Correction to: LIGHTAWE—case studies of LIGHT spreAd in poWder materials: a montE carlo simulation tool for research and educational purposes

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Due to a technical error during the production process, in the originally published online PDF version of this Article part of Appendix B was not published. This error has now been corrected. The Publisher apologizes for this mistake and all related inconveniences caused by this.

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1 Introduction

Research and development of imaging systems can be looked at from two different perspectives: (a) the purpose of image acquisition and (b) the physical principles and technological aspects of the system. For instance, in medical imaging, new innovations are associated either with the radiographer's option and assessment of a particular patient examination for validate diagnosis or with the physical and technological factors that affect the imaging chain and contribute to image formation of improved quality [1]. Regarding the second point of view, one crucial step of the so-called "image chain approach" that lead to the final output (i.e., the image) is the fidelity of the information transfer processes [2, 3]. A variety of imaging techniques with tremendous potential of applications use the branch of light transfer mechanisms with purpose to construct high-performance displays and devices in the visible portion of the electromagnetic spectrum [4–10]. More specifically, intermediate step of the imaging system involves the behavior and properties of light, including its interactions with matter. There are cases where the state of matter (either organic or inorganic) is found in granular structure, that is, as in the form of an ensemble of particles. In such powder materials, subject of interest and examination is the trajectories of light ray tracks, the type of light beam interactions with the particles and the overall optical transmission, reflection and diffusion.

This realm of opportunity for knowledge discovery in imaging information and technology can be still thought of a Pandora's Box since comprehensive quantitative and qualitative understanding is lacking and experimental modalities are extremely costly for such demands. On the other hand, the introduction of computational techniques, the so-called Monte Carlo methods [11], and their widespread use [12, 13], on radiation transport simulations over the last 50 years tender them very promising to solve problems that might be deterministic in principle, however, is difficult or impossible to use other approaches. In particular, the advantage of Monte Carlo method to perform experiments that would be otherwise impossible could be proved crucial for the enhancement of research curiosity which in turn may lead to spectacular scientific discoveries. In this paper, LIGHTAWE Monte Carlo simulation tool is introduced and presented with purpose to insight and further enlighten the study of light spread in powder materials for either research or educational applications. The algorithms of LIGHTAWE are based on Mie scattering theory and Henyey-Greenstein distribution [14–17]. The main issues of LIGHTAWE (design and capabilities) are analytically addressed and described below in terms of the: (i) physics embedded, (ii) treatment of the software, (iii) input data contents (iv) simulation options,

(v) output results, (vi) advantages and benefits and (vii) disadvantages and limitations.

2 Materials and methods

The LIGHTAWE Monte Carlo simulation tool (software as well as corresponding support—if required) is sent to the applicant via e-mail. The main components are briefly presented below including the: (a) physics, and (b) treatment of LIGHTAWE Monte Carlo software.

2.1 The physics of LIGHTAWE

The purpose of LIGHTAWE is to provide optical diffusion studies in granular materials. The powder material was considered as an ensemble of uniformly distributed spherical particles glued together with a binding material and coated in three-dimensional layer. Light quanta are generated and thereafter diffused within the material. Light attenuation is described through light ray interactions (scattering and absorption) with the particles which play the role of "optical scatterers" within the granular structure. A light photon history is considered to start within the phosphor layer with the coordinates of the initial position and the initial direction angles (polar and azimuthal) determined by an isotropic distribution. Thereafter, the intrinsic processes of light propagation are summarized in three stages: (i) first stage: the light photon travels a free path length and afterwards interacts with a phosphor particle, (ii) second stage: the light photons is either absorbed or scattered and finally (iii) third stage: the trajectory of the light photon is terminated (in case of absorption) or the direction of the light photon is changed (in case of scattering). The mathematical expressions of the light quanta interaction mechanisms are analytically provided in a previous article (Appendix B of Ref. [18]). In addition, mathematical analysis of the simulation algorithms requires the evaluation of three optical parameters which correspond to the aforementioned stages: (a) the light extinction coefficient, m_{ext} and (b) the anisotropy scattering factor, g and (c) the percentage light absorption probability p . Their evaluation is carried out within the framework of Mie scattering theory and Henyey-Greenstein distribution, as analytically provided in a previous article (Appendix A of Ref. [18]).

2.2 The treatment of LIGHTAWE

LIGHTAWE has been developed in MATLAB environment and includes a user-friendly guide in the command window divided in two branches: (a) The input data of the desired simulation and (b) The output results of the executable simulation.

