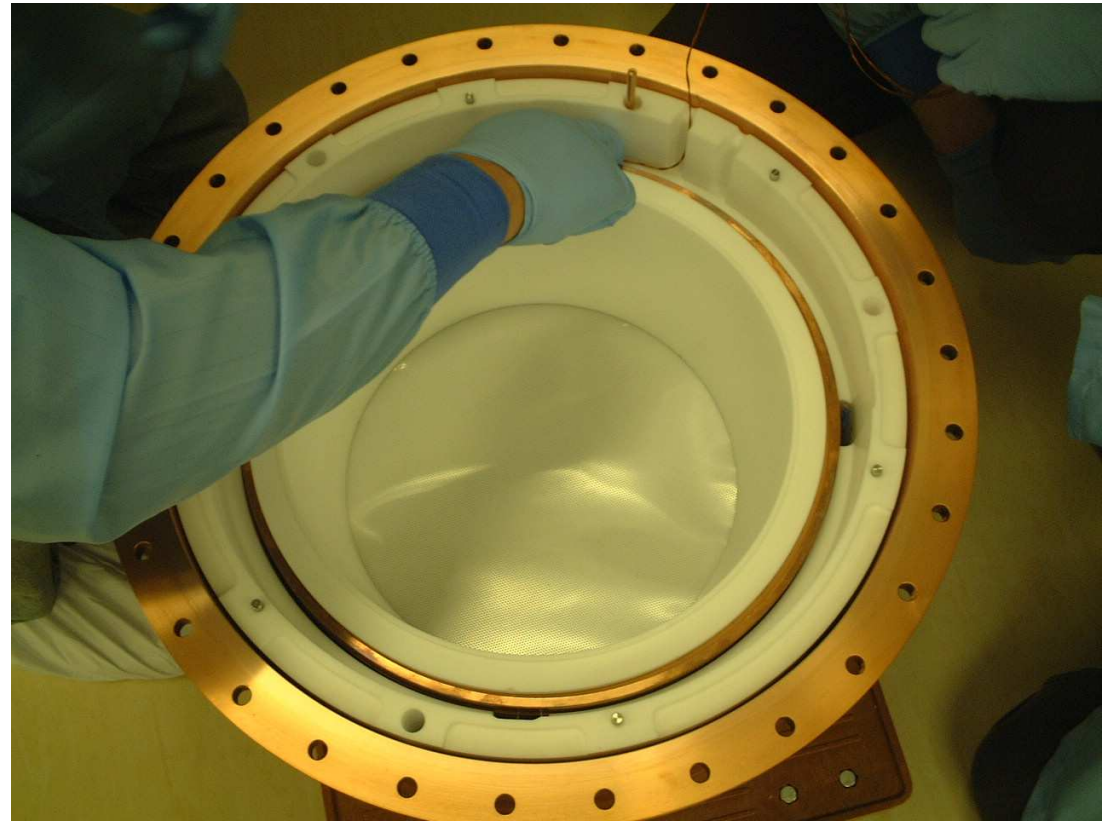
PTFE Reflectance Measurements, Modeling and Simulation for Xenon Detectors

Claudio F. P. Silva
University of Coimbra
LIP Laboratory

Chicago, 11 June 2011



· U · C · LIP

TIPP 2011

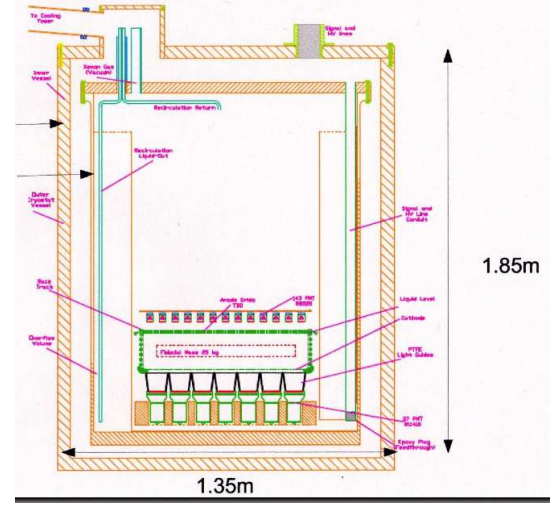
The PTFE in Xenon Detectors

PTFE (polytetrafluoroethylene) is a common choice for the inner walls of liquid/gaseous xenon experiments

- Dark Matter Detectors

LUX

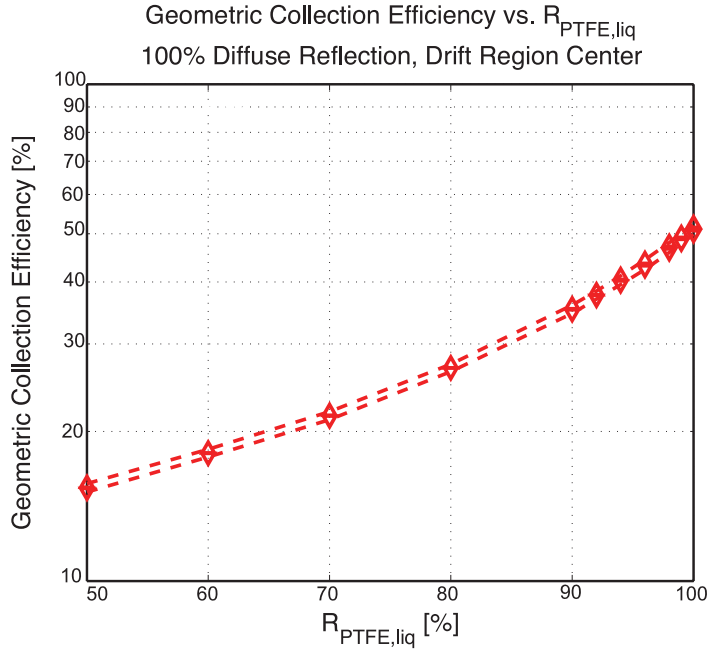
XENON100



Panda-X

- Double-beta decay
  - NEXT (gaseous xenon)

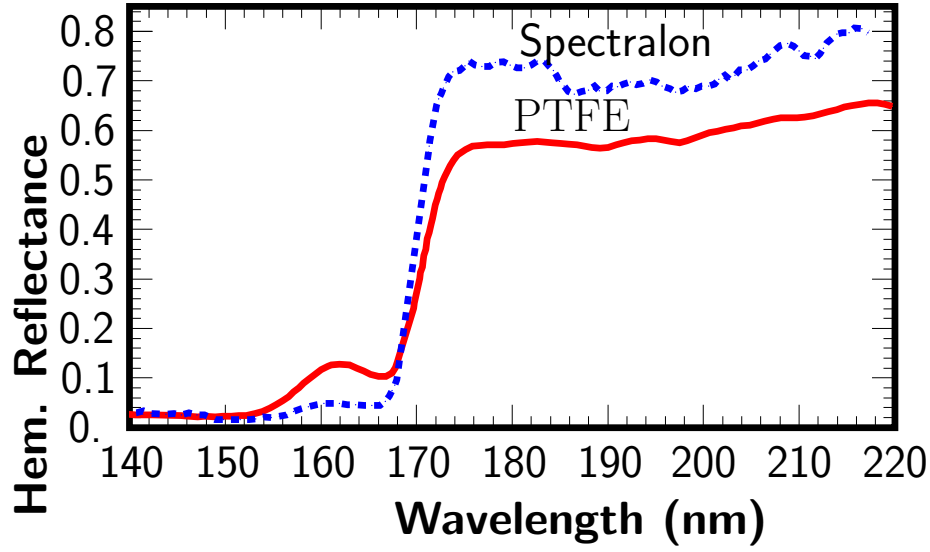
Why the use of PTFE



(LUX collaboration)

PTFE has a high reflectance in the visible spectra ($\simeq$ 99%).
A large reflectance essencial to optimize the light collection.

Xenon emitts in the VUV region (175-178 nm).
Below 250 nm the reflectance of the PTFE is not well known.

