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LETTER

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Letter

Advanced optical simulation of scintillation detectors in GATE V8.0: first implementation of a reflectance model based on measured data

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Abstract

Typical PET detectors are composed of a scintillator coupled to a photodetector that detects scintillation photons produced when high energy gamma photons interact with the crystal. A critical performance factor is the collection efficiency of these scintillation photons, which can be optimized through simulation. Accurate modelling of photon interactions with crystal surfaces is essential in optical simulations, but the existing UNIFIED model in GATE is often inaccurate, especially for rough surfaces. Previously a new approach for modelling surface reflections based on measured surfaces was validated using custom Monte Carlo code. In this work, the LUT Davis model is implemented and validated in GATE and GEANT4, and is made accessible for all users in the nuclear imaging research community. Look-up-tables (LUTs) from various crystal surfaces are calculated based on measured surfaces obtained by atomic force microscopy. The LUTs include photon reflection probabilities and directions depending on incidence angle. We provide LUTs for rough and polished surfaces with different reflectors and coupling media. Validation parameters include light output measured at different depths of interaction in the crystal and photon track lengths, as both parameters are strongly dependent on reflector characteristics and distinguish between models. Results from the GATE/GEANT4 beta version are compared to those from our custom code and experimental data, as well as the UNIFIED model. GATE simulations with the LUT Davis model show average variations in light output of <2% from the custom code and excellent agreement for track lengths with $R^2 > 0.99$. Experimental data agree within 9% for relative light output. The new model also simplifies surface definition, as no complex input parameters are needed. The LUT Davis model makes optical simulations for nuclear imaging detectors much more precise, especially for studies with rough crystal surfaces. It will be available in GATE V8.0.

Keywords: scintillation detectors, diagnostic imaging, GATE, GEANT4, Monte Carlo optical simulation, surface finish, light transport model

S Supplementary material for this article is available online

(Some figures may appear in colour only in the online journal)

1. Introduction

Over the past two decades positron emission tomography (PET) has proven to be a powerful nuclear imaging technique. Researchers have pushed the development of detectors to a point where improvement is as small as hundreds of picoseconds in timing resolution, fractions of a millimetre in spatial resolution, or a few percent in energy resolution. As some of these parameters are approaching theoretical limits, simulation software that can precisely predict the behaviour of the different detector components is needed in order to study potential improvements. Typical PET detectors are composed of a scintillation crystal coupled to a photodetector. Scintillator surface treatments include polished, chemically etched and rough, and are combined with reflectors painted, glued, or wrapped around the crystal.

Variations in material, geometry and surface finish change the behaviour of the scintillation photons at the boundaries of the crystal and their subsequent detection. Variation in polishing or roughening processes between manufacturers further increases complexity in modelling. To obtain realistic simulation results, customized characterization of a surface finish would be a valuable tool.

Nuclear imaging simulations can be carried out in open-source simulation toolkits such as GEANT4 or GATE (Agostinelli *et al* 2003, Jan *et al* 2004) that include a sophisticated model for light propagation in scintillation crystals called the UNIFIED model (Nayar *et al* 1991, Levin and Moisan 1996). In this model, the user must define a surface consisting of micro-facets and set four probabilities to control the reflectance. The micro-facet orientations follow a Gaussian distribution with a standard deviation σ_α. Determining σ_α can be challenging, and even when measured experimentally may lead to inaccurate simulations of non-polished surfaces (Bea *et al* 1994, Janecek and Moses 2010, Roncali and Cherry 2013).

Janecek and Moses developed a more realistic model (GEANT4 plugin RealSurface1.0) based on experimental characterization of crystal surface optical properties. Reflectance data are stored in look-up-tables (LUT) prior to simulation and then used to determine the reflection direction of optical photons travelling in the scintillator during the simulation. Though it produces more accurate light output simulations, this approach has two main limitations. First, it relies on a unique experimental setup requiring 25 mm radius scintillator hemispheres, making it labour-intensive and costly to introduce new surfaces. Only bismuth germanate crystals have been measured and made available in the GEANT4 database. Second, the reflection probability is an arbitrary value defined by the user instead of being extracted from the reflectance data.