Table 1 Table summarizes the customization of LIGHTAWE Monte Carlo software

LIGHTAWE Monte Carlo software

Input data		
Required condition: $0.1 < x < 100$ where $x = \pi d n_{\text{medium}} / \lambda$, x : Mie size parameter, d : particle diameter, n_{medium} : refractive index of the of the medium, λ : light wavelength		
Layer settings		
x-dimension (cm)	0.1–10	
y-dimension (cm)	0.1–10	
Thickness (μm)	1–1000	
Number of pixels	64–512	
Structural properties		
Particle diameter (nm)	10–20,000	
Packing density (%)	10–90	
Optical properties		
Light wavelength (nm)	400–700	
Refractive index of the material (Real part)	1.5–2.5	
Refractive index of the material (Imaginary part)	10^{-6} – 10^{-4}	
Refractive index of the medium (binder)	1.0–1.5	
Light beam properties		
Number of light photons	1 – 10^7	
Simulation options		
(a) Fixed light point source		
Site of light source (% layer depth)	10–90	
(b) Distribution of light sources obtained by X-ray attenuation		
X-ray energy (keV)	10–100	
Material composition	Table 2	
Material density (g/cm^3)	Table 2	
Recommended values apart from the fixed X-ray energy range		
Output data		
Optical parameters	The light extinction coefficient $m_{\text{ext}} (\mu\text{m})^{-1}$	
	The anisotropy factor g	
	The light absorption probability p (%)	
Computation time (min)	According to the setting parameters	
Figure	Light performance (reflected, transmitted, absorbed)	LSF (reflected, transmitted)
	Distribution of light photons per depth of interaction	MTF (reflected, transmitted, pixel)

2.2.1 The input data of LIGHTAWE

The input data required to feed the software of LIGHTAWE are summarized in Table 1. Initially, the user browses for the folder of the code in the MATLAB platform, thereafter the name LIGHTAWE is typed in the command window and the execution of the simulation starts. Basic required condition for the execution of proposed simulations is the Mie size parameter (Table 1) to be more than 0.1 and less than 100 (the so-called “Mie regime”). In such case, the following data are asked from the user: (i) Layer settings: x dimension, y dimension, thickness and number of pixels, (ii) Structural properties: Particle diameter and Packing density, (iii) Optical properties: light wavelength, particle refractive index (real part), particle refractive index (imaginary part), binder refractive index. The numerical values of the aforementioned parameters, provided in Table 1, correspond to representative typical values, however, are recommended (suggestive) for the decision of user’s choice (apart from

the X-ray energy range which is fixed). A point worth commenting is that the selection of particular parameters affect correspondingly the computation time.

2.2.2 The simulation options of LIGHTAWE

After inserting the input data described above, the user sets the number of the light photons used in the proposed simulation. Thereafter, there are two main options of simulations embedded in LIGHTAWE: (a) Fixed light point source (i.e., fixed depth of light photon generation within the layer) and (b) Distribution of light sources obtained from X-ray attenuation (i.e., variable depth of optical photon generation within the layer taken from the penetration of an X-ray beam of particular energy within a specific phosphor material). The first case examines in general the light spread in powder materials (including phosphors) while the second case examines the light spread in specific powder phosphor materials. Therefore, the first case requires the percentage