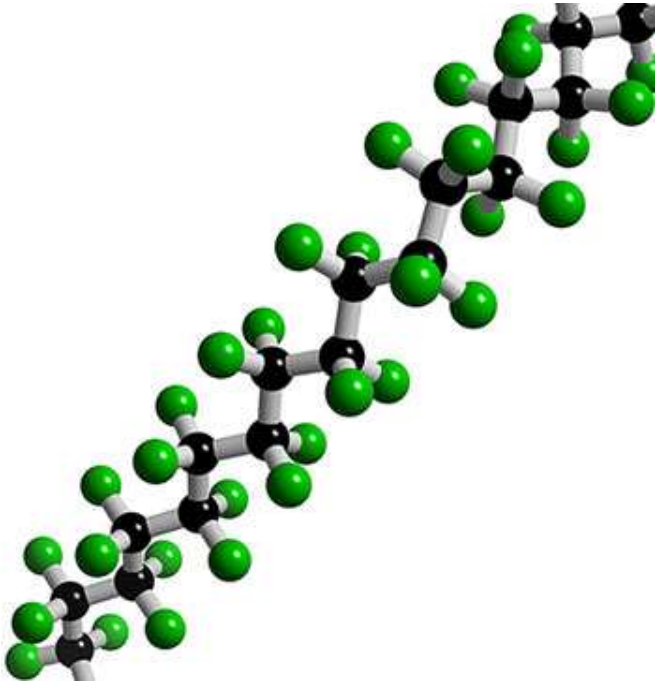


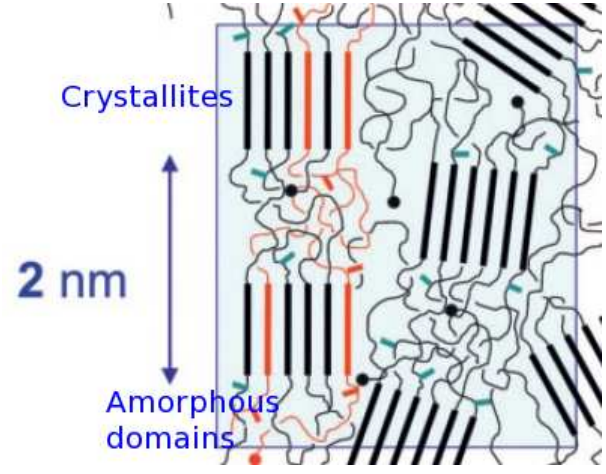
(Kadkhoda et al, SPIE, 3578, 544)

Objectives

- The measurement of the reflectance distributions of various fluoropolymers samples for the xenon scintillation light.
- The modeling of the processes involved and the application to Geant4 simulations.
- Prediction of the reflectance distribution for the liquid xenon/PTFE interface.

The PTFE/Teflon®

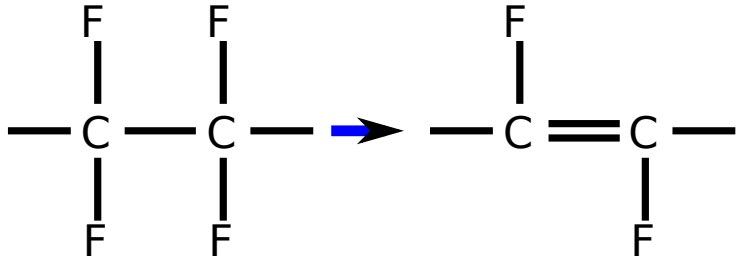


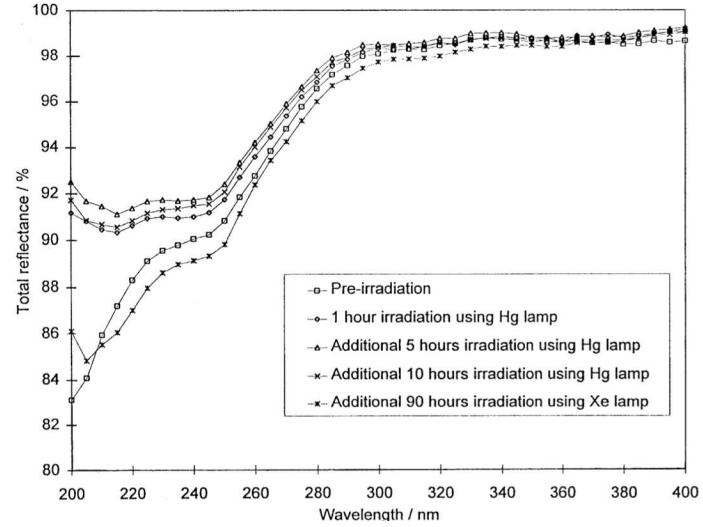


- The simplest fluoropolymer $(-(CF_2)_n-)$
- CF is the strongest bond in organic chemistry (good chemical resistance)
- High temperature resistance -200 °C to 260 °C
- Helicoidal structure (temperature dependent)
- Composed by a crystalline and amorphous phase (usually with different optical properties)

PTFE - What we should be careful

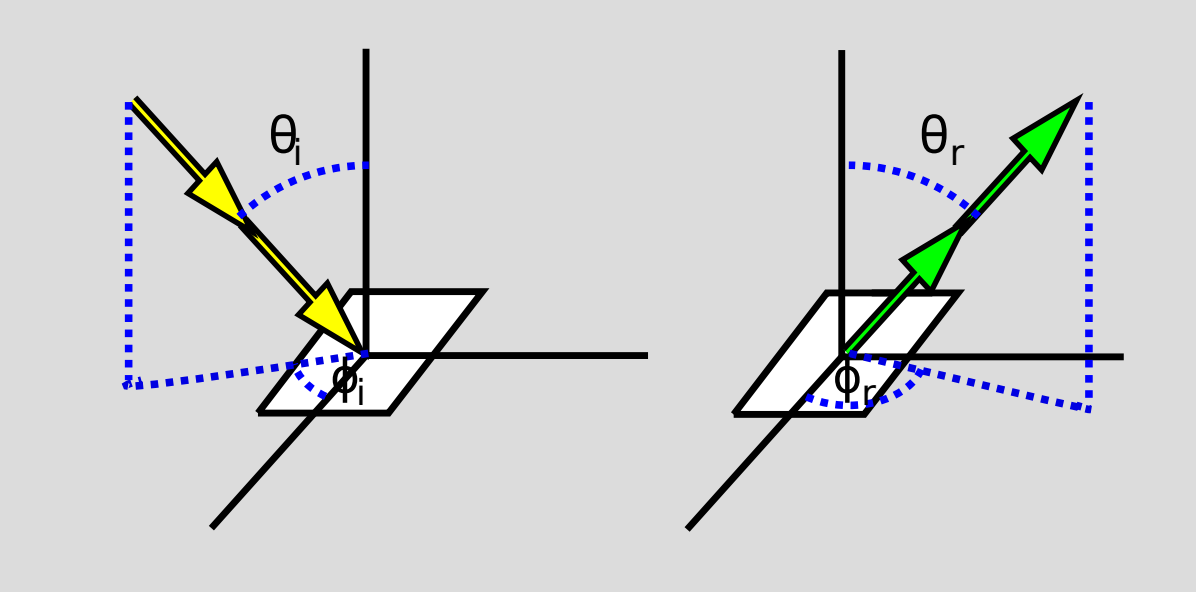
- PTFE degradation under intense VUV radiation





- PTFE absorbs contaminants (hydrocarbonets)
  - Vacuum-baking at about 90 °C for a period of about 48 h recomended
  - It should be left in a sealed container.
  - Plastic containers are not recomended.

What do We Mean by Reflection?

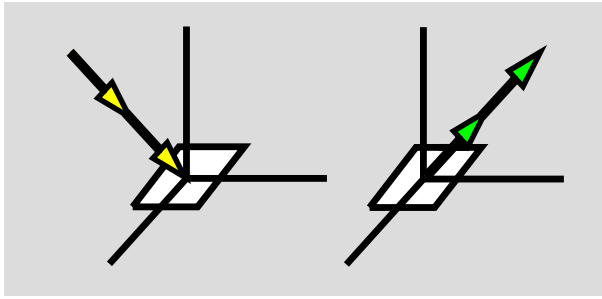


Bidirectional reflectance distribution function

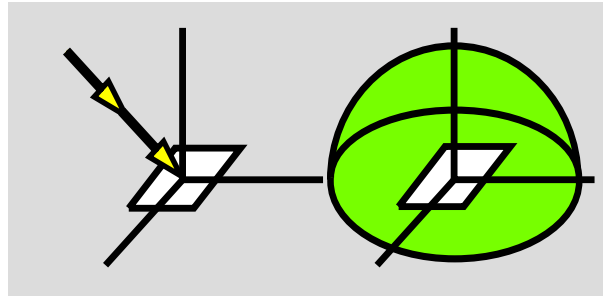
$$\rho\left(\theta_i, \phi_i; \theta_r, \phi_r\right) = \frac{\mathrm{d}I_r\left(\theta_i, \phi_i, \theta_r, \phi_r\right)}{\mathrm{d}\Phi_i\left(\theta_i, \phi_i\right)}$$

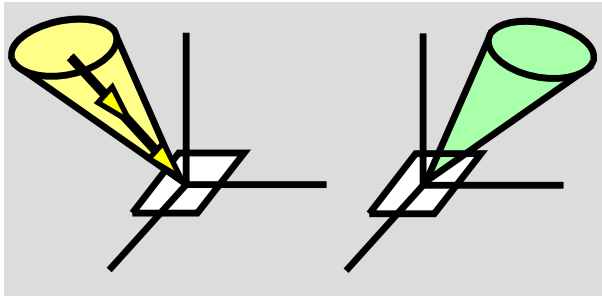
What do We Mean by Reflection?

