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Integration of polarization in the LUTDavis Model for optical Monte Carlo simulation in radiation detectors

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Abstract

Cerenkov photons have distinctive features from scintillation photons. Among them is their polarization: their electric field is always perpendicular to the direction of propagation of light and parallel to the plane of incidence. Scintillation photons are instead considered unpolarized. This study aims at understanding and optimizing the reflectance of polarized Cerenkov photons for optical Monte Carlo simulation of scintillation detectors with Geant4/GATE. First, the Cerenkov emission spectrum and polarization were implemented in the previously developed look-up-table Davis model of crystal reflectance. Next, we modified Geant4/GATE source code to account for scintillation and Cerenkov photons LUTs simultaneously. Then, we performed optical Monte Carlo simulations in BGO using GATE to show the effect of Cerenkov features on the photons' momentum at the photodetector face, using two surface finishes, with and without reflector.

In this work, we describe the new features added to the algorithm and GATE. We showed that Cerenkov characteristics affect their probability to be reflected/refracted and thus their travel path within a material. We showed the importance of accounting for accurate Cerenkov photons reflectance while performing advanced optical Monte Carlo simulations.

Keywords

Cerenkov photons; photon polarization; LUT Davis model; Geant4/GATE

1. Introduction

In recent years, great attention has been given to prompt Cerenkov photons to improve coincidence timing resolution measurement (Lecoq, 2012; Korpar, et al., 2011; Somlai-Schweiger & Ziegler, 2015 ; Ariño-Estrada, et al., 2018; Cates & Levin, 2019; Ota, et al., 2019; Kratochwil, et al., 2020; Gundacker, et al., 2020).

Cerenkov photons differ from scintillation photons by their physical properties. They are emitted at a specific angle with respect to the direction of a charged particle (if the charged particle kinetic energy is above an energy threshold), which defines the so-called

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Cerenkov cone, while scintillation photons are emitted isotropically. The Cerenkov spectrum is continuous and decreases with increasing wavelength, while the scintillation spectrum is usually peaked between 380nm and 480nm, depending on the material. Cerenkov emission is also much faster (a few ps) than atomic or molecular transitions producing scintillation photons (a few ns). Lastly, Cerenkov photons have a specific polarization: their electric field is perpendicular to the surface of the Cerenkov cone, whereas the magnetic field is tangent to it. In contrast, the electric field of scintillation photons does not have a preferred direction, and therefore they are considered unpolarized (Jelley, 1955; Jelley, 1961; Lahoti & Takwale, 1977).

Our group previously developed a crystal reflectance model computed from lutetium oxyorthosilicate (LSO) 3D crystal surface measurement (Roncali & Cherry, 2013; Roncali, et al., 2017), which was implemented in Geant4/GATE since GATE V8.0 (Stockhoff, et al., 2017). Furthermore, this model has been integrated into an open-source standalone application to allow researchers to generate their fully customized crystal reflectance look-up tables (LUTs) (Trigila, et al., 2021).

Cerenkov LUTs were already computed with our algorithm for several materials (bismuth germanate BGO and thallium bromide TlBr) using their Cerenkov emission spectrum and index of refraction as a function of the wavelength (Ariño-Estrada, et al., 2020; Roncali, et al., 2019). However, the crystal reflectance/transmittance was always computed applying Fresnel equations for unpolarized photons.

The first goal of this study was to include polarization within the reflectance algorithm. We studied the influence of Cerenkov photons polarization on the reflectance of polished and rough surfaces in BGO. We generated separate LUTs for unpolarized photons or polarized photons. Geant4/GATE v9.0 source codes were modified to simultaneously simulate scintillation and Cerenkov photons using their specific unpolarized or polarized LUTs. The second goal was to investigate the effect of polarization in BGO crystals using optical Monte Carlo simulations in GATE. We studied the photons' momentum angular distribution at the photodetector face using these new LUTs, testing different surface finishes, with and without reflectors (Teflon).

This work describes the novelties added in the algorithm and GATE, showing the importance of accounting for Cerenkov photons features to perform advanced optical simulations.