Table 2 List of phosphor materials included in LIGHTAWE

Phosphor materials	Typical density (g/cm ³)	Probability of photo-electric effect for X-ray energies 10 keV and 100 keV	Fluorescence yield values ω_K of the heaviest element	Mean Energy of $K\alpha$ X-rays of the heaviest element (keV)	Mean path length of K X-rays of the heaviest element (μm)
1 Ba ₄ Ce ₃ F ₁₇	5.54	0.9993–0.9313	0.9096	34.50	657
2 BaCl ₂	3.89	0.9993–0.9185	0.8997	32.00	831
3 BaF ₂	4.90	0.9993–0.9314	0.8997	32.00	617
4 BaHfO ₃	8.40	0.9994–0.9601	0.9505	55.20	389
5 BaLu ₂ F ₈	7.00	1.0000–0.9568	0.9487	53.52	578
6 BaThF ₆	6.70	0.9842–0.9221	0.9691	91.65	1564
7 BaY ₂ F ₈	5.00	0.9989–0.8756	0.8997	32.00	399
8 Ba ₄ Y ₃ F ₁₇	5.25	1.0000–0.9040	0.8997	32.00	437
9 Bi ₄ Ge ₃ O ₁₂ (BGO)	7.10	0.9993–0.9712	0.9643	75.96	1315
10 CaHfO ₃	7.50	1.0000–0.9574	0.9505	55.20	891
11 CaWO ₄	6.10	0.9990–0.9579	0.9538	58.65	1236
12 CeCl ₃	3.90	0.9993–0.9143	0.9096	34.50	1007
13 CeF ₃	6.20	0.9993–0.9309	0.9096	34.50	578
14 CsF	4.10	1.0000–0.9370	0.8942	30.80	625
15 CsI	4.51	0.9994–0.9434	0.8942	30.80	526
16 CsGd ₂ F ₇	5.50	1.0000–0.9462	0.9320	42.65	464
17 Cs ₂ LiYCl ₆	3.30	0.9991–0.8938	0.8942	30.80	730
18 Cs ₃ LuCl ₆	3.80	0.9993–0.9404	0.9487	53.52	773
19 Cs ₃ Lu ₂ Cl ₉	4.00	0.9992–0.9245	0.9487	53.52	1113
20 Cs ₂ NaCeCl ₆	3.20	1.0000–0.8712	0.9096	34.50	1667
21 Cs ₂ NaLaCl ₆	3.20	0.9993–0.9138	0.9049	33.24	1164
22 Cs ₂ NaLuCl ₆	3.70	0.9993–0.9369	0.9487	53.52	944
23 GdAlO ₃ (GAP)	7.50	1.0000–0.9431	0.9320	42.65	656
24 GdBr ₃	4.60	1.0000–0.9267	0.9320	42.65	689
25 GdBO ₃	6.30	0.9995–0.9473	0.9320	42.65	736
26 Gd ₃ Ga ₅ O ₁₂	7.10	0.9993–0.9244	0.9320	42.65	638
27 Gd ₂ O ₂ S (GOS)	7.30	0.9996–0.9551	0.9320	42.65	554
28 Gd ₂ SiO ₅ (GSO)	6.70	0.9995–0.9484	0.9320	42.65	673
29 Gd ₃ Sc ₂ Al ₃ O ₁₂	5.60	0.9994–0.9309	0.9320	42.65	996
30 K ₂ LaCl ₅	2.90	0.9991–0.8592	0.9049	33.24	1663
31 LaBO ₃	5.20	0.9993–0.9256	0.9049	33.24	674
32 LaB ₃ O ₆	4.20	0.9990–0.8969	0.9049	33.24	1108
33 LaBr ₃	5.30	1.0000–0.9045	0.9049	33.24	334
34 LaCl ₃	3.90	0.9993–0.9094	0.9049	33.24	963
35 LaF ₃	5.90	0.9993–0.9275	0.9049	33.24	586
36 LaLuO ₃	8.40	0.9994–0.9594	0.9487	53.52	349
37 LiBaF ₃	5.30	0.9992–0.9201	0.8997	32.00	650
38 LiLuF ₄	6.00	0.9993–0.9569	0.9487	53.52	1087
39 LiLuSiO ₄	5.50	1.0000–0.9528	0.9487	53.52	1247
40 LiYF ₄	4.00	0.9976–0.7452	0.7155	14.92	382
41 LuAlO ₃ (LuAP)	8.30	0.9994–0.9582	0.9487	53.52	760
42 Lu ₃ Al ₅ O ₁₂	6.70	0.9993–0.9516	0.9487	53.52	1057
43 Lu ₂ O ₃	9.40	0.9995–0.9684	0.9487	53.52	544
44 LuBO ₃	6.90	1.0000–0.9611	0.9487	53.52	863
45 LuBr ₃	4.80	1.0000–0.9433	0.9487	53.52	1066
46 LuCl ₃	4.00	1.0000–0.9531	0.9487	53.52	1688
47 LuF ₃	8.30	0.9994–0.9620	0.9487	53.52	711

Table 2 (continued)