The approach we have developed (Roncali and Cherry 2013) overcomes some of these limitations by calculating the reflectance properties from the crystal topography measured with

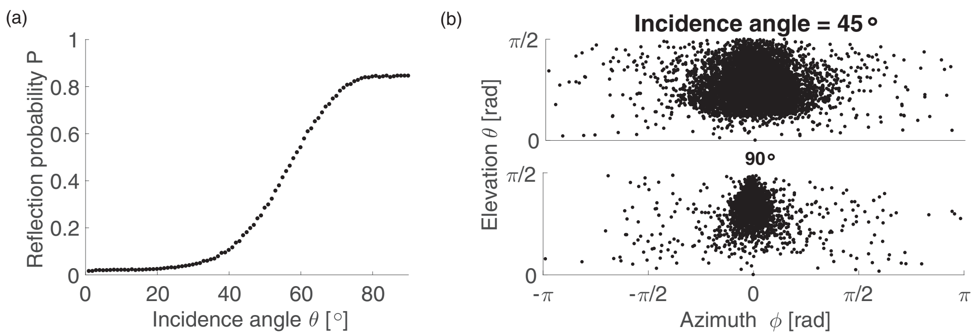

Figure 1. For simulation in GATE/GEANT4, reflectance data for different surface finishes illuminated at incidence between 0° and 90° are stored in two LUTs. (a) Example of a reflection probability LUT from a rough surface without reflector. (b) Direction of reflections (elevation and azimuthal angles in spherical coordinates) for incidence angles of 45° and 90° from a rough surface.

atomic force microscopy (AFM). Here, we implement and validate this model in GEANT4 and GATE including photons transmitted through the reflector. The implementation of our reflectance model gives researchers the tools to accurately predict the light transport in a scintillation crystal with the exact surface definition, which will be instrumental in studies that aim at improving timing resolution, spatial resolution, and depth of interaction (DOI) encoding and involve light transport (Ito *et al* 2011, Lecoq 2012).

2. Materials and methods

2.1. Crystal surface measurements and calculation of look-up-tables

A small number of 45×45 μm² areas of rough 'as cut' and mechanically polished lutetium oxyorthosilicate (LSO) crystals (Crystal Photonics Inc., Florida) was measured using AFM, with 87 nm spatial resolution (Asylum MFP-3D). The surface characterization provides 3D information of the crystal topography. Custom Monte Carlo code is used to compute the reflectance properties of the measured surface by virtually illuminating that surface with ~10^4 photons at each incidence angle. These photons are tracked down to the measured surface, and the probability of reflection is calculated. Next, we calculate the direction of the reflected photons. A detailed explanation of the development of this approach- the LUT Davis model, can be found in Roncali and Cherry (2013) and Roncali *et al* (2017).

Data for incidence angles from 0° to 90° are saved in two LUTs including the reflectivity and the photon reflection directions (figure 1). The reflectance LUTs are computed for crystal surfaces with or without a reflector (figure 2). Lambertian and specular reflectors are modelled: Teflon tape and ESR (Enhanced Specular Reflector Film, Vikuiti™ 3M).

2.2. Implementation in GATE and GEANT4

GEANT4/GATE now include methods to read the LUTs given in table 1, and to apply them to optical photon tracking in the crystal (figure 3). Generated optical data saved in the Hits Tree of the ROOT output (Brun and Rademakers 1997) can be analysed using newly added variables: travel path, travel time, momentum. Details are provided in supplementary figure S1 (stacks.iop.org/PMB/62/L1/mmedia), and in the GATE V8.0 User Guide (OpenGATE Collaboration 2017a, 2017b, 2017c).

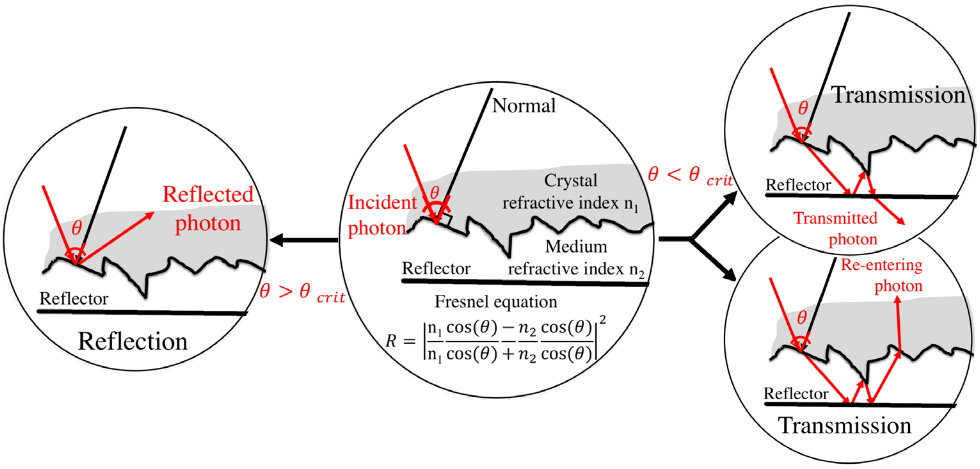

Figure 2. The incident photon reaches a surface and undergoes transmission or reflection with a probability defined by the Fresnel equations. A transmitted photon can re-enter the crystal or be transmitted through the reflector. The angle θ_{crit} sets the limit above which the photon undergoes total internal reflection. Below that angle θ_{crit}, the photon may be transmitted or reflected depending on Fresnel equations.

