MOSAIC: a numerical model for the reflection of photons on a rough dielectric surface.

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ABSTRACT

There are many surface models that describe the comportment of photons when they hit a rough dielectric surface. However, the existing models did not give very good results when used to predict the photoelectron yields produced by BGO crystals. As those models use a slope distribution to describe the roughness of the surfaces, we have designed a new model using a height distribution rather than a slope distribution. MOSAIC uses a Delaunay triangulation to build a static surface. The staticity and the height variation of the surface should correct most of the problems that were not taken in account by a slope variation model such as shading and multiple reflections.

Keywords : Surface model, Optical photon transport model, Corrugated or rough surface, Scintillation counters, Gamma-ray and X-ray detectors, DETECT, UNIFIED, MOSAIC, Monte Carlo.

1. INTRODUCTION

The development of scintillation counters is greatly improved by the use of Monte Carlo simulation techniques. The DETECT[1] program has been developed to assist such development, but this program, despite of many good attempts, still lacks of a reliable surface model. The most complete surface model used within this program is the UNIFIED[2] model which uses a Gaussian distributed slope model to determines the roughness of the surface. The standard deviation used by the model is based on measurements[2,3] made on real BGO crystal, a rough one (BGO-R2) and a smooth one (BGO-S2).

Figure 1 shows the coordinates system that we will use, the suffix i refers to the incident photon or angle, the suffix r to the reflected values, primed variables are measured from the local normal **n'** and non primed variables are measured from the mean normal **n**. The angle between the two normals is α.

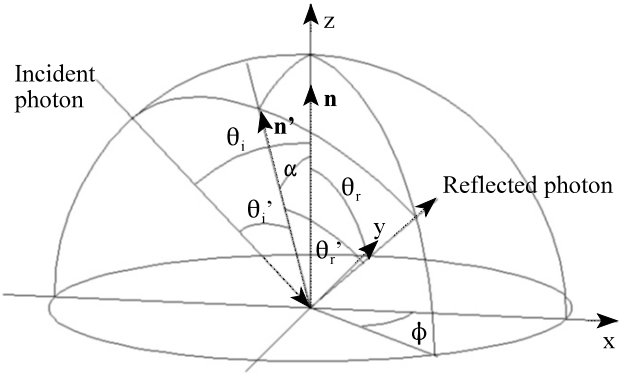

Figure 1: Coordinates system used in the DETECT program.

In this article, we will describe the construction of a height variation based surface model, then we will show and interpret the results obtained by this model and finally we will try to find some others improvements that can make the model more precise. But first, we will discuss why a new model is needed.

2. FLAWS OF A SLOPE BASED MODEL

Moisan et al. have shown[2] that the results of the UNIFIED model when simulating even a simple crystal are not as good as we may want. The modeled photoelectron yields are not accurate on an absolute scale. The UNIFIED model

overestimates the photoelectron yields for the rough crystal and it underestimates it for the smooth crystal. These results show the need for a new, more accurate surface model.

Generally, surface models based on slope variation such as UNIFIED are not static, i.e. the normal of the surface is randomly generated each times a photon interacts with the surface. This is not the case in a real crystal where the surface is definitely static. This difference may or may not change the results of the simulation but it has been used on the UNIFIED model since it is easier not to stock the profile of the surface.

Also, the UNIFIED model does not account for shading or multiples reflections since the simulated surface is completely flat. These effects should modify slightly the reflection of the photons by the surface. For example, enabling multiples reflections should decrease the number of photons that raze the surface since these photons should have a good chance of hitting a ridge of the surface.

Finally, the angular distribution used to determine the local normal of the surface should depend on the incident angle of the photon. In the real world if we suppose that a surface is composed of facets with $\alpha = \pm \delta$ as shown on figure 2, where δ is a constant, the probability for a photon of hitting a type of facet depends on the incident angle.
For the photons with normal incidence on the surface each facet has 50% of probability but when the incidence angle is not 0°, the photon have more probability of hitting one orientation of facet than the other. This aspect should diminish the dispersion of the photons after a reflection or a transmission for a slope based model such as UNIFIED since it would augment the probability of facets for which θ_i' is small.