Phosphor materials	Typical density (g/cm ³)	Probability of photoelectric effect for X-ray energies 10 keV and 100 keV	Fluorescence yield values ω_K of the heaviest element	Mean Energy of $K\alpha$ X-rays of the heaviest element (keV)	Mean path length of K X-rays of the heaviest element (μm)
48 LuPO ₄	6.50	0.9993–0.9543	0.9487	53.52	1038
49 Lu ₂ S ₃	6.25	0.9994–0.9635	0.9487	53.52	894
50 Lu ₂ SiO ₅ (LSO)	7.40	1.0000–0.9622	0.9487	53.52	786
51 Lu ₂ Si ₂ O ₇ (LPS)	6.20	0.9993–0.9560	0.9487	53.52	1049
52 NaI	3.67	0.9993–0.9277	0.8819	28.46	644
53 RbGd ₂ Br ₇	4.80	0.9992–0.9180	0.9320	42.65	646
54 RbGd ₂ Cl ₇	3.70	0.9994–0.9259	0.9320	42.65	1286
55 PbWO ₄ (PWO)	8.28	0.9994–0.9743	0.9634	73.89	461
56 YAlO ₃ (YAP)	5.50	0.9979–0.7515	0.7155	14.92	252
57 Y ₃ Al ₅ O ₁₂ (YAG)	4.60	0.9973–0.7126	0.7155	14.92	339
58 YBO ₃	4.50	0.9979–0.7707	0.7155	14.92	305
59 Y ₂ O ₃	5.00	0.9985–0.8196	0.7155	14.92	215
60 Y ₂ SiO ₅ (YSO)	4.50	0.9983–0.7774	0.7155	14.92	279
61 YTaO ₄	7.50	0.9993–0.9533	0.9522	56.90	801
62 ZnS	4.10	0.9994–0.6361	0.4857	8.63	21

Table provides: (i) the chemical compound, (ii) the typical density of the compound [30–32], (iii) the probability of photoelectric effect for 10 keV and 100 keV, (iv) the fluorescence yield values ω_K of the heaviest element [33], (v) the mean energy of $K\alpha$ X-rays of the heaviest element [34] and (vi) the mean path length of K X-rays of the heaviest element

depth with respect to layer thickness, while the second one, the determination of the X-ray energy (10–100 keV) as well as the chemical compound and the density of the phosphor material.

Regarding the second case, LIGHTAWE includes 62 different chemical compounds with their corresponding density, listed in Table 2. All materials are considered to be in powder form although most of them are commonly and commercially found in other structural forms (e.g., crystal, ceramic, etc.). However, advanced techniques in chemical synthesis methods over the past decade (e.g., chemical vapour deposition, microemulsion route, spray pyrolysis, co-precipitation, sol–gel combustion synthesis, etc.) could replace existing forms of phosphors and give a boost on a new realm of opportunity in granular phosphor development [19] including also powders at submicron and nano scales, even down to 10 nm since in lower sizes a particle size-dependent dielectric function should be considered (usually assuming a Drude–Sommerfeld model) due to the lattice strain effects [20]. A characteristic example is the cerium doped lutetium orthosilicate—Lu₂SiO₅:Ce (LSO) fluorescent material which was initially introduced as a single-crystal scintillator [21] but later was also fabricated in powder coating. Table 2 also provides the probability of photoelectric effect for the two limiting values of X-ray energy (10 keV and 100 keV) to show the domination of photoelectric effect over the scattering (Compton and Rayleigh) phenomena which have been excluded from LIGHTAWE.

To make the code easier and faster, X-ray photons considered to follow only photoelectric absorption and the X-ray energy was considered to be locally absorbed in the interaction site excluding also the emission of fluorescence X-rays (K X-rays). However, relative additional information of the K X-rays effect is provided in Table 2, such as: (i) the probability of K X-rays production though the fluorescence yield ω_K of the heaviest element, (ii) the spread of K X-rays within the material through the mean path length of $K\alpha$ X-rays based on their corresponding energy.

2.2.3 The output results of LIGHTAWE

The output results of LIGHTAWE are summarized in Table 1. The optical parameters, m_{ext} , g and p (%), used to simulate the optical tracks (see Sect. 2.2.1) are provided to the user as output results in the command window. After the termination of the simulation, command window also shows the computation time required to run the proposed simulation and an output figure is observed. The figure illustrates four separate subplots of the following information: (i) the light performance which contains: (a) the percentage of light photons reflected at the upper side of the layer (the back side of the layer also called irradiated side in case of X-ray penetration) (b) the percentage of light photons transmitted at the underside of the layer (the front side of the layer also called non-irradiated side in case of X-ray penetration), and (c) the percentage of light photons absorbed within the material,

(ii) the distribution of light photons per depth of interaction within the layer, (iii) the Line Spread Function (LSF) for reflection and transmission mode and (iv) the Modulation Transfer Function (MTF) for reflection and transmission mode as well as the so-called pixel-MTF due to the pixel size. The mathematical evaluation of LSF and MTF are analytically provided in a previous article (Appendix C of Ref. [18]). After the execution of each simulation, two additional files have been created within the folder of the code. The first one opens with MATLAB and concerns the illustration of the figure and the second one opens with notepad and records all the setting parameters involved in the simulation. In this manuscript, a specific simulation example of LIGHTAWE is presented in [Appendix A](#) (brief physics) and [Appendix B](#) (interface). The computation time corresponds to a single computer of i5 CPU 3.47 GHz processor and 4.00 GB RAM.