2. Materials and Methods

2.1 The Davis LUTs model and the addition of Cerenkov photon polarization

A detailed description of the last version of the LUT model of crystal reflectance can be found in (Trigila & Roncali, 2021). Briefly, the algorithm computes the reflection and transmission probabilities and the ray angular distributions as a function of incidence angles of a given crystal finish (using its topography 3D scanned with atomic force microscopy) coupled to several coupling media (e.g., air or grease). It also includes the possibility of computing the reflectance of a crystal surface coupled to a reflector, modeled as a horizontal plane at a fixed distance from the mean height of the surface. The reflectance properties are then saved in LUTs, which can be used inside optical Monte Carlo simulation using GATE to investigate the light transport and the light collection within crystals.

The algorithm computes the crystal reflectance and the direction of the photons by virtually illuminating the 3D surface with a collimated beam of photons, each with a specific wavelength randomly extracted by the emission spectrum of the selected crystal (figure 1(a)). The beam impinges on the surface with an incident polar angle θ varying between 0° and 90°. For each polar angle the azimuthal angle ϕ is varied from 0° to 360° every 3°. The photon's probability to be reflected or refracted by the crystal surface in contact with the coupling medium at a specific incident angle is locally evaluated using the Fresnel equation.

The Fresnel equation (equation 1) computes the reflectance of an unpolarized photon on a perfectly flat optical interface between two media. An unpolarized photon is an electromagnetic wave whose electric field can be modeled as the sum of two polarization components, one parallel and one perpendicular to the photon plane of incidence, usually called *p*- and *s*- polarization, respectively (figure 1(b)). Unpolarized light reflectance is consequently modeled as the sum of two independent reflectance contributions with polarization, each with half the intensity (R_s and R_p in equation 1). Each contribution depends on the media refractive indices n_1 and n_2 (e.g., BGO, n_1=2.15, in contact with air, n_2=1) and on the photon incident angle θ_1 at the media interface (figure 1). θ_2 represents the refraction angle and is estimated using Snell's law. The sum of the reflectance and transmittance naturally equals 1.

$$R = \frac{1}{2}(Rs + Rp) = \frac{1}{2}\left(\left(\frac{n_1 \cos\theta_1 - n_2 \cos\theta_2}{n_1 \cos\theta_1 + n_2 \cos\theta_2}\right)^2 + \left(\frac{n_1 \cos\theta_2 - n_2 \cos\theta_1}{n_1 \cos\theta_1 + n_2 \cos\theta_2}\right)^2\right) \quad (1)$$

Figure 2 shows the unpolarized light's reflectance R and transmittance T (black lines in figures 2(a–b) respectively) as a function of the incident angle calculated using the Fresnel equation together with the contributions of the *s*- (red lines) and *p*-(green lines) polarizations. As expected from equation1, R and T are the mean value of the R_s and R_p contributions for each incidence angle.

This equation was used within the algorithm to generate LUTs for unpolarized scintillation photons. However, the electric field of Cerenkov photons is always oriented along the plane of incidence, and consequently, we modified the Fresnel equation to include only the p-polarization contribution (R_p) when computing LUT for Cerenkov photons.

We separately computed the *Unpolarized Photons LUTs* and the *Cerenkov Photons LUTs* using BGO polished and rough surfaces, accounting for the scintillation and Cerenkov emission spectra accordingly. For both LUTs, we used a wavelength-dependent index of refraction (Roncali, et al., 2019).

2.2 New Geant4/GATE code to use scintillation and Cerenkov reflectance LUTs simultaneously

Unpolarized Photons LUTs and *Cerenkov Photon LUTs* were merged into a *Scintillation-Cerenkov LUT* to account for scintillation and Cerenkov photon reflectance simultaneously during GATE simulations.

The current version of GATE (Sarrut, et al., 2021) does not support LUTs containing information for different photon types. We modified the Geant4/GATE source code to use these new LUTs. During a simulation, an optical photon is tagged based on its nature (figure 3): 1 for scintillation and 2 for Cerenkov photon. Once a photon arrives on the crystal edge, the tag is used to extract the correct reflectance and angular distribution within the *Scintillation-Cerenkov* LUTs.

2.3 Optical Monte Carlo simulation with Geant4/GATE v9.0

To test the effect of polarization, we performed optical Monte Carlo simulations in a $3 \times 3 \times 20\ mm^3$ BGO crystal with the toolkit GATE v9.0 (figure 4). We defined the radiation sources as the 0.420 MeV electrons corresponding to electrons generated by 511 keV photoelectric interactions in BGO. We used the same simulation seeds so that the scintillation and Cerenkov photons were generated from the same electrons to only consider the effect of Cerenkov photon characteristics on their transport and detection using different LUTs.