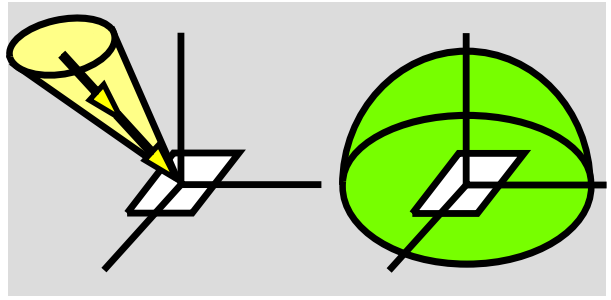
Bidirectional



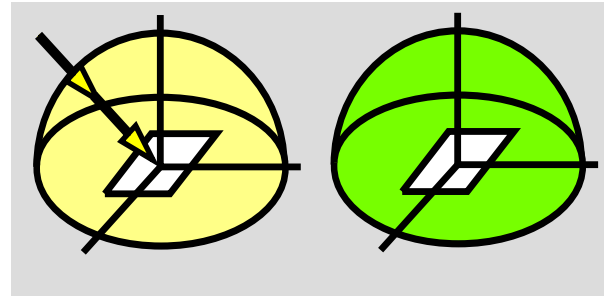
Directional-Hemispherical



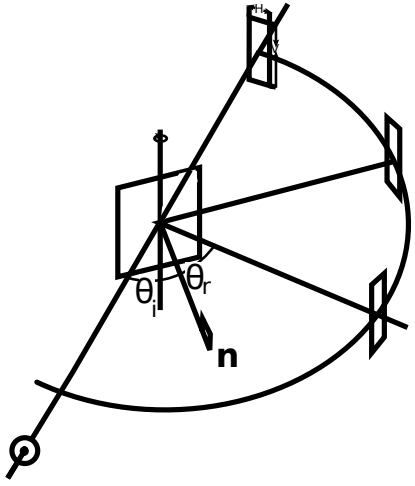




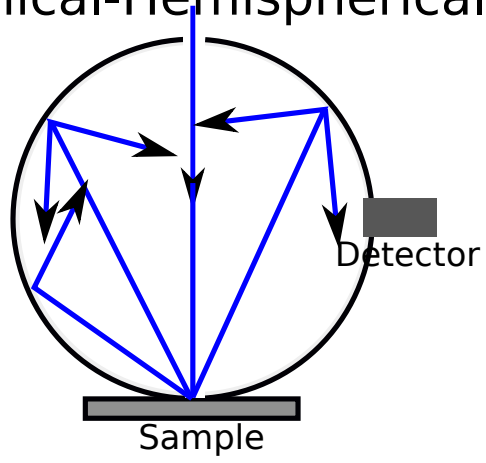
Bi-Hemispherical



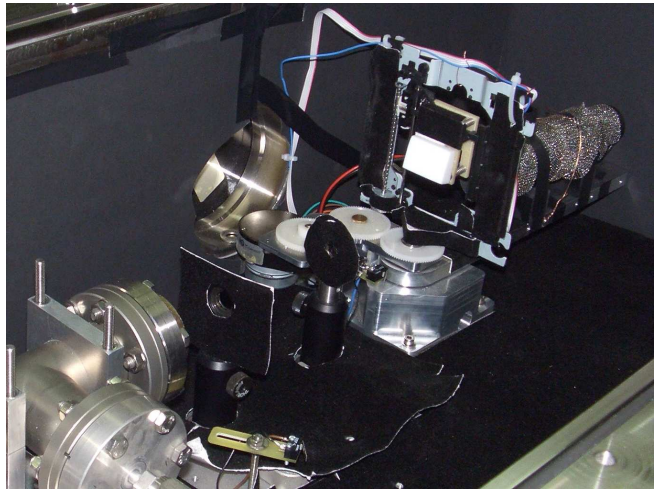
Biconical

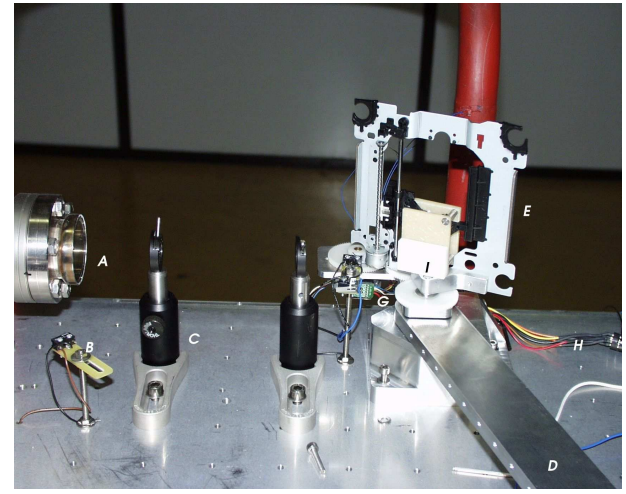


Conical-Hemispherical



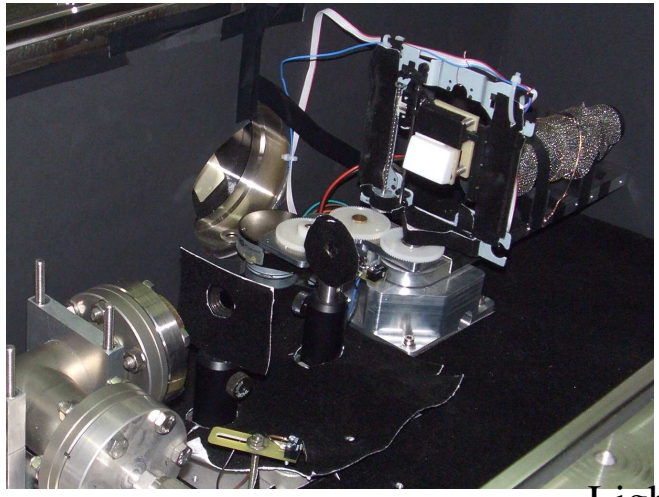
The Angle Resolution System

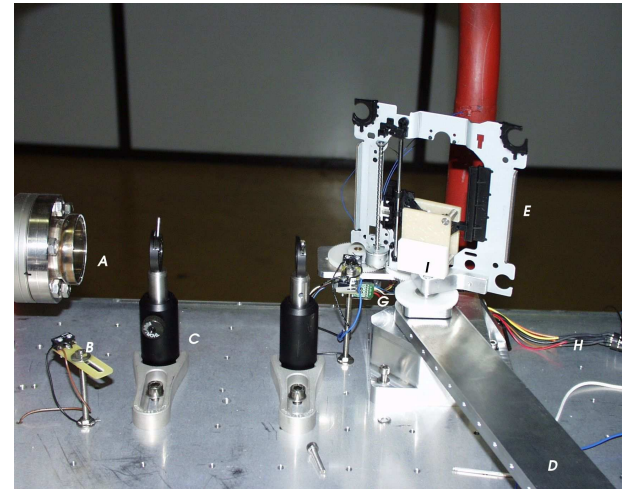


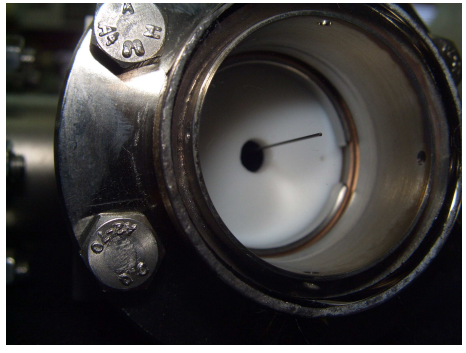


- The Angle Resolution System (ARS) is placed inside an air tight chamber.
- The light of 175 nm is emitted by a xenon proportional counter.

