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A More Physical Approach to Model the Surface Treatment of Scintillation Counters and its Implementation into DETECT

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Abstract

DETECT is a Monte Carlo simulation capable of realistically modeling the optics of scintillation detectors. A limitation of this widely used program is its lack of realism and flexibility in dealing with the surface finish and reflector coating of photon counters. To address these limitations, we initiated the implementation into DETECT of a more physical model to treat the interactions of scintillation photons with dielectric surfaces. Inspired from the initial work of Nayar *et al.*, this approach has the particular advantage of unifying, into a single parameterization, models that usually apply over a very limited range of surface roughness values. This flexibility is ensured by using the standard deviation of the surface slope as a model parameter that can be extracted from simple measurements.

I. INTRODUCTION

The design of scintillation counters assisted by Monte Carlo simulation can be a time and cost effective approach provided the simulation model allows for a detailed treatment of the counter's geometry as well as of the propagation, absorption, loss or detection of scintillation photons through that geometry. The program DETECT [1] is a Monte Carlo simulation capable of realistically modeling the optics of scintillation detectors. The program isotropically generates a number of scintillation photons in a volume element of the detector and individually tracks their surface interactions and passage within the components of the detector. Optical tracking of a scintillation photon is pursued until it is either absorbed, reaches a detection element, or escapes from the detector volume. The geometry of the detector can be described with a very general syntax. However, an actual limitation of DETECT is its lack of realism and flexibility in modeling the surface finish and reflector coating of photon counters. These limitations become particularly important when addressing the impact of the average roughness, or reflective coating of the counter's surface on the position and energy resolution.

We present here work in progress to implement into our local version of DETECT a more physical model, called the UNIFIED model, to treat the interactions of scintillation photons with dielectric surfaces. We first motivate this work by exposing the options available in DETECT to treat scintillator surfaces and by outlining their limitations. We then outline the UNIFIED surface model, inspired from the work of Nayar *et al.* [2], and discuss how it can be implemented to address these limitations. We then provide a prescription to constrain the model's free parameters with a simple set of characterization data.

II. SURFACE MODELS IN DETECT

The public domain version of DETECT [1] offers four options: METAL, PAINT, POLISH or GROUND to specify the optical properties of individual surfaces in a scintillation counter. Each of these options relates to a different effective model to treat the reflection and transmission of light at surface boundaries, with a reflection coefficient as the only free parameter.

In the METAL model, the surface is assumed to be smooth and covered with a metallized coating representing a specular reflector of Reflection Coefficient, RC. A random check against the value of RC determines whether the photon is absorbed at the surface or undergoes reflection at an angle equal to the angle of incidence. The PAINT model simulates a surface painted with a diffuse reflecting material characterized by reflection coefficient RC. If random sampling shows that reflection occurs, it is assumed to be Lambertian. In these two models, transmission is not considered and so a jump in the index of refraction at the surface interface is of no relevance. For this reason their application is somewhat limited.

The POLISH and GROUND models represent surfaces that may or may not be in optical contact with another component. In these models, one may consider a surface to be made up of micro-facets with normal vectors that follow a given distribution. Figure 1 shows the coordinate system used in these models along with the definition of the following geometrical parameters:

- $\vec{d}_i$ - the direction vector of the incident photon,
- $\vec{d}_r$ - the direction vector of the reflected photon,
- $\vec{d}_t$ - the direction vector of the refracted photon,

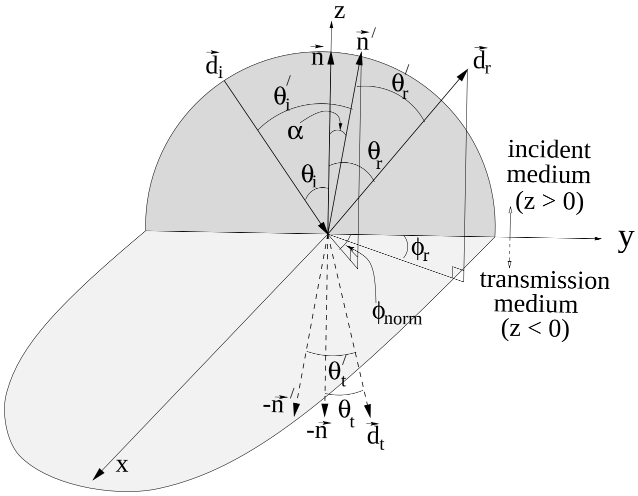

Figure 1: Coordinate system used in DETECT surface models along with the definition of geometrical parameters.

