NE 697: GEANT4 Simulations of Light Transport in ^{6}Li Glass Scintillator

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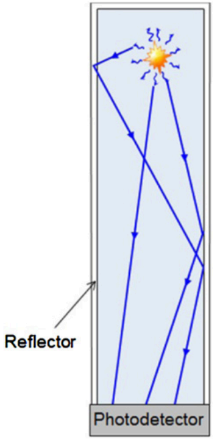
Outline

Introduction

Understanding and optimizing light collection is critical for achieving high performance in scintillation detectors.

The light transport in the crystal is dependent on

- the crystal geometry,
- the bulk absorption and scattering of the material,
- the surface treatment of the crystal faces.



Reflection of optical photons within a scintillator. Image obtained from [7].

GEANT4 Surface Treatment Models

- glisur (GEANT3)
  Users indicate the value of polish, where a random point is generated in a sphere of radius (1-polished), and the corresponding vector is added to the average surface nominal normal as the micro-facet normal. A specular reflection is thereafter calculated based on the microfacet orientation. [2] [5]

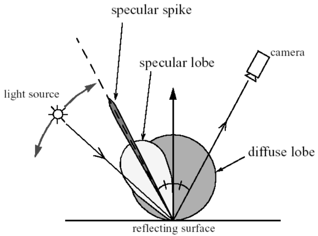
- unified
  Users specify a parameter *SigmaAlpha*, which defines the standard deviation of the Gaussian distribution of micro-facets around the average surface normal. [2] Four kinds of surface reflections are possible: specular, spike, lobe, backscatter and Lambertian. [5]

  Note: Geant4 assumes that the four reflection type probabilities are constants, and not functions of incidence angles, which does not fully agree with measured data in Ref. [5]

- LUT
  Model is based on measured surface data with rough and polished finishes that can be coupled without reflectors, or in combination with a specular reflector (e.g. ESR) or a Lambertian reflector (e.g. Teflon). Coupling method can be air or optical grease. [2]

Types of Reflection

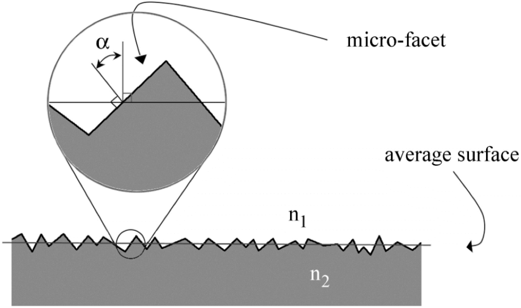
Surface reflections components:



Terminology [5]

Specular spike	the reflected photon is reflected about the average surface normal
Backscatter	the photon is reflected by into the direction the photon came from
Lambertian	the photon will be reflected with a Lambertian distribution (cosine distribution) about the average surface normal
Specular lobe	the surface is assumed to consist of micro-facets, which are oriented around the average surface with a Gaussian distribution defined by *SigmaAlpha*. A micro-facet is randomly selected from the distribution defined by *SigmaAlpha*, and a specular reflection is thereafter calculated based on the micro-facet orientation.

Micro-Facets



For a ground surface in the unified model, the parameter *SigmaAlpha* defines the standard deviation of the Gaussian distribution of micro-facets around the average surface normal. Image obtained from [5].

Note

Optical Monte Carlo software such as DETECT, Litrani, Geant4 or GATE allow the operator to set the surface reflections as purely specular, purely diffuse (Lambertian), or a linear combination of specular and Lambertian, which might not be a true representation of the real world. [4]

- Janecek, 2008

Outline

GEANT4 Simulation Model

Goals:

- Light collection efficiency based on crystal geometry, surface finish, reflector type and coupling method.
- Light sharing of monolithic and pixelated scintillators across array of photodetectors

Key Model Parameters:

- Source: monoenergetic neutron beam at 25 meV (1.8 Å)
- Geometry: single pixel and pixel array (8×8 pixels)
- Material: ^{6}Li-enriched glass scintillator (GS 20, Scintacor)
- Physics list: $\leq$ 20 MeV neutron, G4OpticalPhysics

