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

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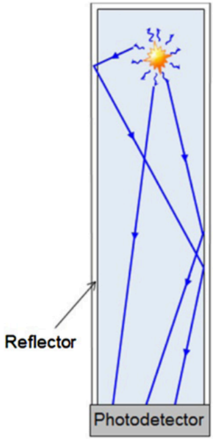
Outline

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]

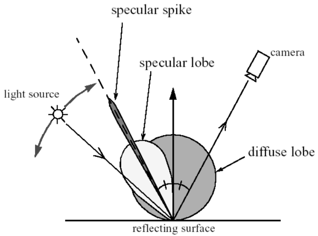
- unified
  Users specify a parameter *SigmaAlpha*, which defines the standard deviation of the Gaussian distribution of micro-facets around the average surface normal. [2] Four kinds of surface reflections are possible: specular, spike, lobe, backscatter and Lambertian. [5]

  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

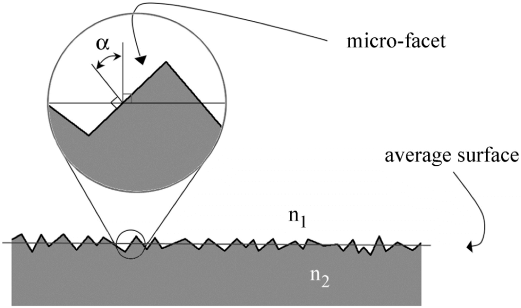
Surface reflections components:



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:

- Compare light collection based on different surface treatments (surface roughness, reflector type, coupling method)
- Estimate light sharing of monolithic scintillators over pixelated photodetectors

Key Model Parameters:

- Source:
  - monoenergetic neutron beam at 25 meV (1.8 Å)
  - optical photons at 3.19 eV (395 nm)
- Geometry: single pixel and pixel array (8×8 pixels)
- Material: ^{6}Li-enriched glass scintillator (GS20, Scintacor)
- Physics lists:
  - QGSP_BERT_HP
    energy of primary particle < 5 GeV, detailed neutron transport (< 20 MeV)
  - G4OpticalPhysics
    optical photon transportation
- Output: ROOT files
- Data Analysis: Python (Use uproot to read ROOT files)

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

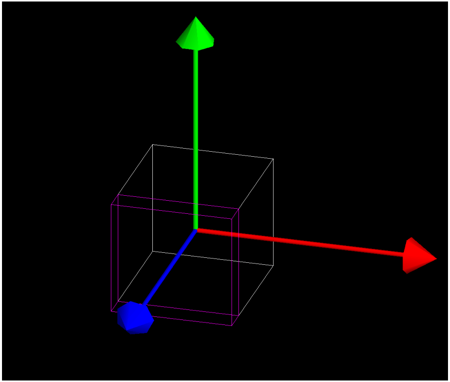
Example GPS setup using macro

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

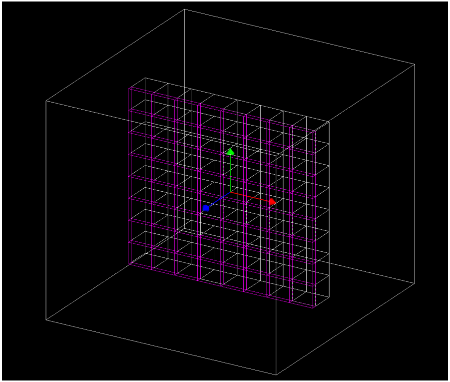
Detector Geometry

Two detector geometry configurations:

single pixel



8 × 8 pixel array



scintillator (white wiring), photodetector (magenta wiring)

Scintillator Material Composition and Properties

Material Composition [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
model	unified
surface finish	rough, polished
reflector type	air, TiO_2
crystal thickness	2 mm

Parameters for unified model [5]

SigmaAlpha	0.0227 rad/1.3^o (polished) 0.209 rad / 12^o (rough)
REFLECTIVITY †	0.05 (air) 0.89 (TiO_2)
RINDEX †	1.0 (air) 1.35 (TiO_2)
Reflection Type Probability †	100% Diffuse lobe, 0% specular lobe 0% specular spike, 0% backscatter

