Counterintuitive MCNPX Results for Scintillator Surface Roughness Effect

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Why a Surface Roughness Study?

- Scientific Curiosity
 - Most solid radiation detection materials, in particular solid scintillation materials, produced by current industrial processes have smooth surfaces. No one has looked at alternative surface types.
- Common Sense Analogies
 - Sanded glass is less reflective than smooth glass. Could this mean more energy is deposited on the sanded glass (or is there simply more scattering)?
 - An open window in a distant wall appears dark. Apparently this traps more photons than a flat wall. Can we create some tiny windows on a detector's surface to trap more incoming particles?
 - Blackbodies (practically a deep cavity) absorb incoming photons and converts their energy into thermal energy (increased temperature + thermal emission output). Could some kind of surface cavity structure help to improve the scintillation output?

Why Choose Inorganic Scintillation Detectors

- Scientific / Technical / Industrial Considerations
 - Scintillators convert the kinetic energy of charged particles into detectable light—more energy deposited implies more scintillation light output. (G. Knoll, 2000)
 - Scintillation detectors, in particular NaI detectors, are the most widely-used radiation detectors. Therefore, a surface roughness study, if successful, would have an immediate industrial impact.
 - LaBr_3 somehow represents a current trend in inorganic scintillator studies. If a roughness study proves useful for LaBr_3 , then its application base is broadened.

Primarily Considering $\phi 1'' \times 1''$ Scintillation Crystals

$\Phi 1'' \times 1''$ Scintillation Crystal Geometrical Properties

MCNPX Settings

Aluminum Casing

MCNPX Settings

Source – Detector Relationship

MCNPX Settings

Importance Space

Crystal Surface Geometry

Outside of the Box Considerations

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Consider Three Possible Surface Processing Methods

- Sanding or Micro-sanding
- Drilling or Micro-drilling
- Cutting or Micro-cutting
 - Parallel Cutting
 - Cross Cutting
- These processes can be easily adapted by industry, if proven useful
- Correspondent MCNPX modeling schemes will be created

Crystal Surface Geometry

Micro-sanding Pattern

This setup may simulate a surface sanding process

Micro-sanding MCNP Geometrical Parameters

- For LaBr_3 and NaI detectors
- Run parameters with
 - Micro-sphere radius $r = 100 \mu\text{m}$ and $50 \mu\text{m}$
 - Micro-sphere distance $d = 4 \times$ sphere radius
 - Roughness height $h = 1 \times$ sphere radius

Micro-sanding Modeling Experimental Design Table

Experimental Parameters and Values				
Pattern Code	μ -sphere radius	μ -sphere Distance	μ -Roughness Height	# Particles
Sand050	50 μm	200 μm	50 μm	1×10^6
Sand100	100 μm	400 μm	100 μm	1×10^6

Crystal Surface Geometry

Micro-drilling Pattern

Micro-drilling MCNP Geometrical Parameters

- For LaBr_3 and NaI detectors
- Run parameters with:
 - Micro-cylinder radius $r = 100 \mu\text{m}$ and $50 \mu\text{m}$
 - Micro-cylinder height $h = 8 \times \text{radius}$
 - Micro-cylinder distance $d = 4 \times \text{sphere radius}$
 - Roughness height $h = 4 \times \text{sphere radius}$

Micro-drilling Modeling Experimental Design Table

Experimental Parameters and Values

Pattern Code	μ -cylinder radius	μ -cylinder Distance	μ -cylinder Height	μ -roughness Height	# Particles
Drill050	50 μm	200 μm	400 μm	200 μm	1×10^6
Drill100	100 μm	400 μm	800 μm	400 μm	1×10^6

Crystal Surface Geometry

Micro-cutting (Parallel Cutting) Pattern

Four design parameters to consider

a = Base ellipsoid short radius

b = Base ellipsoid long radius

d = Micro-cylinder distance

h = Roughness height

This setup may simulate a parallel surface cutting process

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Micro-cutting (Parallel Cutting) MCNP Geometrical Parameters