Table 1. Available surface finishes and reflector combinations in GATE V8.0.

	Bare	Teflon	ESR + air	ESR + Optical grease
Rough	Rough_LUT	RoughTeflon_LUT	RoughESR_LUT	RoughESRGrease_LUT
Polished	Polished_LUT	PolishedTeflon_LUT	PolishedESR_LUT	PolishedESRGrease_LUT

2.3. Validation

2.3.1. Validation against custom Monte Carlo code. The LUT Davis model is applied in custom code similarly to Roncali *et al* (2017). A $3 \times 3 \times 20\,\text{mm}^3$ LSO crystal coupled to a $3 \times 3\,\text{mm}^2$ detector is modelled with the following parameters: light yield 35 photons/keV, absorption length 800 mm for all wavelengths, refractive index 1.82, decay time 40 ns, broad LSO emission spectrum, and detector efficiency 1. The light pulses in the custom code are generated in 2.5 mm bins. In the GATE simulation, two monoenergetic 511 keV sources irradiate the crystal from opposing sides at each DOI (2, 6, 10, 14, and 18 mm from the detector face). No depth bin is modelled. The number of detected photons per pulse, or light output (LO), is a useful validation parameter because it is strongly dependent on the number of reflections per photon and on the reflectance model used to process each reflection. The photon track length (distance from scintillation emission to detection point) is also analysed. It is proportional to the number of reflections per photon and can reveal potential discrepancies if the model does not work reliably.

2.3.2. Validation against experimental data. The setup consists of a reference detector and a test detector. A crystal is coupled to an SiPM with silicone optical grease (Bicron BC-630). The reference detector is irradiated with a Na-22 source from its top face. The test detector is irradiated from the side every 4 mm from the detector, starting at 2 mm. We estimate the bin

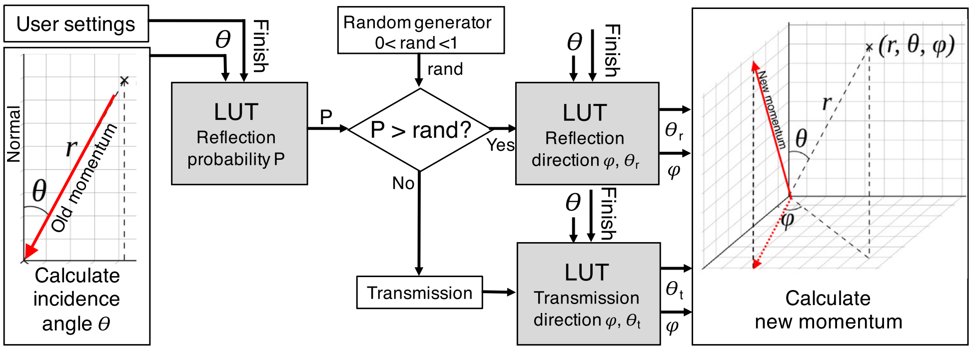

Figure 3. The old momentum is a unit vector describing the incident photon. From left to right: the angle θ between the incident photon (old momentum) and the surface normal is calculated, and the reflection probability is extracted from the LUT corresponding to the surface finish set by the user. A Bernoulli test determines whether the photon is reflected or transmitted, and two angles (φ, θ) are drawn from the reflection/transmission direction LUT. A sequence of geometrical operations produces the new momentum from the selected (φ, $\theta_{r,t}$).

size to be ~2.5 mm (Kwon *et al* 2016). Two rough and two polished crystals are measured with and without attached reflector (same crystals as characterized with AFM to generate the LUTs). The reflector is air-coupled Teflon, wrapped 5 times, or ESR, coupled with air and optical grease, respectively. The LO in the experimental setup is given by the photopeak position and is an indirect measure of the number of detected photons.

Results are also compared to simulations with the UNIFIED model for a crystal with no reflector or Teflon tape. The setup is the same as in section 2.3.1. The model is set to a ground finish with parameters derived from our measured surfaces: σ_α of 18° and 1.3° for rough and mechanically polished surfaces, respectively. For surfaces with Teflon reflector the finish is set to *groundbackpainted* and the reflectivity is set to 0.99 (Levin and Moisan 1996, Janecek and Moses 2010).