3 Discussion

3.1 LIGHTAWE advantages and benefits

LIGHTAWE has been developed to perform dedicated Monte Carlo simulations of light spread in powder materials. An advantage of LIGHTAWE for optical diffusion studies is the separation of two different branches: (i) the study of light spread within a granular layer based only on its structural and optical properties, (ii) the examination of particular powder phosphor materials taking into account the depth of the X-ray penetration. The above options make LIGHTAWE an available and useful tool for a variety of instrumentations which incorporate granular structured materials, such as medical and storage phosphor imaging, radioluminescent and fluorescence sensing, detecting tools of biological structures, and phosphor-based white LED devices. The performance of optical diffusion could also enhance research on particle characterization methods, microscopy techniques, homeland security as well as national defense applications and finally could have an impact on several scientific fields including chemical, energy, optoelectronic and space industries.

The investigation of optical diffusion can be thought of a Pandora's Box since comprehensive quantitative and qualitative understanding is lacking and experimental set-ups are extremely costly for such demands. However, the option of LIGHTAWE to alter a set of parameters (listed in [Table 1](#)) and perform a countless number of probable and comparable simulations, can insight and further enlighten the research of light spread performance. In addition, based on the Monte Carlo methodology, LIGHTAWE can overcome cumbersome analytical modelling, inconvenience and fussiness [22] and can take advantage of computer science to perform experiments that would be otherwise impossible

(i.e., the capability to design, evaluate and optimize “virtual” experimental set-ups of “zero cost” or with “low risk” actions) enhancing curiosity-driven future research [23].

An objective disadvantage of Monte Carlo packages is the lack of making user-friendly software with the result the corresponding difficulty of the users to treat the structure of the code. In academic institutions, the majority of PhD students need particular training on Monte Carlo packages by more experienced researchers or they are called to attend particular workshops [24] to adapt to the setting parameters demands of ‘black box’ simulation tools. The ease to use treatment of LIGHTAWE is one of its major advantages and can also be a useful computational tool for educational purposes in academic institutions. The study of light spread under the variability of several parameters offers pedagogic ways of learning optical diffusion in powder structures and also provides important information about statistical phenomena that would be impossible to assess otherwise.

3.2 LIGHTAWE disadvantages and limitations

Due to the programming algorithms that rely on repeated random sampling to obtain numerical results and reproduce stochastic processes statistically, high computation time is required for precision achievement. Like in most Monte Carlo codes and packages, LIGHTAWE depends on the computation time via the number of light photons and the corresponding simulation of long light tracks. Particular parameters increase dramatically the trajectories of light photons within the material, such as: (i) the increase of the layer thickness, (ii) the increase of the packing density, which expresses the spatial distribution of phosphor particles within the phosphor layer, (iii) the size of the particle diameter (mainly in the submicron scale). However, acceleration of the simulation runs can be accomplished by the availability of advanced calculating tools (e.g., clusters or powerful CPUs). Of course, Monte Carlo is an average method, i.e., the average expectation of one observable is computed, however, this approach is fine if the system is ergodic [25].

LIGHTAWE provides a series of capabilities on studying the optical diffusion, however, light propagation modeling is subject of several limitations. The investigation of light spread in real powder structures is limited to the considerations of X-ray and light beam characteristics, such as (i) the absence of X-ray scattering, K X-rays and Auger electrons, polychromatic light photons, reflection at the boundaries, and absorbing dyes incorporation. The modelling of light spread is based on specific methodology (Mie-scattering algorithms) and the accuracy is related to Riccati–Bessel functions. The assumption of spherical particles in contrast to arbitrary sized and shaped particles in real structures is also an issue worth commenting.