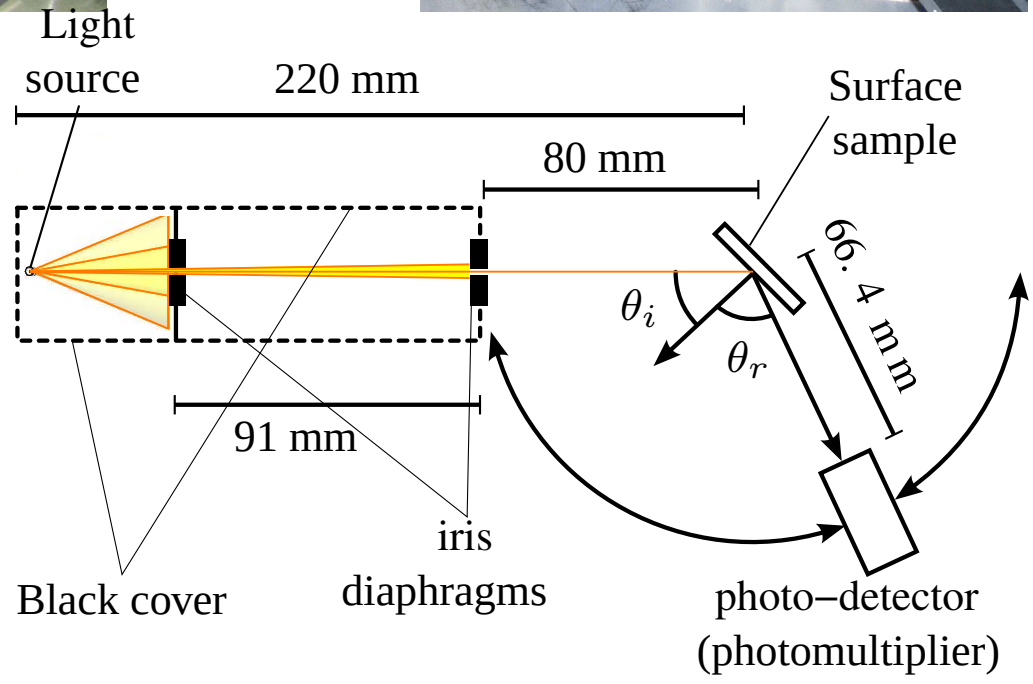
The Angle Resolution System





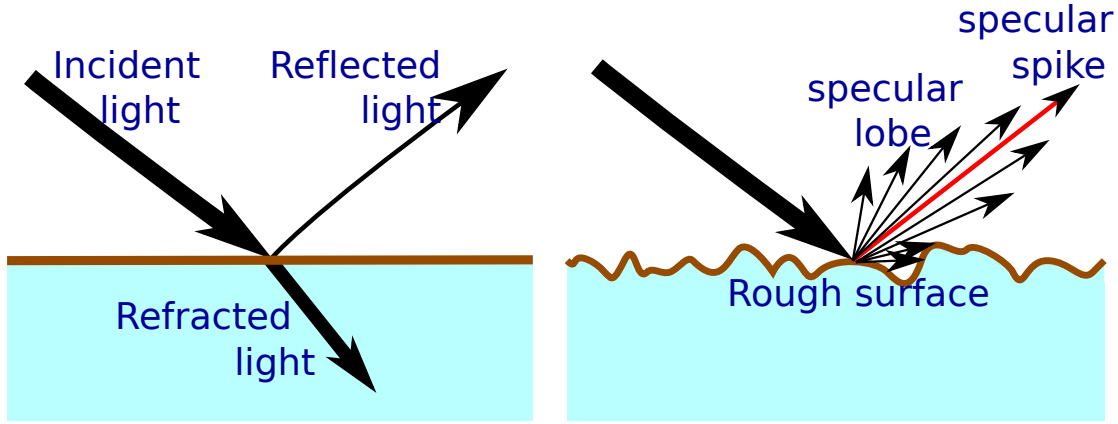


Xenon scintillation light source

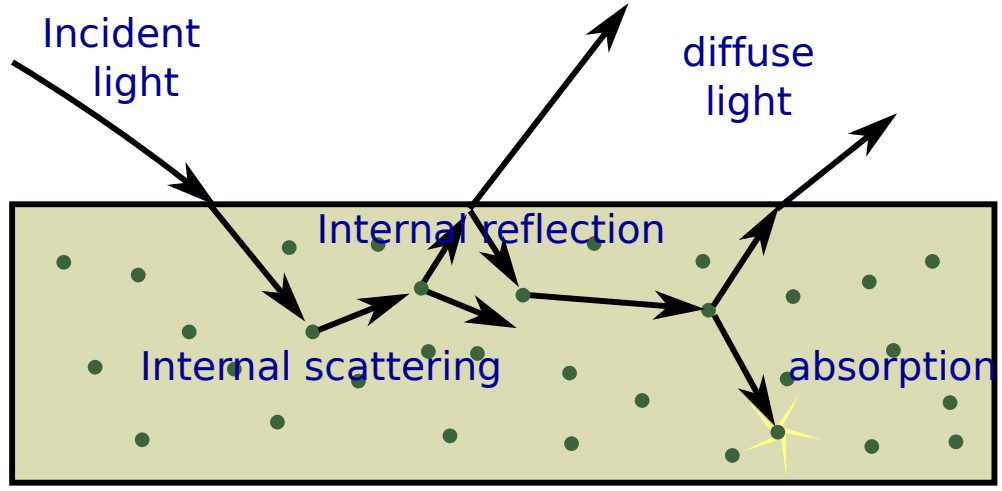


Reflectance Components

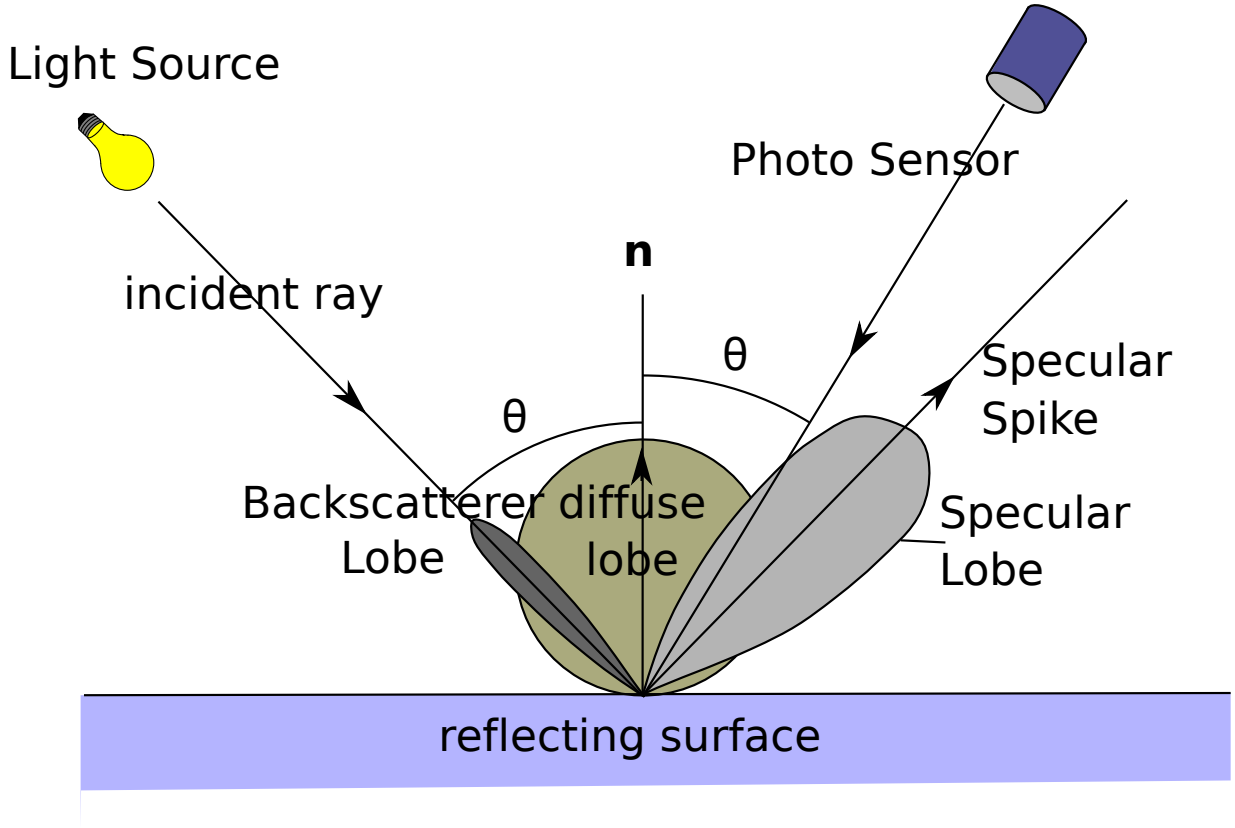
- Specular:



- Diffuse:



Reflectance Components



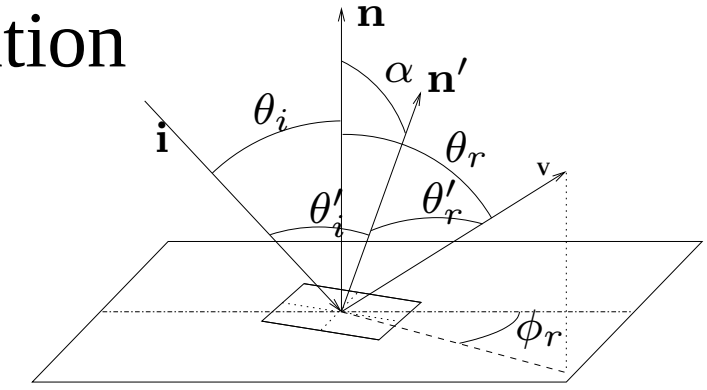
$$\rho = \rho_l + \rho_s + \rho_d + \rho_b$$

- $\rho_l \longrightarrow$ specular lobe
- $\rho_d \longrightarrow$ diffuse lobe
- $\rho_s \longrightarrow$ specular spike
- $\rho_b \longrightarrow$ backscatterer lobe

The Specular Reflection

$$\rho = F\left(\theta_i\right)\chi_1\chi_1^*\delta\left(\mathbf{i}-\mathbf{r}\right) + \left(1-\chi_1\chi_1^*\right)F\left(\theta'\right)\frac{P_\alpha\left(\alpha\right)G\left(\theta_i,\theta_r\right)}{4\cos\theta_i}$$

- F - the Fresnel equations, dependent of n and κ
- χ_1 - the characteristic function of the probability distribution of heights $P_1\left(z\right)$
- $P_\alpha\left(\alpha\right)$ - the probability distribution of the slopes α
- $G\left(\theta_i,\theta_r\right)$ - shadowing-masking attenuation coefficient



The Specular Lobe

The following distributions P_α were considered

- Cook-Torrance - *Gaussian Like*

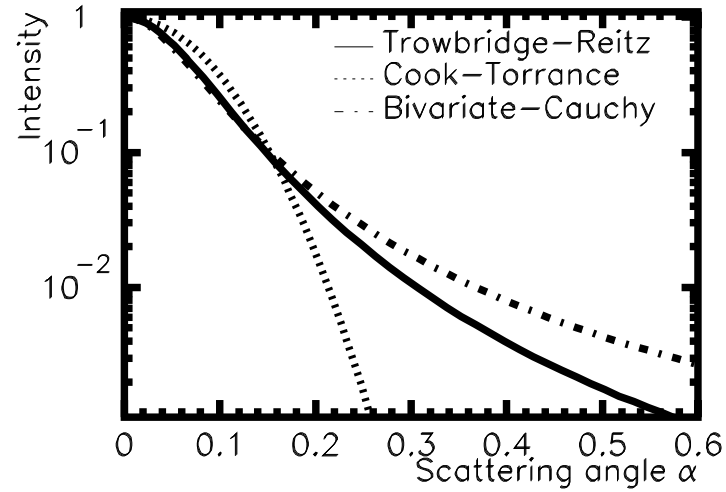
$$P_{CT}(\alpha, m) = \frac{1}{\pi m^2 \cos^4 \alpha} \exp\left(-\frac{\tan^2 \alpha}{m^2}\right)$$

