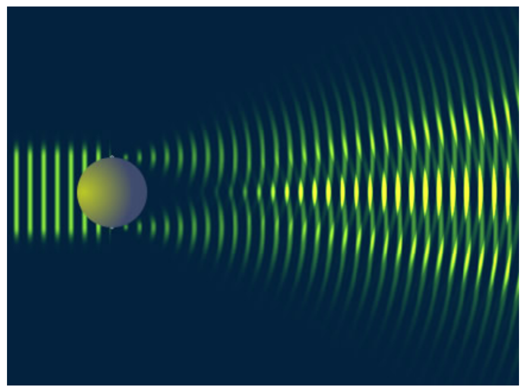
Laser Diffraction Theory



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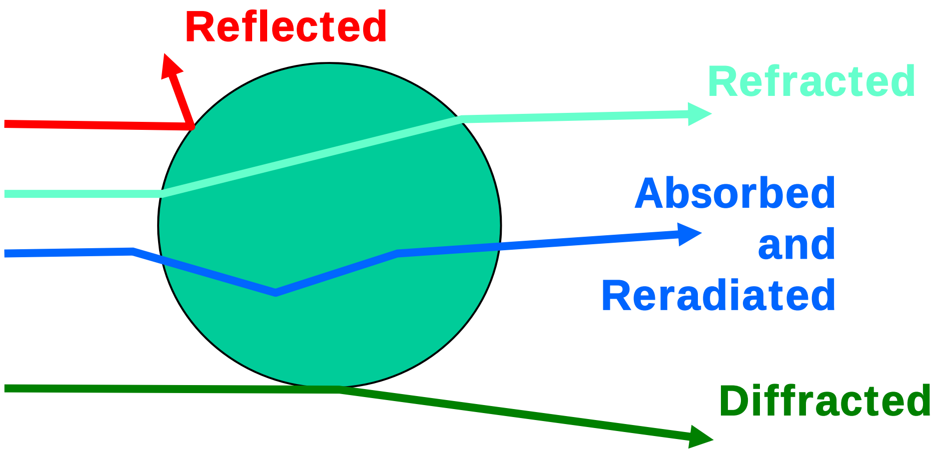
HORIBA Scientific
www.horiba.com/us/particle

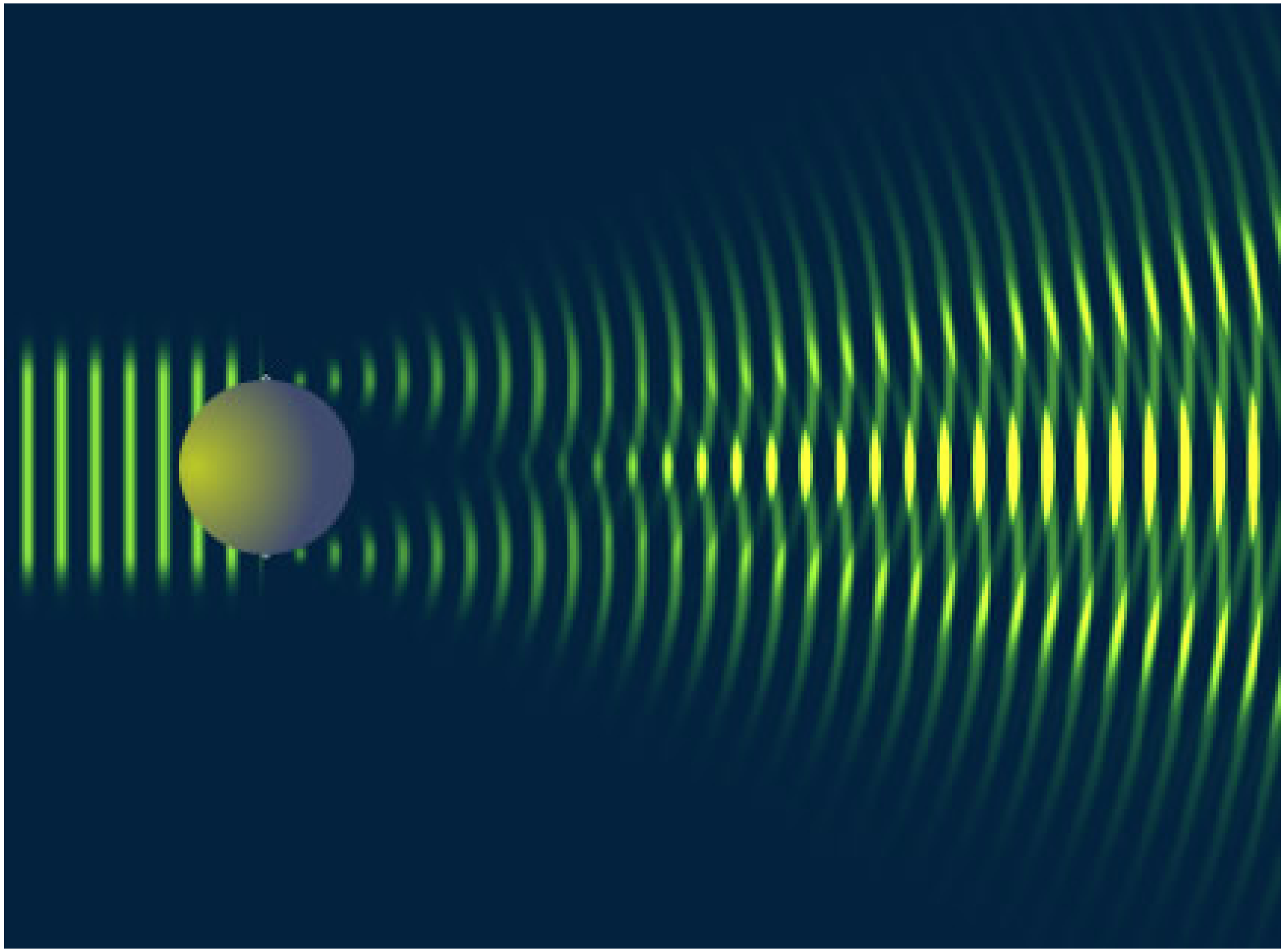
When a Light beam Strikes a Particle

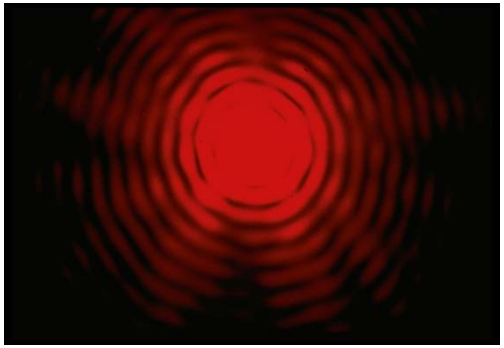
- Some of the light is:
  - Diffracted
  - Reflected
  - Refracted
  - Absorbed and Reradiated



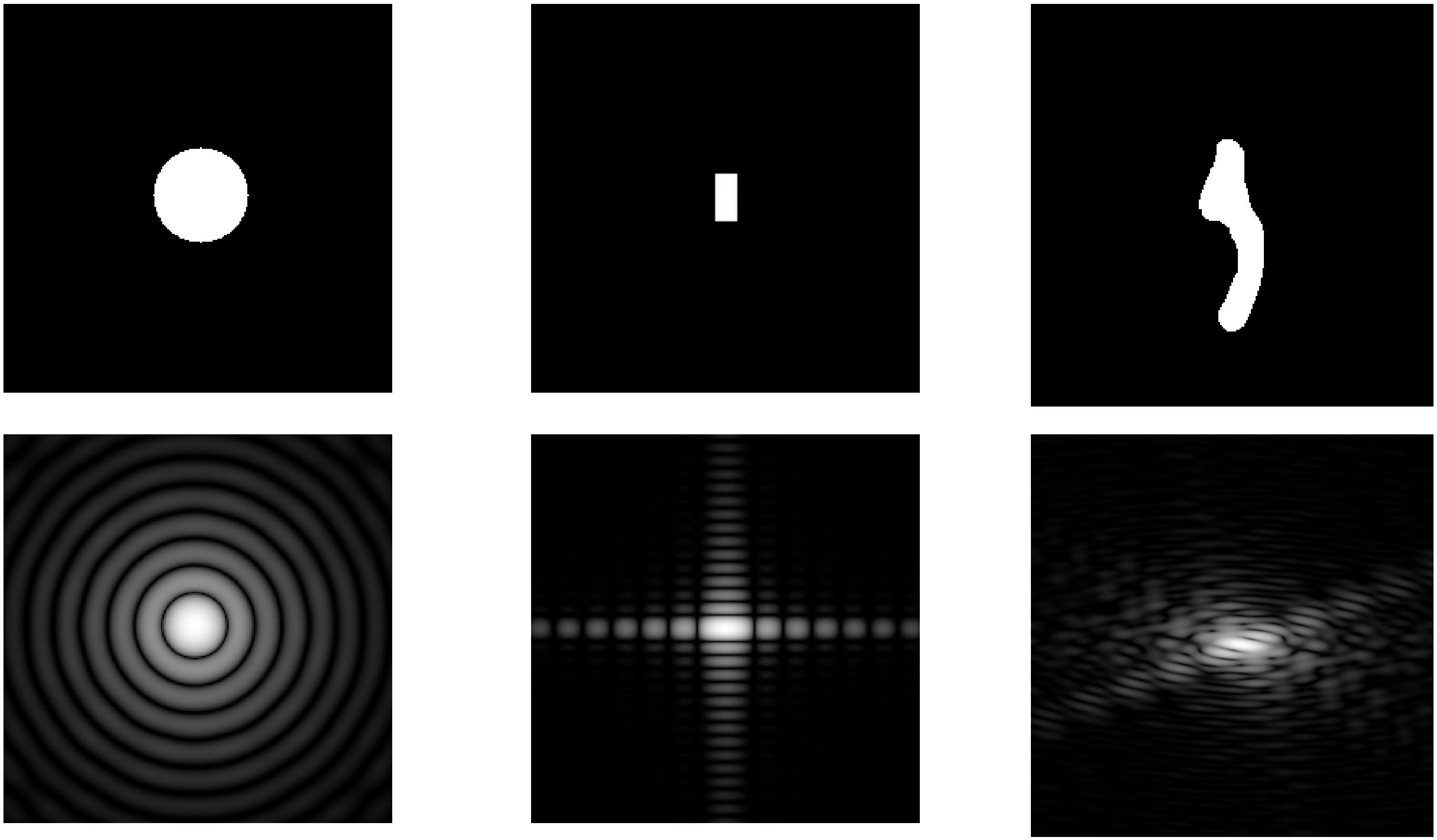
- Small particles require knowledge of optical properties:
  - Real Refractive Index (bending of light)
  - Imaginary Refractive Index (absorption of light within particle)
  - Refractive index values less significant for large particles
- Light must be collected over large range of angles

Diffraction Pattern





Diffraction Patterns



Using Models to Interpret Scattering

- Scattering data typically cannot be inverted to find particle shape.
- We use optical models to interpret data and understand our experiments.

The Calculations

- There is no need to know all of the details.
- The LA-950 software handles all of the calculations with minimal intervention.
- This talk is to improve your understanding of the results.

