On the mirror roughness: A first case study

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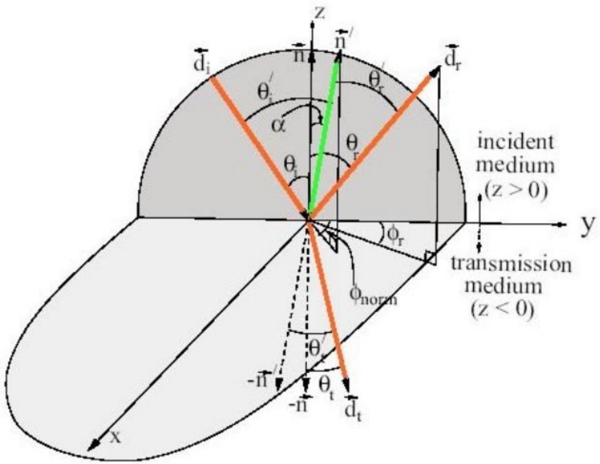
Geant4 modeling on mirror roughness

- Optical surfaces are either of *dielectric-dielectric* or *dielectric-metal* type.
- The types are described in two *models*: unified and glisur. The glisur model is inherited from Geant3.
- In dielectric-metal case: the surface *finish* can either be polished or grounded.
  There are other models, but less relevant for our discussion.
- A ground finish allows to add surface roughness. The two models have different implementation methods.
  - Unified: *SetAlphaSigma(parameter)*
  - Glisur: *SetPolish(parameter)*

Microfacet theory

The assumption is that a rough surface is a collection of 'micro-facets'



Coordinate system used for ***ground*** surfaces along with the definition of geometrical parameters.

Surface effects

POLISHED: In the case where the surface between two bodies is perfectly polished, the normal used by the G4BoundaryProcess is the normal to the surface defined by:

(a) the daughter solid entered; or else
(b) the solid being left behind

GROUND: The incidence of a photon upon a rough surface requires choosing the angle, α, between a 'micro-facet' normal and that of the average surface.

The UNIFIED model assumes that the probability of micro-facet normals populates the annulus of solid angle sin(α)dα will be proportional to a gaussian of SigmaAlpha:

```
theOpSurface -> SetSigmaAlpha(0.1);
```

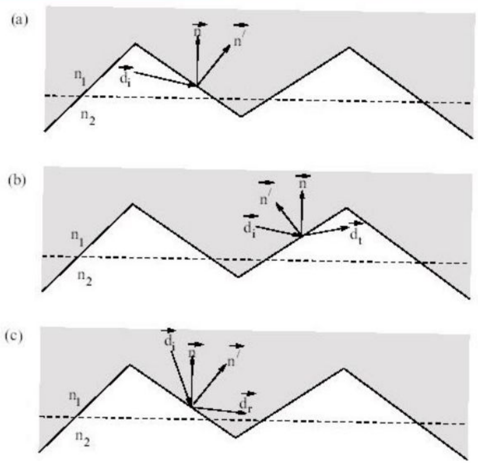
where sigma_alpha is in [rad]

In the GLISUR model this is indicated by the value of polish; when it is <1, then a random point is generated in a sphere of radius (1-polish), and the corresponding vector is added to the normal. The value 0 means maximum roughness with effective plane of reflection distributed as cos(α).

```
theOpSurface -> SetPolish(0.0);
```

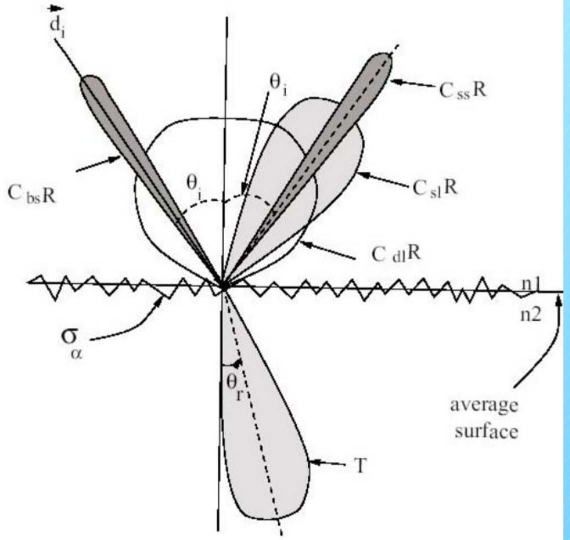
The 'facet normal' is accepted if the refracted wave is still inside the original volume.