Primary particles

Utilize a built-in primary particle generator → G4GeneralParticleSource:

- Offers many pre-defined options
  - particle type (neutron, gamma, proton, etc.)
  - position distribution (point, plane, beam, etc.)
  - angular distribution (isotropic, cosine-law, etc.)
  - energy distributions (mono-energetic, power-law etc.)
- Can be used via C++ or command line (or macro) UI

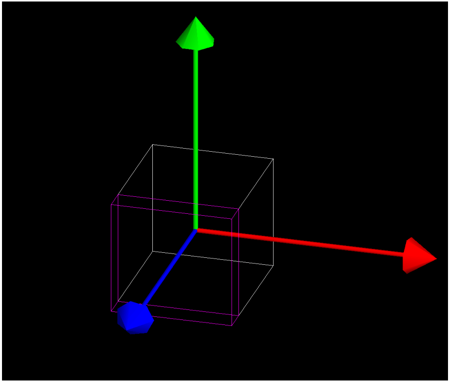
Example GPS setup using macro

$/gps/energy\ \ 0.025\ eV$
$/gps/particle\ \ neutron$
$/gps/direction\ \ 0.\ \ 0.\ \ 1.$
$/gps/pos/type\ \ Beam$
$/gps/pos/shape\ \ Circle$
$/gps/pos/sigma_r\ \ 4\ mm$
$/gps/pos/centre\ \ 0.\ \ 0.\ \ -10.\ cm$

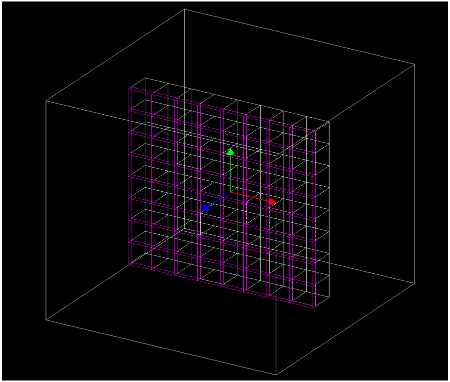
Detector Geometry

Two detector geometry configurations:

single pixel



8×8 pixel array



scintillator (white wiring), photodetector (magenta wiring)

Scintillator Material Composition and Properties

Material Composition [9]

	SiO_2	MgO	Al_2O_3	Ce_2O_3	Li_2O	Li	^6Li
Weight %	57	4	18	4	17.1	7.9	7.87

Material Properties [1]

Density (g/cm^3)	2.50
Wavelength† (nm)	395
Refractive index†	1.55
Decay time‡ (ns)	18/57/98
Scintillation yield†† (photons/MeV)	~1,276
Linear attenuation coefficient‡‡ (cm^{-1})	14.85
Photon absorption length (cm)	100 (assumed)
Yield ratio	1.0
Resoution scale	1.0

† at maximum emission. Full emission spectrum will be needed in simulation

‡ Fast component, slow component and 90% to 10% respectively

†† About 6,000 photons per absorbed neutron is normalized by the Q-value (4.73 MeV)

†† at thermal neutron energy (2meV)

Scintillator Boundary Interaction

Surface treatment

surface type	dielectric-dielectric, dielectric-LUT † dielectric-LUTDAVIS ‡
model	unified, LUT, DAVIS
surface finish	rough, polished
reflector type	teflon (lambertian), ESR (specular)
coupling method	air
crystal thickness	1, 2, 6, 20 mm

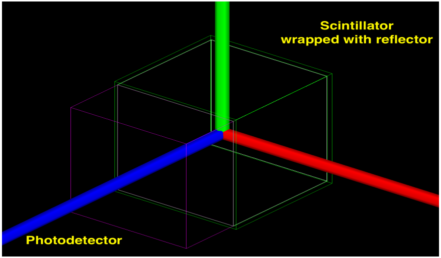
† LUT model is based on BGO crystal. [4]
‡ DAVIS model is based on LYSO crystal [7]