We generated 200,000 electrons at the center of the crystal cross-section, 5, 10, and 15 mm away from the photodetector face and towards it. The photodetector was placed in one of the $3\times3\ mm^2$ crystal faces and its geometric efficiency and quantum efficiency were set to 1.

We used the *Unpolarized Photons LUTs* or merged *Scintillation-Cerenkov LUTs* on all crystal surfaces: air-coupled polished or rough surface with and without a reflector (Teflon) at the edges, and grease-coupled polished surface for the photodetector face.

For all these configurations, we studied the distribution of the detected photons' incident angle on the photodetector face, estimated from their momentum before detection and the surface normal. We divided the detected optical photons into three families to investigate the effect of Cerenkov features on the photodetector face and the lateral edges (figure 4): photons directly detected (no reflections), photons detected after one reflection, and photons detected after more than one reflection.

3. Results

3.1 Cerenkov photons characteristics effect on reflectance

Figure 5 shows the angular distribution of reflectance without reflector, for the polished (figure 5(a)) and rough surface (figure 5(b)) when considering unpolarized and p-polarized photons.

With the polished surface, the reflectance follows the Fresnel equation (shown in figure 2). Polarization primarily affects the reflectance at intermediate incident angles, with both coupling media (10–35° with air; 20–43° with grease). Of interest is the effect with a grease-coupling (blue) representing the interface in contact with the photodetector, which is expected to change the distribution of detected Cerenkov photons. With the rough surface, the polarization effect is lower compared to the polished surface, although it affects a larger range of incident angles, mainly when considering a grease coupling. Similar results are obtained with the air- and grease-coupled surfaces with Teflon (not-shown).

Cerenkov photon features included in the LUTs also slightly change the angular distribution of reflected/transmitted rays (not shown). The changes in the reflectance and in the angular distribution are expected to alter the photon travel path inside the crystal.

3.2 Optical Monte Carlo simulations with GATE

3.2.1 Effect of polarization on the detected photons' incident angle on the photodetector face—The directly detected photons' incidence angles distribution on the photodetector face (not shown) hinges on the source position compared to the photodetector face. Photons emitted at the center of the crystal at ~5, ~10 and ~15 mm arrive on the photodetector face with a maximum incident angle of ~17°, ~9° and 6°, respectively. In this angular range, their reflectance is slightly affected by polarization (polished-grease, figure 5), and consequently, their incidence angle distribution. However, the closer the photons are emitted to the photodetector, the larger the solid angle on the photodetector face and consequently the effect of polarization.

Figure 6 shows the normalized distribution of the incidence angles on the photodetector face after one (figure 6(a)) or more reflections (figure 6(b)) when emitted 5 mm far from this face and when using LUTs with reflectors.

All distributions follow the reflectance trends (polished-grease, figure 5). Photons arriving with an angle lower than ~42° (critical angle for a BGO/grease interface) undergo transmissions on the photodetector face and are detected. All distributions steeply decrease around this angle. At greater angles, photons experience internal reflections.

As expected, the scintillation and Cerenkov distributions are similar when using the *Unpolarized LUTs* (bold lines in figures 6) since the photon fate is determined by the same LUTs, regardless of their nature. In contrast, the detected Cerenkov photon distributions obtained using the *Scintillation-Cerenkov LUTs* show a shift towards lower incident angles in all configurations. The behavior is expected from the reflectance changes when considering polarization and is due to the combined effect of the polarization on the lateral edges and on the photodetector face when photons arrive with an incident angle higher than ~20°, where its effect starts to be important (figure 5). It is already evident after only one reflection (figure 6(a)) and becomes even more important when photons undergo more than one reflection. Similar results are obtained when using LUTs without reflector and when considering 10 mm and 15 mm as emission depth (not shown).

Since the effect of polarization was already clear at 5 mm, we did not investigate emission points closer to the photodetector face. Moreover, we did not move the electron source emission point on the x-y plane. By moving the source on the x-y plane, we expect the directly detected photons to arrive on the photodetector face with a larger range of incident angles than those emitted at the crystal center. This could lead to an increased polarization effect on their angular distribution on the photodetector face and an increased number of internal reflections. For what concerns the photon detected after one or multiple reflections, we expect to have a similar trend as the one shown with the photons emitted at the center of the crystal (figure 6(b)). This distribution depends, indeed, on the LUT used on the photodetector face. Thus, the effect should be the same, although there could be a difference in the number of detected photons.

