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Comparison of different rough surface models for computer simulation of light collection in a scintillator/light guide system

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A model of the reflecting surface has been developed that takes into account the data of the microface slope distribution for glass surfaces treated by various abrasives. These distributions were used to simulate the light collection in the scintillators. The proposed model efficiency has been confirmed by the agreement between the calculated light scattering indicatrices for the surfaces with various roughness degree and the experimental results obtained before. The comparison between the calculated results of the light collection for different rough surface models and the experimental ones in a scintillator/conical light guide system with different types of lateral surfaces indicates that the best agreement is obtained when the developed model is used.

Разработана компьютерная модель отражающей поверхности на основе данных о распределении наклонов микрограней для поверхностей стекол, обработанных различными абразивами. Эти распределения использовались для моделирования светособирания в сцинтилляторах. Эффективность модели подтверждается совпадением между расчетными индикатрисами рассеяния света для поверхностей с разной степенью шероховатости с ранее полученными экспериментальными результатами. Сравнение расчетов коэффициента светособирания для разных моделей поверхности в системе "сцинтиллятор — световод" с экспериментальными результатами показало, что разработанная модель дает наилучшее согласие.

The problems of light collection are relevant for all the application fields of scintillation engineering. The numerical calculations are widely used to elucidate the influence of different factors on the light collection processes. When simulating the light collection processes in detectors, the selection of proper surface model is the crucial issue [1–5]. There is a common approach for the simulation of the specular surface, but the situation is quite different in the case of rough surface. One of main problems of the existing rough surface models is the absence of unambiguous relationship between the parameters of the real surface and the model one. In this work, an attempt is made to overcome this drawback by proposing a new model of rough surface that links the distribution nature of microfaces with the surface treatment conditions (abrasive size). Distributions of microfaces for different surface treatment conditions were obtained before experimentally in [6].

A comparative study of light collection for the proposed model and several other models has been carried out in this work. The light collection simulation results have been compared to experimental studies of the relative light output change in a scintillator/light guide system to evaluate the effectiveness of models.

It is well known that light guide transmits the light flow emitted by the scintillator without focusing it and at minimum losses [1]. At the same time, the change of the reflector type and the surface treatment of the light guide will result in the modification of the light collection coefficient of the whole scintillator/light guide system. When studying such system experimentally, it is easier to reveal the influence of the surface treatment character and the reflector on the light collection process.

To modify the optical parameters of the lateral light guide surfaces is an easier, faster and cheaper task as compared to similar modifications on the scintillator. That is why the scintillator/light guide system was selected here for a detailed study.

Several models of the rough surface exist today that differ in the description method of scattering indicatrix and surface profile. The main features thereof are summarized below.

Lambert description (cosine approximation). This model is based on the assumption of the scattering indicatrix independence of the light incidence angle. Usually, the scattering indicatrix is assumed to be in proportion to cosine (Lambert Law). In practice, the Lambert Law is met satisfactorily only for the incidence angles smaller than 60° [1]. The drawbacks of the Lambert description are the absence of the scattering indicatrix maximum along the mirror reflection that was observed for real rough surfaces and the impossibility to take into account the roughness degree of the reflecting surface.

Effective reflectivity. This model takes into account the basic properties of the real scattering indicatrix: its dependence on the incidence angle and existence of a well-defined maximum along the mirror reflection direction. The model scattering indicatrix consists of cosine and mirror components. Integral intensities of these components are equal to $1-p$ and $\bar{p}$, respectively. The surface microrelief is specified by the unique parameter — effective reflectivity

$$\bar{p} = \overline{p(\theta)} = \int_{\pi/2} p(\theta)\sin\theta d\theta,$$

where θ is the angle between the incidence angle direction and the normal to the general surface [2].

Approximation by the micro-facets. This model is based on the Bouguer approach [3]. The reflecting rough surface is represented as a set of flat micro-facets randomly oriented with respect to the normal to the general surface. It is assumed that each elementary micro-facet reflects the incident light as a mirror. The model does not take into account the existing diffraction discrepancy of the light, because it is rather small in comparison with full width of the scattering indicatrix. The last one is defined as a width of the micro-facet distribution function with respect to normal orientations. This approach is effective when the micro-facet size is larger than the incident light wavelength [4, 5].