- For LaBr_3 and NaI detectors
- Run parameters for the cutting blade with:
 - Micro-ellipsoid short radius $a = 50 \mu\text{m}$ and long radius $b = 100 \mu\text{m}$
 - Micro-ellipsoid blade length $h = 1"$ (enough for the detector size)
 - Micro-ellipsoid blade distance $d = 4 \times \text{short radius}$
 - Roughness height $h = 1 \times \text{long radius}$

Micro Parallel Cutting Modeling Experimental Design Table

Experimental Parameters and Values

Pattern Code	μ -blade Short radius	μ -blade Long radius	μ -blade Distance	μ -rough Height	# Particles
PCut050	50 μm	100 μm	200 μm	100 μm	1×10^6
PCut100	50 μm	150 μm	200 μm	150 μm	1×10^6

Crystal Surface Geometry

Micro-cutting (Cross-Cutting) Pattern

Micro-Crosscutting Parameters (Cross Cutting - X-cuts followed by Y-cuts)

- For LaBr3 and NaI detectors
- Run parameters for the cutting blade with:
 - Micro-ellipsoid short radius $a = 50 \mu\text{m}$ and long radius $b = 100 \mu\text{m}$
 - Micro-ellipsoid blade length $h = 1''$ (enough for the detector size)
 - Micro-ellipsoid blade distance $d = 4 \times \text{short radius}$
 - Roughness height $h = 1 \times \text{long radius}$

Micro Cross Cutting Modeling Experimental Design Table

Experimental Parameters and Values

Pattern Code	μ -blade Short radius	μ -blade Long radius	μ -blade Distance	μ -rough Height	# Particles
XCut050	50 μm	100 μm	200 μm	100 μm	1×10^6
XCut100	50 μm	150 μm	200 μm	150 μm	1×10^6

Energy Deposition Summary

F6 Tally (MCNPX)

Surface type	CdSe	CeBr ₃	CeF ₃	LaBr ₃	LaCl ₃	LaF ₃	Nal	SiO ₂
Smooth	2.6941E-05	2.7244E-05	2.7610E-05	2.7097E-05	2.7752E-05	2.7645E-05	2.8022E-05	2.6710E-05
Sand050	2.6927E-05	2.7458E-05	2.8072E-05	2.7559E-05	2.8134E-05	2.7831E-05	2.9260E-05	2.7761E-05
Sand100	2.6630E-05	2.7125E-05	2.7644E-05	2.7227E-05	2.7222E-05	2.7364E-05	2.8346E-05	2.6899E-05
Drill050	2.7299E-05	2.7810E-05	2.8585E-05	2.7710E-05	2.8442E-05	2.8077E-05	2.9307E-05	2.8537E-05
Drill100	2.7526E-05	2.8157E-05	2.8404E-05	2.7907E-05	2.8568E-05	2.8262E-05	2.9099E-05	2.7993E-05
PCut050	2.7804E-05	2.7862E-05	2.8874E-05	2.7960E-05	2.8256E-05	2.8682E-05	2.9688E-05	2.8133E-05
PCut100	2.8637E-05	2.8808E-05	2.9482E-05	2.8714E-05	2.8730E-05	2.9171E-05	2.9218E-05	2.9048E-05
XCut050	2.6934E-05	2.7491E-05	2.7878E-05	2.7281E-05	2.7510E-05	2.7874E-05	2.9070E-05	2.7650E-05
XCut100	2.7147E-05	2.7836E-05	2.7984E-05	2.7527E-05	2.7970E-05	2.7657E-05	2.8786E-05	2.7433E-05

Average Energy Deposition

- 3D view of the data in the previous slide
- Front line shows the data for smooth surfaces

Difference in Energy Deposition

- Differences in average energy deposition as compared with correspondent crystals with smooth surfaces
- Front line data are zeroes for smooth surfaces.