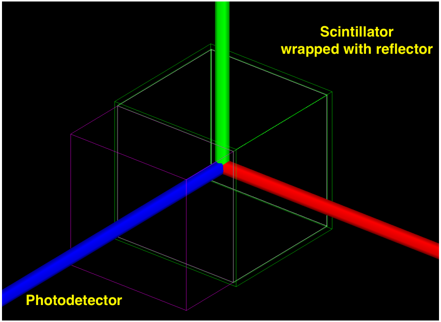
† Assume constant over all optical photon energies

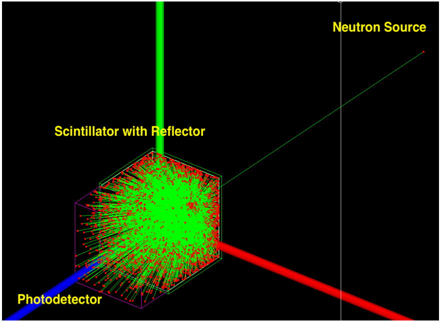
Outline

Detector Setup: Light Collection

A single pixel is used to study the light collection with different surface treatments and scintillator thicknesses. Figure below shows a 2 mm x 2 mm x 2 mm scintillator cube with polished surfaces coupled to a layer of reflective coating.

A neutron is emitted a distance away from the scintillator. Neutron is captured in the scintillator and approximately 6,000 photons are emitted isotropically.

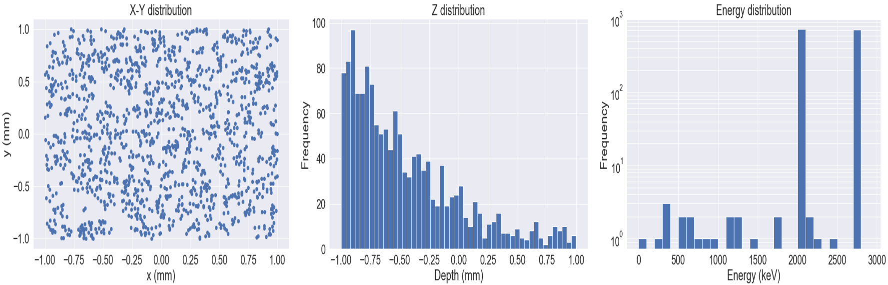




Validation: Neutron Capture

Here are an additional few plots that illustrate the expected results of neutron capture and energy deposited in the scintillator:

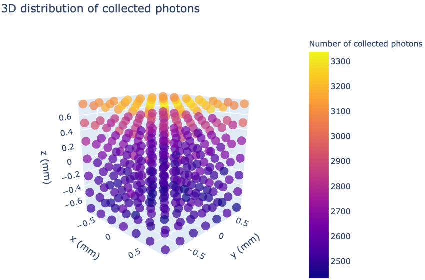
X-Y distribution: uniform distribution of neutron capture
Z distribution: neutron attenuation of GS20 at 25 meV
Energy distribution: energy deposited by the reaction productions of neutron capture
^{3}H (2.73 MeV) and α (2.05 MeV)

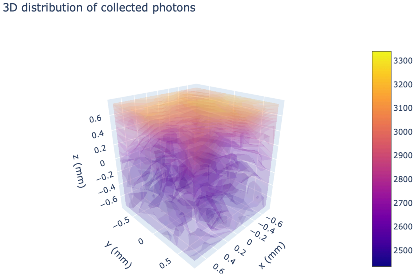


Validation: Optical Transport

To make sure that the simulation of optical transport behaves as expected, 6,000 photons are emitted isotropically at $7 \times 7 \times 7 = 343$ positions within the scintillator volume. Optical photons are used instead of neutrons to speed up simulation.

Photodetector is positioned at $z = 1.0$ mm, where most photons are detected, as expected. The scintillator cube has a polished surface with no reflectors coupled to it.