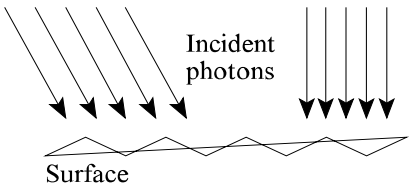

Figure 2: Incident photons on a rough surface

3. DEVELOPING A HEIGHT BASED MODEL

In this paper we present our approach to develop a height based surface model. This method allows us to use a random generated static surface, i.e. the surface used to simulate the reflection of photons is randomly generated in a first step of the simulation then it is used so the surface is exactly the same during all the simulation.

This static random generated surface should represent adequately a real rough dielectric surface. Also, the height distribution will allow the existence of some surface artifacts like scratches. The measurements made on real BGO crystals[2,3], rough and polished, will be used to gauge the new model.

To model a three dimensional surface, we assumed that the surface is covered by triangular facets. Each vertex of these facets is generated randomly so that the triangular facets are also distributed randomly. To build the facets with the randomly distributed vertex, we used a Delaunay triangulation[4]. This method consists to build triangles from a set of points (vertex) so that each triangle is as equilateral as possible. To be sure of this, we have to verify that no vertex is inside a circle circumscribing any of the triangles. There are many algorithm that can perform rapidly a Delaunay triangulation such as a "divide and conquer" method and a method that uses a tree structure to store the triangulation called "Delaunay tree". We used this last method to compute the triangulation since it allows to find quickly over which triangle a point is located.

As these techniques have already been developed by some others, we did not want to do the job again, so we have used an algorithm made by the INRIA Prisme Project that is probably better than what we could do. For the needs of our program we must modify the triangulation to add a third dimension to the vertices of triangulation, which will add roughness. This addition does not change the algorithm of the triangulation, it just ensures that the surface is not flat. The height of the vertices is added following a Gaussian distribution of parameter σ_h centered on the mean height of the surface. The standard deviation σ_h will be fixed following some measurements taken on BGO crystals.

As we have seen before, the triangulation is included in a tree structure. The first triangle in the triangulation is the mother, or root, since the triangulation is included in a tree structure, and all the following triangles are her sons. So when a triangle is destroyed it will be declared dead and the triangles generated will be called his sons, but the information concerning the dead triangle is kept. This structure allows fast research within the triangulation. The first step, when searching in which triangle is a point, is to verify if the point is in the root, then if it is the case, to search in which of his sons the point is located and repeat until we find a triangle that isn't dead. All the points in the surface are in the root since we fixed the vertices of the triangle root so that it encloses all the surface. This structure offers a great advantage but it also have a drawback. As we kept all information on the dead triangles, this needs a great quantity of memory. Each new vertex added create at least three new triangles, so the memory needed will cause some problems when simulating large surfaces. With the density of points used and for a computer equiped with 256 Mb of memory, the surface simulated cannot exceed a few square millimeters. We need to find a technique that will allow to expand the possibilities since the common dimensions of crystals are of the order of some square centimeters.

The method retained to expand the surface of the triangulation consist of doing a mosaic with a triangulation that serves as the base element. To keep some diversity, the orientation of each element of the mosaic will be randomly determined. The x, y and z axis can be inverted or not, this will give 8 different possibilities. We will not allow 90° rotations on z axis, which should permute x and y axis, since the base element of the mosaic does not usually have same dimensions on x and y axis.

To be sure that the surface generated corresponds to the surface that we want to simulate, we have to be sure that the simulated surface has the same distributions, height and angular, than the real surface. We first use the height distribution to generate the triangulation of the surface, but we must be sure that the generated surface also follows the angular distribution of the real surface. To do so, we must add a correlation between the height of neighboring vertices. The correlation length is added with the following equations:

$$Z = \frac{1}{s\,\sigma_h\sqrt{2\pi}}\exp^{\frac{-(z-\mu)^2}{2(s\,\sigma_h)^2}}$$

$$\text{where}\quad \mu = \frac{\sum_{i=1}^{n} z_i \exp^{\frac{-dist_i^2}{T^2}}}{n} \qquad \text{and} \qquad s = \prod_{i=1}^{n}\left(1-\exp^{\frac{-dist_i^2}{T^2}}\right) \tag{1}$$

where " Z " is the distribution used to generate the height " z " of a vertex, " T " is the correlation length, " z_i " is the height of vertex " i ", " $dist_i$ " is the distance in the x-y plane between the vertex " i " and the vertex that we want to generate the height and " n " is the number of points used to compute the correlation. The vertex which are used to compute the correlation are those in the neighborhood of the new vertex, so we use the vertices of all the triangles destroyed by the new point. If there where no correlation, or the correlation length where 0, the center of the Gaussian distribution " μ " would be 0 and " s " a factor reducing the standard deviation would be 1. So " Z " would be a Gaussian