Laser Diffraction Models

- Large particles -> Fraunhofer
  - More straightforward math
  - Large, opaque particles
  - Use this to develop intuition

- All particle sizes -> Mie
  - Messy calculations
  - All particle sizes

Light

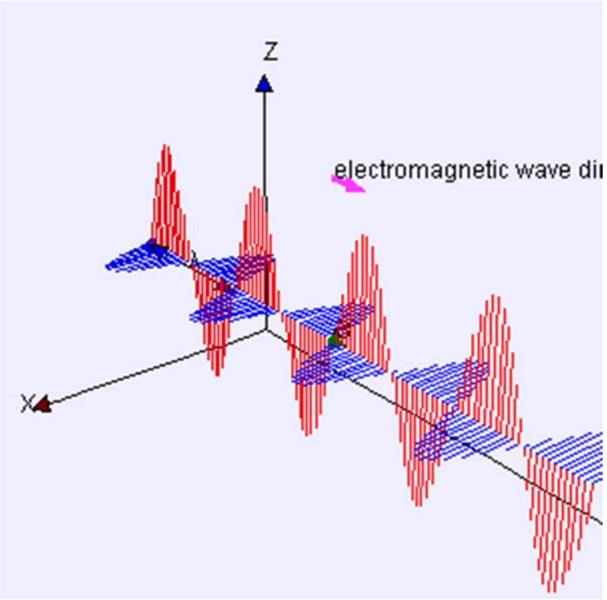
Expressed in just in y-direction

$$E = E_0 \sin(ky - \omega t)$$

Oscillating electric field

$$H = H_0 \sin(ky - \omega t)$$

Oscillating magnetic field (orthogonal to electric field)



Cheat by using vector notation (for 3 dimensions) and real part of complex numbers (because it makes the trig easier).

$$\mathbf{E} = \mathbf{E}_0 \exp(i\mathbf{k} \bullet \mathbf{x} - i\omega t)$$

$$\mathbf{H} = \mathbf{H}_0 \exp(i\mathbf{k} \bullet \mathbf{x} - i\omega t)$$

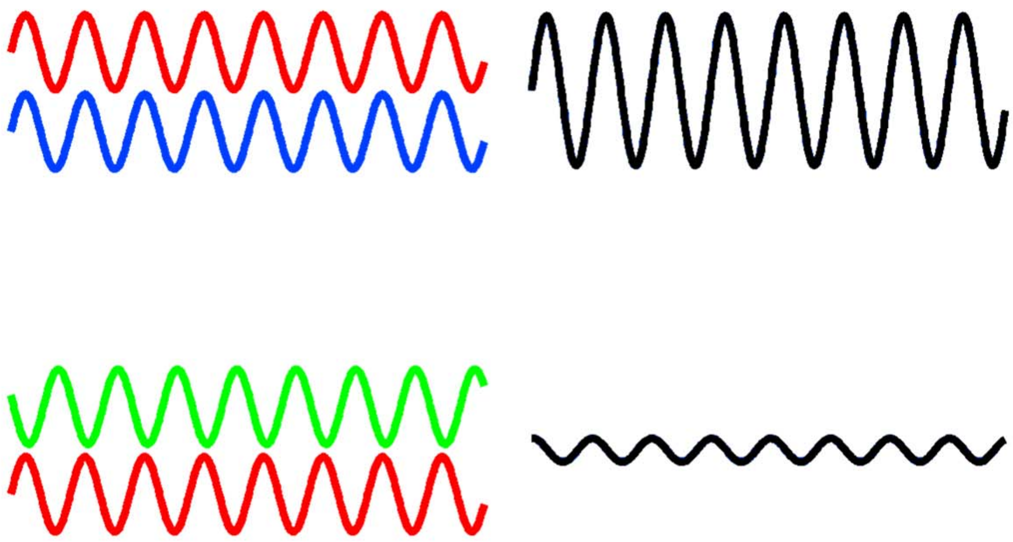
Complements of Lookang @ weelookang.blogspot.com

Light: Interference

Look at just the electric field.

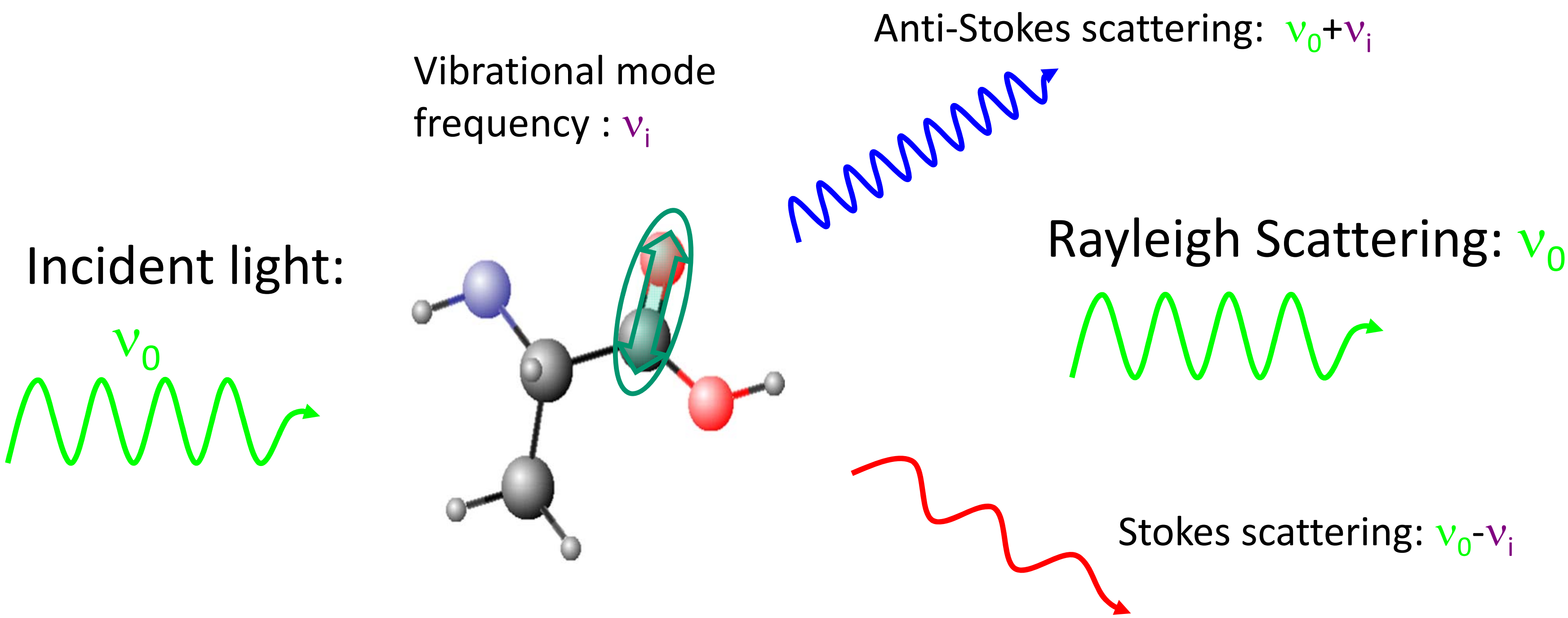
$E = E_0 \sin(kx - \omega t)$ Oscillating electric field

$E = E_0 \sin(kx - \omega t + \phi)$ Second electric field with phase shift



We will use interference to develop an intuitive understanding later.

Microscopic View of Scattering



Today we discuss the scattered photons that do not change wavelength. Also, we treat everything as a continuum.

About 1 scattered photon in a million has a wavelength shift that depends on the molecule. These extra photons are the basis for Raman spectroscopy. Horiba makes Raman instruments too!

Fraunhofer Diffraction

A good approximation to develop intuition

Fraunhofer Diffraction

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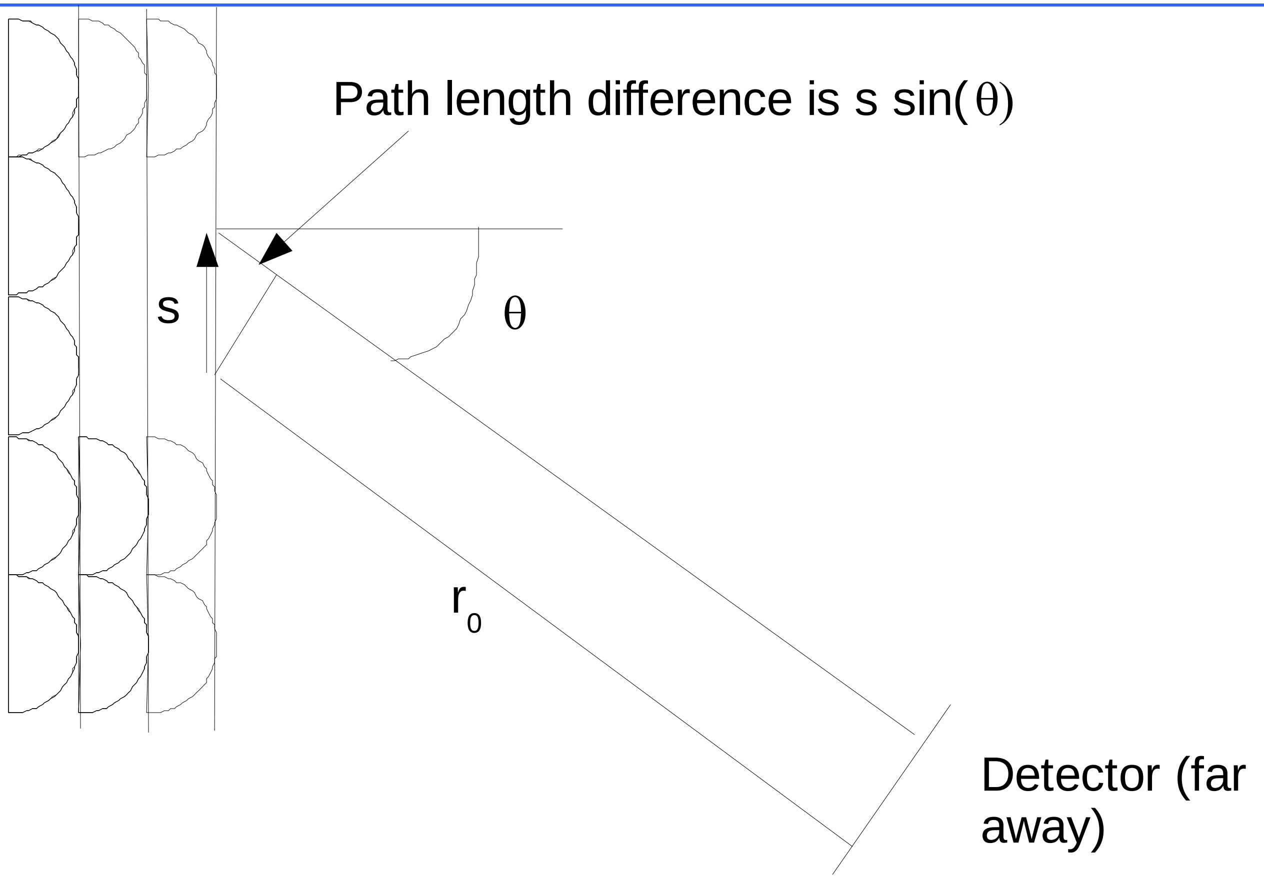


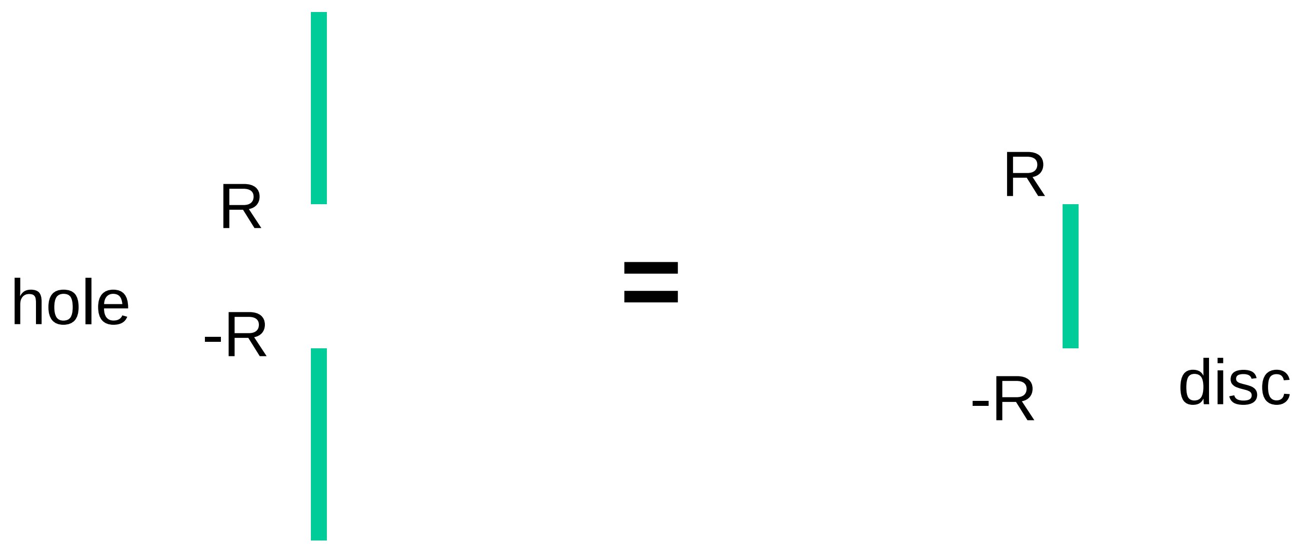
$k = 2\pi/\lambda$

Electric field at target from each position s:

$$\exp(ik(r_0 + s\sin(\theta)) - \omega t)$$

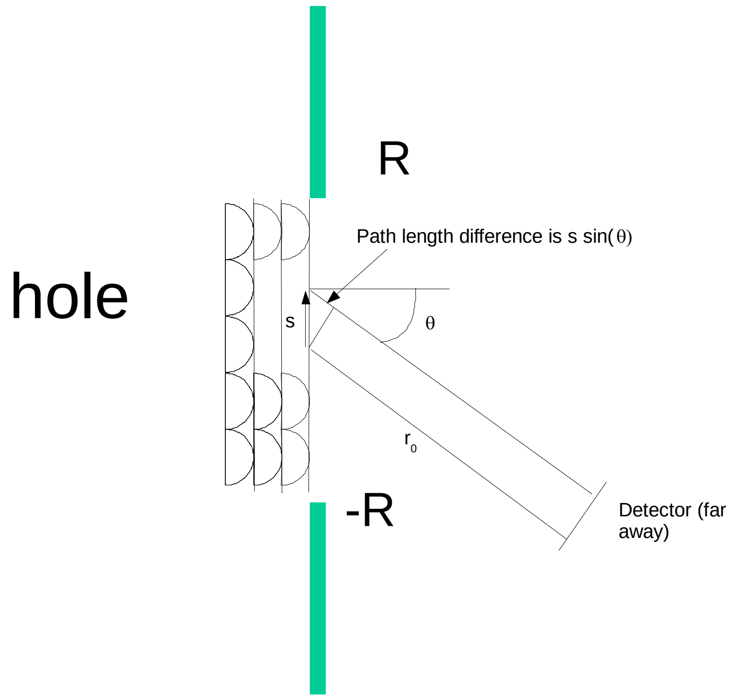
Fraunhofer Diffraction

We want to treat a hole because it is easy. We need a trick.