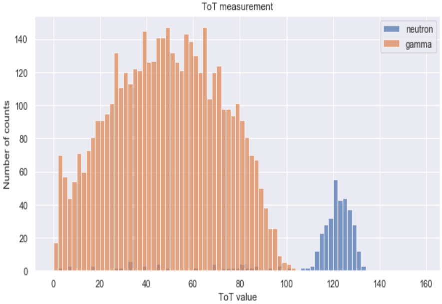




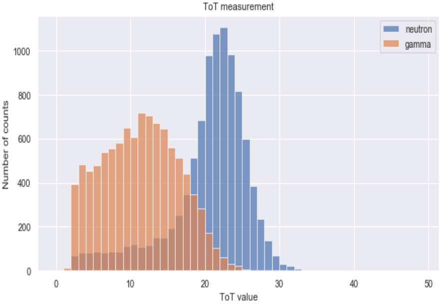
Metric: Which is Better?

In Time-over-Threshold (ToT) spectrum, neutron peak with higher ToT values is better as it gives a better separation between neutron peak and gamma peak.

Experimental data:



6×6 mm^2 SiPM



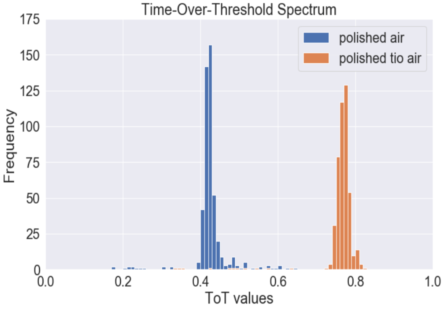
1×1 mm^2 SiPM

* The separation difference between neutron peak and gamma peak has to do with the active area of the SiPM. If the active area of SiPM is smaller than the area of the scintillator surface coupled to the SiPM (2×2 mm^2), less photons are collected as a results.

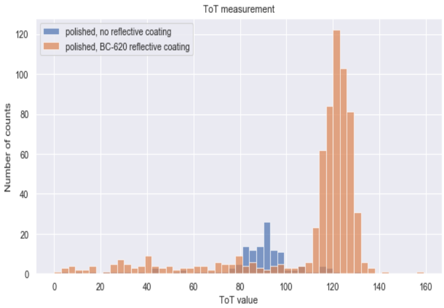
Results: Surface Treatments I

The simulation model is able to produce results that are consistent with experimental data when the scintillator surface is polished.

Since the experimental data is not normalized, results can only be compared in relative. Both experimental and simulated results show that scintillator coupled with reflective coating have higher ToT values than the ones without.



Simulated result

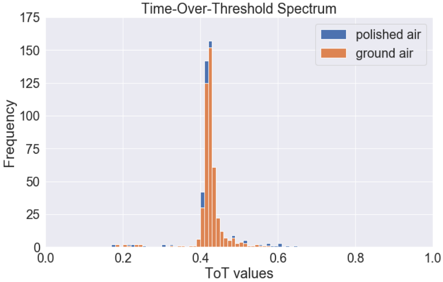


Experimental result

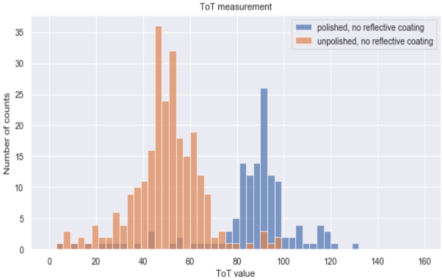
Results: Surface Treatments II

The simulation model is not able to model rough surfaces well. This result is expected and published in numerous articles. [4] [5] [7] [8]

The next slide will show published result from [5] that shows the discrepancy between simulated data and experimental data using Geant4 unified model.



Simulated result



Experimental result

Results: Surface Treatments III

The original code (using Geant4 unified model) perform better in simulating polished surfaces than rough surfaces as the discrepancies between simulated data and measured data are smaller.

Using Geant4 unified model, the simulated light yield tends to be higher for rough surfaces than for smooth surfaces. Meanwhile, measured data generally shows that the light yield for polished surfaces are higher than rough surfaces.