One of the advantages of the micro-facet model is the additional possibility to consider the light transmission into the external medium, that, in particular, allows to simulate the rough output window of the detector. This model enables also to examine the consecutive transmission of a ray through several interfaces, thus providing to take into account the influence of various film coatings and external reflectors on the light collection process.

Developed model. Authors of the papers [7, 8] extracted the micro-facet distribution from the measurements of the surface profile by means of a profilometer. In our model, to determine the micro-facet orientation distribution, we have used conclusion from [6] that this distribution is almost independent of the microhardness and elastic properties of the processed materials, and is only defined by treatment conditions and abrasive powder size. This conclusion is valid when the hardness of the abrasive exceeds considerably that of the processed material. This implies that the experimental data of the micro-facet slope distribution for the surfaces of IKS-3 glasses, treated by various abrasives and given in [6], will be similar for other materials such as scintillators and light guides. That approach excludes the necessity of the surface profile measurement, since already known results of the micro-facet slope distribution for each abrasive will be used. Moreover, it enables to link directly the light scattering indicatrices obtained by the simulation with the surface treatment conditions.

Comparison of the experimental [6] and calculated indicatrices of reflected light, obtained for the same objects, was carried out to check the efficiency of the proposed model. Experimental and model indicatrices

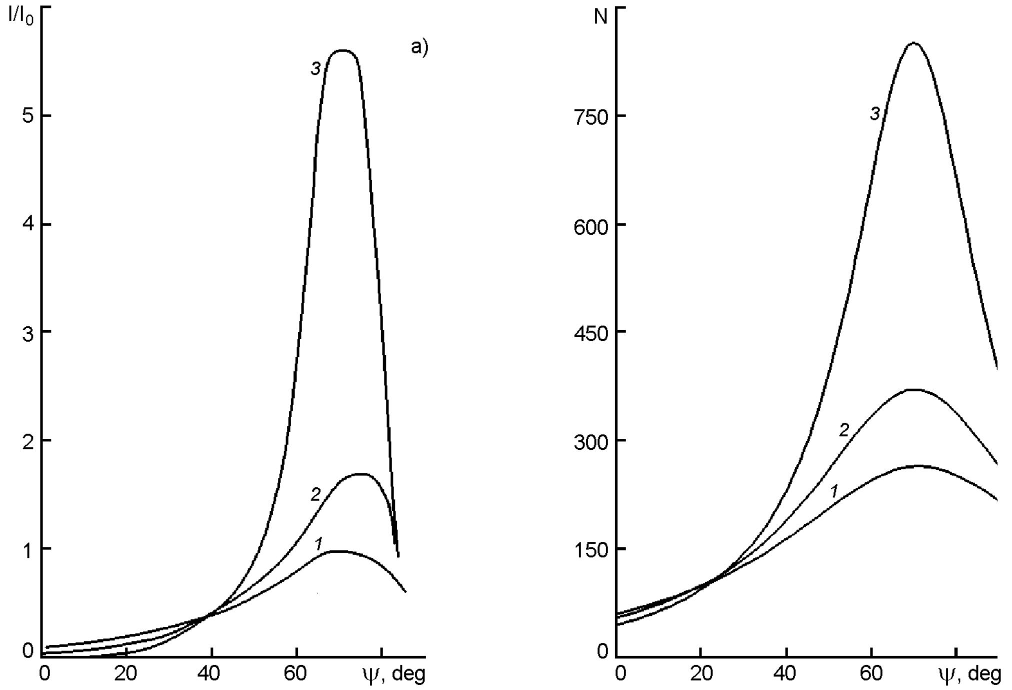

Fig. Experimental (a) and simulated (b) light scattering indicatrices of the IKS-3 glasses treated by abrasives with various grain size: 120 μm (*1*), 10 μm (*2*), 7 μm (*3*). Incidence angle is 70°.