- n_1 - the index of refraction of the incident medium,
- n_2 - the index of refraction of the transmission medium,
- $\vec{n}$ - the average normal of the surface,
- θ_i - the angle of incidence relative to the average normal,
- θ_r - the angle of reflection with respect to the average normal,
- θ_t - the angle of refraction with respect to the average normal,
- ϕ_r - the angle between the projection of the reflected or refracted photon onto the average surface and the plane of incidence,
- $\vec{n'}$ - the normal of a particular micro-facet,
- α - the angle between a given micro-facet and the mean surface,
- ϕ_{norm} - the angle between the projection of the micro–facet normal onto the average surface and the plane of incidence,
- θ_i' - the angle of incidence relative to the micro–facet normal,
- θ_r' - the angle of reflection with respect to the micro–facet normal,
- θ_t' - the angle of refraction with respect to the micro–facet normal.

Note that when $\phi_r = 0$ or 180 degrees, the reflected or refracted photon is in the plane of incidence. Also note that the yz plane forms the plane of incidence, and that all vectors are of unit length. Variables that are primed are values with respect to the micro–facet normal.

The POLISH model is meant to account for a perfectly polished surface that may or may not be in optical contact with another component. If no other component is specified, the surface is assumed to interface with vacuum. Photons incident on the surface are assumed to have random polarization, and are first tested for the possibility of Fresnel reflection if a change in refractive index occurs at the surface. This probability is given by [3]:

$$R = \frac{1}{2}\left[\frac{\sin^2(\theta_i' - \theta_t')}{\sin^2(\theta_i' + \theta_t')} + \frac{\tan^2(\theta_i' - \theta_t')}{\tan^2(\theta_i' + \theta_t')}\right], \qquad (1)$$

where θ_i' and θ_t' are respectively the angles of incidence and refraction with respect to a local micro-facet's normal which is always taken to be parallel to the average surface normal, α=0, to treat a perfectly polished surface interface. Note that R can be conveniently re–expressed as a function of n_1, n_2, and any of θ_i', θ_r', or θ_t', using the laws of reflection and refraction. If reflection is selected, the angle of reflection is set equal to the angle of incidence. If reflection does not occur, the photon is transmitted with the complementary probability of:

$$T = 1 - R, \qquad (2)$$

and assumed to follow Snell's law of refraction. Depending on the refractive index change and the angle of incidence, this may result in total internal reflection of the photon back into the incident component. A reflection coefficient, RC, may be specified to simulate an external diffuse reflector for those photons that pass through the surface interface. If a coat of diffuse reflector has been specified the transmitted photon may be reflected back across the surface. The value of the reflection coefficient gives the probability of a transmitted photon to be returned to the original medium by Lambertian reflection. The photon is again refracted as it crosses the surface back into the original medium. When the reflected photon fails to cross the surface on its first attempt, additional reflection angles are randomly selected until the reflected photon successfully re-enters the original component.

Finally, the GROUND option is available to simulate a roughened or ground optical surface. It is treated in the same way as the polished surface described above, except that the angle, α, between a given micro-facet and the mean surface used to define θ_i' and θ_t' in equation (1) follows a Lambertian distribution. To prevent unrealistic cases in which a photon travelling at an oblique angle could arrive on the wrong side of one of the micro-facets, a test is made of the dot product of the reflected photon direction with the local surface normal. For those cases in which the result is negative, a new local normal is randomly selected until this dot product is positive. As in the case of the POLISH model, a reflection coefficient, RC, may be specified to simulate an external diffuse reflector for those photons that pass through the rough surface.