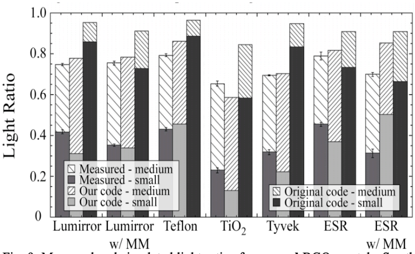


Fig. 9. Measured and simulated light ratios for **ground** BGO crystals. See the text for Fig. 7 for detailed description of the figure.

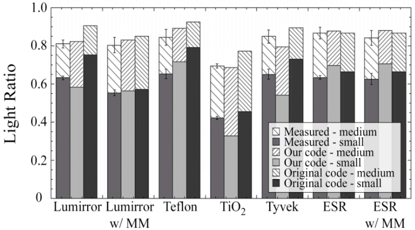


Fig. 7. Measured and simulated light ratios for **polished** BGO crystals. The measured data (with standard deviation error bars) is the leftmost columns, our code simulations are the middle columns, and the original code simulations are the rightmost columns for each attached reflector material. The 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™".

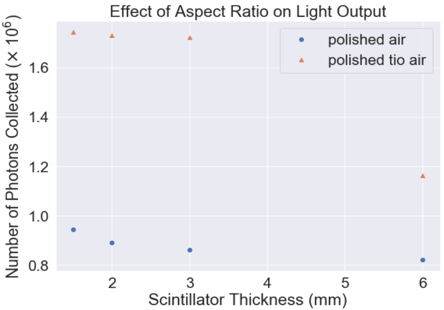
Rough

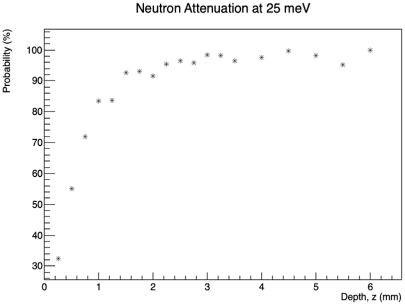
Polished

Results: Scintillator Thickness

The effect of aspect ratio on the light output of scintillator. It has been demonstrated that crystals shaped in thin rods have a lower light output as compared to bulky or sliced crystals. [6]

Since our simulation model works well with polished surfaces, we only investigated two polished surface treatments. The simulated result is consistent with the result published in [6].



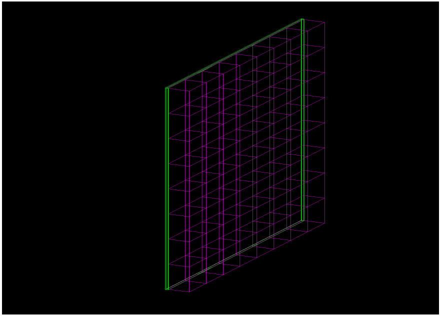


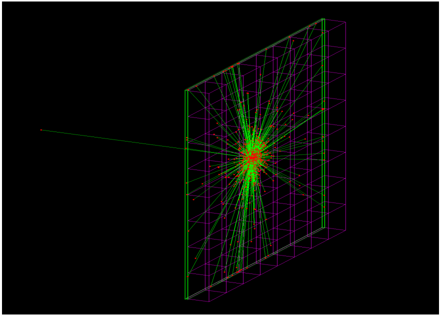
Experimental validation is needed to find the optimum scintillator thickness for maximum light output.

