side faces.

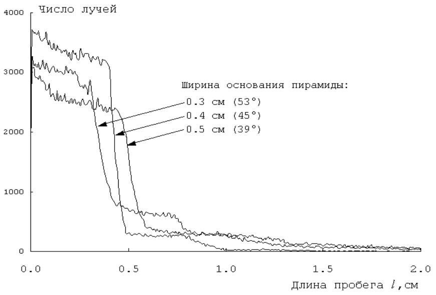

*Fig.3. Distribution of beams over path lengths in a tetrahedral pyramid with side faces at ~ 45° to the base*

The value of $l_{\max}$ obtained from (2) is in agreement with that obtained by Monte-Carlo calculations. Thus, beams with $l > l_{\max}$ go to the photoreceiver, intersecting with the base not less than twice. Let us denote the number of such beams as $N_1$, and the total number of beams - as $N$. In the angular reflector, in each subsequent incidence onto the base the angle remains the same. If the inclination angle differs from 45°, the incidence angle will change, and the beam can come to the output cone. In Table 3, calculated data are presented on the light collection fraction that is due to such beams. The situation of angular reflector causes light capturing, leading to worsening of the light collection coefficient.

Table 3.

Relationship between beams of different spatial orientation in the tetrahedral pyramid

| Size of pyramid base, cm | Light collection, τ | Fraction of "long" paths, $\frac{N_1}{N}$ | Additional light collection, $\tau\frac{N_1}{N}$ |
|---|---|---|---|
| 0.3 | 0.568 | 0.335 | 0.190 |
| 0.4 | 0.479 | 0.100 | 0.048 |
| 0.5 | 0.592 | 0.199 | 0.118 |

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## ОБ ОПТИМАЛЬНЫХ ГЕОМЕТРИЧЕСКИХ ФОРМАХ СЦИНТИЛЛЯЦИОННЫХ ЭЛЕМЕНТОВ НА ОСНОВЕ ZnSe

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С использованием метода Монте-Карло проведены расчеты коэффициента светособирания для различных форм сцинтилляторов на основе ZnSe. Теоретически показано, что оптимизация светосбора достигается в сцинтилляторах с геометрией, для которой реализуется хаотическое собирание световых лучей. Это предположение экспериментально подтверждено на примере детекторов прямоугольного и цилиндрического типа со скругленными вершинами или ребрами, для которых обнаружено повышение светового выхода до 20% при изменении регулярной динамики световых лучей на хаотическую.

## ПРО ОПТИМАЛЬНІ ГЕОМЕТРИЧНІ ФОРМИ СЦИНТІЛЯЦІЙНИХ ЕЛЕМЕНТІВ НА ОСНОВІ ZnSe

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З використанням методу Монте-Карло проведені розрахунки коефіцієнта світлозбирання для різних форм сцинтиляторів на основі ZnSe. Теоретично показано, що оптимізація світлозбирання досягається у сцинтиляторах з геометрією, у якій реалізується хаотичне збирання світлових променів. Це припущення експериментально підтверджено на прикладі детекторів прямокутного і циліндричного типу з округленими вершинами та ребрами, для яких виявлено підвищення світлового виходу до 20 % при заміні регулярної динаміки світлових променів на хаотичну.