The radiant intensity can be used to mathematically express the distribution of light created by the POLISH or GROUND surface models. The radiant intensity J is defined as the photon flux, dΦ, passing through the solid angle dω, J=dΦ/dω. A perfectly diffuse or Lambertian surface which appears equally bright from all directions is characterized by the radiant intensity: $J_L = \cos(\theta_r)$. Similarly, the radiant intensity for the POLISH and GROUND surface models, J_P and J_G, may be respectively expressed as follows:

$$\begin{aligned} J_P(\theta_i, \theta_r, \phi_r) &= [R(\theta_i, n_1, n_2)\delta(\theta_i - \theta_r) \\ &+ T(\theta_i, n_1, n_2)\delta(\theta_t - \theta_s)]\delta(\phi_r) \quad (3) \\ J_G(\theta_i, \theta_r, \phi_r) &= \cos(\alpha_r)R(\theta_r', n_1, n_2) \\ &+ \cos(\alpha_t)T(\theta_t', n_1, n_2), \quad (4) \end{aligned}$$

with $\theta_s = sin^{-1}(\frac{n_1}{n_2}\sin\theta_i)$. Note that J_P and J_G are both functions of θ_i, θ_r, and ϕ_r only, since α_r, α_t, θ_r', and θ_t' may all be expressed in terms of these three variables alone.

A polar plot of the radiant intensity of the GROUND and POLISH surface models is shown in Figure 2.

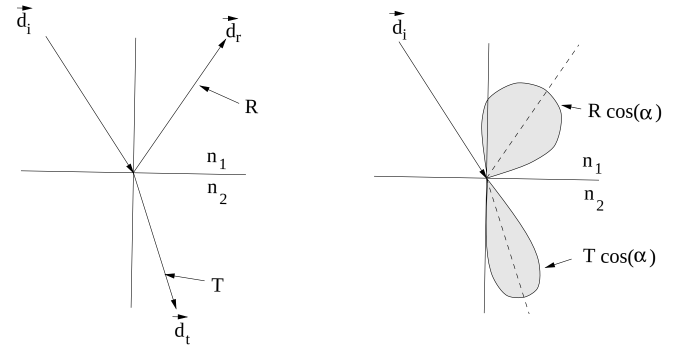

Figure 2: Polar plot of the radiant intensity of the POLISH (left) and GROUND (right) models.

III. Unified Model for Rough Surfaces

Two limitations affect the realism of the GROUND and POLISH models in describing the surface finish of scintillation counters. Firstly, the distribution of micro-facet slopes is fixed in these models, which restrict their use over a limited range of surface roughness values. Secondly, a vacuum is always assumed to be between the dielectric and a diffuse reflective coat. A more physical surface model would allow the user to specify the average roughness of the surface being modelled as well as allow to change the index of refraction of its reflective coat depending on its specific nature.

Detailed models of optical reflections on rough dielectric surfaces have been long available for pattern recognition in robotic vision. These are generally derived from the laws of geometrical optics or classical electrodynamics and will be appropriate depending on the relative ratio of the optical wavelength and the surface's average roughness. Recently, Nayar *et al.* showed in [2] that geometrical and physical models of surface reflectivities can conveniently be unified. There it was recognized that the physical approach of Beckmann–Spizzichino; which derives the radiant intensity of random surfaces from the laws of classical electrodynamics; and that of Torrance–Sparrows; which relies on geometrical optics and the assumption that a rough surface is a collection of micro–facets, converge to identical forms for the non-specular contributions to the radiant intensity of rough surfaces. From this convergence, a unified model of the reflection of light on dielectric surfaces was prescribed by the authors to allow a parameterization over a wide range of wavelength and roughness. The UNIFIED model introduced here is inspired from Nayar *et al.*'s initial prescription but extends the formalism to consistently include light transmission at surface interfaces.

A. *Model Outline*

In the UNIFIED model, the angle between a micro–facet normal and the average surface normal, α, is assumed to follow a gaussian distribution of standard deviation of σ_α. In contrast to the POLISH or GROUND models of DETECT, the UNIFIED model therefore allows, through σ_α, the simulation of a wide range of surface roughness values. Like the other surface models in DETECT, the UNIFIED model also allows a reflection coefficient, RC, to be specified to simulate an external diffuse reflector. The UNIFIED model treats this reflection coefficient in the same manner as POLISH or GROUND, with the addition that an index of refraction, $n_2 = N_{rc}$, can be specified for the reflective coat.

In addition to σ_α and N_{rc}, the UNIFIED model allows for the use of the following four constants to control the radiant intensity of the surface:

- C_{sl}, the specular lobe constant, controls the probability of specular reflection about the normal of a micro-facet;
- C_{ss}, the specular spike constant, controls the probability of specular reflections about the average normal of the surface;
- and finally, C_{bs}, the backscatter spike constant, controls the probability of backward reflection. This occurs when a photon hits a micro-facet at a normal angle, after several reflections within a deep groove, and is reflected back along its original path. This process is enhanced on very rough surfaces [4].
- C_{dl}, the diffuse lobe constant, controls the probability of internal Lambertian reflection;

Note that the sum of the four constants is constrained to unity to preserve the relative probabilities of reflection or transmission at the surface interface.