Microfacet theory



Special cases handled by the UNIFIED model:
(a) when the incident photon does not aim toward the local micro-facet; or when the transmitted (b) or reflected (c) photon heads in the wrong direction with respect to the average surface normal.

In cases (b) and (c), multiple interactions with the boundary are possible within the Process itself and without the need for relocation by the G4Navigator.



Polar plot of the radiant intensity in the UNIFIED model

Csl: Reflection prob. about the normal of a micro facet
Css: Reflection prob. about the average surface normal
Cdl: Prob. of internal Lambertian reflection
Cbs: Prob. of reflection within a deep grove with the ultimate result of exact back scattering.

Microfacet theory

ChatGPT

Microfacet Theory: Microfacet theory models a surface as a collection of tiny, randomly oriented facets (microfacets) that scatter light. Each microfacet is a small planar surface that reflects light according to the laws of reflection. The overall appearance of the surface is determined by the distribution and orientation of these microfacets.

Microfacet Angle: The microfacet angle refers to the angle between a microfacet's normal and the overall surface normal. The distribution of these angles is critical in determining how light is reflected from the surface.

The relationship can be described mathematically using the microfacet distribution function, often represented by models such as the Beckmann or GGX distribution. These functions define the probability density of microfacet normals given a certain surface roughness parameter:

Beckmann Distribution: Often used for modeling surfaces with Gaussian distribution of microfacet slopes.

GGX (Trowbridge-Reitz) Distribution: A more modern and widely used distribution that handles high roughness levels better, providing a more physically plausible model.

Both distributions use a roughness parameter (often denoted as α\alphaα) that controls the spread of microfacet angles:

- **Low alpha (smooth surface)**: The distribution is sharply peaked around the surface normal, indicating a small range of microfacet angles.
- **High alpha (rough surface)**: The distribution is wider, indicating a larger spread of microfacet angles.

2. Microfacet Angle in Terms of Roughness Parameter

To express the microfacet angle in terms of the roughness parameter, consider that:

$$\theta_m \approx \arctan\left(\frac{\alpha \cdot x}{\lambda}\right)$$

where:

- x is a random variable representing the distribution of surface slopes.
- λ is a characteristic length scale (e.g., related to the measurement or the wavelength of incident light).

This implies that as the roughness parameter α increases, the potential microfacet angles θ_m also increase, meaning that more microfacets deviate significantly from the macroscopic surface normal.

3. RMS Roughness and Microfacet Angle

If you connect α with the RMS roughness σ_h:

$$\sigma_h = \alpha \cdot \lambda$$

Then, for small θ_m:

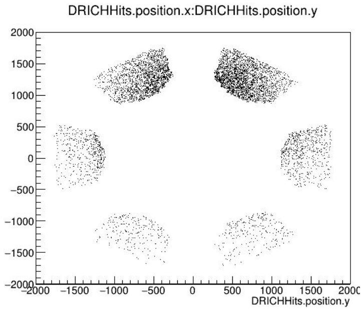
$$\theta_m \approx \arctan\left(\frac{\sigma_h}{\lambda}\right)$$

As α (and thus σ_h) increases, the microfacet angles θ_m increase, highlighting a rougher surface.

Testing of the two models (unified and glisur)

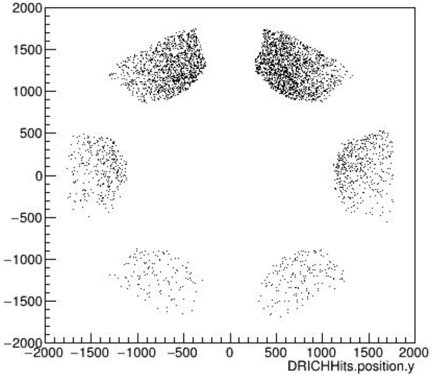
```
<opticalsurface name="MirrorSurface_DRICH" model="unified" finish="ground" type="dielectric_metal">
      <property name="REFLECTIVITY" coldim="2" values="
        1*eV  0.9
        7*eV  0.9
        "/>
</opticalsurface>

mirrorSurf->SetSigmaAlpha(0) // it means perfectly polish!
```