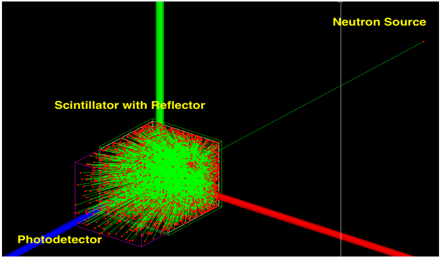
Parameters for unified model

SigmaAlpha	0.0227 rad/1.3^o (polished) 0.209 rad / 12^o (rough)

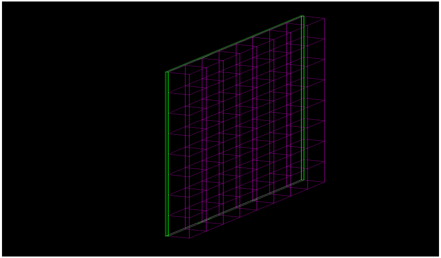
Simulated Detector Setup

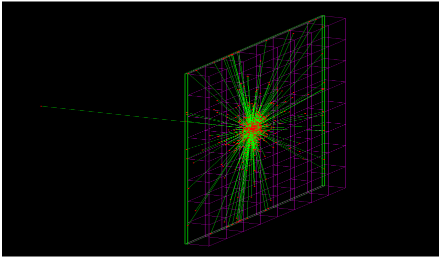
single pixel (light collection efficiency)





pixel array (light sharing)

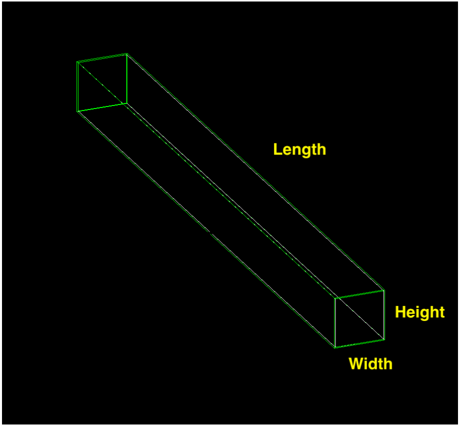




Outline

Results: Light Collection Efficiency

To optimize scintillator parameters to maximize the light collection efficiency, the light collection efficiency is compared for different scintillator surface treatments and aspect ratios.

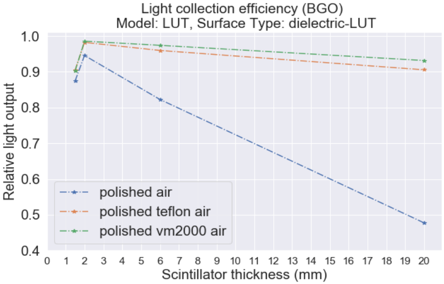


The aspect ratio of a geometric shape is the ratio of its sizes in different dimensions.

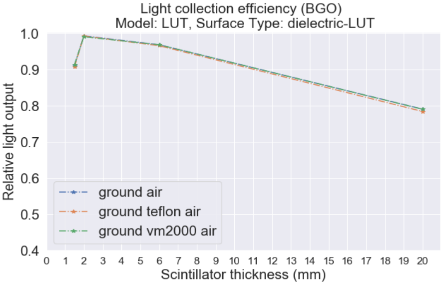
Here, we will talk about the aspect ratio of a cuboid (assume that width and height are of equal dimension)

$$aspect\ ratio = \frac{length}{width}$$

Results: Validation Using Published Results



Polished crystal



Rough crystal

Findings

- For polished surfaces, having optical reflectors generally provides better light collection.
- For rough surfaces, having reflectors does not necessary help with better light collection.
- "Surface roughness proved to be the most important parameter when choosing crystal setup. The reflector choice was of less importance and of almost no consequence for rough-cut surfaces." [4]

Below shows the comparison between experimental measurements (*Measured*), simulated results using LUT (*Our code*)and Geant4 unified model (*Original code*), from Berkeley Lab. [3]
The BGO crystal used has a dimension of $3 \times 10 \times 30$ mm^3.