Babinet's principle: Scattering from an aperture is the same as scattering from its complement

Fraunhofer Diffraction

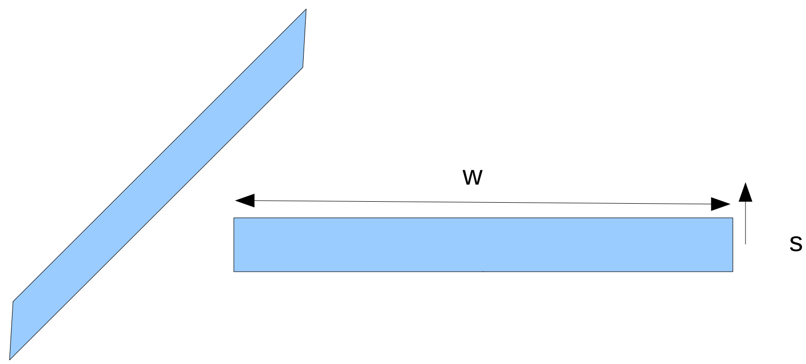


$$E(\theta) = \int_{-R}^{R} A \exp(iks \sin\theta) ds$$

Fraunhofer Diffraction

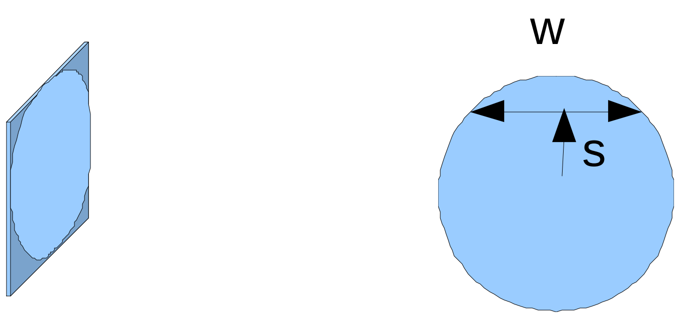
Need to figure area of each strip of aperture to integrate.
For a slit it is easy (and we usually ignore length):

$$A = wds$$

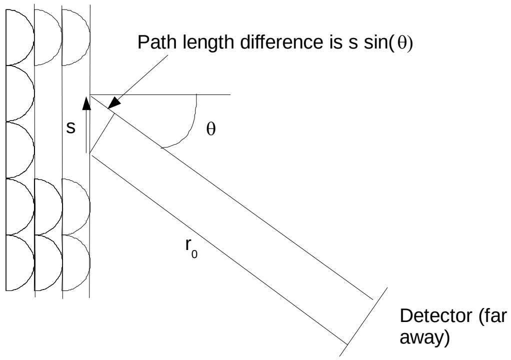


For a circle, it is a bit messy:

$$A = 2\sqrt{R^2 - s^2}\,ds$$



Fraunhofer Diffraction

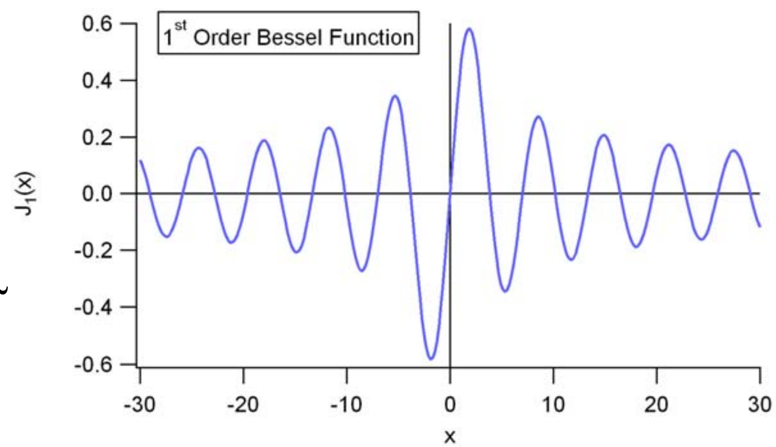


Now integrate over s from –R to R

$$\int_{-R}^{R} 2\sqrt{R^2 - s^2}\,\exp(iks\sin\theta)\,ds$$

dimensionless size parameter $\alpha = \pi D / \lambda$

$$E = \frac{2E_0}{r} R^2 \frac{J_1(\alpha \sin\theta)}{\alpha \sin\theta}$$



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Fraunhofer Approximation

$$(S_1)^2 = (S_2)^2 = \alpha^4 \left[\frac{J_1(\alpha \sin\Theta)}{\alpha \sin\Theta} \right]^2$$

$$I(\Theta) = \frac{I_0}{k^2 a^2} \alpha^4 \left[\frac{J_1(\alpha \sin\Theta)}{\alpha \sin\Theta} \right]^2$$

dimensionless size parameter $\alpha = \pi D/\lambda$;

J_1 is the Bessel function of the first kind of order unity.

Assumptions:

a) all particles are much larger than the light wavelength (only scattering at the contour of the particle is considered; this also means that the same scattering pattern is obtained as for thin two-dimensional circular disks)

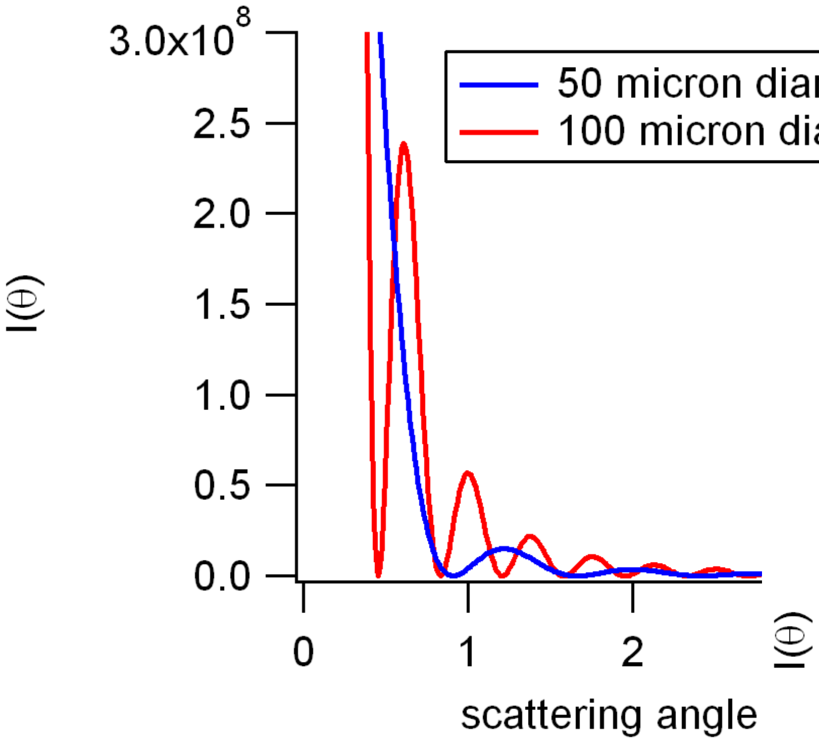
b) only scattering in the near-forward direction is considered (Q is small).

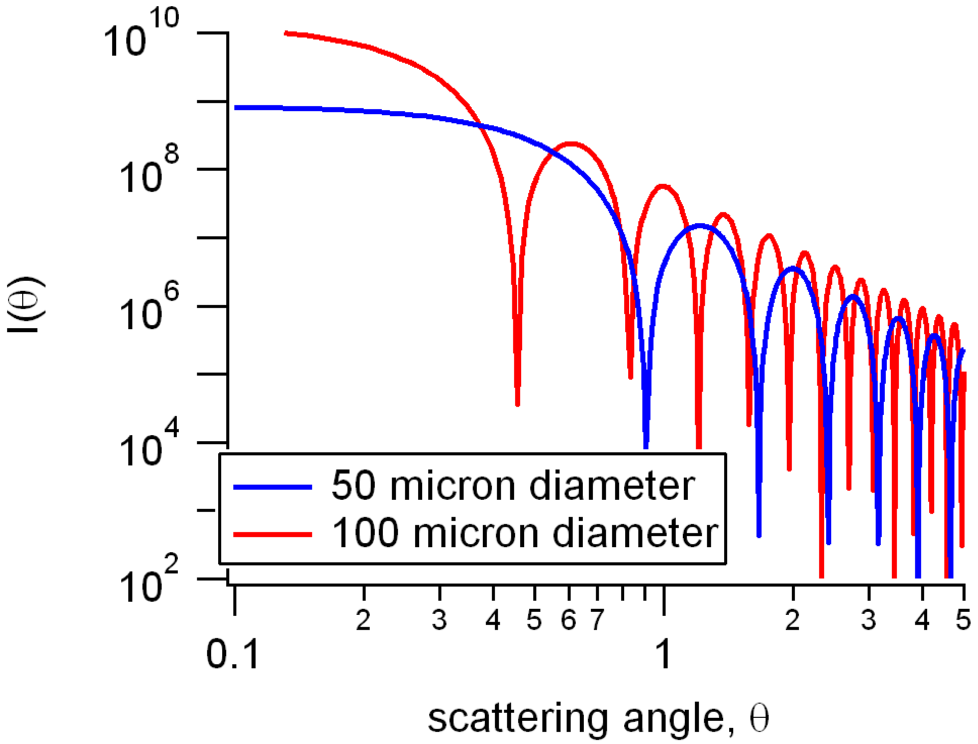
Limitation: (diameter at least about 40 times the wavelength of the light, or $\alpha >> 1$)*

If λ=650nm (.65 μm), then 40 x .65 = 26 μm

If the particle size is larger than about **26 μm**, then the Fraunhofer approximation gives good results. Rephrased, results are insensitive to refractive index choice.

Fraunhofer: Effect of Particle Size

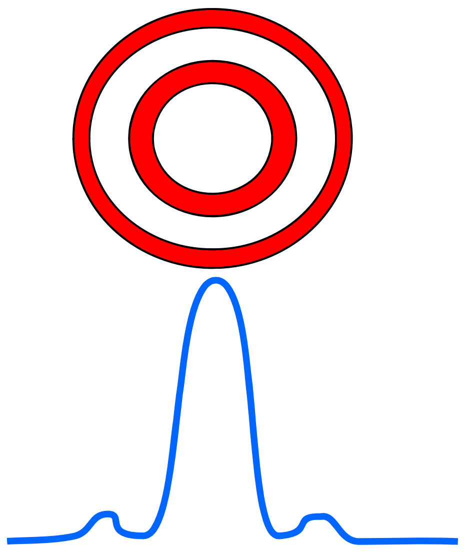




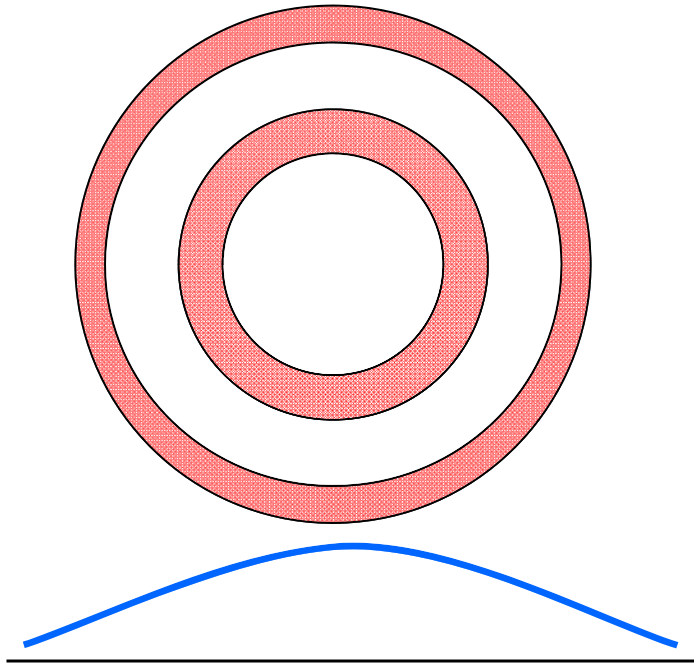
Diffraction Pattern: Large vs. Small Particles

LARGE PARTICLE:

- Peaks at low angles
- Strong signal



Narrow Pattern - High intensity



Wide Pattern - Low intensity

SMALL PARTICLE:

- Peaks at larger angles
- Weak Signal

Poll

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- How many of you work with particles with sizes over 1 mm?
- How many of you work with particles with sizes over 25 microns and less than 1 mm?
- How many of you work with particles with sizes over 1 micron and less than 25 microns?
- How many of you work with particles with sizes less than 1 micron?