4. Discussion and Conclusions

In this work, we presented the implementation of Cerenkov polarization inside the previously developed LUT Davis model (Roncali & Cherry, 2013; Roncali, et al., 2017; Trigila & Roncali, 2021). We generated LUTs for both scintillation (unpolarized) and Cerenkov (p-polarized) photons, accounting for their emission spectra accordingly. We showed that, for both polished and rough finish, Cerenkov characteristics affect the surfaces' reflectance.

We carried out Monte Carlo simulations using GATE v.9.0 (Sarrut, et al., 2021) modified to simultaneously account for scintillation and Cerenkov photons. Until now, there was no possibility to use separate LUTs for each photon type. We showed that Cerenkov photons physical features integrated into the LUTs changed the photon angular distribution on the photodetector face, affecting the results of optical simulations in several configurations.

The obtained simulation results suggest that considering the physical characteristics of scintillation and Cerenkov photons separately during the LUTs generation is important to carry out more accurate optical Monte Carlo simulations. The changes in the photons' momentum are expected to affect the photon travel path towards the photodetector and subsequently the detection efficiency, timing performance and other detector characteristics in a way that will be thoroughly analysed in future work.

The LUT Davis model has been previously integrated into GATE (Stockhoff, et al., 2017). We developed a standalone open-source application to allow researchers to generate their fully customized crystal reflectance LUTs (Trigila, et al., 2021). In the next release, it will allow generating fully customized Cerenkov LUTs. Last, Geant4/GATE changes will be added in their next releases and are currently available upon request to the authors.

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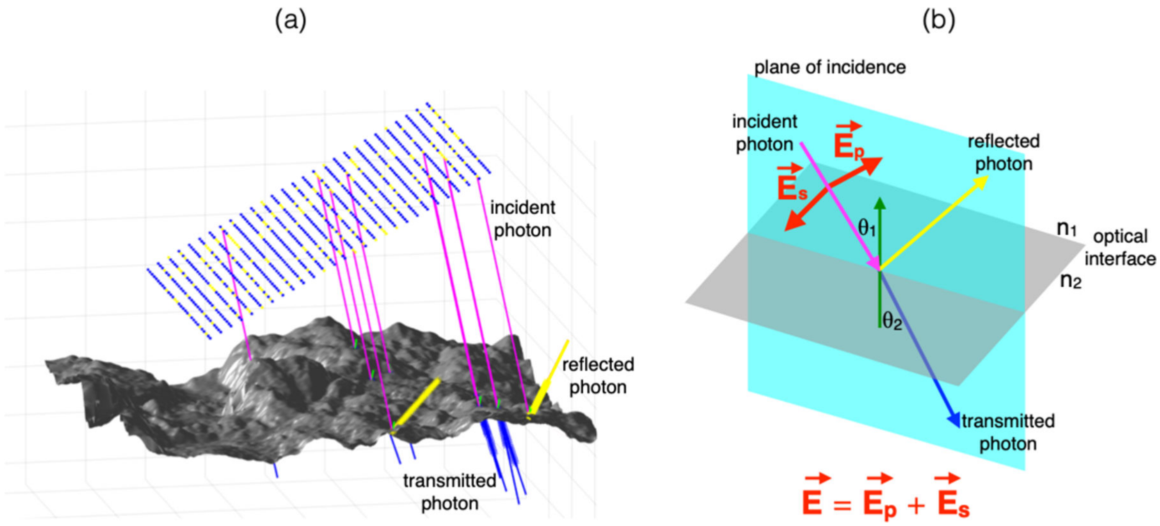

Figure 1:
(a) In the algorithm, a 3D surface is virtually illuminated with a collimated beam of photons (magenta) to compute the crystal reflectance. These photons can be reflected (yellow) or transmitted (blue). For a given surface-coupling-reflector combination, two LUTs are saved: the reflectance and the transmittance LUT. (b) The photon's probability of being reflected or refracted by an optical interface between two media with different indexes of refraction (n_1 and n_2) at a specific incident angle Θ_1 is locally evaluated using the Fresnel equation for unpolarized light. Unpolarized light is an electromagnetic wave whose electric field can be modeled as the sum of two polarization components, one parallel to the photon plane of incidence and one perpendicular, usually called *p-* and *s-* polarization, respectively.