The validity of the present computational program has been provided in terms of: (a) the algorithms applied for the sampling

of physical parameters, such as (i) the free path length, (ii) the optical attenuation (scattering and absorption) coefficients, and (iii) the scattering angles, [26] (b) the absorption and scattering efficiency factors and the complex elements of Mueller scattering matrix [26, 27] (c) the prediction and comparison of the optical parameters (light extinction coefficient m_{ext} , anisotropy factor g , probability of light absorption p) with other Mie calculators [28] for a variety of grain sizes [29]. Particular comparisons with experimental data have also been carried out for $\text{Gd}_2\text{O}_2\text{S}:\text{Tb}$ phosphor material [26].

However, matter of fact, most of the times the construction of the real powder layers has remained trade secrets from the manufacturers and comparison with experimental measurements (apart from the weakness of different experimental set-ups to re-produce identical results for similar samples) is always subject of various types of uncertainties on the material synthesis, development and construction, such as: (i) the precise concentration of activator dopant, (ii) the type of the binding material and the incorporation of unknown additional substances (e.g., absorbing dyes), (iii) the exact particle size and shape, etc.

4 Appendix A: brief physics of the simulation example

The geometry of the simulation model considers a phosphor layer modeled as a three-dimensional powder material consisting of uniformly distributed particles (phosphor grains of equal size) of $\text{Gd}_2\text{O}_2\text{S}$ luminescent material (case 27 of the list of materials) embedded within a binding medium (Na_2SiO_3). The geometry of the layer contains (a) phosphor dimensions: (i) surface dimensions: 1 cm (length) and 1 cm (width), (ii) number of pixels of surface area: 127 and (iii) layer thickness: 200 μm ; (b) structural properties: (i) density: 7.3 g/cm^3 , (ii) packing density: 50%, and (iii) particle size: 7 μm , (c) optical properties: (i) light wavelength: 545 nm, (ii) refractive index of the phosphor grains: (real part: 2.3, imaginary part: 10^{-5}), (iii) refractive index of the surrounding medium: 1.35. The phosphor layer surface was assumed to be irradiated by a pencil monoenergetic X-ray beam with energy 20 keV. This energy corresponds to mass attenuation coefficient 36.88 cm^2/g for $\text{Gd}_2\text{O}_2\text{S}$ and determines the distribution of the X-ray photon absorbed (i.e., the interaction sites) and, therefore, the distribution of light photons produced (10^6 light photons were chosen) per depth of interaction within the layer. The Monte Carlo simulation involves the following steps:

4.1 Step A: X-ray attenuation

To simulate the X-ray transport within the phosphor layer, the model initially determines the free path length (fpl) of

each X-ray quantum of energy E , according to the following expression:

$$\text{fpl} = \frac{1}{\mu(E) \rho \rho_p} \ln R \quad (1)$$

where $\mu(E)$ is the mass attenuation coefficient of the phosphor material, ρ is the bulk density, and ρ_p is the packing density.

4.2 Step B: X-ray to light conversion and diffusion

For each X-ray photon interaction event leading to energy deposition, light photons are produced following an isotropic spatial distribution. After their creation, light photons are transmitted through material towards the layer surfaces according to the following stages:

4.2.1 First stage: light travel until interaction

Light photon travels a free path length and afterwards interacts with a phosphor particle. This distance determined according to the following equation:

$$\text{fpl} = \frac{1}{m_{\text{ext}}} \ln R \quad (2)$$

where R is a random number uniformly distributed in the interval $(0, 1]$ and m_{ext} is the Mie light extinction coefficient which is computed by the following formula:

$$m_{\text{ext}} = V_d A Q_{\text{ext}} \quad (3)$$

where V_d is the volume density of the phosphor material, A is the geometrical cross-section of the grain and Q_{ext} is the extinction efficiency factors. For the presented geometry, the m_{ext} coefficient was evaluated equal to 0.216 μm^{-1} .

4.2.2 Second stage: light interaction

Light photon is either absorbed or scattered. At the site of light photon interaction, the type of interaction is expressed by the probability of light absorption p . This probability is calculated using the Mie light absorption and scattering coefficients m_{abs} , m_{sct} , as follows:

$$p = \frac{m_{\text{abs}}}{m_{\text{abs}} + m_{\text{sct}}} \quad (4)$$

For a random number R , if $R \leq p$ light photon is absorbed and the photon track within the material terminates, otherwise if $R > p$ light photon is scattered and the photon track continues in a new direction. For the presented geometry, the p coefficient was evaluated equal to 0.08111%.