- Trowbridge-Reitz

$$P_{TR}(\alpha, \gamma) = \frac{\gamma^2}{\pi\left(\gamma^2 \cos^2 \alpha + \sin^2 \alpha\right)^2}$$

- Bivariate-Cauchy

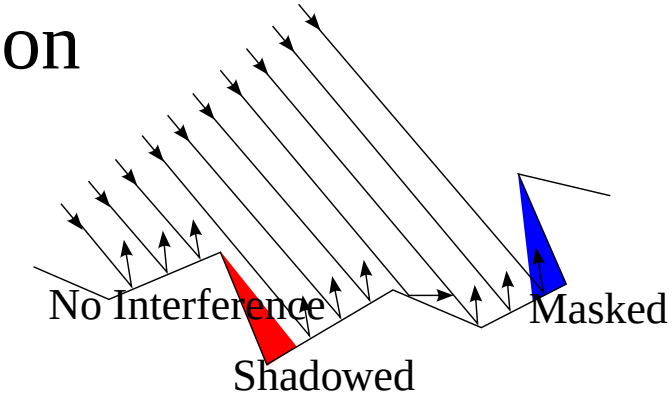
$$P_{BC}(\alpha, \gamma) = \frac{\gamma^2 + \gamma}{\pi\left(\gamma^2 \cos^2 \alpha + \sin^2 \alpha\right)^{\frac{3}{2}}}$$



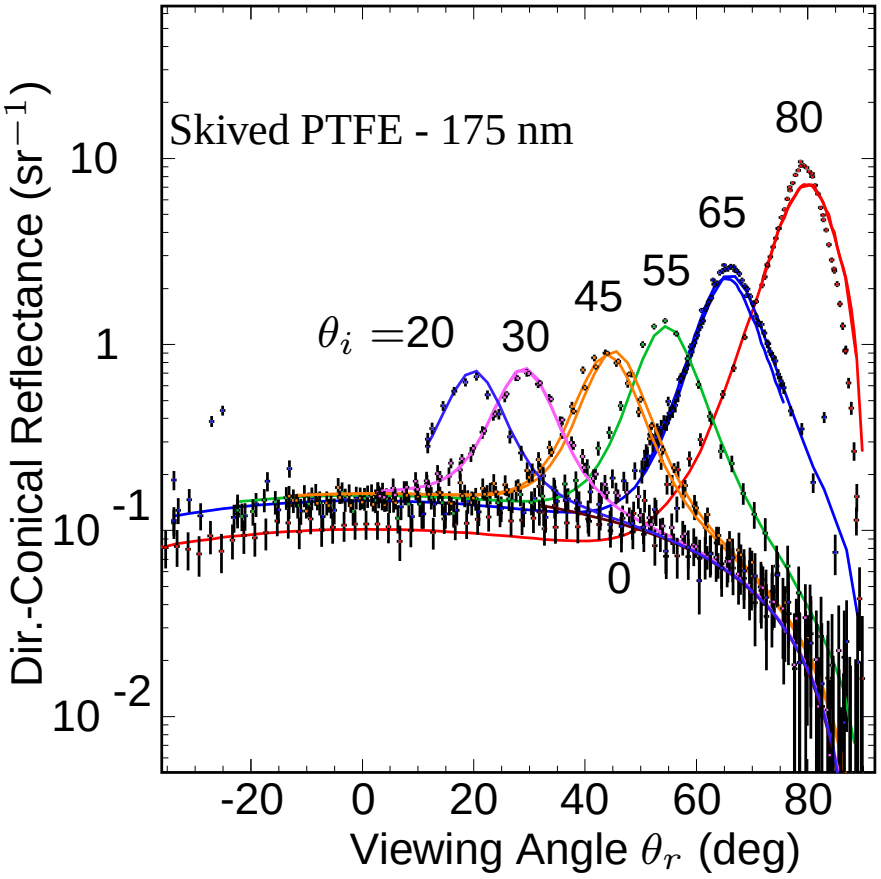
The Specular Reflection

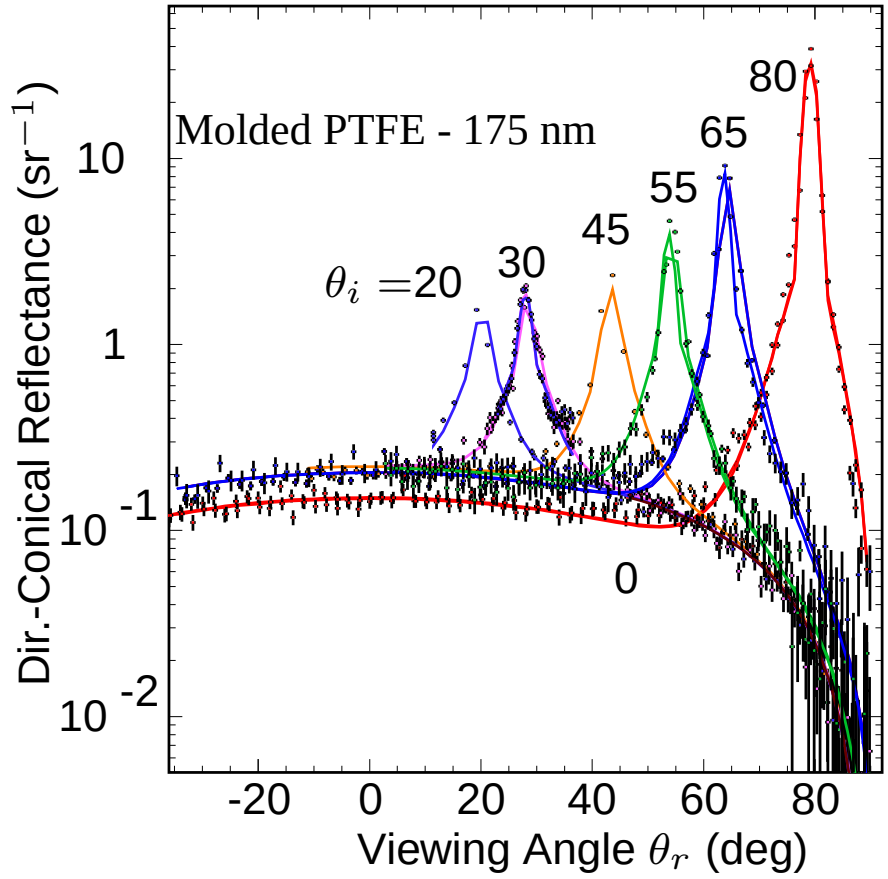
$$\rho = F\left(\theta_i\right)\chi_1\chi_1^*\delta\left(\mathbf{i}-\mathbf{r}\right) + \left(1-\chi_1\chi_1^*\right)F\left(\theta'\right)\frac{P_\alpha\left(\alpha\right)G\left(\theta_i,\theta_r\right)}{4\cos\theta_i}$$

- F - the Fresnel equations, dependent of n and κ
- χ_1 - the characteristic function of the probability distribution of heights $P_1\left(z\right)$
- $P_\alpha\left(\alpha\right)$ - the probability distribution of the slopes α
- $G\left(\theta_i,\theta_r\right)$ - shadowing-masking attenuation coefficient