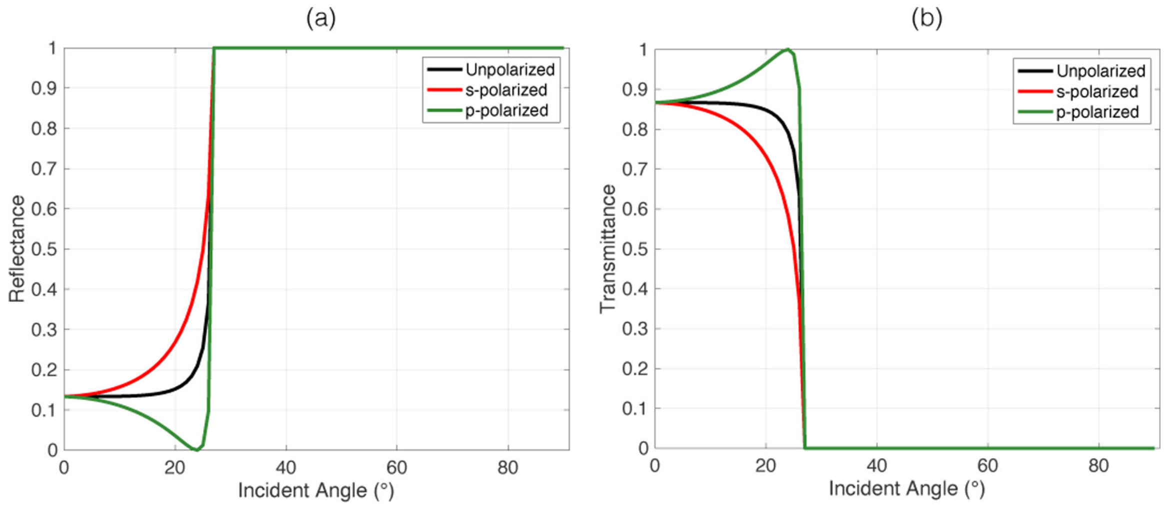

Figure 2:
(a) Reflectance and (b) transmittance as a function of the incident angle in BGO in contact with air. The black lines represent the reflectance and transmittance obtained using the Fresnel equation for unpolarized light (equation 1). The red and green lines represent the *s*-polarization and *p*-polarization contributions, respectively.

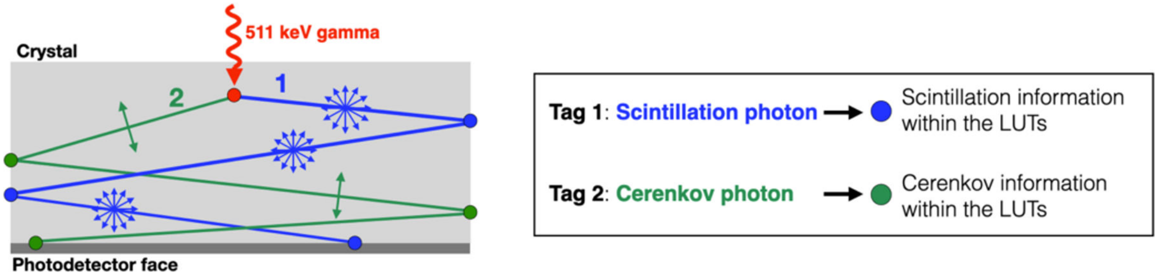

Figure 3:
Geant4/GATE codes were modified to read Scintillation-Cerenkov LUT. A tag was added to identify the photon nature: 1 for scintillation and 2 for Cerenkov photons. The tag is used to read the corresponding information within the LUT.