Polished crystal

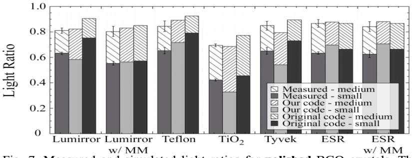


Fig. 7. Measured and simulated light ratios for **polished** BGO crystals. The measured data (with standard deviation error bars) is the leftmost columns, our code simulations are the middle columns, and the original code simulations are the rightmost columns for each attached reflector material. The striped columns show the light collected from a medium surface normalized to the light collected from a large surface, while the solid color columns show the light collected from a small surface normalized to the light collected from a large surface. The abbreviation "w/ MM" stands for "with MeltMount™".

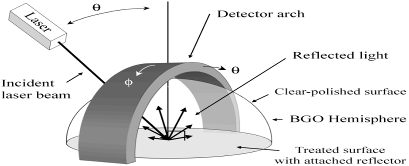


Fig. 1. Sketch to illustrate the principle used for measuring reflectance distributions. An incident laser beam is reflected off the bottom (flat) surface of a BGO hemisphere, and the reflected light is measured by an array of PIN photodetectors, which are mounted on an arch. The detector arch moves from theta -90° to +90°, thus enabling measurements of the full 2π of solid angle. All light entering and exiting the hemisphere is perpendicular to the surface, thus enabling all reflection angles to be measured. The laser is mounted on the outside of the detector arch and is movable from theta -90° to +90°, with phi = 0°.

Rough crystal

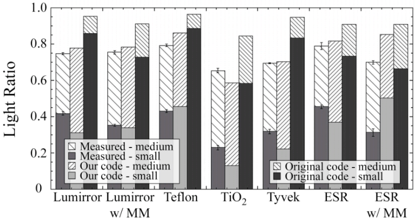


Fig. 9. Measured and simulated light ratios for **ground** BGO crystals. See the text for Fig. 7 for detailed description of the figure.

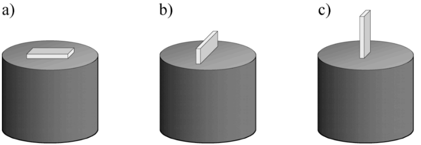


Fig. 4. The same crystal is positioned in three different orientations onto a PMT to validate the results of the simulations. By using the same crystal to measure ratios of the light output in three different orientations – through the large surface (a), the medium surface (b), and the small surface (c) – we avoid crystal-to-crystal variations in light output and get self-calibrated measurements.

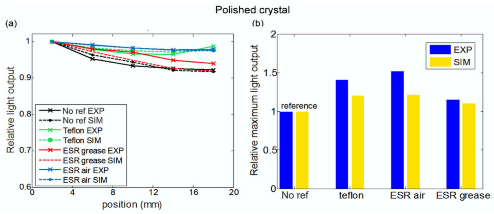


Figure 12.
Light output for polished crystals with no reflector, Teflon, or ESR (air-coupled or grease-coupled). a) Normalized outputs for experiments (EXP) and simulations (SIM). b) Maximum light outputs, taken at the depth closest to the photodetector (2 mm).

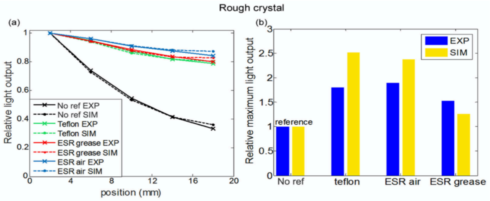


Figure 10.
Light output for rough crystals with no reflector, Teflon, or ESR (air-coupled or grease-coupled). a) The normalized outputs show excellent agreement between experiments (EXP) and simulations (SIM) for all types of reflectors. b) The maximum light output, taken at the depth closest to the photodetector show reasonable agreement.

