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

Su-Ann Chong

July 31st, 2020

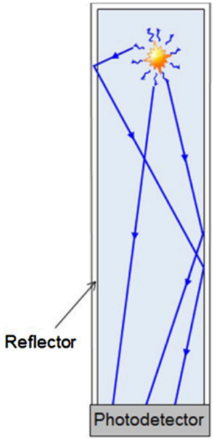
Outline

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 [6].

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]

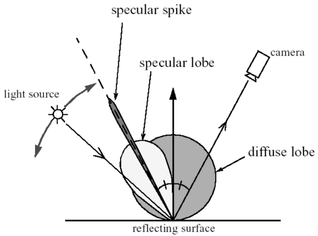
- unified
  Users specify a parameter *SigmaAlpha*, which defines the standard deviation of the Gaussian distribution of micro-facets around the average surface normal. [2] Four kinds of surface reflections are possible: specular, spike, lobe, backscatter and Lambertian. [5]

  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

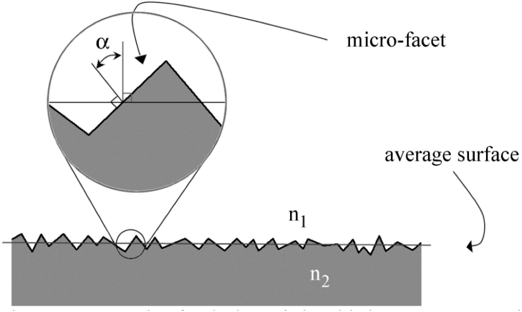
Surface reflections components:



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

1. Introduction
2. **Simulation Model**
3. Results and Discussions
4. Conclusion and Future Work

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 $\rightarrow$ 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

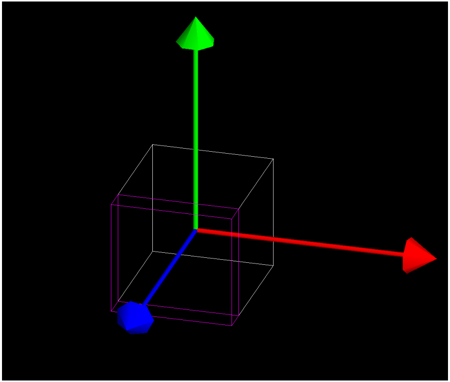
Example GPS setup using macro

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

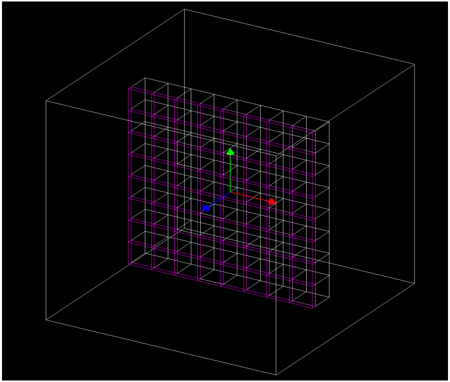
Detector Geometry

Two detector geometry configurations:

single pixel



8×8 pixel array



scintillator (white wiring), photodetector (magenta wiring)

Scintillator Material Composition and Properties

Material Composition [8]

	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

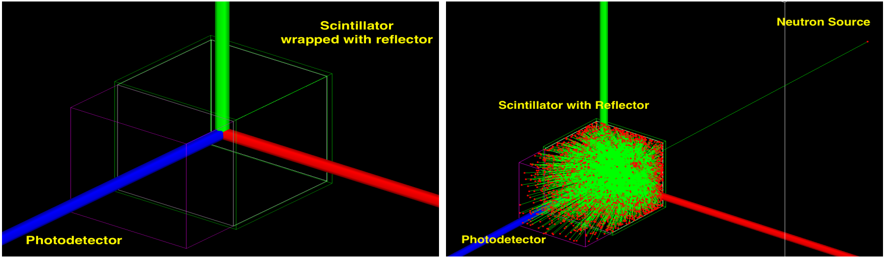
† LUT model is based on BGO crystal. [4]
‡ DAVIS model is based on LYSO crystal [6]