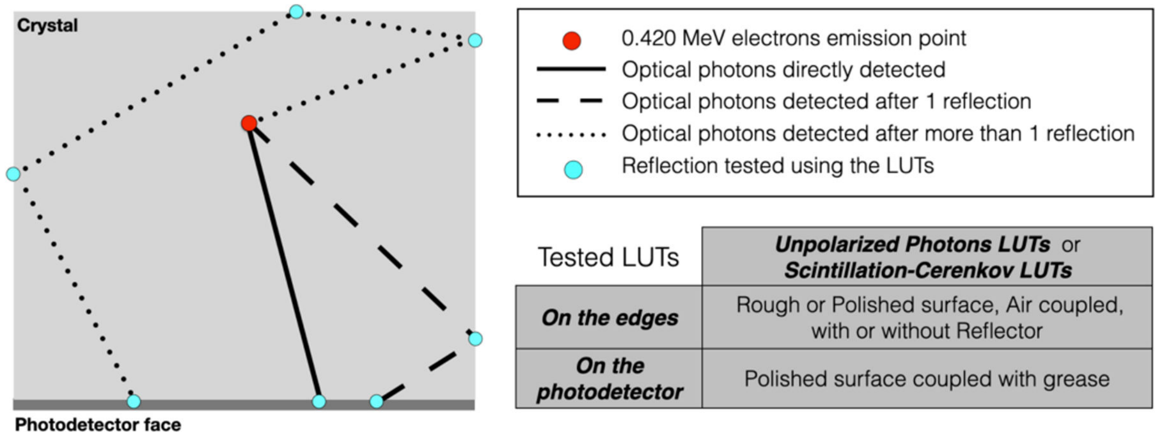

Figure 4:

Schematic view of the simulation performed with GATE. 0.420 MeV electrons were emitted in a 3 × 3 × 20 mm^3 BGO crystal towards the photodetector face. The electrons were emitted 5, 10, and 15 mm far from the photodetector. We tested several LUTs, with and without polarization. The optical photons generated by both scintillation and Cerenkov radiation were separated into different families to investigate the effect of polarization on the crystal edges and the photodetector face. The image is not to scale.

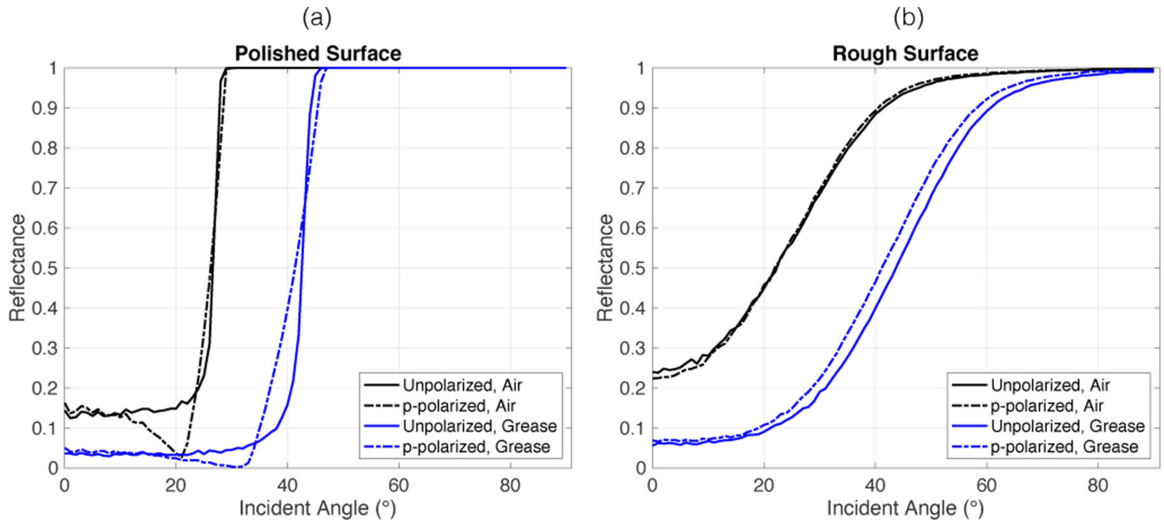

Figure 5:

Reflectance for the (a) polished and (b) rough surface, both air- (black) or grease- (blue) coupled, when considering unpolarized (scintillation, bold lines) or p-polarized (Cerenkov, dotted lines) photons.

Relative percentage variation of the p-polarized reflectance with respect to the unpolarized reflectance at 20°,40° and 60°: −66.1%, 0%, 0% for the polished surface air-coupled; −24.8%, +158.5%, 0% for the polished surface grease-coupled; −0.1%, +1.4%, 0.3% for the rough surface air-coupled; 18.6%, 18.4%, 3.8% for the rough surface grease-coupled.