PTFE Reflectance Distributions



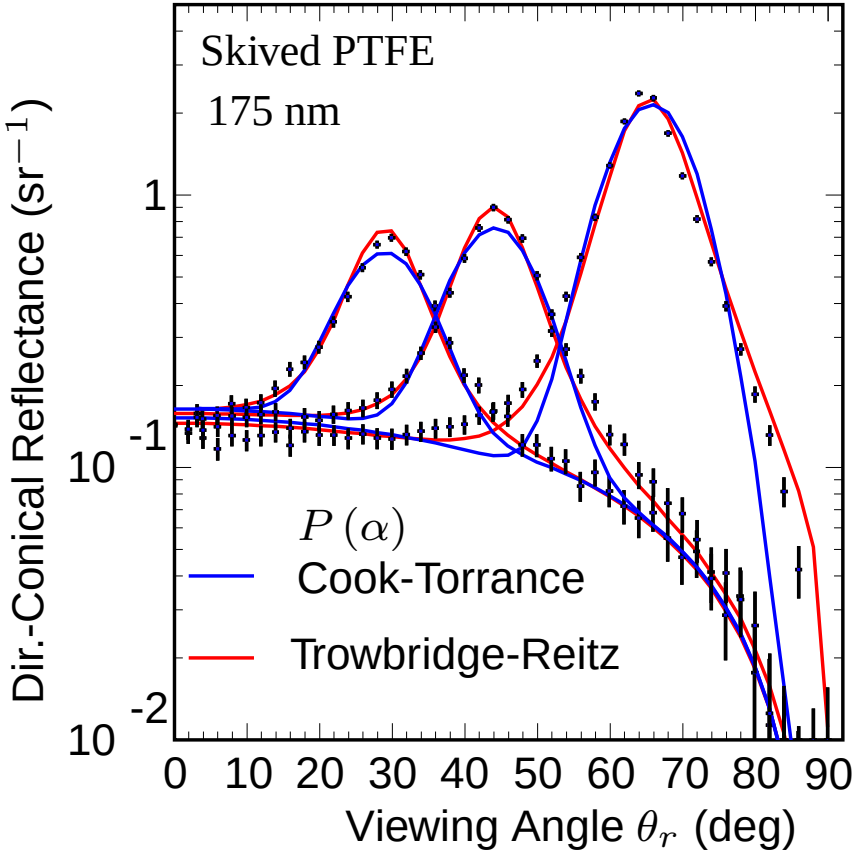


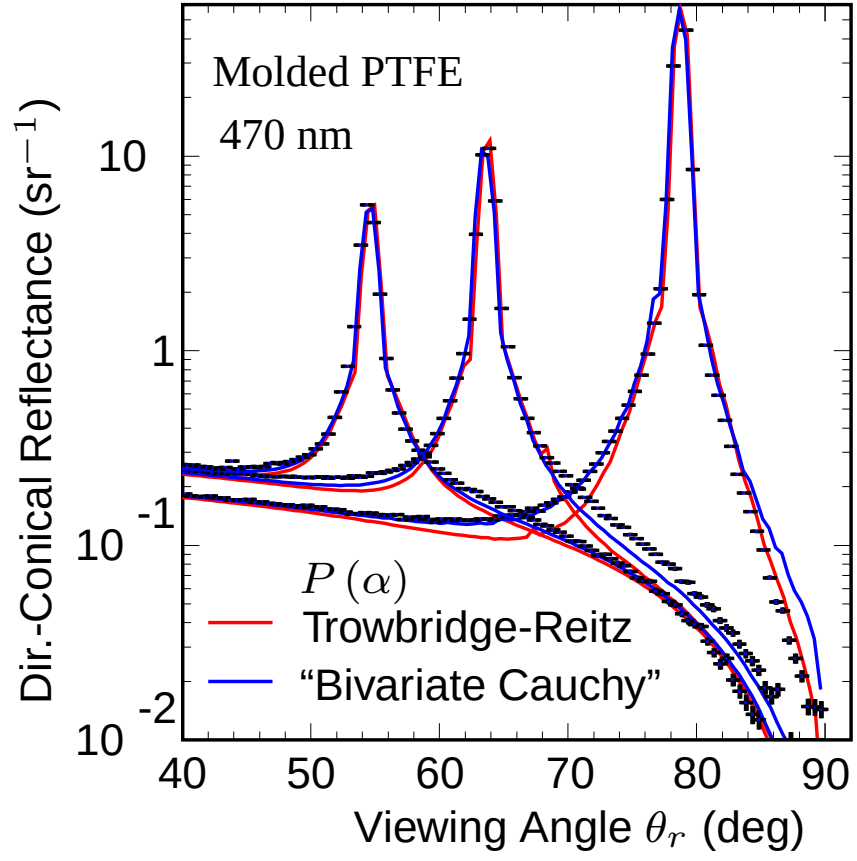
We observe three different components

- Diffuse Lobe
- Specular Lobe
- Specular Spike

The Specular Lobe

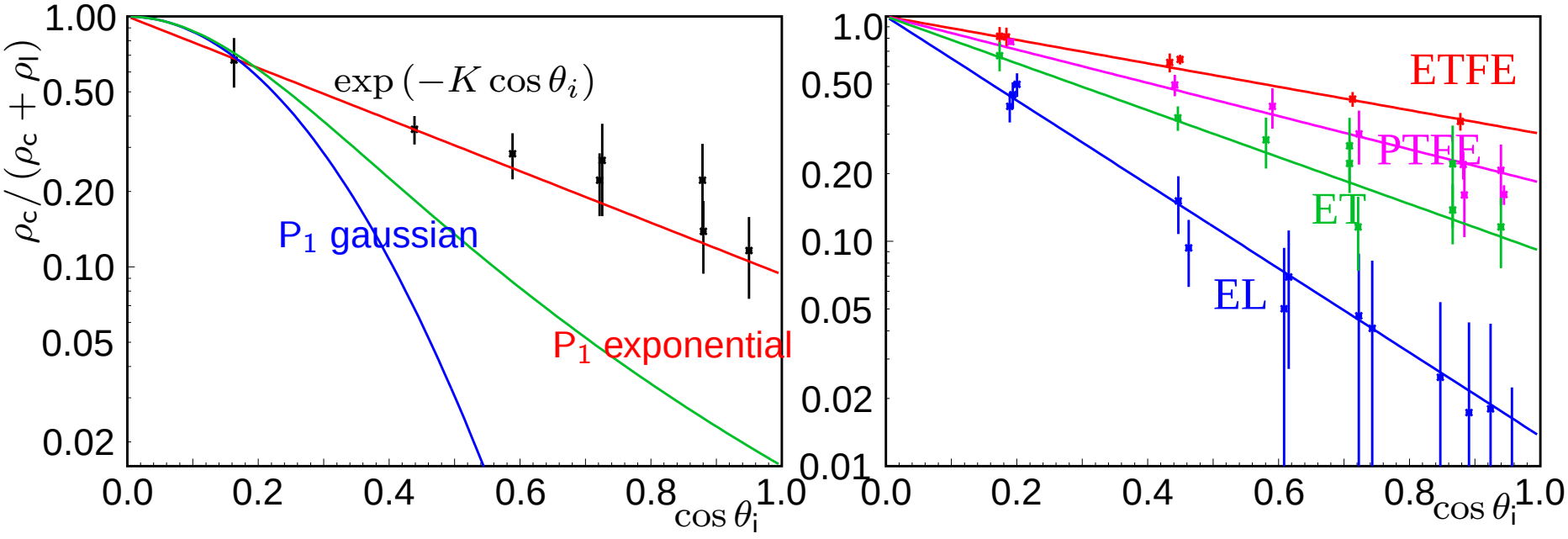
- The “bivariate-cauchy” has the best description
- γ is constant with θ_i and decreases with λ.





The Specular Spike

The intensity of the specular spike ($\rho_c / (\rho_c + \rho_l)$) changes with the roughness, wavelength of the light and angle of incidence.



- The usual distributions p_1 do not describe the data. $\Lambda = \exp(-K\cos\theta_i)$ is an empirical function.

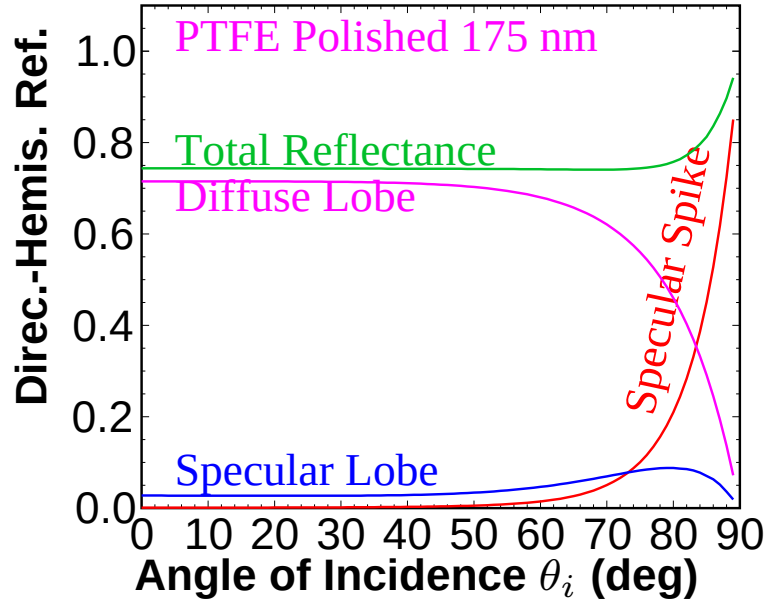
The Fits

A global fit is applied to results with only three or four parameters. For the different samples we obtain

$\lambda = 175\,\mathrm{nm}$	n refractive index	a_d albedo	γ sp. lobe width	K spike intensity
Skived PTFE	1.49±0.07	0.58±0.02	0.064±0.006	-
PTFE (not polished)	1.51±0.07	0.52±0.06	0.057±0.008	-
Extruded ($\perp$) PTFE	1.50±0.03	0.69±0.07	0.055±0.007	3.0±0.3
Extruded ($\parallel$) PTFE	1.46±0.04	0.63±0.07	0.066±0.008	4.3±0.5
Molded PTFE	1.45±0.04	0.74±0.07	0.049±0.015	1.7±0.2

The Hemispherical Reflectances

- Directional-Hemispherical



- Bi-Hemispherical Reflectance

	Diffuse.	S. Lobe	S. Spike	Total
Skived PTFE	0.488±0.009	-	0.089±0.008	0.577±0.007
Molded Polished	0.625±0.034	0.040±0.004	0.0438±0.024	0.71±0.04