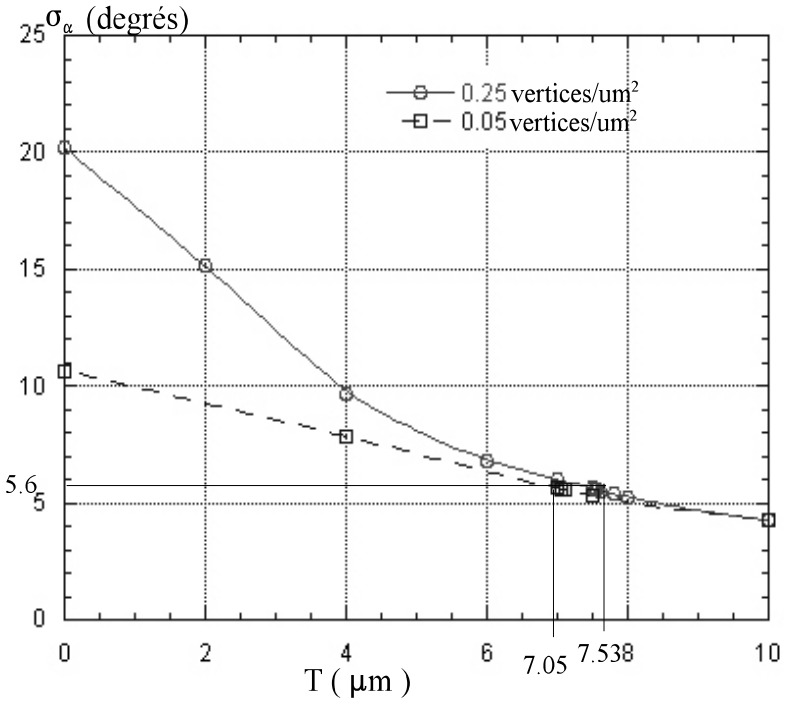

Figure 3: Graph of the standard deviation σ_α in function of the correlation length.

distribution centered on 0 with parameter " σ_h ". The correlation changes the center of the Gaussian distribution which will be " μ " and reduce the standard deviation by a factor " s ", which is always between 0 and 1.

The correlation length T has been determined by constructing many surfaces with the same parameters except for their correlation length and by checking which fits the best the angular distribution. The results of this process are shown in the figure 3.

On figure 3 we see that in order to obtain an angular distribution like the one of the rough BGO crystal, $\sigma_\alpha = 5.6°$, we have to fix the correlation length at 7.53 μm for a vertice density of 0.25 vertex/μm^2. This density of vertex have been used since the measurements made on the BGO crystals have been made with a 2 μm step which leads to a vertex by $(2\ \mu m)^2$. However, to be able to cover a greater surface, we have used a second density. This second density of vertices was fixed to 0.05 vertex/μm^2 to still have more than one vertex by T^2. As we can suppose, the correlation length needed to achieve the same angular distribution will change when changing the vertices density, so we had to recompute the correlation length. The new value has been fixed to 7.05 μm.

To verify rapidly if a photon goes through a triangular facet, we have used Plücker coordinates[5,6]. The Plücker coordinates system have six dimensions where each point represent a directed line in common 3D space. These coordinates allow to greatly simplify some calculations. Suppose a line going from point A (a_x, a_y, a_z) to point B (b_x, b_y, b_z), the Plücker coordinates for this line will be:

$$\begin{aligned} L_1 &= b_x - a_x \\ L_2 &= b_y - a_y \\ L_3 &= b_z - a_z \\ L_4 &= b_y a_z - a_y b_z \\ L_5 &= b_z a_x - a_z b_x \\ L_6 &= b_x a_y - a_x b_y \end{aligned} \qquad \textbf{(2)}$$

The use of this coordinates system allows, with a simple calculation, to know if two lines go through one another or if they passes by in a clockwise or counter clockwise manner. The first step is to make the following calculation:

$$C = L_1M_4 + L_2M_5 + L_3M_6 + L_4M_1 + L_5M_2 + L_6M_3 \quad (3)$$

where L and M are lines in Plücker coordinates. If C is zero then the lines L and M crosses. If C is positive then L passes by M in a clockwise fashion and finally if C is negative then L passes by M counterclockwise. Knowing this, we compute the Plücker coordinates for the photons direction and for the tree sides of the facet, and by doing the calculation given in (3) with the photon direction and each of the tree sides, we can find if the photon pass inside the facet or not.