Mie Scattering

An exact treatment for a spherical particle.

Maxwell's Equations

- Solve these and the universe's secrets are yours.
- Notation from Bohren and Huffman Absorption and Scattering of Light by Small Particles

$$\nabla \bullet \mathbf{E} = 0$$

Net charge is zero

$$\nabla \bullet \mathbf{H} = 0$$

No magnetic monopoles

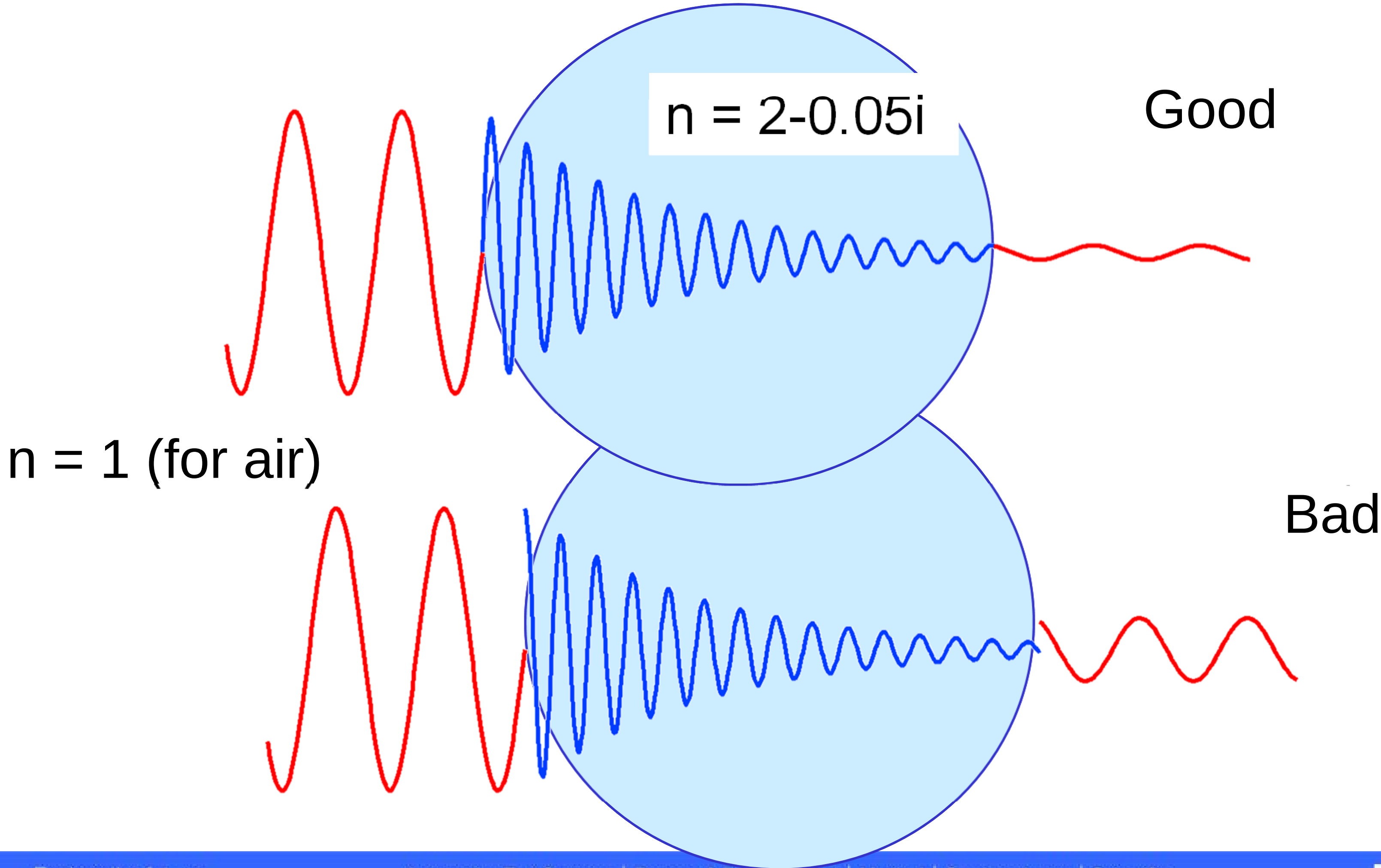
$$\nabla \times \mathbf{E} = i\omega\mu \cdot \mathbf{H}$$

$$\nabla \times \mathbf{H} = -i\omega\varepsilon \cdot \mathbf{E}$$

Time varying magnetic field gives electric field and vice versa. No current flows through system.

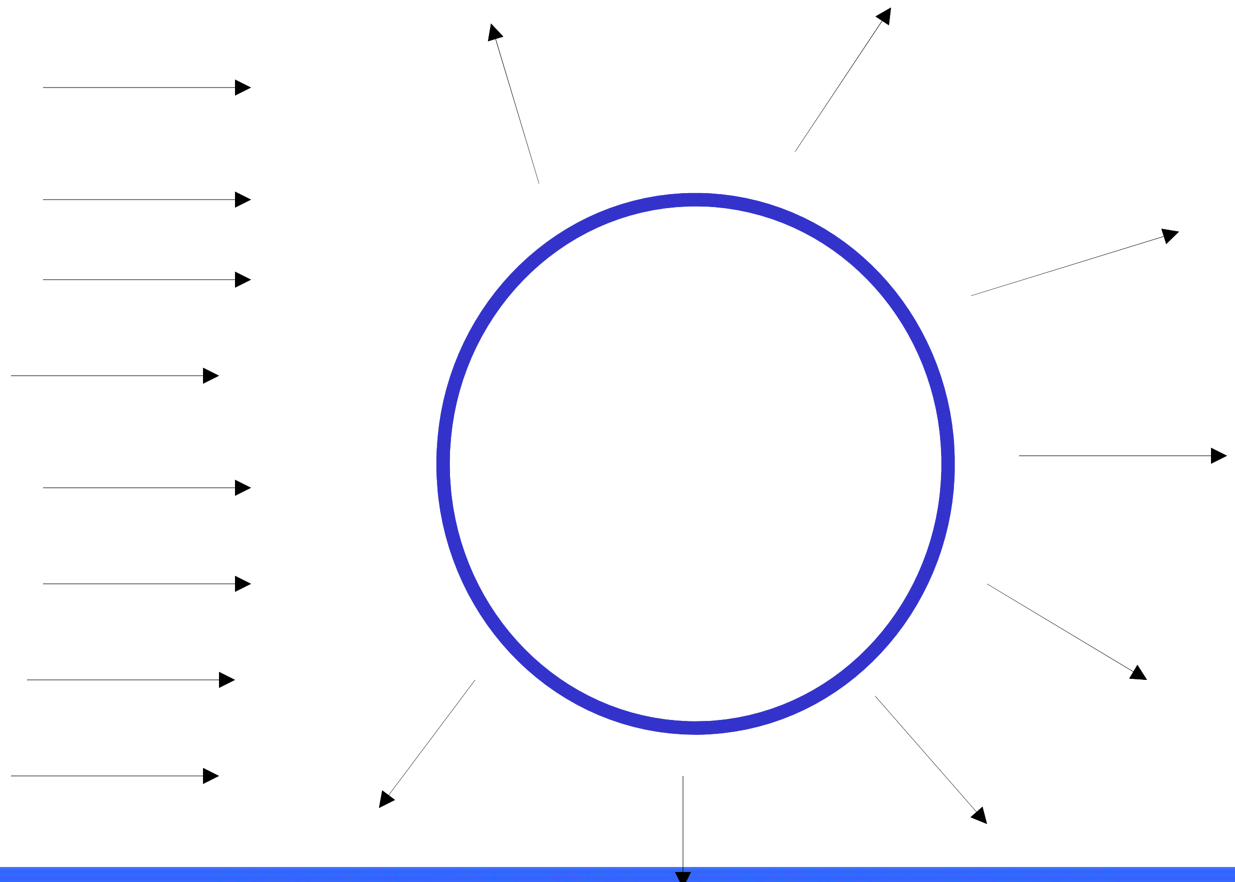
Boundary Conditions

- Properties of particle different from surrounding medium
- Tangential components of E and H are continuous at boundary



Overview of Solution

- Sum of incoming plane wave and scattered waves.
- We also get information on extinction and so on.



Mie Scattering

$$I_s(m,x,\theta) = \frac{I_0}{2k^2r^2}\left(\left|S_2\right|^2 + \left|S_1\right|^2\right)$$

Use an existing computer program for the calculations!

$$S_1(m,x,\theta) = \sum_1^\infty \frac{2n+1}{n(n+1)}\{a_n\pi_n + b_n\tau_n\}$$

$$S_2(m,x,\theta) = \sum_1^\infty \frac{2n+1}{n(n+1)}\{a_n\tau_n + b_n\pi_n\}$$

$$\pi_n = \frac{P_n^1(\cos\theta)}{\sin\theta}$$

$$\tau_n = \frac{d}{d\theta}\left(P_n^1(\cos\theta)\right)$$

$$a_n = \frac{m\psi_n(mx)\psi_n'(x) - \psi_n(x)\psi_n'(mx)}{m\psi_n(mx)\xi_n'(x) - \xi_n(x)\psi_n'(mx)}$$

$$b_n = \frac{\psi_n(mx)\psi_n'(x) - m\psi_n(x)\psi_n'(mx)}{\psi_n(mx)\xi_n'(x) - m\xi_n(x)\psi_n'(mx)}$$

ξ, ψ: Ricatti-Bessel functions

P_n^1: 1st order Legendre Functions

Mie

The equations are messy, but require just three inputs which are shown below. The nature of the inputs is important.

$$x = \pi D / \lambda$$

Decreasing wavelength is the same as increasing size. So, if you want to measure small particles, decrease wavelength so they "appear" bigger. That is, <u>get a blue light source for small particles</u>.

$$m = n_p / n_m$$

We need to know relative refractive index. As this goes to 1 there is no scattering.