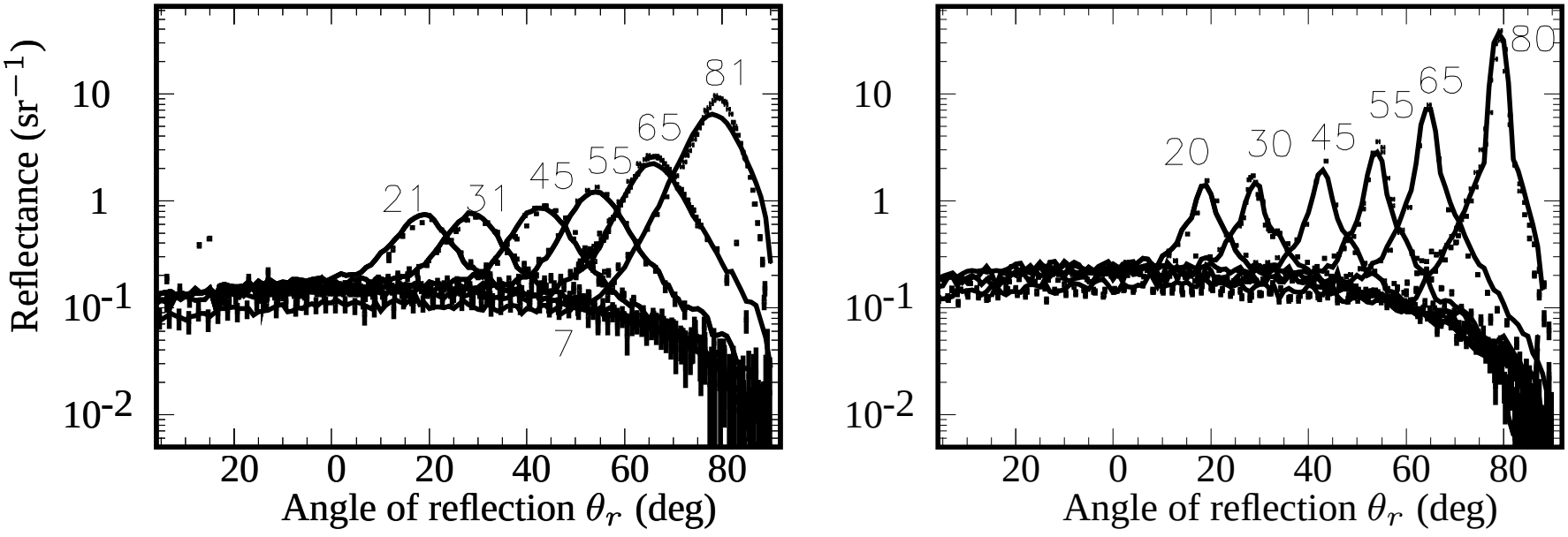
Geant 4 - Current

The current descriptions (Unified and Glisur) do not agree in many ways with our measurements

- Diffuse lobe proportional to the reflected light
- The intensity of the specular spike is independent of the angle of incidence
- It is restricted to gaussian statistics
- The shadowing and masking are not fully considered

Geant 4 - New

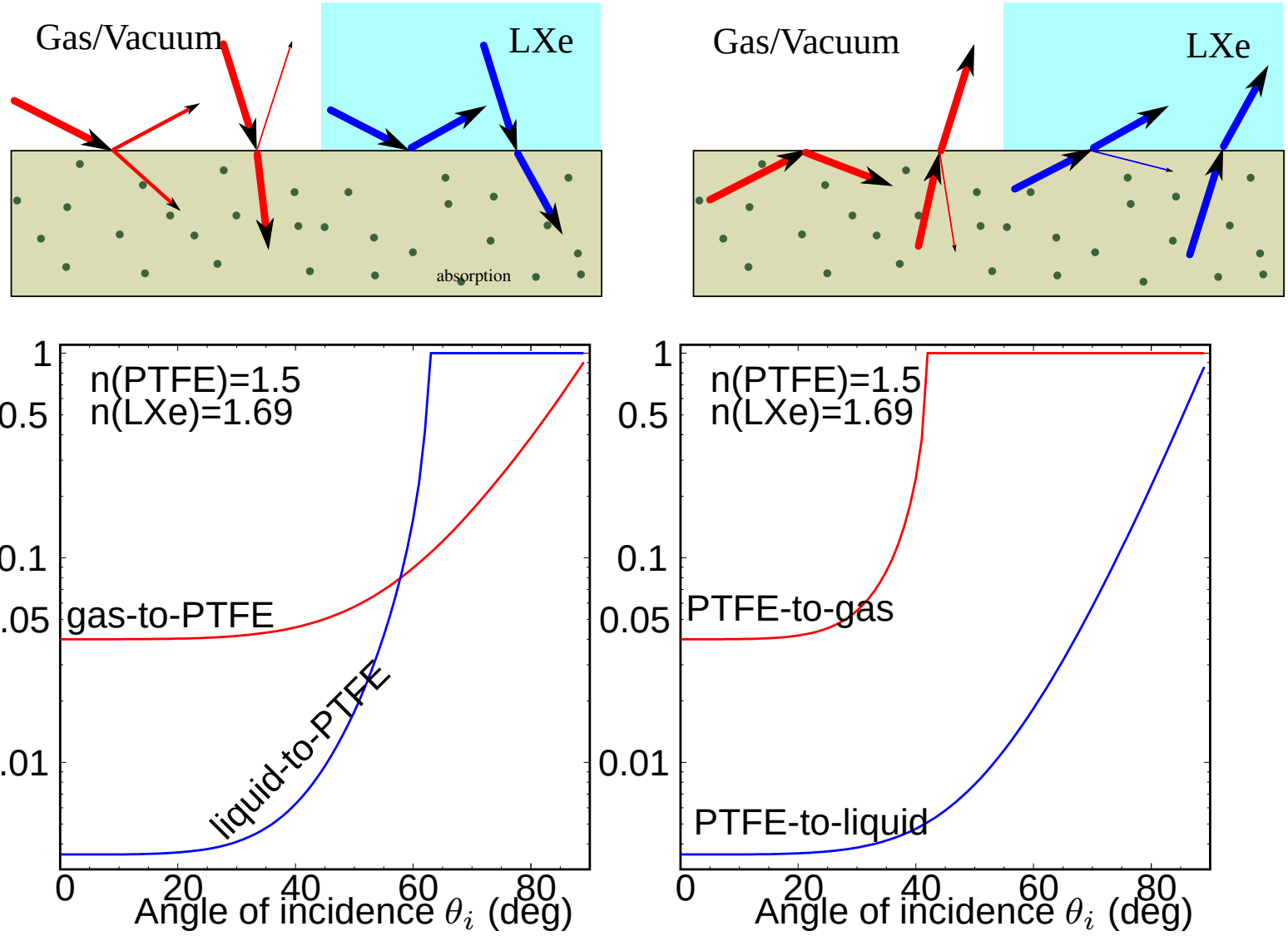
- This model of reflection was included in the Geant4 as new method of the class G4BoundaryProcess.
- Inverse cumulative functions are used to generate the direction of both the diffuse reflected and specularly reflected light.



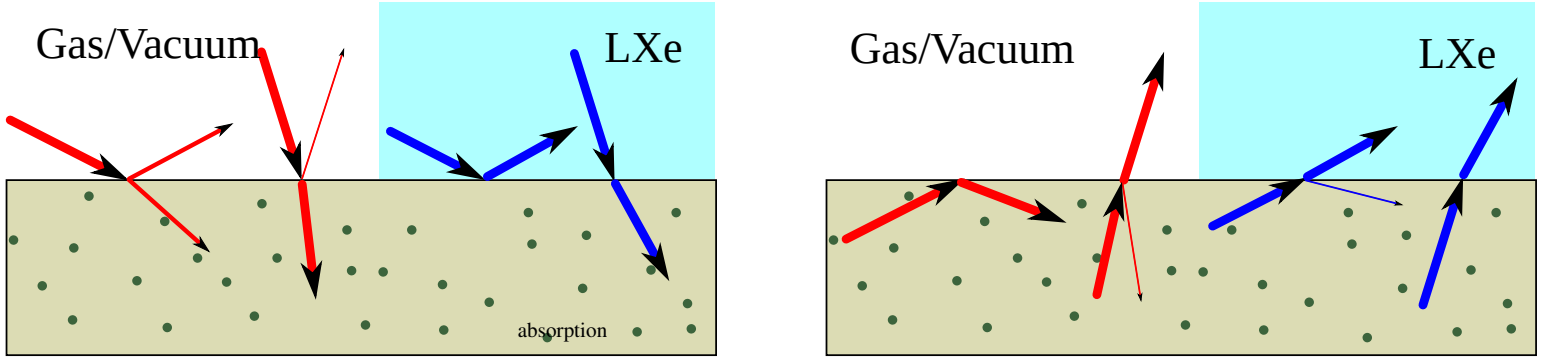
Reflection in a Liquid Interface

- The reflectance obtained in the gas/PTFE is between 60-80%. There are strong indications that the reflectance in the liquid xenon is much higher ($>$80%).
- The liquid xenon has a higher index of refraction ($n \simeq 1.69$) comparatively to the air or vacuum