The LYSO crystal used has a dimension of $3 \times 3 \times 20$ mm^3. These measurements were published from UC Davis.[8]

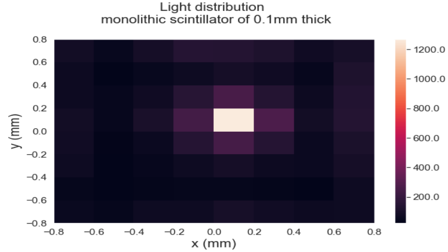
Findings

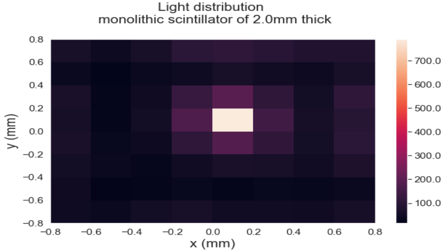
- Showed consistent results that thicker scintillators (larger aspect ratio) has better light collection with the coupling of optical reflectors to polished surfaces.
- It was also measured that as the thinner scintillators (smaller aspect ratio) collect light better in rough surfaces.
- However, it showed that coupling of optical reflectors makes a different in light collection for rough surfaces. This observation is supported by another publication from CERN on LYSO scintillator. [6]

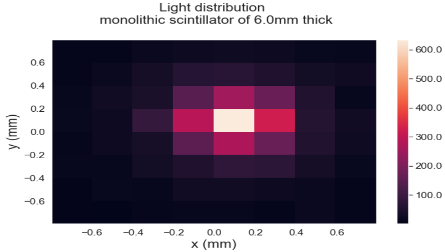
Discussion

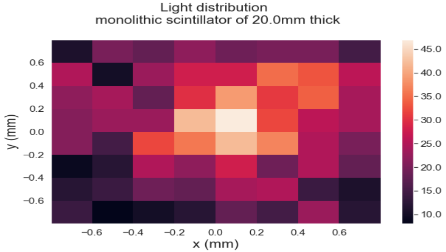
- Both publications agree that scintillators with larger aspect ratio performs better in light collection when the scintillator surfaces are polished and coupled to optical reflectors.
- Simulated and measured results seem to suggest that scintillators with smaller aspect ratio may perform better in rough surfaces in certain cases.
- Discrepancy in light collection is found in both publications for rough scintillator surfaces with and without optical reflectors.

Results: Light Sharing / Crosstalk







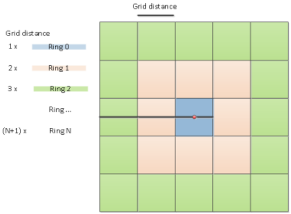


Light Sharing Between Pixels

Quantify cross talk using the percent difference in count rates between the first nearest neighbors and the second nearest neighbors.

Results

Scintillator thickness (mm)	Crosstalk (%)	Target (counts)
0.1	65.93	1268
2.0	65.25	790
6.0	75.42	634
20.0	73.36	47



Discussion

- The overall crosstalk using monolithic scintillator is still much larger than segmented scintillator (experimentally measured to be about 5.64%)
- Monolithic scintillator results in the whole detector area to be dead during scintillations → lower detection rate

Outline

Conclusion

Key results:

- Scintillators with larger aspect ratio have higher light collection efficiency when the scintillator surfaces are polished and coupled to optical reflectors
- Scintillators with smaller aspect ratio may have better light collection when the scintillator surfaces remain unpolished, rough-cut.
- Monolithic scintillator in a pixel array configuration results in much larger cross talk between photodetector pixels than pixelated scintillator, even with scintillator thickness of 100 μm.

Challenges in optical simulation using GEANT4:

- A simplified description of rough surfaces as an ensemble of micro-facets determined by the distrubution of Gaussian distribution may not be the true representation of surface roughness.
- Optical reflectance of a material may not be a linear combination of backscatter spike, specular spike, specular lobe and Lambertian reflections.
- Two published results demonstrated the discrepancies between GEANT4 unified models and experimental data and obtained better accuracy by using measured reflectance data in simulation modelling without making assumptions about the surface roughness.

Future Work

The simulation model developed was able to produce consistent results with published data when using BGO as the scintillator. If experimental reflectance data of GS20 is obtained, correct optical transport modelling can be made.