$$\theta$$

Scattering Angle

Effect of Size

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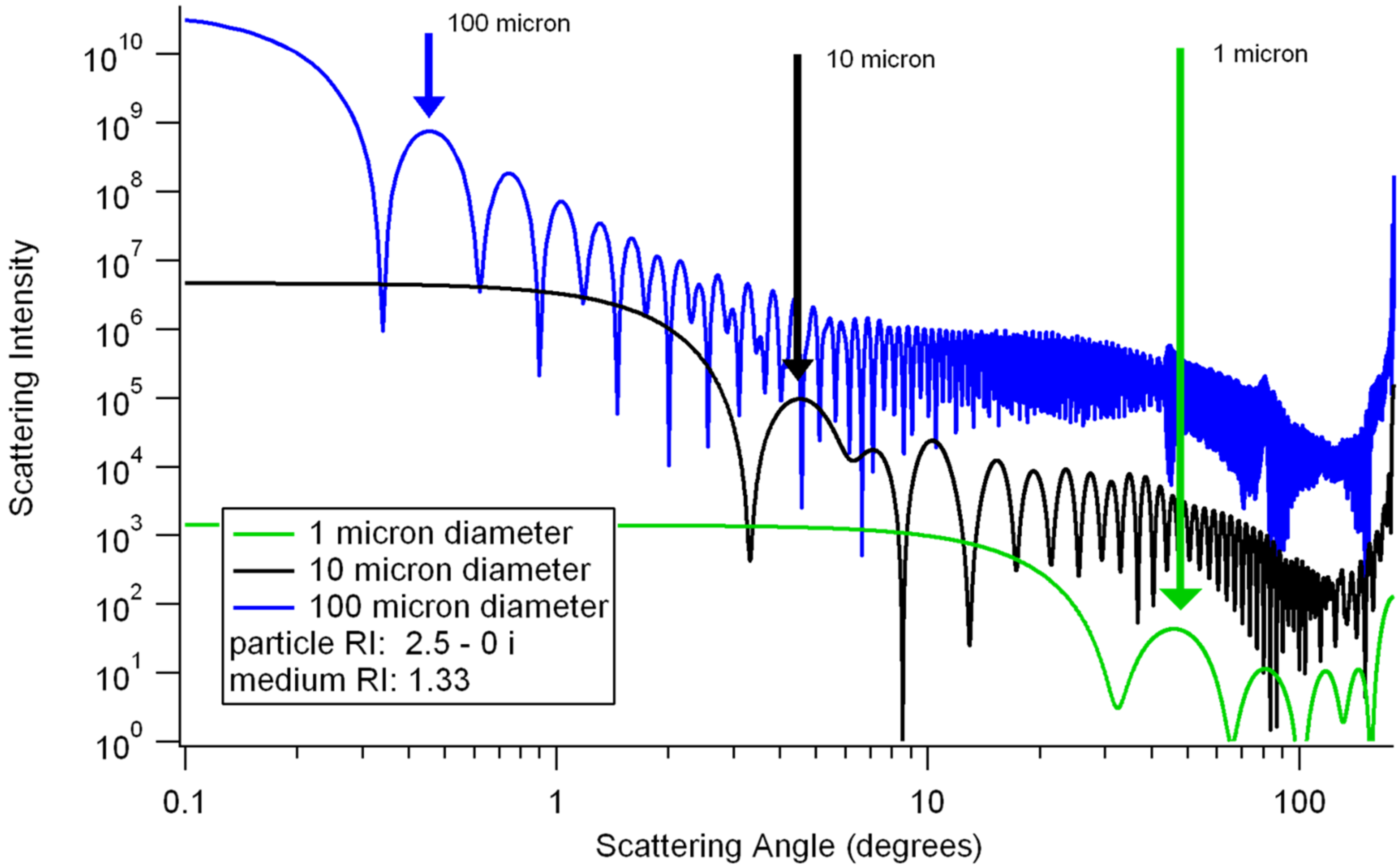
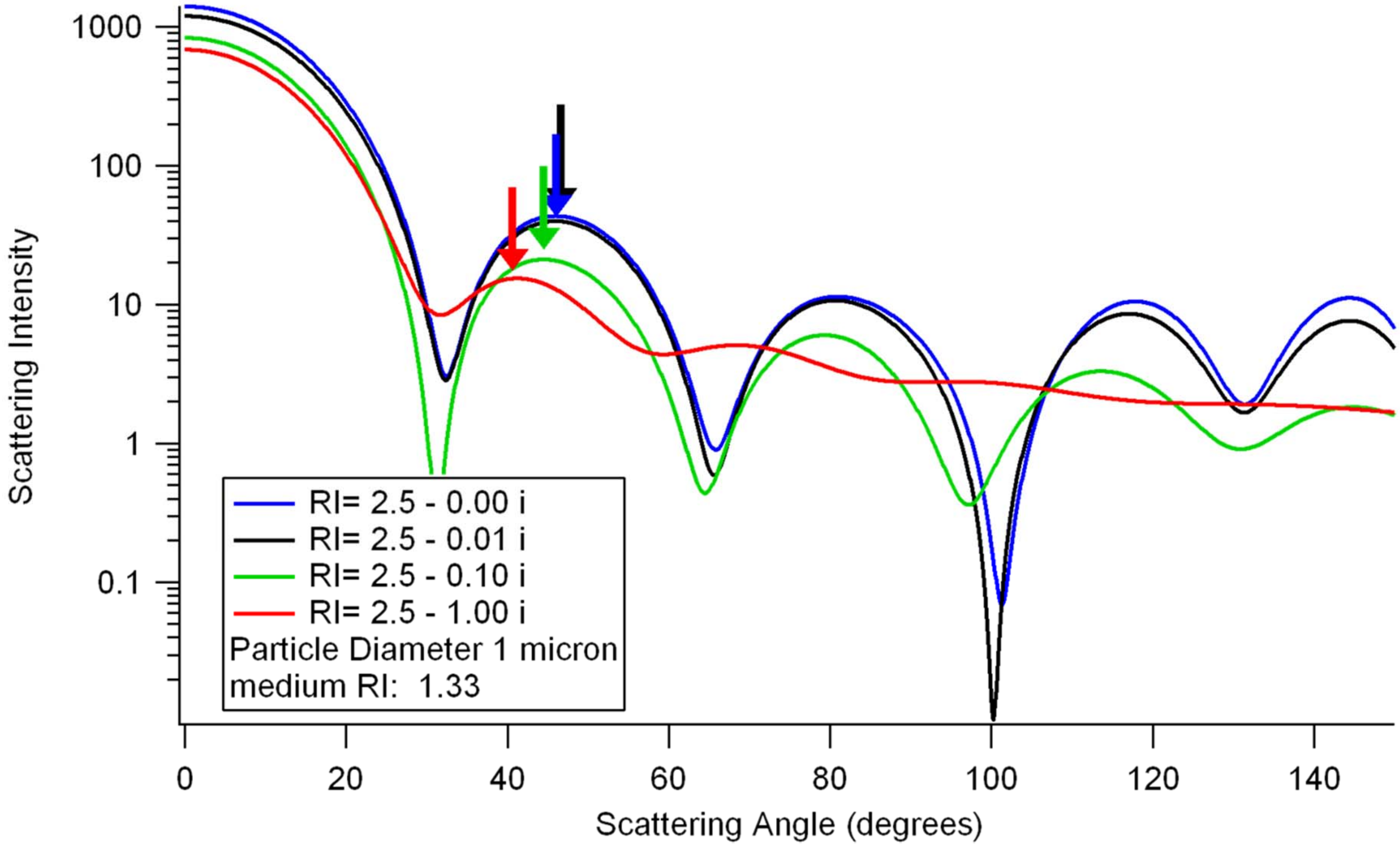


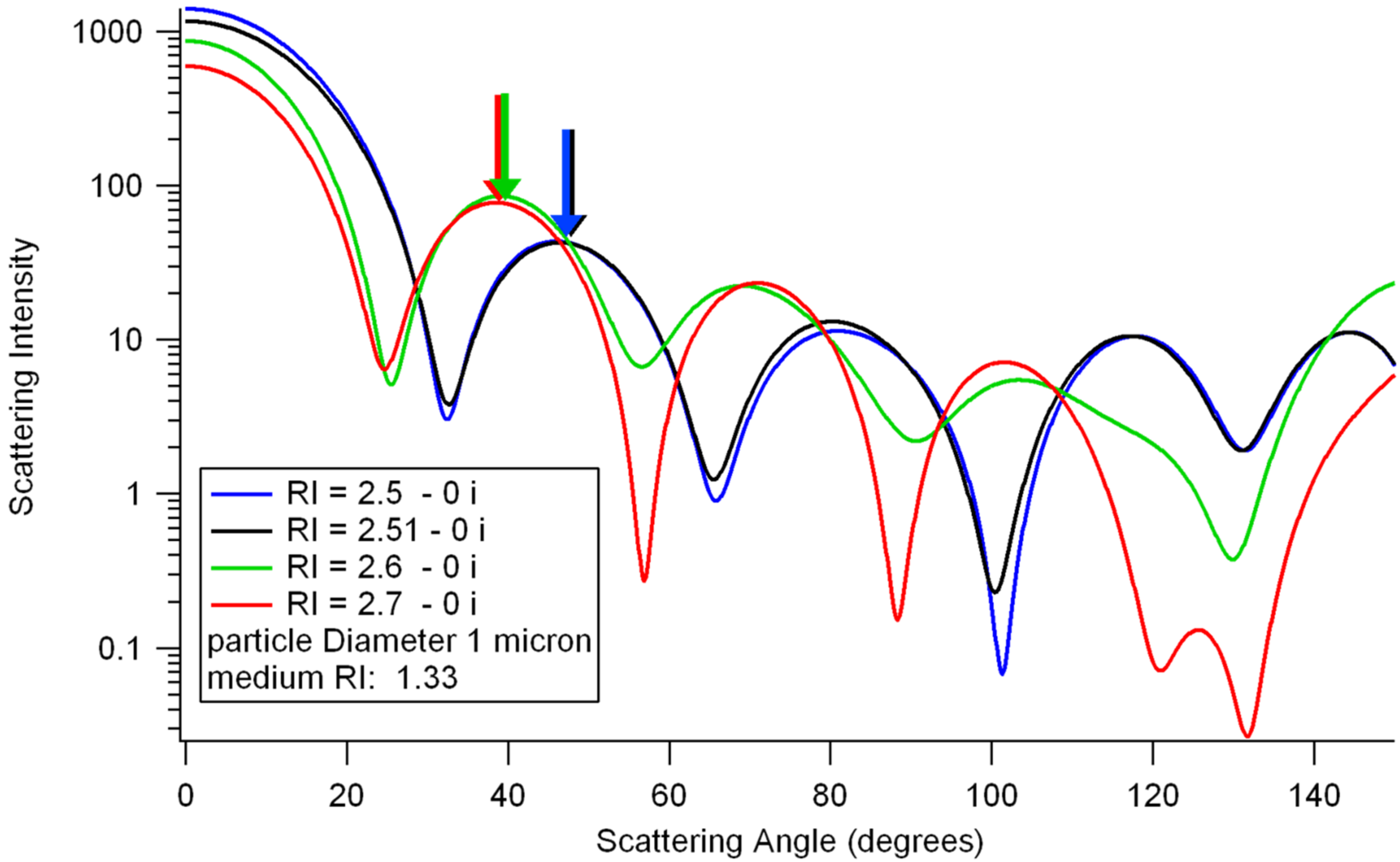
As diameter increases, intensity (per particle) increases and location of first peak shifts to smaller angle.

Effect of RI: imaginary term



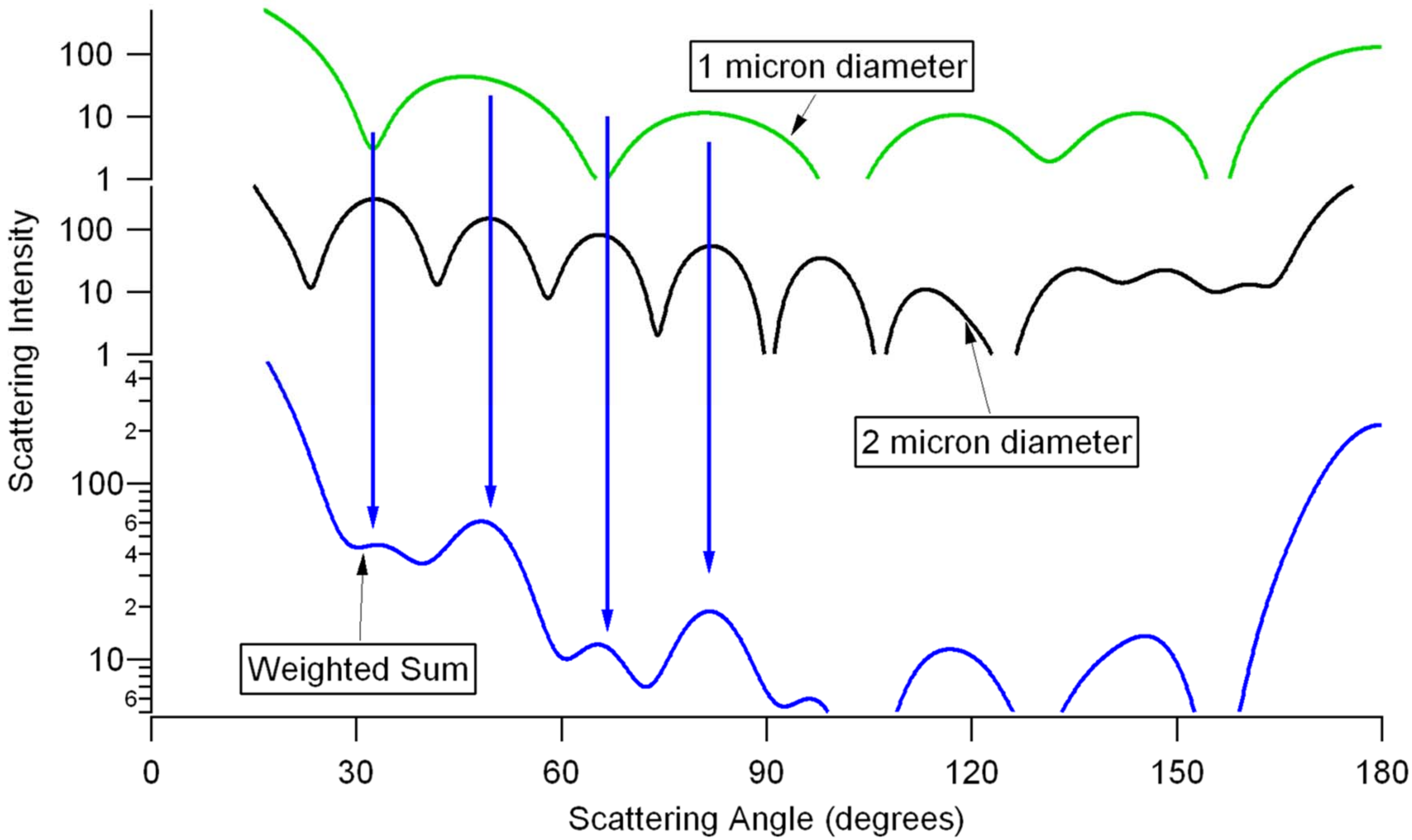
As imaginary term (absorption) increases location of first peak shifts to smaller angle.