of light reflection of IKS-3 glasses, processed by the abrasives with grain size of 7, 10, and 120 μm, are presented in Figure. The beam incidence angle on the sampleis equal to 70°. The curves are drawn in Cartesian rectangular coordinates. The abscissa axis represents the observation angles ψ. For the left panel, the ordinate axis represents the ratio of the light intensity scattered by the sample to the light intensity scattered on magnesium oxide under normal illumination and observed at the angle of 5 degrees, whereas for the right panel it represents the number of reflections in the given direction *N*. As one can observe from Fig. 1, the shape and the position of the scattering indicatrice maxima obtained using the developed model are in a good agreement with experimental data.

Monte Carlo simulation [9] was used in our study. The general simulation algorithm for light reflection from the diffuse surface of a scintillator consists of the following steps (the step 2 is repeated many times):

1. The direction of the incident ray on the reflecting surface is specified.

2. Reflection laws are defined for the selected type of the model:

2.1. Model of diffuse reflection: uniform reflection direction to the upper hemisphere is sampled under Lambert law.

2.2. Model of effective reflectivity:

1) the probability of specular or diffuse reflection is sampled;

2) depending on the reflection type (specular or diffuse), the ray is directed in accordance with specular reflection law or Lambert law, respectively.

2.3. Model of micro-facets:

1) orientation of micro-facet normal is sampled from the uniform distribution within limits with respect to the general surface normal;

2) taking into account the incident ray orientation with respect to a randomly oriented micro-facet, the reflected ray direction is determined in accordance with the specular reflection law.

2.4. Developed model:

1) orientation of micro-facet normal with respect to the general surface is sampled from the experimental distribution defined by the surface treatment conditions;

2) taking into account the incident ray orientation with respect to randomly orientated micro-facet, the reflected ray direction is determined in accordance with the specular reflection law and total internal reflection.

3. The reflected rays are sorted by homogeneously specified directions. The obtained distribution represents the scattering indicatrix of the light incident at a specified angle on the reflecting surface.

The relative changes of the light output in the scintillator/conical light guide system were determined experimentally for different light collection conditions at the lateral light guide surface. The light output of a scintillator is known to be determined by the expression $V = \eta \cdot \tau$, where η is the light yield defined by the scintillator material, τ is the light collection coefficient defined by the detector optical properties. The scintillator light yield was fixed in the experiment. In this case, all the light output variations are associated with the changes in the light collection conditions (i.e. τ).

Six light guides of the same shape were used in our study (samples Nos. 1–6). Initially, all the sample surfaces were polished. Then the following changes of the lateral surfaces were introduced to the samples Nos. 2–6:

— matting by an abrasive with grain size of 10 μm (sample No.2);

— white enamel coating (sample No.3);

— black enamel coating (sample No.4);

— wrapping with one layer of TETRATEX film by "Tetratec Europe Ltd", England (sample No.5);

— wrapping with one layer of aluminum foil (sample No.6).

The light output relative change was determined from the change of full absorption peak position during the uniform excitation of the scintillator volume by 662 keV γ-ray photons from a ^{137}Cs source. A packed NaI:Tl scintillator without immersion of ∅ 25 mm×25 mm size and 20 mm high conical light guides with the top and bottom face diameters of 30 mm and 67 mm, respectively, made of acrylic plastic were used to carry out the measurements. The light guide bottom face was placed on a photomultiplier tube (PMT), the scintillator was placed on the light guide top face. Vaseline oil was used as the optical contact at the scintillator/light guide/PMT interfaces. The radioactive source was placed 85 mm above the scintillator/conical light guide system. The measurements were performed using a scintillation spectrometer unit consisting of the studied scintillator and light guide, Hamamatsu R1307 PMT, PU-1 preamplifier, analog-digital converter (ADC) with EVT-SP-4p amplifier. The spectra were collected and processed by a personal computer. The results of the light collection coefficient measurements for all the samples are presented in Table.