3. Results

3.1. Validation against custom Monte Carlo code

3.1.1. Light output. Maximum LO differences for rough surfaces are <1.3%, except for ESR grease which diverges by 5.3% at 18 mm (figure 4). For polished surfaces the maximum absolute difference is less than 100 photons (1.5%). These differences are within statistical variation for such Monte Carlo simulations and codes are considered in excellent agreement. Small discrepancies in the LUTs are likely amplified when using a specular reflector such as ESR, because it reflects a photon according to its incidence angle, while the Lambertian reflection is independent on the incident direction.

3.1.2. Track lengths. Figure 5 shows that the photon track length for custom and GATE simulation is extremely close for all combinations of surface finish and reflector, indicating that the transport of optical photons is modelled similarly in both codes. Results are also in good agreement with results from (Cates *et al* 2015).

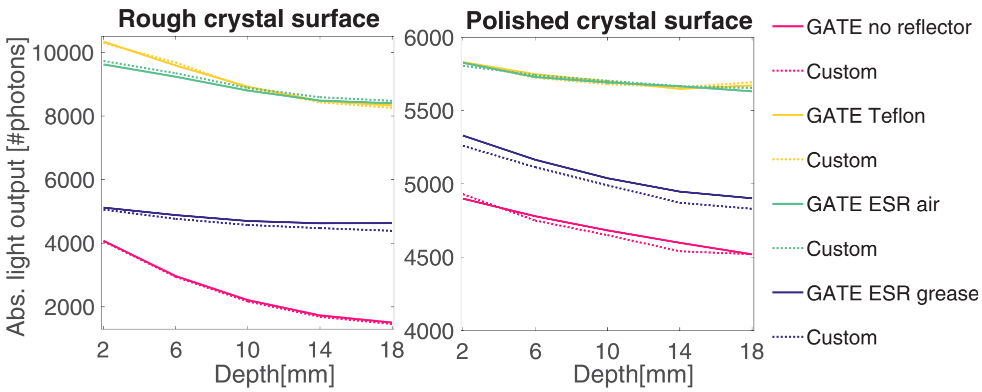

Figure 4. Light collected at different DOIs for a rough and for a polished surface, coupled to various reflectors. The GATE/GEANT4 simulation of the LUT Davis model shows excellent agreement with our validated custom Monte Carlo simulation code.

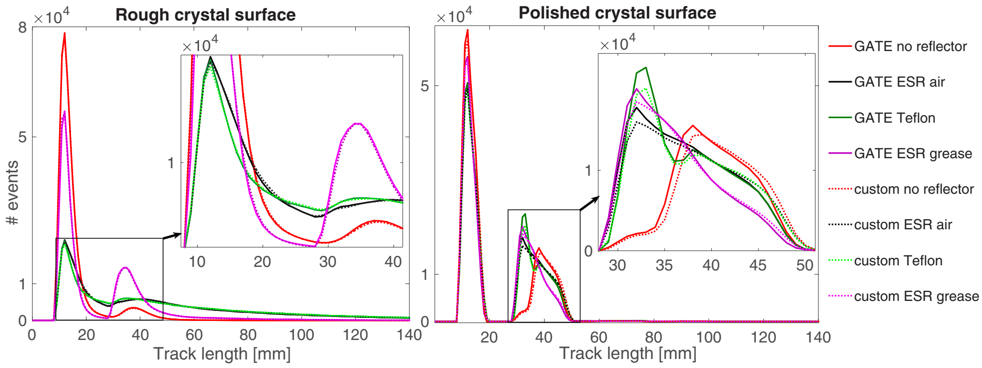

Figure 5. Track length (total distance travelled in the crystal) of $5 \cdot 10^5$ scintillation photons emitted at a DOI of 10 mm and detected by the photodetector. The impact of the crystal surface finish is reflected by the change in the peak shape and amplitude. The track lengths simulated with GATE are very similar to those generated with custom code ($R^2 > 0.99$), indicating excellent agreement of the codes.

3.2. Validation against experimental data

For polished surfaces, the maximum difference is less than 2% for all configurations. For all rough surfaces but ESR-grease the GATE simulation produces LO values close to experimental data, with a maximum difference of 3.9% (figure 6). The LUT for ESR-grease diverges by 9% at 18 mm.