Effect of RI: Real Term



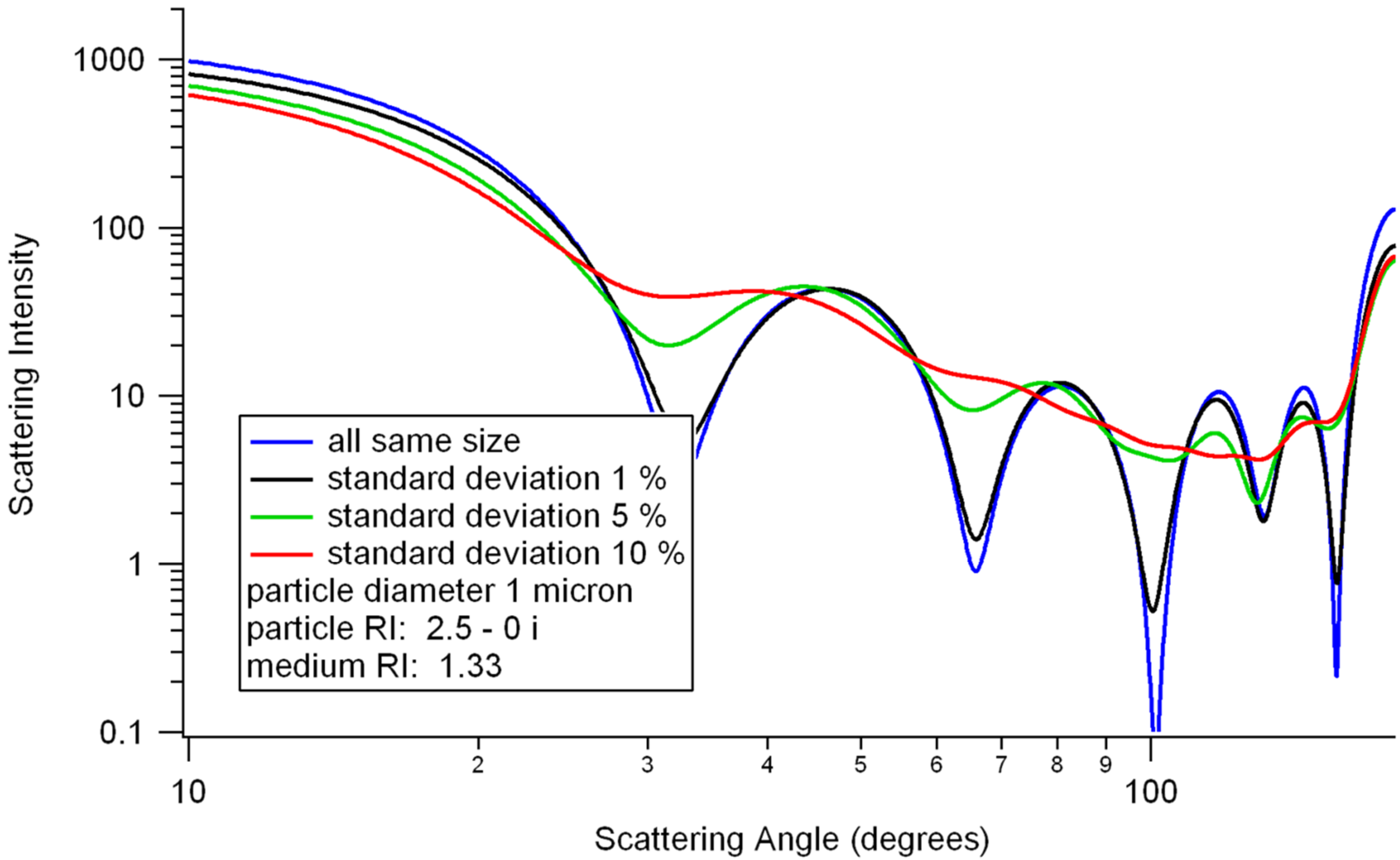
It depends….

Mixing Particles? Just Add



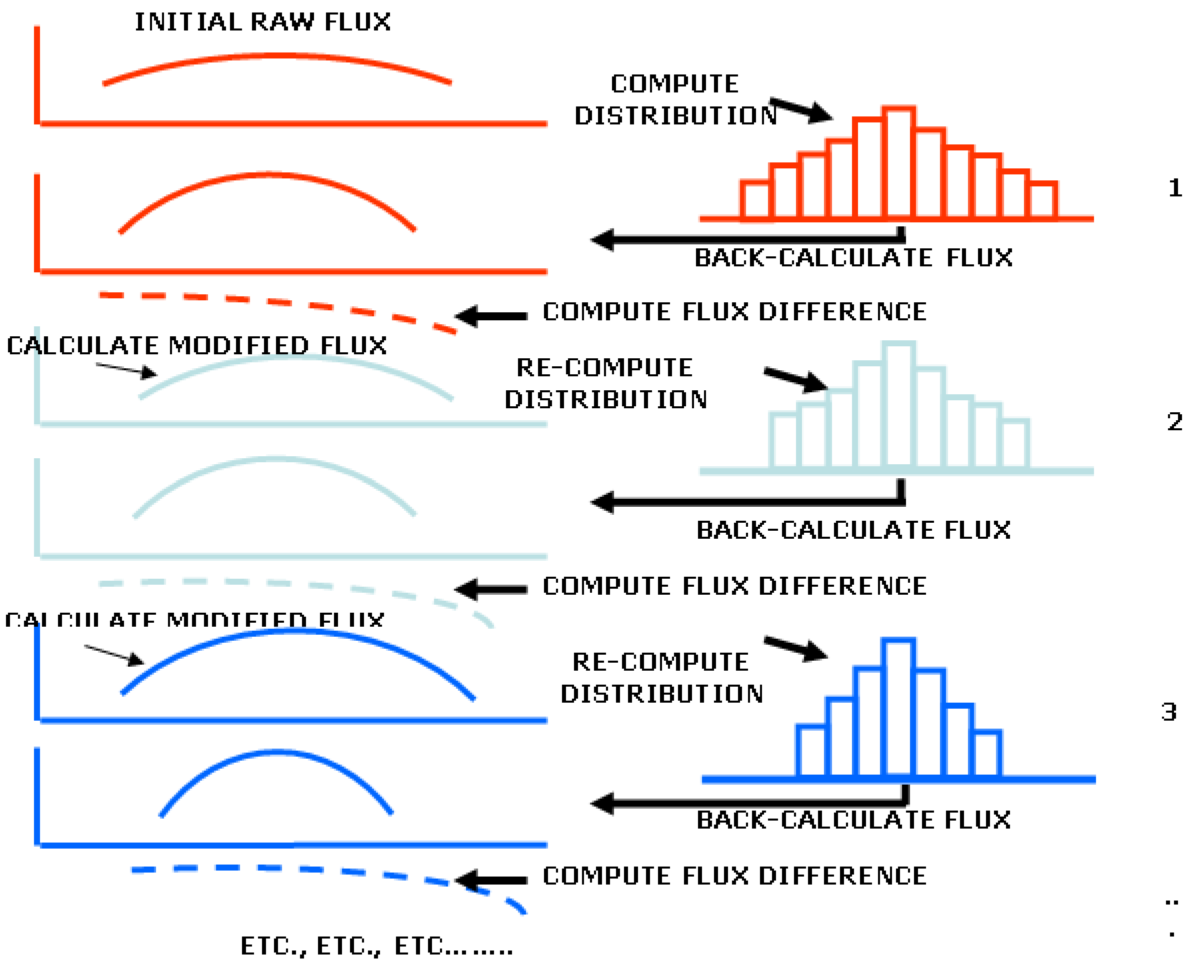
The result is the weighted sum of the scattering from each particle. Note how the first peak from the 2 micron particle is suppressed since it matches the valley in the 1 micron particle.

Effect of Distribution Width



As distribution becomes wider, the peaks become less distinct.

Iterations



INITIAL RAW FLUX
COMPUTE DISTRIBUTION
1
BACK-CALCULATE FLUX
COMPUTE FLUX DIFFERENCE
CALCULATE MODIFIED FLUX
RE-COMPUTE DISTRIBUTION
2
BACK-CALCULATE FLUX
COMPUTE FLUX DIFFERENCE
RE-COMPUTE DISTRIBUTION
3
BACK-CALCULATE FLUX
COMPUTE FLUX DIFFERENCE
ETC., ETC., ETC……..

Pop Quiz

- As particle size increases:
  - Peaks shift to smaller angles
  - Peaks shift to larger angles
  - Nobody said there would be a quiz!

Pop Quiz

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- As particle size increases:
  - Peaks shift to smaller angles
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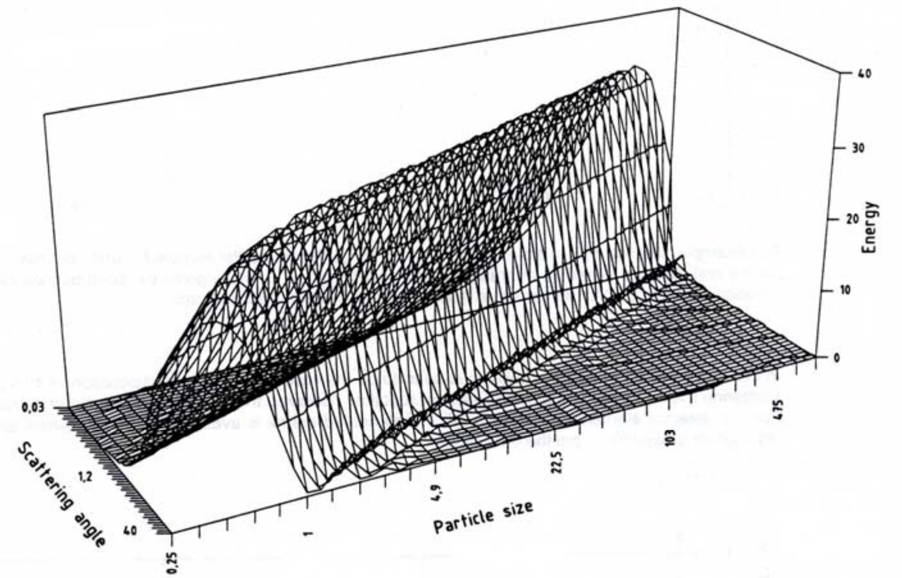
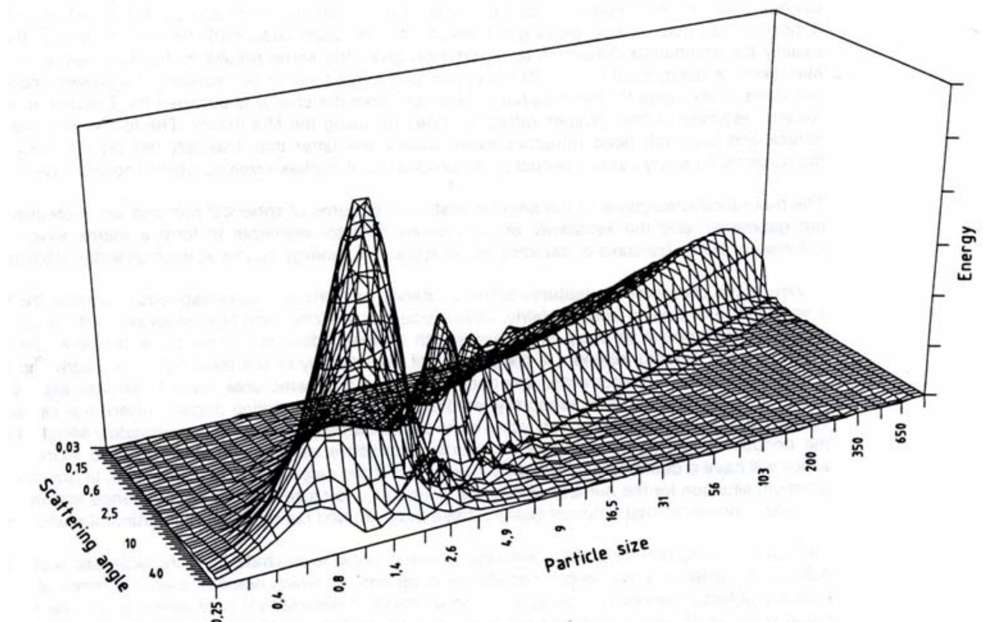
½ credit

Comparison of Models



Light energy scattering patterns for an arbitrary detector configuration against particle size (µm) and scattering angle (°) for equal volumes of particles (Fraunhofer theory)



Light energy scattering patterns for an arbitrary detector configuration against particle size (µm) and scattering angle (°) for equal volumes of particles (Mie theory, latex particles RI 1.60 - 0.0i, in water RI 1.33)

- Fraunhofer (left) vs. Mie (right)