Reflection in a Liquid Interface



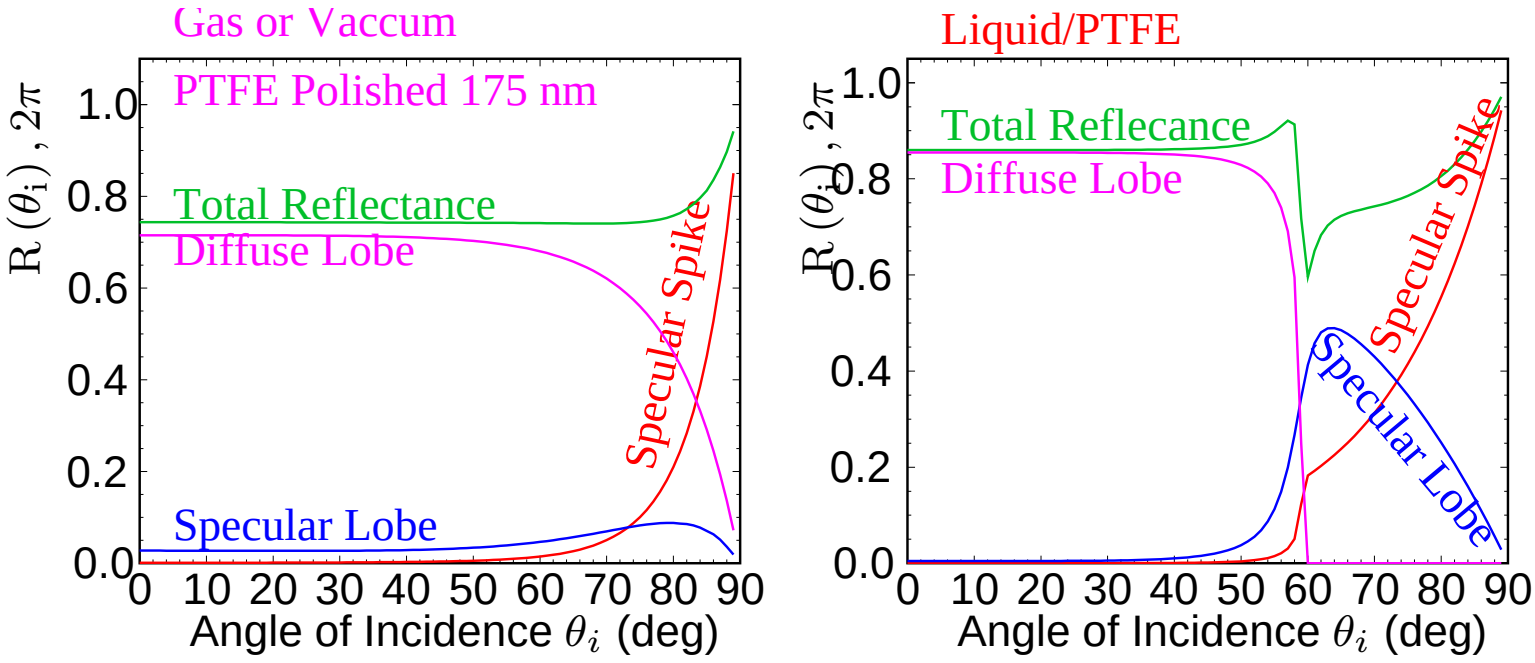
Reflection in a Liquid Interface



In the liquid:

- The internal reflection probability is smaller.
- Less light returns to the bulk to be internally scattered where it can be eventually absorbed.
- The multiple-diffuse albedo a_d will be larger.

Reflection in a Liquid Interface



	Diffuse Lobe		*Specular Lobe*		*Specular Spike*		*Total Ref*	
	Gas	Liq.	Gas	Liq.	Gas	Liq.	Gas	Liq.
Skived PTFE	0.49	0.55	0.089	0.25	0.0	0.0	**0.58**	**0.80**
Molded PTFE	0.63	0.59	0.040	0.13	0.04	0.16	**0.77**	**0.89**

Conclusion

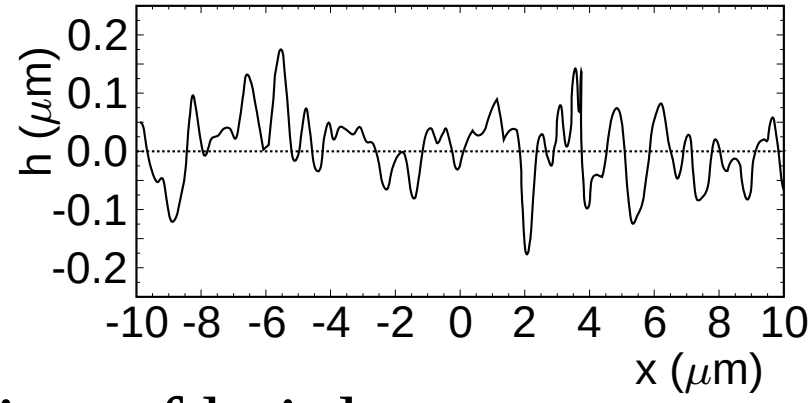
- We developped an angle resolution system to measure the reflectance distribution in vacuum.
- The reflectance distribution of the PTFE is composed by three contributions (diffuse lobe, specular lobe and specular spike).
- Four free parameters reproduces fairly well the details of the measured reflectance distributions.
- A new simulation of the reflectance processes was included in Geant-4
- The reflectance distributions were estimated to a Liquid-PTFE interface.


Thank you!

Surface Statistics

- $h\,(x,y)$ the height function

  $z = h\,(x,y) \quad \langle h\,(x,y)\rangle$=0



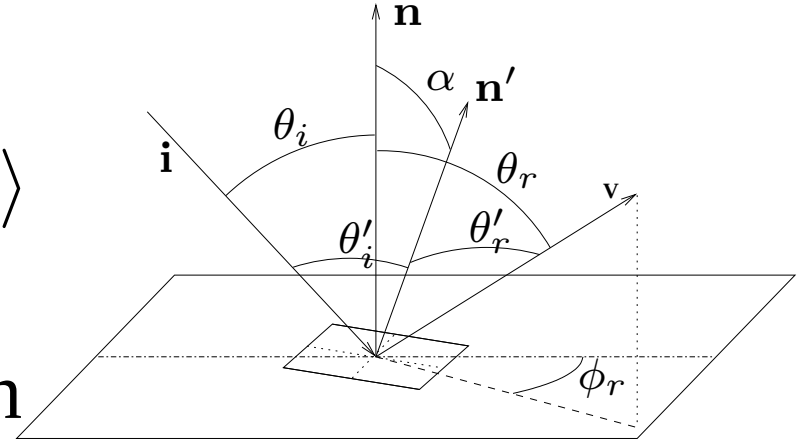
- $P_2\,(z,z')$, bivariate distribution of heights

$$P_2\,(z,z') = \frac{1}{\sqrt{2\pi[1-C(\tau,T)]}\sigma_h} \exp\left\{-\frac{z^2-2C(\tau,T)zz'+z'^2}{2\sigma_h^2[1-C(\tau,T)]}\right\}$$

- $C\,(r,T)$ correlation function

$$C = \frac{1}{\sigma_h^2}\left\langle h\,(x_1,y_1)\,,h\,(x_2,y_2)\right\rangle$$

- $P_\alpha\,(\alpha,\sigma_\alpha)$ - slope distribution



The Specular Reflection in a Rough Surface

- A complex diffraction problem

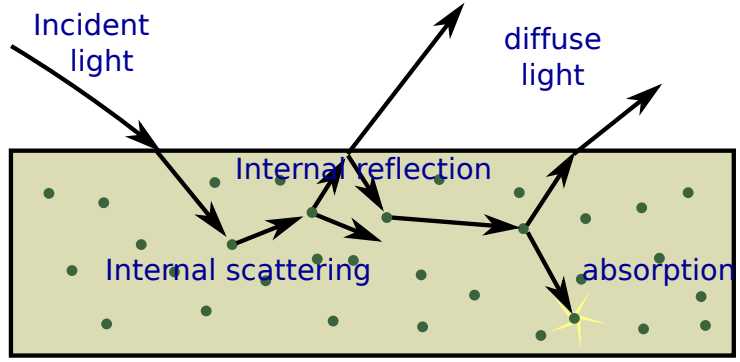
$$\rho = \frac{R^2 \cos^2 \theta'}{\cos \theta_i \lambda^2} \int_0^\infty \chi_2 (\tau) J_0 (k_z \tau) \tau \mathrm{d}\tau$$

χ_2 is the characteristic function of P_2

- For a bivariate gaussian distribution

$$\begin{aligned} \rho &= \frac{E_0^2 R^2 \cos^2 \theta'}{\lambda^2} \chi_1 \chi_1^* \left\{ \int_0^\infty J_0 (k_z \tau) \tau \mathrm{d}\tau \right. \\ &\left. + \sum_{n=1}^{\infty} \frac{k_z^{2n} \sigma_h^{2n}}{n!} \int_0^\infty [C (\tau, T)]^n J_0 (k_z \tau) \tau \mathrm{d}\tau \right\} \end{aligned}$$

The Diffuse Component



$$\rho_d = \frac{a_d}{\pi} \cos\theta_r \Upsilon\left(\theta_i, \theta_r, \phi\right) \left[1 - F\left(\theta_i, \right)\right] \left[1 - F\left(\theta_r\right)\right]$$

- The light is scattered isotropically in the bulk.
- The Fresnel factors account with the two refractions of the light, Air-to-PTFE and PTFE-to-Air.
- a_d is the multiple-diffuse albedo of the surface.
- Oren-Nayar factor Υ accounts for the roughness of the surface.