To a good approximation, the radiant intensity for the UNIFIED surface model may be expressed as:

$$\begin{aligned} J_U(\theta_i,\theta_r,\phi_r) &\approx R(\theta_r', n_1, n_2)[C_{sl}\, g(\alpha_r; 0, \sigma_\alpha) \\ &+ C_{ss}\delta(\theta_i - \theta_r)\delta(\phi_r) + C_{bs}\delta(\theta_i + \theta_r)\delta(\phi_r) \\ &+ C_{dl}\, cos(\theta_r)] \\ &+ T(\theta_t', n_1, n_2) g(\alpha_t; 0, \sigma_\alpha), \end{aligned} \tag{5}$$

where $g(\alpha; 0, \sigma_\alpha)$ is a gaussian with a mean of 0^o and a standard deviation of σ_α, for $\alpha \epsilon\ [0, 90^o]$, and is equal to 0 otherwise. A polar plot of the radiant intensity of the reflected and transmitted components of the UNIFIED model along with the terms that control their probability is shown in Figure 3.

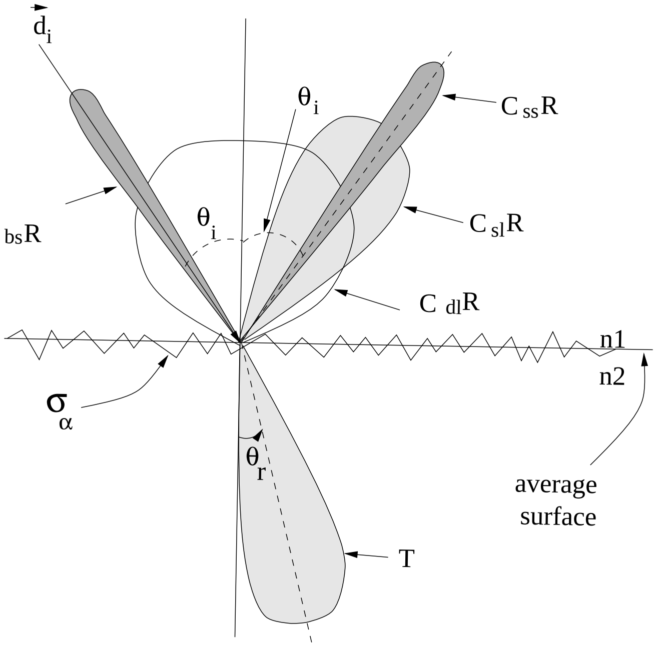

Figure 3: Polar plot of the radiant intensity in the UNIFIED model.

The previous expression of the radiant intensity, J_U, stresses well the unification of several surface models into a single parameterization. For instance, when $n_1 = n_2$ in equation (5), the transmission coefficient T is equal to 1 and the UNIFIED model reverts to DETECT's PAINT option. Similarly, setting $C_{sl} = 1$ and $\sigma_\alpha = 0$ leads to the radiant intensity of the POLISH model. In treating a rough interface between two dielectric surfaces, the model will be used in its most physical representation by setting $C_{sl} = 1$ and constraining σ_α to surface roughness data, as will be further discussed in the last section.

B. Model Implementation in DETECT

The implementation of the UNIFIED model into our local version of DETECT builds on the design of the standard POLISH and GROUND options. The incidence of a photon upon a surface specified as UNIFIED first requires choosing the angle, α, between the micro–facet normal and that of the average surface, as well as the azimuthal angle ϕ_{norm}. The UNIFIED model assumes that the probability of micro–facet normals to populate the annulus of solid angle $\sin(\alpha)d\alpha d\phi_{norm}$ will be proportional to a gaussian of standard deviation σ_α. Accordingly, ϕ_{norm} is chosen from a uniform probability distribution between 0 and 2π, while values of α are randomly sampled from the probability distribution $sin(\alpha)g(\alpha; 0, \sigma_\alpha)$.

Given the chosen values of α and ϕ_{norm}, a check is made to make sure that $\vec{d_i} \cdot \vec{n'} > 0$. If this is not true, then new values α, and ϕ_{norm} are chosen until the test is satisfied to ensure that the incident photon aims toward the local micro–facet. A case where this condition is not satisfied is shown schematically in Figure 4(a).