Comparison, Large Particles

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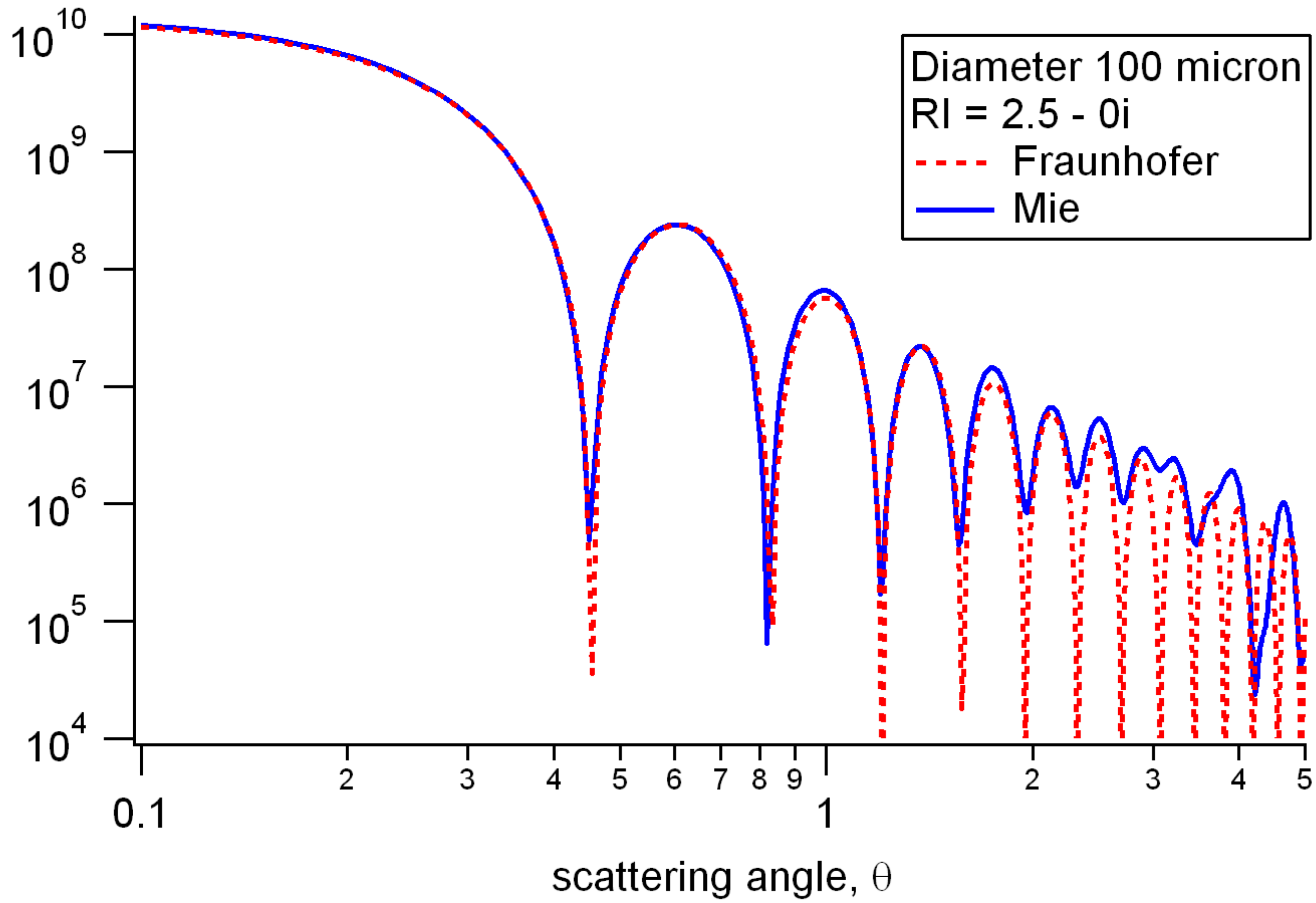
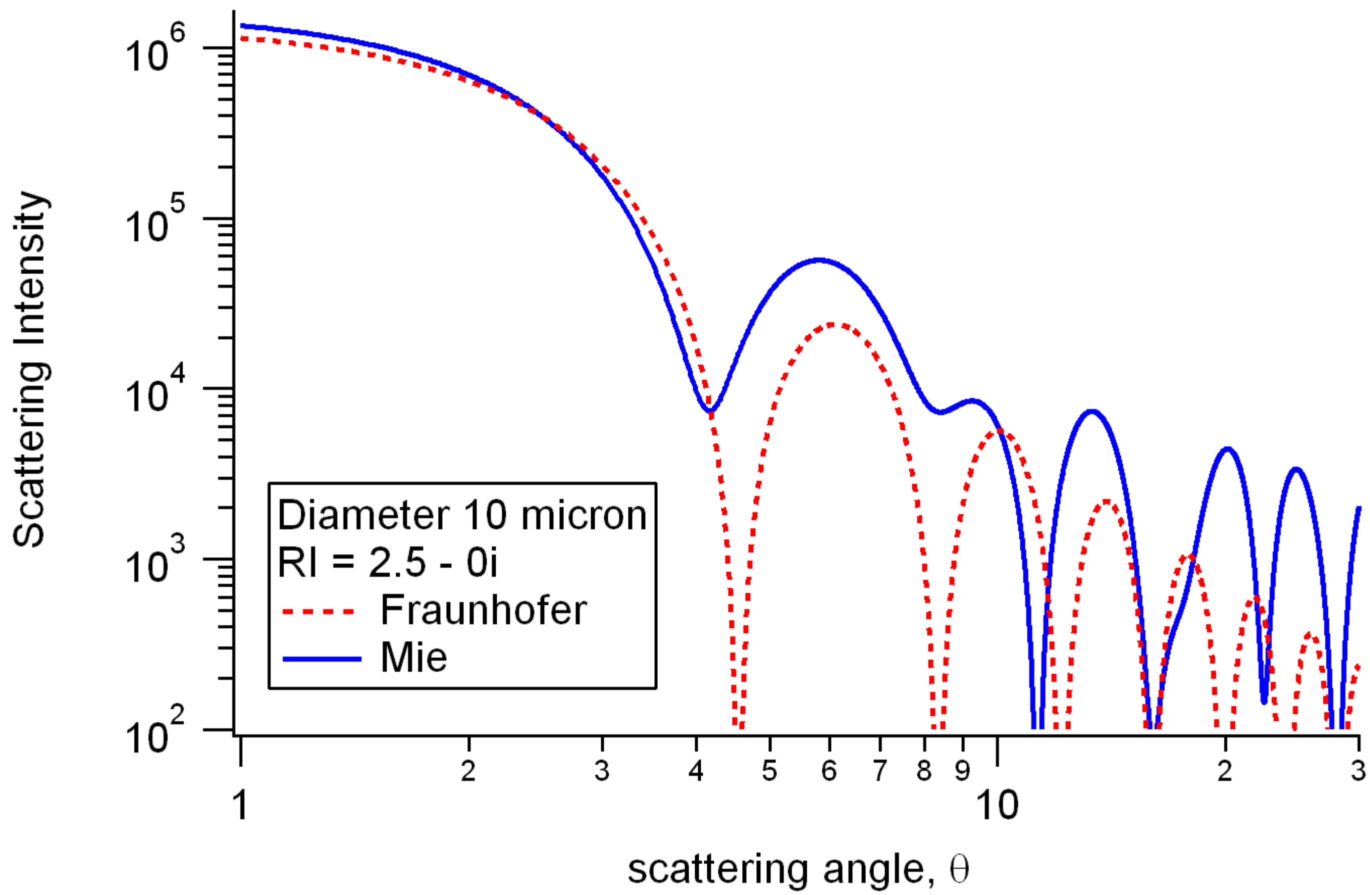


For large particles, match is good out to through several peaks.

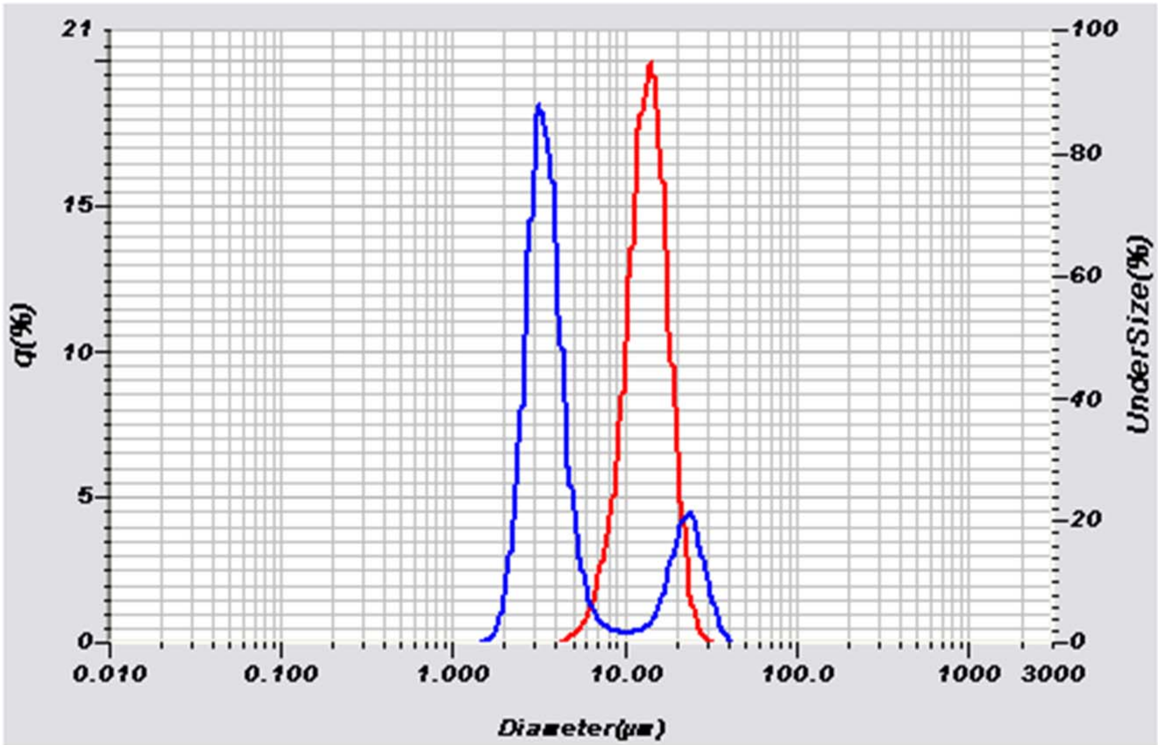
Comparison, Small Particles



For small particles, match is poor.

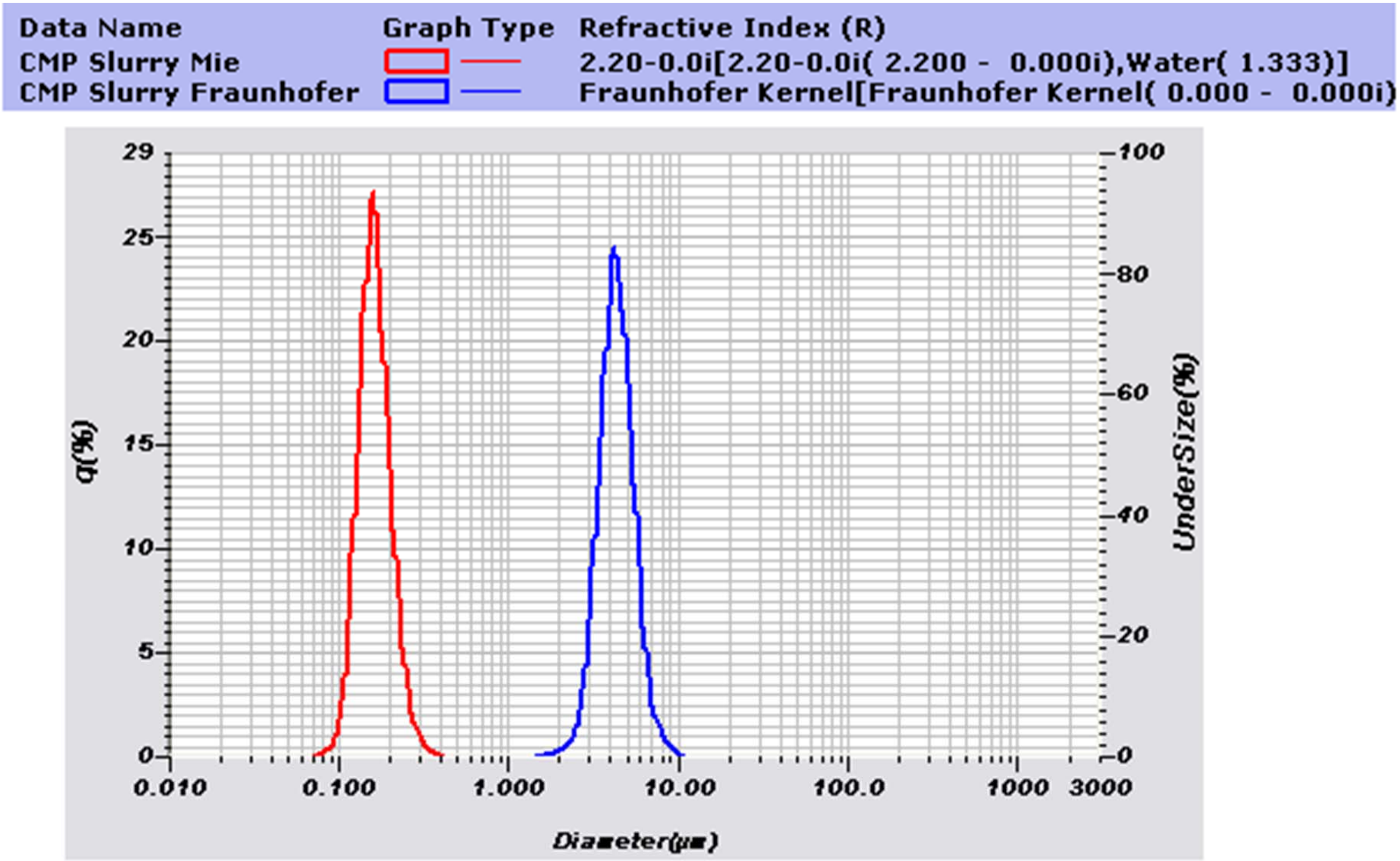
Practical Application: Glass Beads

Data Name	Graph Type	Refractive Index (R)
Standard Glass Beads Mie	red	STD-GLASSBEADS[STD-GLASSBEADS(1.510 - 0.000i),
Standard Glass Beads Fraunhofer	blue	Fraunhofer Kernel[Fraunhofer Kernel(0.000 - 0.000i