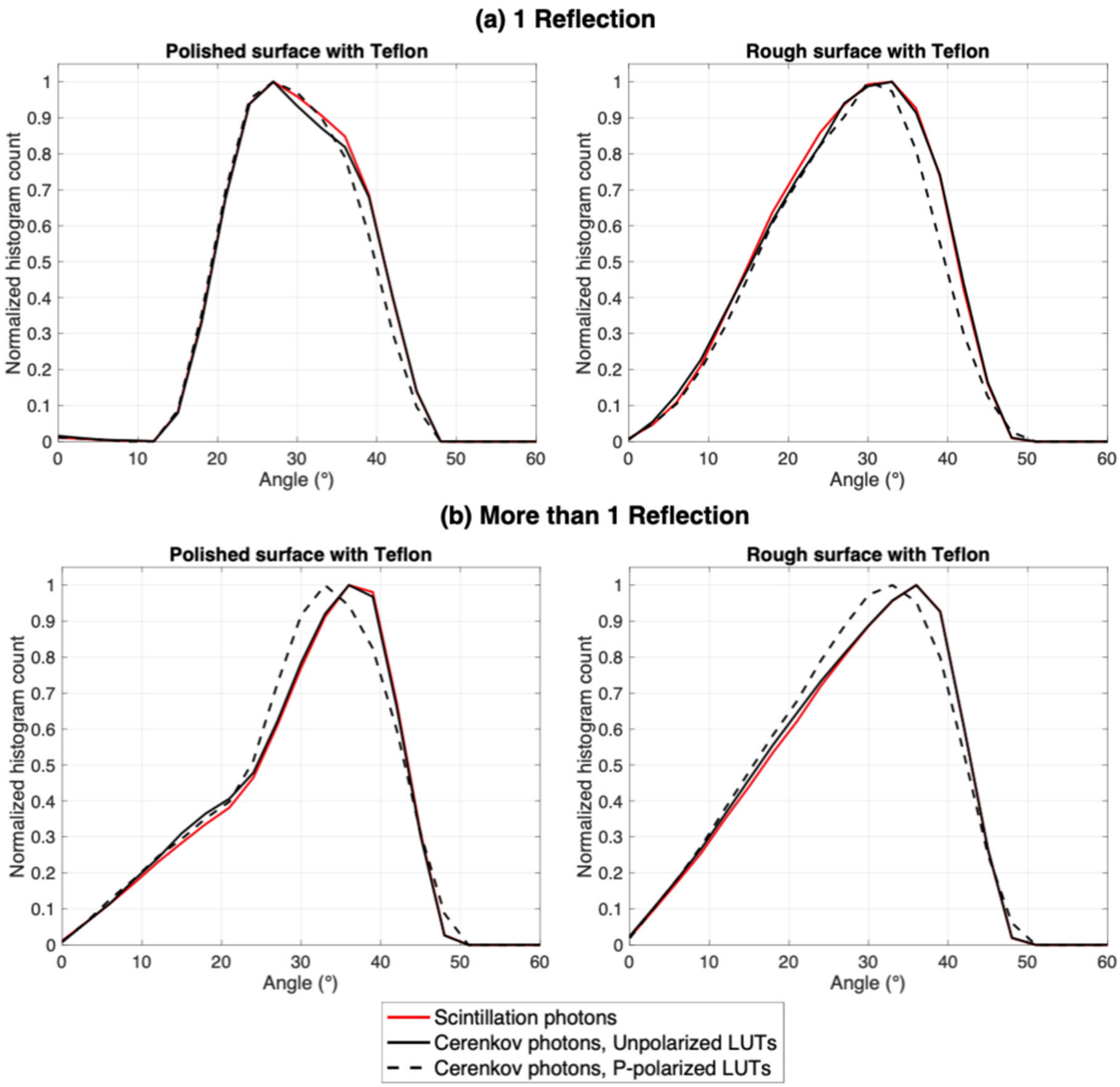

Figure 6:

Distribution of the detected photons' incident angle on the photodetector face for several simulated configurations for (a) the photons detected after one reflection or (b) after more than one reflection. In bold, the scintillation and Cerenkov photons distribution when using Unpolarized LUTs. The dotted lines show the results when using the Scintillation-Cerenkov LUTs. These LUTs cause the Cerenkov photon distribution to be shifted towards lower incident angles in all configurations.