Since there aren't published result that a direct comparison can be made, experimental data is needed in order to validate the simulation model:

- Measure the reflectivity of GS20 crystal with different surface treatments
- Perform experimental measurements on actual detector setup with different scintillator surface treatments and aspect ratios

References

[1] 6-lithium enriched glass scintillators: Products: Scintacor.

[2] Geant4 book for application developers.

[3] M. Janecek.
Reflectivity spectra for commonly used reflectors.
IEEE Transactions on Nuclear Science, 59(3):490–497, 2012.

[4] Martin Janecek and William W. Moses.
Measuring light reflectance of bgo crystal surfaces.
IEEE Transactions on Nuclear Science, 55(5):2443–2449, 2008.

[5] Martin Janecek and William W. Moses.
Simulating scintillator light collection using measured optical reflectance.
IEEE Transactions on Nuclear Science, 57(3):964–970, 2010.

[6] Kristof Pauwels, E. Auffray, S. Gundacker, A. Knapitsch, and P. Lecoq.
Effect of aspect ratio on the light output of scintillators.
IEEE Transactions on Nuclear Science, 59(5):2340–2345, 2012.

[7] Emilie Roncali and Simon R Cherry.
Simulation of light transport in scintillators based on 3d characterization of crystal surfaces.
Physics in Medicine and Biology, 58(7):2185–2198, 2013.

[8] Emilie Roncali, Mariele Stockhoff, and Simon R Cherry.
An integrated model of scintillator-reflector properties for advanced simulations of optical transport.
Physics in Medicine and Biology, 62(12):4811–4830, 2017.

[9] A.r. Spowart.
Neutron scintillating glasses: Part 1.
Nuclear Instruments and Methods, 135(3):441–453, 1976.

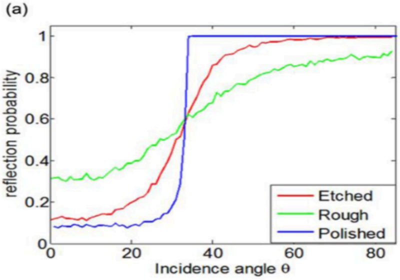
Outline

5. **Backup Slides**

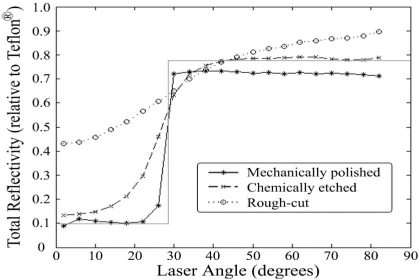
Relevant Published Data

Scintillator crystal without any reflectors:

	GS20	LYSO	BGO
Refractive Index	1.55	1.81	2.15
Critical angle (^{o})	40.18	33.53	26.23
Wavelength at maximum emission (nm)	395	420	480



LYSO [8]

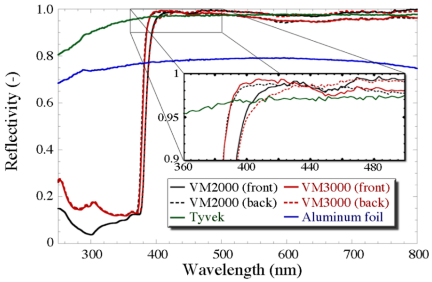


BGO [5]

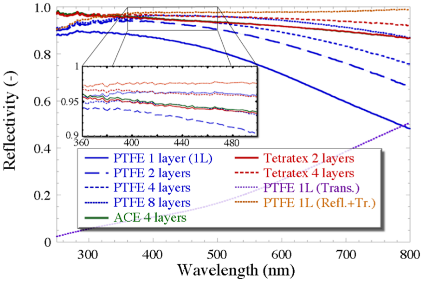
Relevant Published Data

Several reflectors exhibits ”cut-offs” for the reflectivity for shorter wavelengths, such as TiO_2 (420 nm) and ESR film (395 nm). [3]

Reflectivity curve as a function of wavelengths:



VM2000 [3]



Teflon [3]