Fig. 1 Figure illustrates four separate subplots of the: (i) light performance which contains: **a** the percentage of light photons reflected at the upper side of the layer, **b** the percentage of light photons transmitted at the underside of the layer, and **c** the percentage of light photons absorbed within the material, (ii) distribution of light photons per

depth of interaction within the layer, (iii) LSF for reflection and transmission mode and (iv) MTF for reflection and transmission mode as well as the so-called pixel-MTF due to the pixel size effect. The setting parameters are provided in the [Appendix A](#) and [Appendix B](#) sections

4.2.3 Third stage: light scattering

In case of scattering, the new direction of light photon is determined from the Henyey-Greenstein distribution, as given below:

$$\cos \theta = \frac{1}{2g} \left[1 + g^2 - \left(\frac{1 - g^2}{1 - g + 2gR} \right)^2 \right] \text{ when } g \neq 0 \quad (5)$$

The free parameter g is the anisotropy factor, which implies isotropic distribution of light for $g = 0$ and sharply forward direction of light for $g = 1$. R is a random number uniformly distributed in the interval $(0, 1]$. The anisotropy factor was calculated using the following equation:

$$g = \frac{\int_0^\pi 2\pi S_{11}(\theta) \cos \theta \sin \theta d\theta}{\int_0^\pi 2\pi S_{11}(\theta) \sin \theta d\theta} \quad (6)$$

where $S_{11}(\theta)$ is the first element of the so-called Mueller matrix, which implies that light extinction is independent of the light polarization state. For the presented geometry, the g factor was evaluated equal to 0.736. Results are illustrated in Fig. 1 which includes the following subplots: (i) the light performance, (ii) distribution of light photons per depth of interaction within the layer, (iii) LSF for reflection and transmission mode and (iv) MTF for reflection and transmission mode as well as the so-called pixel-MTF due to the pixel size effect.

5 Appendix B: interface of the simulation example

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1 .....
2 WELCOME TO LIGHTAWE - START THE SIMULATION
3 .....
4 .....
5 .....
6 INPUT DATA - START
7 .....
8 .....
9 .....
10 LAYER SETTINGS
11 .....
12 SET THE X-AXIS DIMENSION OF THE LAYER IN CENTIMETERS
13 CHOOSE BETWEEN 0.1 - 10
14 X-AXIS (CENTIMETERS):1
15 SET THE Y-AXIS DIMENSION OF THE LAYER IN CENTIMETERS
16 CHOOSE BETWEEN 0.1 - 10
17 Y-AXIS (CENTIMETERS):1
18 SET THE THICKNESS OF THE LAYER IN MICROMETERS
19 CHOOSE BETWEEN 1 - 1000
20 THICKNESS (MICROMETERS):100
21 SET THE NUMBER OF PIXELS OF THE IMAGE (LAYER OUTPUT)
22 CHOOSE 64 - 512
23 NUMBER OF PIXELS:127
24 .....
25 .....
26 .....
27 STRUCTURAL PROPERTIES OF THE MATERIAL
28 .....
29 SET THE PARTICLE DIAMETER IN NANOMETERS
30 CHOOSE BETWEEN 10 - 20000
31 PARTICLE DIAMETER(NANOMETERS):7000
32 SET THE PARTICLE PACKING
33 CHOOSE BETWEEN 0.10 - 0.90
34 PACKING DENSITY: 0.50
35 .....
36 .....
37 .....
38 OPTICAL PROPERTIES OF THE MATERIAL
39 .....
40 SET THE LIGHT WAVELENGTH IN NANOMETERS
41 CHOOSE BETWEEN 400 - 700
42 LIGHT_WAVELENGTH (NANOMETERS):545
43 SET THE REFRACTIVE INDEX OF THE MATERIAL - REAL PART
44 CHOOSE BETWEEN 1.5 - 2.5