The experimental and simulation results of the scintillator/light guide system were compared to estimate the efficiency of the models described above and to define the optimal application conditions thereof. The following refraction indices were used in our simulations: $n_a = 1$ for the air, $n_o = 1.5$ for the vaseline oil, $n_g = 1.48$ for the acrylic plastic, $n_e = 1.48$ for the binder of the black and white enamel, $n_s = 1.85$ for the NaI:Tl single crystal. The point of the scintillation appearance was set in the center of the scintillator. The number of photons per one scintillation at the 662 keV energy absorption was set to 26480 that corresponds to the NaI:Tl scintillation efficiency of 40000 photons/MeV. The simulation results are presented in Table. Normalization of the light collection coefficients were normalized to the τ value for the completely polished surface.

The wide spread in the calculated of τ values for the white and black enamels in comparison to the experimental ones is explained by the lack of knowledge of a diffuse reflection coefficient (R) for these materials. Indeed, the R value depends on the

Table. Experimental and calculated normalized light collection coefficients for the scintillator/light guide system

Lateral surface	Light collection coefficient, τ				
	Experiment	Surface model			
		Lambert	Effective reflectivity	Micro-facets	Developed
Polishing	1.00	1.00	1.00	1.00	1.00
Matting	1.02	1.43	1.09	1.25	0.98
Tetratex	1.16	1.52	1.18	1.09	1.15
Foil	1.15	1.10	1.10	1.09	1.10
White enamel	1.14	1.76	1.24	1.24	1.32
Black enamel	1.00	1.09	1.09	1.09	1.17

incident light wavelength and an abrupt change of R by several times is observed in the wavelength range of 300 to 400 nm [1]. The τ value depends also on the condition of the enamel dispersed phase [6]. That is why these two materials were excluded from the comparative analysis. Comparison of the obtained τ values for the four remaining types of the surfaces has shown that the best agreement with the experiment is provided by the developed model (less than 4 % deviation from experimental values) and by the effective reflectivity model (less than 7 % deviation). The worst agreement with experiment is observed in case of Lambert description (deviation up to 31 %).

The best agreement between the simulation and experimental results is achieved under two conditions: (a) taking into account the residual roughness of the polished surface in the simulation; (b) proper selection of reflection coefficients for the reflectors. The reflection coefficients of TETRATEX film R_t = 0.78 and aluminum foil R_f = 0.75 were used in the calculations. The reference reflection coefficients of these materials are somewhat higher and the use thereof in routine results in a deviation from the experiment. Similar fitting conditions between the model and the experiment were used in [7] and gave also a beneficial effect.

Thus, a model of reflecting surface has been developed that takes into account the real state of the surface treatment. The known results of the micro-facet orientation distributions for glass surfaces treated by different abrasives were used in the model. Basing on the fact that these distributions are almost independent of the microhardness and elastic properties of the treated scitillators and are only defined by the treatment conditions and abrasive powder size, those distribution data were used to simulate the light collection in the materials with different hardness.

The efficiency of the proposed model is confirmed by agreement of the shape and the position of maxima between the calculated light scattering indicatrices for the surfaces with various roughness degree and the experimental results [6]. Comparison between the calculated results of the light collection for different rough surface models and the experimental ones in a scintillator/conical light guide system with different types of lateral surfaces indicates that the best agreement is obtained when the developed model is used. This is provided under conditions of the proper reflection coefficient choice for the reflectors and by the introduction of the residual roughness for the polished surface.

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Порівняння моделей шорсткуватої поверхні при комп'ютерному моделюванні світлозбирання у системі "сцинтилятор — світловод"

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Розроблено комп'ютерну модель відбиваючої поверхні на основі даних про розподіл нахилів мікрограней для поверхонь стекол, оброблених різними абразивами. Ці розподіли використовувалися для моделювання світлозбирання у сцинтиляторах. Ефективність моделі підтверджується збігом між розрахованими індикатрисами розсіювання світла для поверхонь із різним ступенем шорсткості з раніше отриманими експериментальними результатами. Порівняння розрахунків коефіцієнта світлозбирання для різних моделей поверхні у системі "сцинтилятор — світловод" з експериментальними результатами показало, що розроблена модель дає найкраще узгодження.