Parameters for unified model

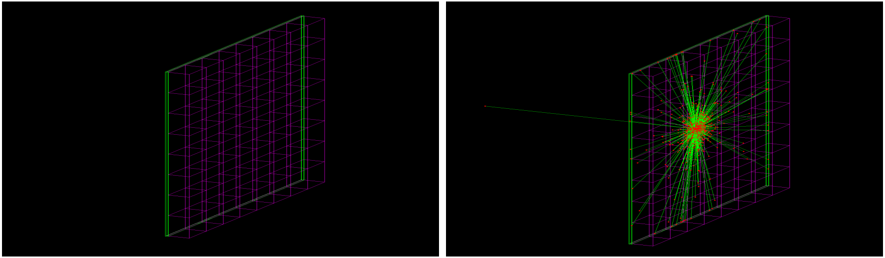
SigmaAlpha	0.0227 rad/1.3^o (polished)
	0.209 rad / 12^o (rough)

Simulated Detector Setup

single pixel (light collection efficiency)



pixel array (light sharing)



Outline

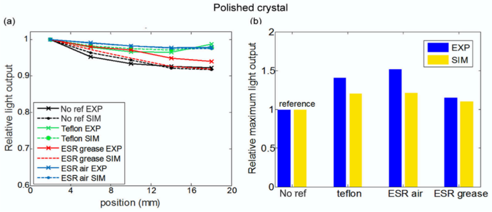


Figure 12.
Light output for polished crystals with no reflector, Teflon, or ESR (air-coupled or grease-coupled). a) Normalized outputs for experiments (EXP) and simulations (SIM). b) Maximum light outputs, taken at the depth closest to the photodetector (2 mm).

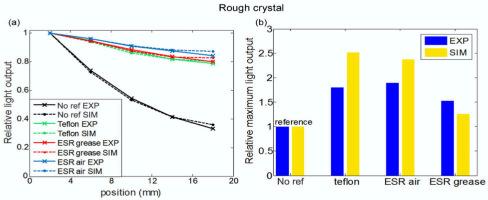


Figure 10.
Light output for rough crystals with no reflector, Teflon, or ESR (air-coupled or grease-coupled). a) The normalized outputs show excellent agreement between experiments (EXP) and simulations (SIM) for all types of reflectors. b) The maximum light output, taken at the depth closest to the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

The LYSO crystal used has a dimension of $3 \times 3 \times 20$ mm^3. These measurements were conducted by another publication.[7]

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.

Results: Light Sharing / Crosstalk

Outline

Conclusion

Future Work

Measure experimental data Measure our own LUT

Acknowledgement

Most of the framework can be obtained from Dr. Micah Folsom's public Github repository. (https://github.com/micahfolsom/mgg4)

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] 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.

[7] 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.

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

Outline

5. **Backup Slides**

Equations

Snell's law:

$$n_i\ sin(\theta_i) = n_t\ sin(\theta_t)$$

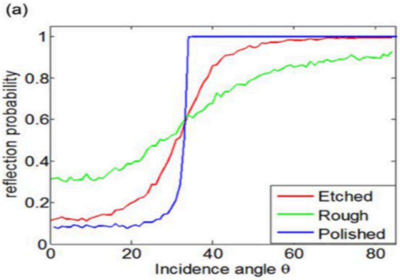
Critical angle:

$$\theta_c = sin^{-1}(n_t/n_i)$$

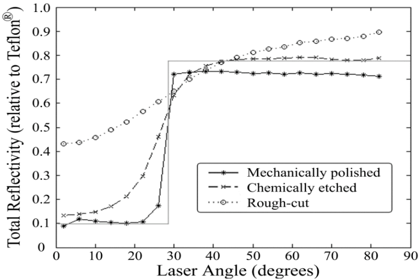
Relevant Published Data

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 [7]

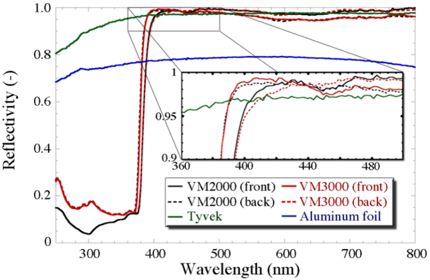


BGO [5]

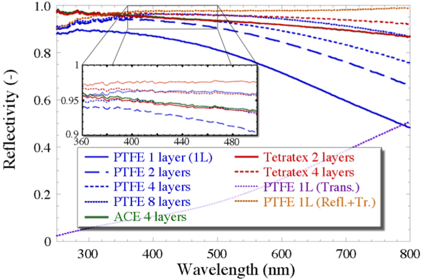
Relevant Published Data

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]