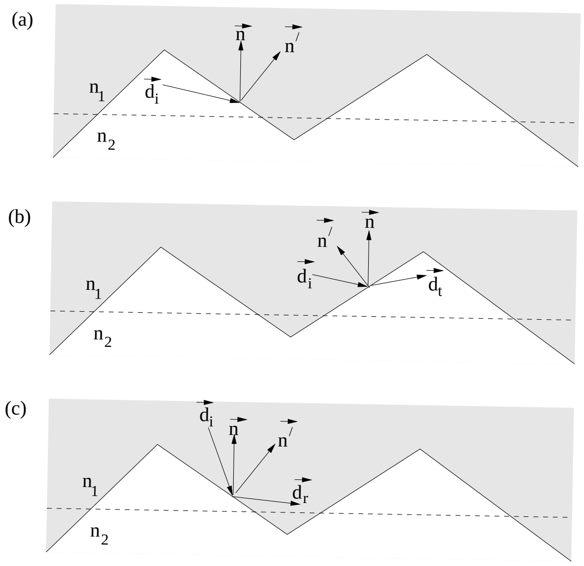

Figure 4: Special cases handled by the UNIFIED model: (a) when the incident photon does not aim toward the local micro–facet; or when the transmitted (b) or reflected (c) photon heads in the wrong direction with respect to the average surface normal.

In this first implementation of UNIFIED photons are assumed to have random polarization, and are then tested for the possibility of reflection if a change in refractive index occurs at the surface. The angle, θ_i', between the direction of incident photon and the local micro–facet normal $\vec{n'}$ is considered to calculate the Fresnel's reflection coefficient $R(\theta_i', n_1, n_2)$. When a reflective coat has been specified, R is calculated using $n_2 = N_{rc}$. Based on the value of R, reflection or refraction is randomly chosen. If refraction is chosen the photon is transmitted and its direction with respect to the local normal $\vec{n'}$ is computed using Snell's law and the values of n_1 and n_2. If reflection occurs then a choice is made between the four different types of reflection according to the values of C_{sl}, C_{ss}, C_{bs} and C_{dl}. When the specular lobe is chosen, the photon is reflected specularly with respect to the local normal. If the specular spike is chosen, then the photon reflects specularly with respect to the average normal. If the backscatter spike is chosen, the photon returns on its original path. Finally, if the diffuse lobe is chosen then the photon is distributed according to a Lambertian distribution.

Two special cases may happen when after reflection or refraction a photon still aims at the surface again. These two cases will happen when $\vec{d_t} \cdot \vec{n} > 0$ or $\vec{d_r} \cdot \vec{n} < 0$ respectively, and are shown schematically in Figure 4(b) and (c). In the occurrence of any of these two cases, a new local micro–facet normal $\vec{n'}$ is chosen and the incident photon is forced to interact again with the surface.

As with POLISH and GROUND a reflection coefficient, RC, may be specified to simulate an external diffuse reflector for those photons that are transmitted through the surface interface. If a coat of diffuse reflector has been specified the transmitted photon may be reflected according to a Lambertian distribution. When the reflected photon fails to cross the surface on its first attempt, additional reflection angles are selected until the photon successfully re-enters the original component. The photon is finally refracted with respect to the local micro–facet normal as it crosses the surface back into the original medium.

C. A Prescription to Constrain the Model

The implementation of the UNIFIED model through equation (5) requires the specification of seven free parameters: n_1, σ_α, C_{sl}, C_{ss}, C_{bs}, C_{dl}, n_2, and RC. A simple prescription can be followed to constrain these parameters for a given surface. For instance, one may consider the modeling of a plastic or inorganic scintillator, with a refraction index n_1 that is known from the fabricant, and which is coated by a white reflector and coupled to a photomultiplier tube to serve as a simple scintillation counter.

An input value for σ_α can be directly obtained by taking a profile of the crystal surface using a stylus probe as discussed in Ref. [5]. The top panel of Figure 5 shows such a surface stylus profile measured for a very rough BGO crystal. The data provides the surface height variation as a function of the stylus position. Projection of the data onto the Y-axis directly leads to the height distribution shown in the middle panel of Figure 5. A gaussian fit to that distribution shows a standard deviation of σ_h=45 kÅ with respect to the average surface. Similarly, the surface profile data can be differentiated in steps of $\sim 2\mu$m to obtain the distribution of micro–facet slopes, α, shown in the bottom panel of the figure. The distribution is found to be in good agreement with a gaussian with standard deviation σ_α of 11.8^o.