Simulated Detector Setup

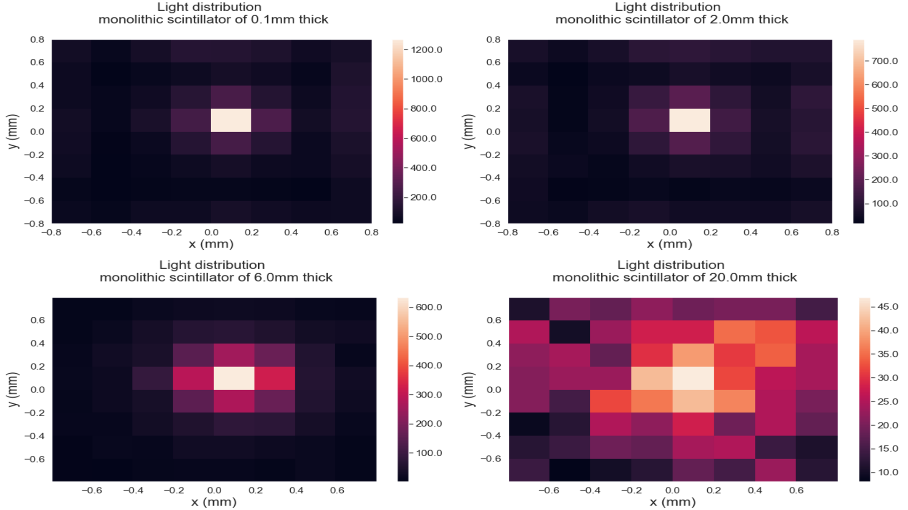
Having pixelated scintillator arrays often requires cutting, polishing, applying reflective coating and optical grease and assembling scintillator arrays to couple to SiPM, hence results in higher cost and more laborious.

We are interested to investigate the effect of monolithic scintillator thickness on the crosstalk/light sharing between pixels.





Results: Light Sharing / Crosstalk

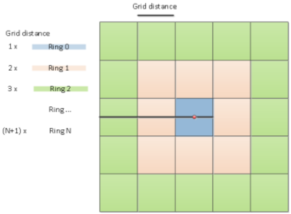


Light Sharing Between Pixels

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

- Geant4 unified model can model polished surfaces relatively well, but performs rather poorly on rough surfaces. This may be due to the model description on surface roughness is not a true representation of the actual surfaces.
- The aspect ratio of the scintillator affects the light output. Crystal shaped in thin rods have a lower light output as compared to bulky or sliced crystals.
- 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.

Key results

- Coupling of reflective coating helps with light collection for polished surfaces, evidenced by both experimental and simulated results.
- Segmentation in scintillator is necessary to prevent crosstalk/light sharing between pixels and increase the counting rate of the detector.

Future Work

- Lack of experimental data
  - Light output of different scintillator thicknesses to find the optimal scintillator thickness for maximum light collection
  - Effect of monolithic scintillator thickness on crosstalk/light sharing between pixels to validate that pixelation in scintillator is necessary for minimal crosstalk and high counting rate
- Interest of time
  - The reflectance and transmitance of light on the scintillator with different surface treatments can be measured and incorporated in the look up table (LUT) model in Geant4.
  - Better results has been shown in modelling rough surfaces.
  - Future optical transport simulation on GS20 can be available to public.

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.

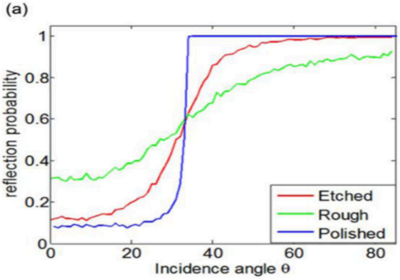
Outline

5 **Backup Slides**

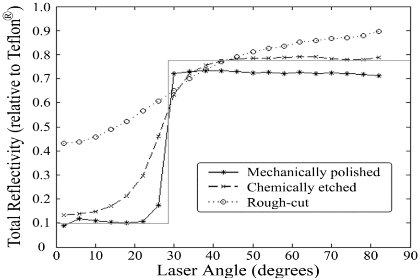
Relevant Published Data

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]

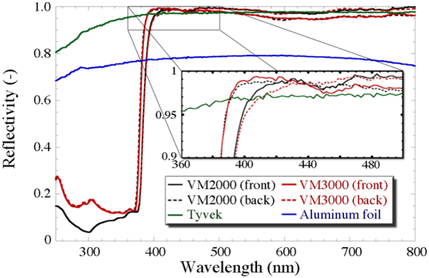


BGO [5]

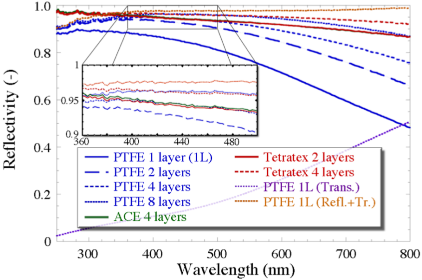
Relevant Published Data

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]