<u>**More direct estimate, but currently not working!**</u>

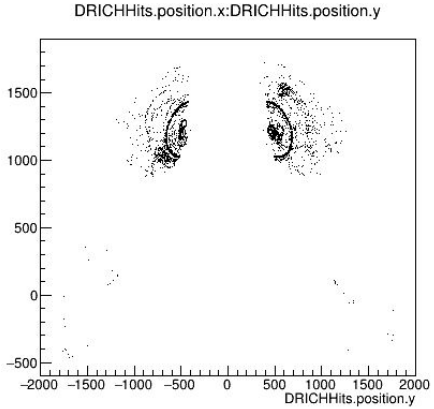



```
<opticalsurface name="MirrorSurface_DRICH" model="glisur" finish="ground" type="dielectric_metal">
      <property name="REFLECTIVITY" coldim="2" values="
        1*eV  0.9
        7*eV  0.9
        "/>
    </opticalsurface>
```

<u>**Less direct estimate, but working!**</u>



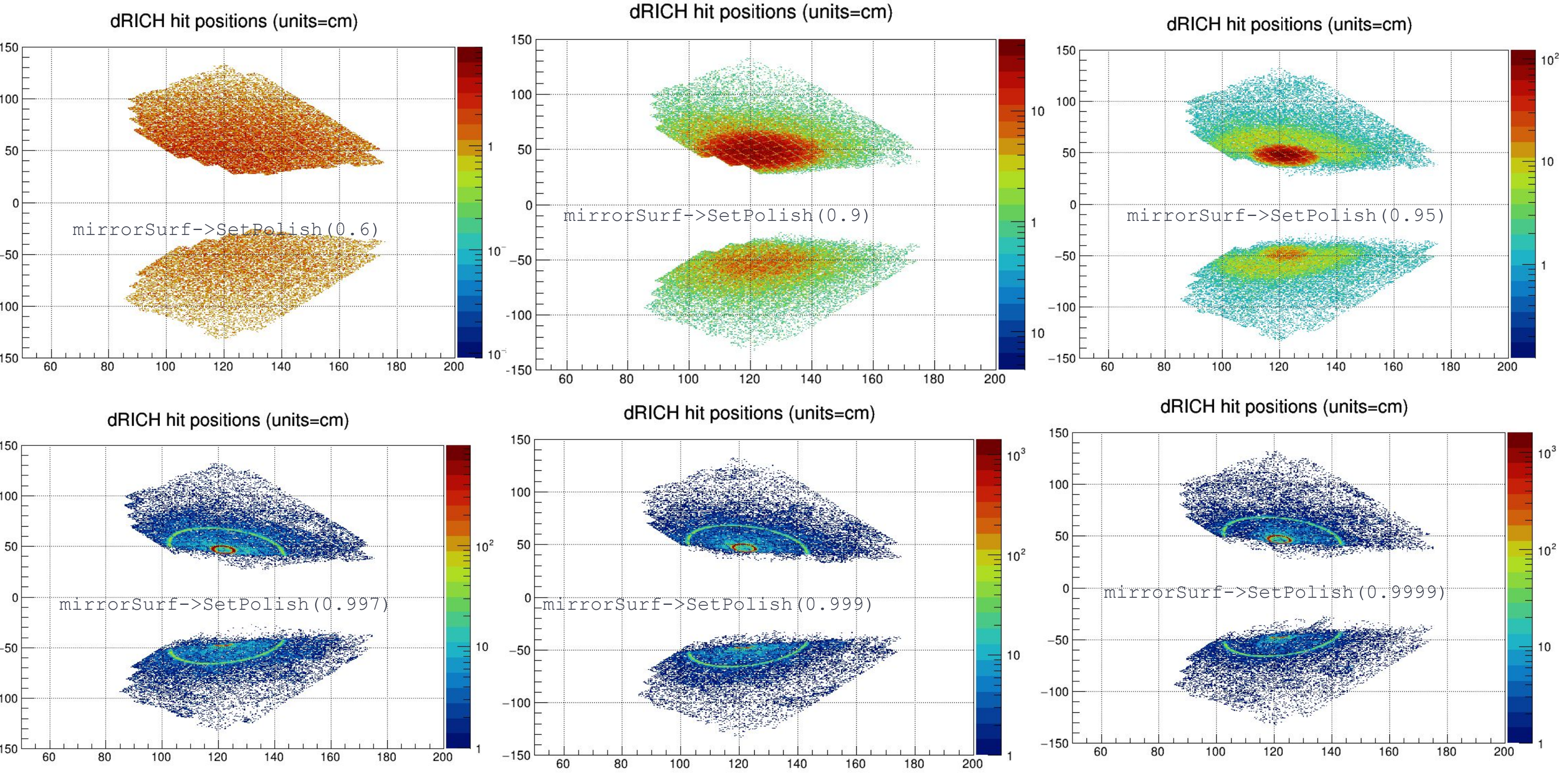

```
mirrorSurf->SetPolish(0) // no polish
```