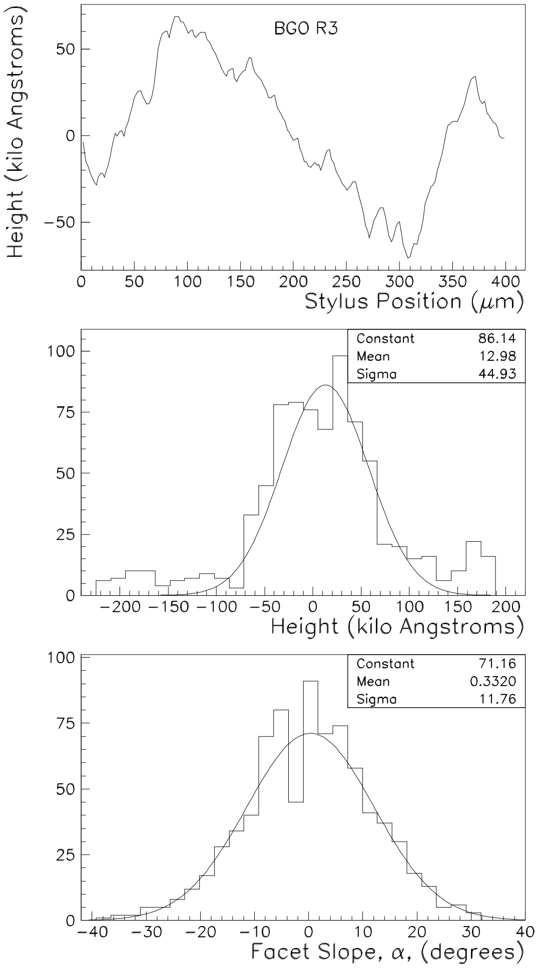

Figure 5: Surface profile (top), height distribution (middle), and micro–facet slope distribution (bottom) measured for a very rough BGO crystal.

Values of C_{sl}, C_{ss}, C_{bs} and C_{dl} are constrained by the relative values of the scintillation light wavelength, λ and the standard deviation of the surface height distribution, σ_h [2]. For instance, when $\sigma_h/\lambda \leq 0.025$ the crystal may be considered as highly polished and can be modeled by using $\sigma_\alpha = 0$ along with C_{ss} or C_{sl} =1.0. As σ_h become increasingly significant in comparison with the scintillation wavelength, photons incident at the surface interface will start to interact with respect to local micro–facet. According to [2], as soon as $\sigma_h/\lambda > 1.5$, the specular spike vanishes and the radiant intensity is dominated by the specular lobe. In that regime the scintillator surface will be accounted for with the UNIFIED model by setting C_{sl}=1 and using a measured value for σ_α.

The index of refraction of the reflective coat, n_2 or N_{rc}, is also determined quite easily. If the coat does not bound to the surface, as with a teflon tape wrap, an air layer is present between the scintillator and the reflector and N_{rc} must be set to 1. If the coat chemically reacts with, or wets, the surface; its index of refraction is that of the solvent binding to the scintillator. This will be the case if titanium or magnesium oxide powders are mixed with an optical epoxy to act as reflective coat. Finally, the reflection coefficient of the coat, RC, can be constrained by considering the absolute number of photoelectrons produced by the scintillation counter.

IV. Discussion and Conclusion

In this paper we presented a first report of the implementation, in the widely used program DETECT, of a more physical model to treat the interactions of scintillation photons with dielectric surfaces. Motivation for this work was found in the practical limitations of the effective surface models offered by the public domain version of DETECT. Inspired from the initial work of Nayar *et al.*, the UNIFIED surface model was designed to merge, into a single parameterization, models that usually apply over a very limited range of surface treatments. This flexibility was ensured by using the standard deviation of the surface slope as a model parameter that can be extracted from simple measurements.

A thorough test of this new model can be achieved by confronting its predictions of the absolute number of photoelectrons obtained from pencil–like scintillation crystals under different surface conditions. Such a validation of the model is currently under progress and will be reported in future work.

V. Acknowledgments

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VI. References

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