To simplify the model, the polarisation of the photon is not defined. This way, the photon is entirely defined by his position, direction and wavelength. To determine the reflection coefficient at each interaction of the photon with the dielectric surface, we use an average on all the possible polarisation, which gives the reflection coefficient R as:

$$R = \frac{1}{2}\left(\frac{\sin^2(\theta_i'-\theta_t')}{\sin^2(\theta_i'+\theta_t')} + \frac{\tan^2(\theta_i'-\theta_t')}{\tan^2(\theta_i'+\theta_t')}\right) \quad \textit{where} \quad \sin(\theta_t') = \frac{n_1}{n_2}\sin(\theta_i') \quad (4)$$

4. RESULTS

The figure 4 shows the angular distribution of probability of reflection of a photon for some incidents angles θ_i. All the other parameters of the models are kept constant and are fixed to represent the rough BGO crystal: $n_1 = 2.15$, $n_2 = 1$, $\sigma_h = 0.58\ \mu m$, $T = 7.53\ \mu m$ and the vertice density is $0.25/\mu m^2$. Each graph gives the angular probability of reflection of a photon, the angle θ_r is represented radially and the deviation angle ϕ is represented angularly with the probability of not being deviated from the plane of incidence plotted to the right. The scale of each graph is plotted on the right of the graph.

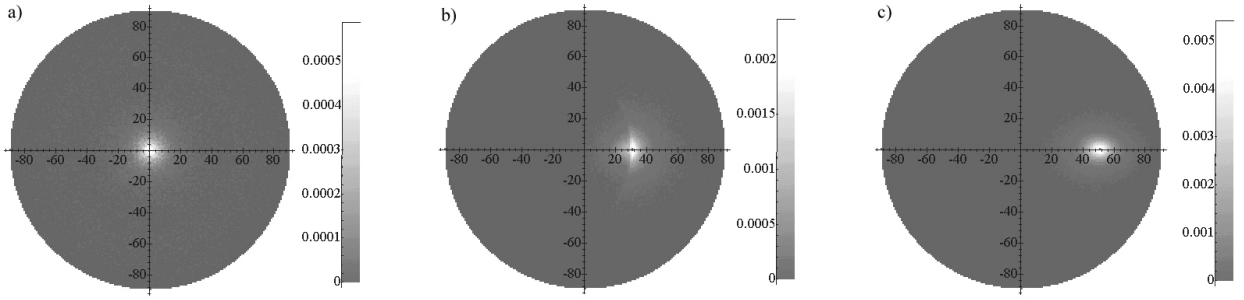

Figure 4: Graphs of angular distribution made with the MOSAIC model and the following parameters $n_1=2.15$, $n_2=1$, $\sigma_h=0.58\ \mu m$ with a) $\theta_i=0°$, b) $\theta_i=25°$ and c) $\theta_i=50°$.

We see on the graph of figure 4 that the maximum probability of reflection is always around $\theta_r=\theta_i$ and $\phi=0°$ which corresponds to a reflection by a facet with a normal parallel to the mean normal. The graphs a) and c) show Gaussian-like distribution but it is not the case for the graph b). The difference in the graph b) comes from the total internal reflection which occurs for reflected angles greater than 30.4°, so for reflected angles smaller than this, the probability of being reflected is small and for angles greater than 30.4° the probability is one which causes this discontinuity in the distribution. The probability for the photon to be reflected is smaller when $\theta_i = 0°$ (graph a)) and it's near one when $\theta_i = 50°$ (graph c)).