The coupling to the photodetector and reflector wrapping are inherently variable processes, with limited reproducibility, and have a strong effect on the light collection (Roncali *et al* 2017). As we assume perfect crystal-reflector assemblies in the simulation, discrepancies with experiments might occur. The crystal transmittance increases when optical grease is used as a coupling medium instead of air, due to a smaller index mismatch. Imperfect assumptions for reflector coupling thus have a larger effect in the case of a ESR-grease reflector (figure 6).

The polished surface is reasonably well described by the UNIFIED model, with a maximum deviation of 9% with Teflon wrapping. However, the error for rough bare surfaces is 20% and 16% with Teflon. This is because both the reflection probability and direction of reflection

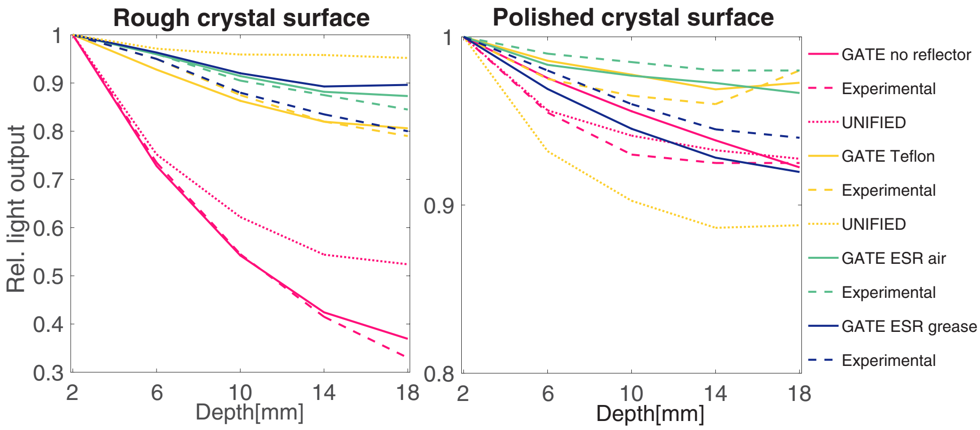

Figure 6. The relative LO as a function of DOI is shown for experimental data and the implemented LUT Davis model in GATE. Trends for different surfaces are normalized by their maximum LO. In contrast, the UNIFIED model shows large variations from the experimental data past the 6 mm DOI position, because inaccuracies in the reflection model add up as the photons undergo more reflections.

depend on multiple factors such as the thickness of the reflector, its refractive index, and the wavelength of the reflected photon, which cannot be reliably simulated with the UNIFIED model.

4. Discussion

The LUT Davis model enables the user to simulate more realistic optical data in scintillators for polished and also rough surfaces. The implementation of the model in GATE/GEANT4 was validated for the upcoming release in 2017. Excellent agreement was achieved between our custom simulation code and GATE code for all rough and polished surfaces, with an average of <2% difference. Both codes showed good agreement with experimental data in terms of relative LO: <2% difference for polished surfaces and <4% for rough surfaces, except ESR-grease (9%). This deviation is quite likely explained both by the large influence of the reflector properties and by the assumption that reflectors are perfectly coupled to the crystal.

The differences of the newly implemented model compared to existing solutions in GATE are fundamental in terms of approach, but pass almost unnoticed to the user in practice, and actually simplify the simulation setup. The modelling of a reflector coupled to the crystal is combined into one single optical surface, and the surface definitions are reduced to one parameter, the finish, set from table 1. This is a tremendous simplification over the UNIFIED model. It is also important to note that the LUT-based approach significantly decreased the computation time by 30% in the configurations presented in this paper.

To facilitate the analysis of optical data, additional variables were implemented in the ROOT Hits tree in GATE V8.0. For instance, the track length of each individual photon can be used to study transit time in the crystal to improve timing performance for time-of-flight detectors, or to improve collection of the scintillation light (e.g. optimizing reflector properties to minimize light loss, or increase light extraction through the photodetector face). The momentum direction of detected photons is also now available, which can be applied to optimize the coupling to the photodetector (e.g. light guide design, anti-reflective coating on the photodetector).

5. Conclusion

The LUT Davis model implementation will be included in GATE V8.0 (April 2017) and GEANT4 (June 2017). LUTs describing rough and polished crystal surfaces without reflector, with a Lambertian reflector (Teflon) and an air- and grease-coupled specular reflector (ESR) have been validated and will be included in the release. The model is based on measurements of actual crystal surfaces. A tool for users to calculate custom LUTs for additional surfaces will be provided in future developments in the form of a graphical user interface.

Acknowledgments

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