**Difference in Average Energy Deposition (Mev/g)
Between Rough and Smooth Scintillators**

Energy Deposition Improvement

Energy deposition improvement as compared with crystals with smooth surfaces

Improve%	CdSe	CeBr3	CeF3	LaBr3	LaCl3	LaF3	NaI	SiO2	Rank	Min	Mean	Max
Smooth	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	8	0.00%	0.00%	0.00%
Sand050	-0.05%	0.78%	1.67%	1.71%	1.38%	0.67%	4.42%	3.94%	5	-0.05%	1.81%	4.42%
Sand100	-1.16%	-0.44%	0.13%	0.48%	-1.91%	-1.02%	1.15%	0.71%	9☹	-1.91%	-0.26%	1.15%
Drill050	1.33%	2.08%	3.53%	2.26%	2.49%	1.56%	4.58%	6.84%	4	1.33%	3.08%	6.84%
Drill100	2.17%	3.35%	2.88%	2.99%	2.94%	2.23%	3.84%	4.80%	3	2.17%	3.15%	4.80%
PCut050	3.20%	2.27%	4.58%	3.19%	1.82%	3.75%	5.94%	5.33%	2	1.82%	3.76%	5.94%
PCut100	6.30%	5.74%	6.78%	5.97%	3.53%	5.52%	4.27%	8.75%	1☺	3.53%	5.86%	8.75%
XCut050	-0.02%	0.91%	0.97%	0.68%	-0.87%	0.83%	3.74%	3.52%	7	-0.87%	1.22%	3.74%
XCut100	0.77%	2.17%	1.36%	1.59%	0.79%	0.04%	2.73%	2.71%	6	0.04%	1.52%	2.73%
Rank	7	5	3	4	8☹	6	2	1☺	Global	-1.91%	2.24%	8.75%
Min	-1.16%	-0.44%	0.00%	0.00%	-1.91%	-1.02%	0.00%	0.00%	-1.91%	Yellow =0		
Mean	1.39%	1.87%	2.43%	2.10%	1.13%	1.51%	3.41%	4.07%	2.24%	Green >0		
Max	6.30%	5.74%	6.78%	5.97%	3.53%	5.52%	5.94%	8.75%	8.75%	Red <0

Percentage Improvement in Energy Deposition

- 3D view of data in previous slide
- Shows percentage improvement as compared with correspondent smooth surfaces

Percentage Improvement
in Average Energy Deposition (Mev/g)

Discussion

- MCNPX results suggest that a rough surface generally improves the detectors photon detection efficiency
- Of all 64 rough surfaces and scintillator couplings, about 57 showed some improvement (89%)
- The rough surfaces demonstrated systematic advantages for scintillators NaI, LaBr₃, LaCl₃, CeBr₃, and LaF₃
- The mean improvement is about 2.5% for all crystals, with a maximum improvement of 8.75% for SiO₂

Discussion

Reasons for the these types of simulation results are not explained by this work; however, the following are suspected:

- Increased gamma capturing may be due to the periodicities (or wave patterns) of the evaluated roughness patterns, as compared with those studied in optics for diffraction gratings or other fields.
- Increased gamma capturing may be to due to the increase of the effective surface areas of the scintillators under various surface-roughness schemes.
- The increase in internal reflection of the photons in the visible wavelengths resulting from scintillation may be an outcome or benefit of roughening the crystal surface.

Discussion

Caveats:

- Statistical uncertainties in real-world data and in these MCNPX simulations are present. A high precision statistical analysis is required to ascertain the true statistical significance of these findings.
- The MCNPX results presented here are for tallies of energy deposition.
- The effects of rough surfaces on photon internal reflection have not yet been studied.
- A more detailed analysis that incorporates the incoming gamma-ray energy deposition, internal reflection of visible photons, depth of interaction, and rough surfaces on photon internal reflection, etc., is required in order to explain the overall comprehensive picture.

Summary

- We have reported on our recent MCNPX simulation results of energy deposition for a group of 8 scintillation detectors, coupled with various rough surface patterns.
- The MCNPX results generally favored the detectors with various rough surface patterns.
- The observed MCNPX results are not fully explained by this work.
- The MCNPX results are reported for stimulating further investigations.