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45 **REFRACTIVE INDEX OF THE MATERIAL (REAL PART):2.3**
 46 **SET THE REFRACTIVE INDEX OF THE MATERIAL - IMAGINARY PART**
 47 **CHOOSE BETWEEN 10^{-6} - 10^{-4}**
 48 **REFRACTIVE INDEX OF THE MATERIAL (IMAGINARY PART): 10^{-5}**
 59 **SET THE REFRACTIVE INDEX OF THE MEDIUM (BINDER)**
 50 **CHOOSE BETWEEN 1.0 - 1.5**
 51 **REFRACTIVE INDEX OF THE MEDIUM (BINDER):1.35**
 52
 53
 54
 55 **LIGHT BEAM PROPERTIES**
 56
 57 **SET THE NUMBER OF LIGHT PHOTONS**
 58 **CHOOSE BETWEEN 1 - 10^7**
 59 **NUMBER OF LIGHT PHOTONS:1000000**
 60
 61 **SET THE OPTION OF SIMULATION**
 62
 63 **CASE 1: FIXED LIGHT POINT SOURCE**
 64 **CASE 2: DISTRIBUTION OF LIGHT SOURCES - X-RAY PENETRATION**
 65 **CHOOSE 1 OR 2**
 66 **CASE:2**
 67
 68
 69 **SET THE X-RAY ENERGY (keV)**
 70 **CHOOSE BETWEEN 10 - 100**
 71 **X-RAY ENERGY (keV):20**
 72
 73
 74 **SET THE MATERIAL COMPOSITION**
 75 **CHOOSE BETWEEN 1 - 62**
 76
 77 **CASE 1: Ba₄Ce₃F₁₇**
 78 **CASE 2: BaCl₂**
 79 **CASE 3: BaF₂**
 80 **CASE 4: BaHfO₃**
 81 **CASE 5: BaLu₂F₈**
 82 **CASE 6: BaThF₆**
 83 **CASE 7: BaY₂F₈**
 84 **CASE 8: Ba₄Y₃F₁₇**
 85 **CASE 9: Bi₄Ge₃O₁₂ (BGO)**
 86 **CASE 10: CaHfO₃**
 87 **CASE 11: CaWO₄**
 88 **CASE 12: CeCl₃**
 89 **CASE 13: CeF₃**
 90 **CASE 14: CsF**

91	CASE 15: CsI
92	CASE 16: CsGd₂F₇
93	CASE 17: Cs₂LiYCl₆
94	CASE 18: Cs₃LuCl₆
95	CASE 19: Cs₃Lu₂Cl₉
96	CASE 20: Cs₂NaCeCl₆
97	CASE 21: Cs₂NaLaCl₆
98	CASE 22: Cs₂NaLuCl₆
99	CASE 23: GdAlO₃ (GAP)
100	CASE 24: GdBr₃
101	CASE 25: GdBO₃
102	CASE 26: Gd₃Ga₅O₁₂
103	CASE 27: Gd₂O₂S (GOS)
104	CASE 28: Gd₂SiO₅ (GSO)
105	CASE 29: Gd₃Sc₂Al₃O₁₂
106	CASE 30: K₂LaCl₅
107	CASE 31: LaBO₃
108	CASE 32: LaB₃O₆
109	CASE 33: LaBr₃
110	CASE 34: LaCl₃
111	CASE 35: LaF₃
112	CASE 36: LaLuO₃
113	CASE 37: LiBaF₃
114	CASE 38: LiLuF₄
115	CASE 39: LiLuSiO₄
116	CASE 40: LiYF₄
117	CASE 41: LuAlO₃(LuAP)
118	CASE 42: Lu₃Al₅O₁₂
119	CASE 43: Lu₂O₃
120	CASE 44: LuBO₃
121	CASE 45: LuBr₃
122	CASE 46: LuCl₃
123	CASE 47: LuF₃
124	CASE 48: LuPO₄
125	CASE 49: Lu₂S₃
126	CASE 50: Lu₂SiO₅ (LSO)
127	CASE 51: Lu₂Si₂O₇
128	CASE 52: NaI
129	CASE 53: RbGd₂Br₇
130	CASE 54: RbGd₂Cl₇
131	CASE 55: PbWO₄
132	CASE 56: YAlO₃ (YAP)
133	CASE 57: Y₃Al₅O₁₂ (YAG)
134	CASE 58: YBO₃
135	CASE 59: Y₂O₃
136	CASE 60: Y₂SiO₅ (YSO)

```

137  CASE 61: YTaO4
138  CASE 62: ZnS
139  .....
140  MATERIAL COMPOSITION - CASE:27
141  .....
142  SET THE DENSITY OF THE MATERIAL (g/cm^3)
143  MATERIAL DENSITY (g/cm^3):7.3
144  .....
145  INPUT DATA - END
146  .....
147
148  .....
149  OUTPUT DATA - START
150  .....
151
152  LIGHT EXTINCTION COEFFICIENT ( $\mu\text{m}^{-1}$ ):
153  0.216
154  ANISOTROPY FACTOR:
155  0.736
156  PROBABILITY OF LIGHT ABSORPTION (%)
157  0.08111
158  COMPUTATION TIME(MIN)
159  20.61
160  .....
161  OUTPUT DATA - END
162  .....

```

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