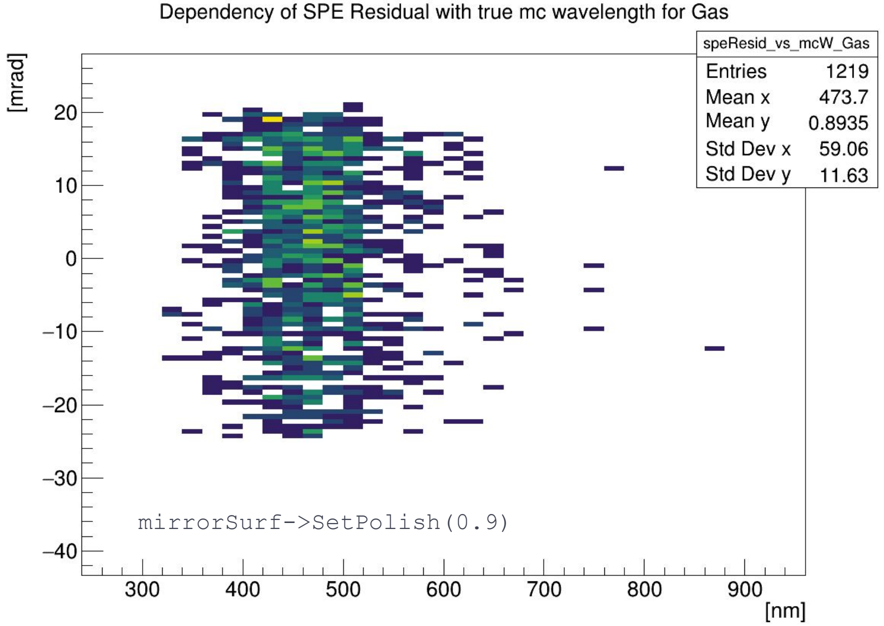

```
mirrorSurf->SetPolish(1) // fully polished
```

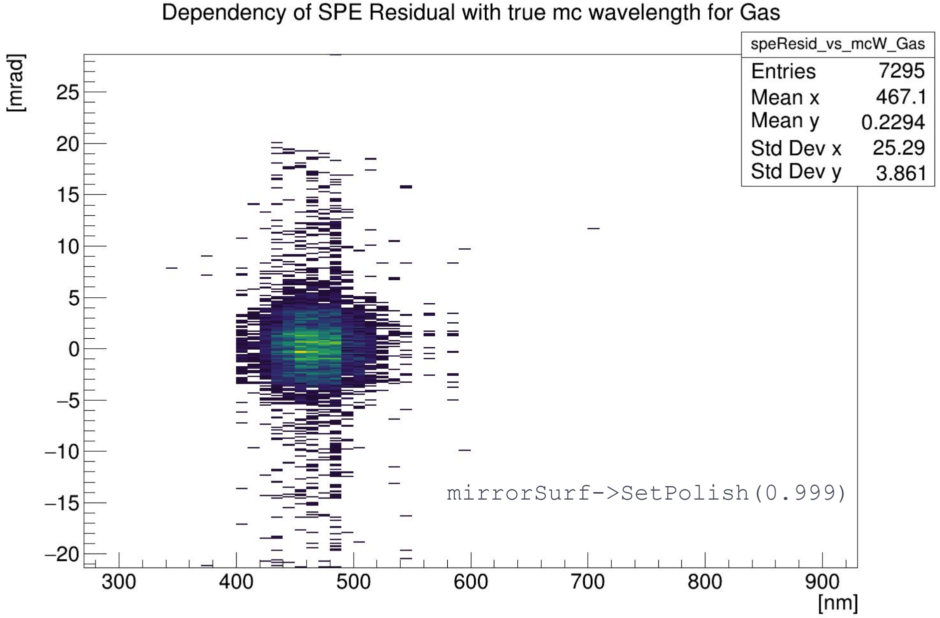
Images

Eta 2.0, 500 Saturated pions



Lambda Dependency





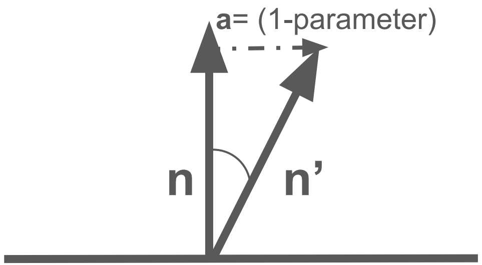
No clear dependency!