Figure 5 shows the differences between the angular distribution of probability of reflection of the MOSAIC model and the UNIFIED model. It gives the distribution of probability obtained with the new model minus the one obtained with the UNIFIED model. Again the parameters have been fixed to represent the rough BGO crystal: $n_1 = 2.15$, $n_2 = 1$, $\sigma_h = 0.58\ \mu m$ for MOSAIC and $\sigma_\alpha = 5.6°$ for UNIFIED and the different graphs are plotted with different incident angle.

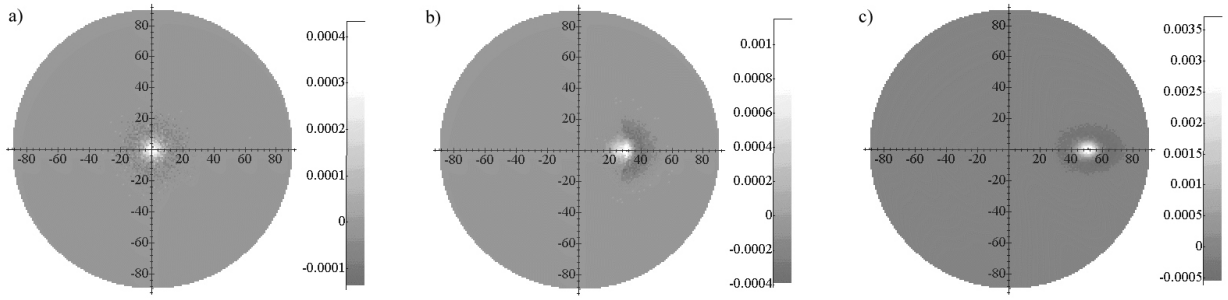

Figure 5: Graphs showing the differences betweenthe the angular distributions of the MOSAIC and UNIFIED models for n_1=2.15, n_2=1, σ_h=0.58 μm or σ_α = 5.6° and for a) θ_i=0°, b) θ_i=25° and c) θ_i=50°.

The first thing to notice on the graphs of figure 5 is that the MOSAIC model scatters the photons less than the UNIFIED model since there is a negative ring (darker) and a positive center (lighter) on each graph. This result was expected since the angular distribution used in the UNIFIED model does not have any dependence on the incident angle θ_i. The real angular distribution should have probabilities smaller when the incident photon direction is not parallel with the normal of the facet. By adding this dependency on the angular distribution of the UNIFIED model, we should have results looking like those of the MOSAIC model. This is good since it shows that the new model corrects at least an error of the UNIFIED model.

5. CONCLUSION

The results of the MOSAIC model are differents from those obtained with other models, principally for rough surfaces. These results show that the errors came, at least in part, from the surface modelization. However, to decide if this new model is really better than the existing models, we will have to try to simulate a complete crystal.

Also, to have a better model, we should add wavelenght dependancies, which didn't change the surface model in itself, it just changes the refraction index of the cristal and, when simulating a complete crystal, others aspects of the simulation may be dependant in wavelenght. The polarisation of the photon can also change somehow the results since we have used a reflection coefficient that is a mean over all polarisations. So furthers results will be presented as soon as possible to determine if MOSAIC can predicts experimental results better than existing models.

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REFERENCES

1. C. Moisan, E. M. Hoskinson, A. Levin and D. Vozza, "A Public Domain Platform to Model Scintillation Counters for Gamma-Ray Imaging Applications", SPIE Proc., vol. 3115, pp. 21-29, 1997.
2. C. Moisan, A. Levin and H. Laman, "Towards a Model Accounting for the Impact of Surface Treatment on the Performances of Scintillation Counters", SPIE Proc. vol. 3141, pp. 324-325, 1997.
3. C. Moisan, A. Levin and H. Laman, "Testing Scintillation Transport Models with Photoelectron Yields Measured under Different Surface Finishes", 1997 IEEE nuclear Science Symposium, vol .1, pp.824-829, november 1997.
4. J.-D. Boissonnat and M. Teillaud. "On the randomized construction of the Delaunay tree", Theoret. Comput. Sci. Vol. 112, pp. 339-354, 1993.
5. S. Avidan and A. Shashua, "Trajectory Triangulation of Lines: Reconstruction of a 3D point Moving along a Iine from a monocular image Sequence", IEEE Conf. on Computer Vision and Pattern Recognition (CVPR), June, 1999.
6. N. Andreff, B Espiau and R Horaud, "Visual Servoing from Lines", Proc. IEEE Int. Conference on Robotics and Automation, 2000.