First simulation cases

Eta 2.0, 500 Saturated pions

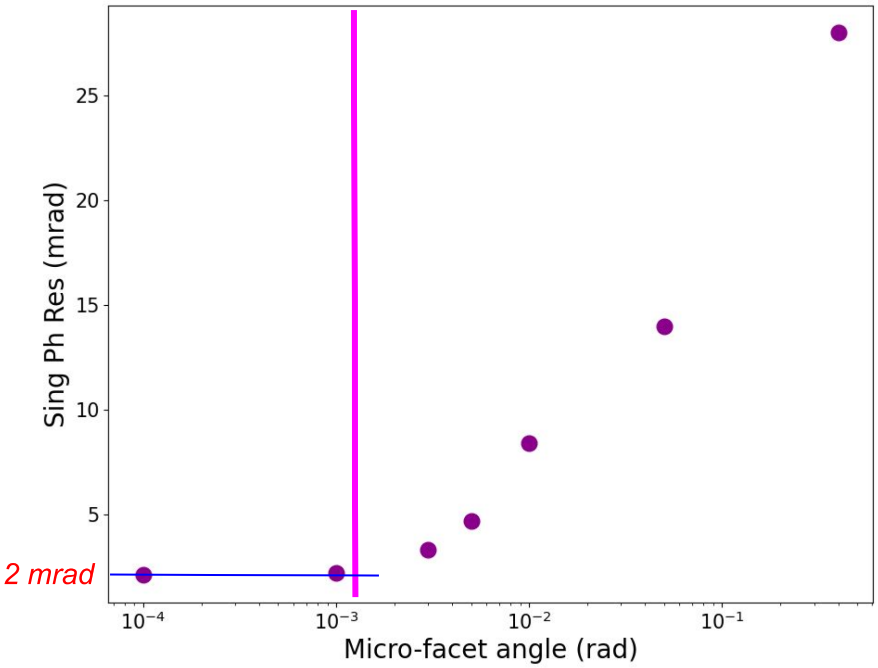
As mentioned earlier, the micro-facet angle is fed from the set polish parameter as (1-parameter) in the form of addition to the overall surface normal.

I assumed, that if the adding vector is small, then we can assume, that the mirco-facet angle is proportional to the norm of the vector.



n' = n + a

theta ~ a/n → ||n|| =1



Intuitively the results make sense:

For a focusing mirror, the parallel beams are falling on different surface of the mirror. If we assume the normals across the surface vary by *k* mrad, the image should disperse ~ *k* mrad, as long as other things do not dominate.

My guesses (may even be an *educated* one)

- The micro facet angle(rad) is related to the surface roughness (nm).
- Roughness ~ lambda*tan(m-f-angle)
- We need an estimate of this lambda. Depending on the measurement methods the lambda can be either the wavelength of the light or even the profilometer accuracy.
- Typical profilometer accuracy is 1-2 micron, this leads to a roughness (1 mrad limit from simulation) O(1 nm), if we are talking about wavelength scale resolution then 0.45 nm~ 4.5 Angstrom. An atomic/molecular level smoothness (The average bond length between carbon atoms… diameter of DNA double helix is 20 angstrom). Does it make sense?
- COMPASS mirror roughness is around 1.65 nm, measured on sampling basis. But, how was it measured? We will discuss with mirror experts in Elettra Sychrotron at Trieste, where COMPASS mirrors were measured 20 years ago.

What to do next?

- ❑ We have a tool (may not be the best one) to play with some parameters.
- ❑ How does the requirement change with polar and azimuthal angles?
- ❑ How does it change with the wavelength? (first impression there is nothing, which is definitely not the case)
- ❑ How does it depend on pseudorapidity?
- ❑ Experimentally, how can we determine the roughness? How close our simulations models are?
- ❑ How does the mirror thickness play a role?