Graph Type	D(v,0.1)	D(v,0.5)	D(v,0.9)
red	8.98783(μm)	13.47741(μm)	18.8536
blue	2.58072(μm)	3.62044(μm)	22.3174

Practical Application: CMP Slurry



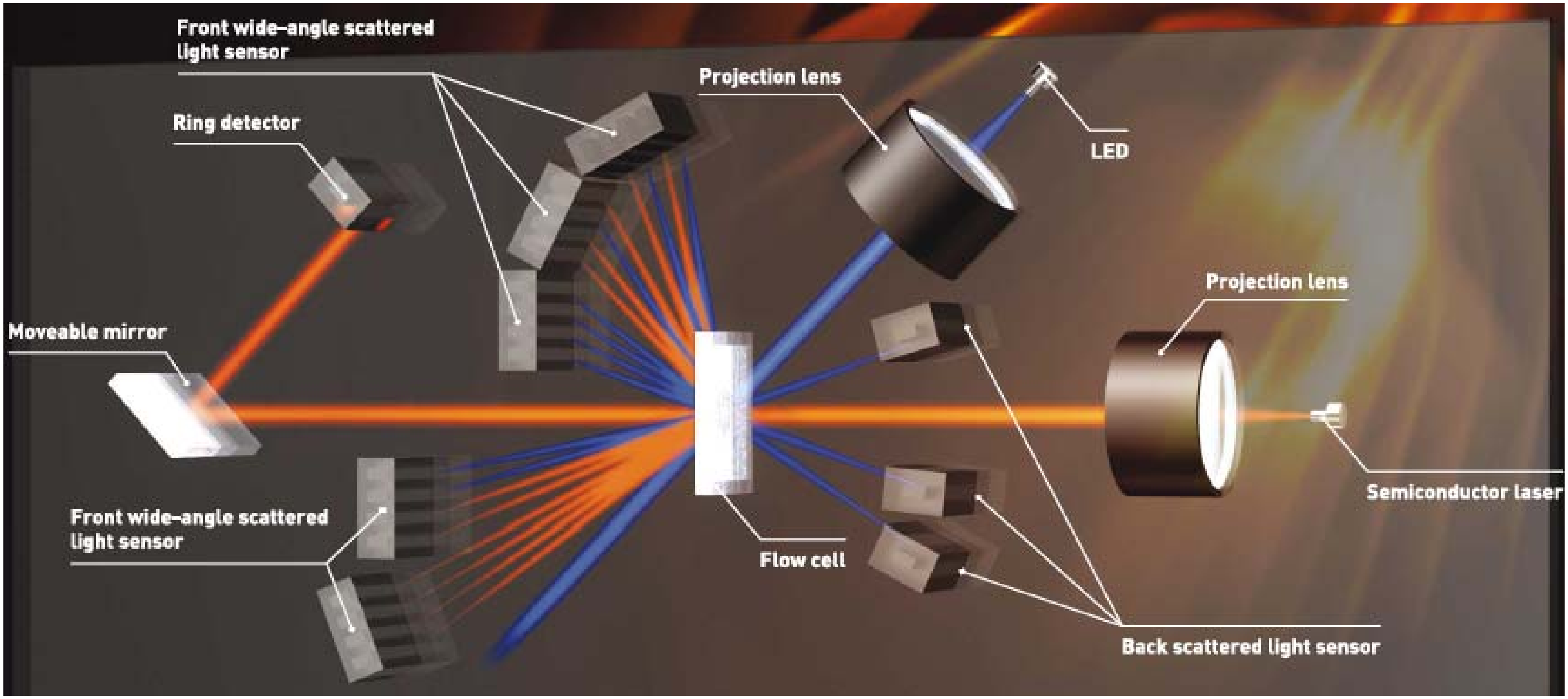
What about background (blank)?

Even pure liquids scatter. Also, there is often some constant background signal due to stray light. And, the detectors will always show a background signal. These effects are small, but they should be corrected.

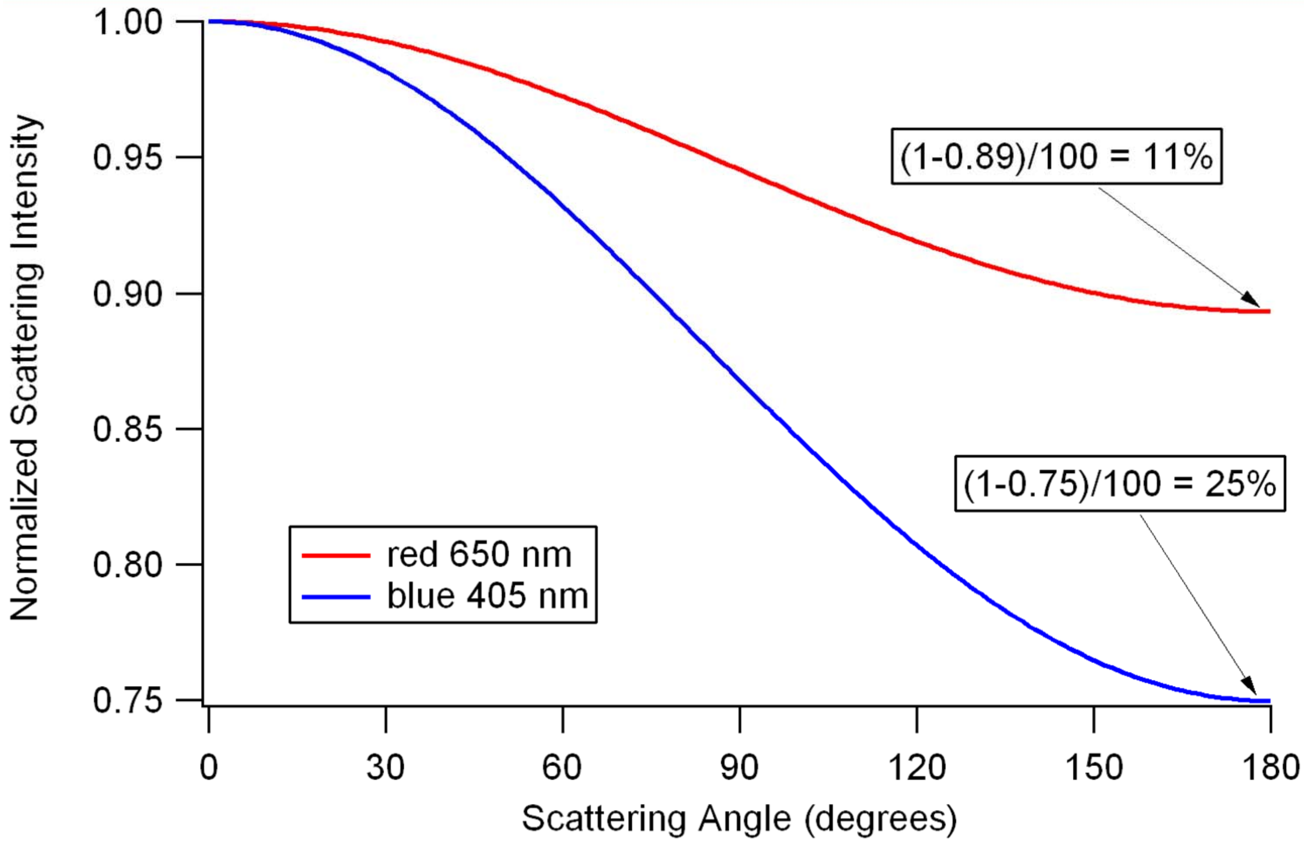
The background is subtracted before applying any of analysis mentioned before.

As the background becomes smaller, the analysis becomes easier.

LA-950 Optics

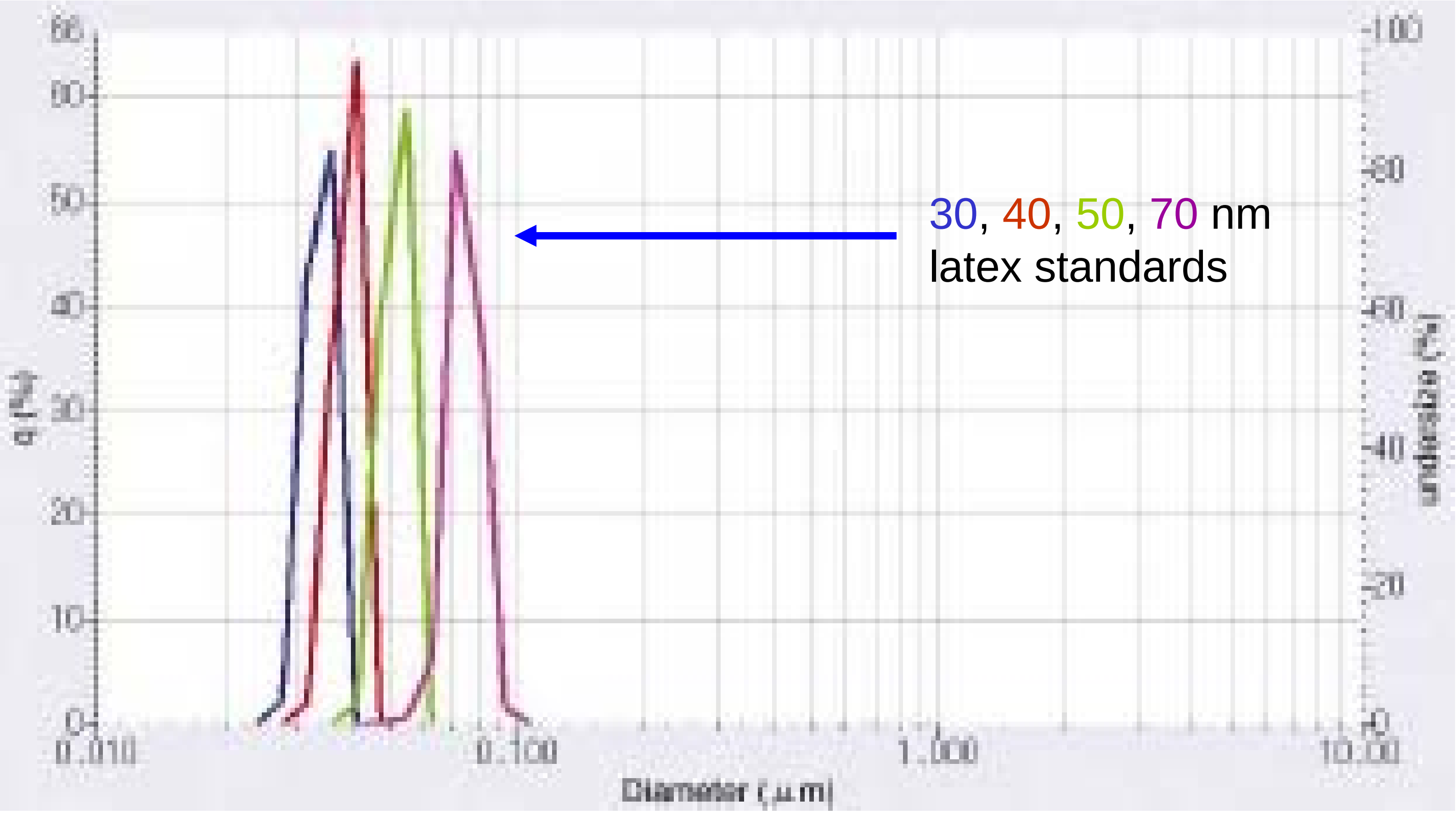


Short Wavelengths for Smallest Particles



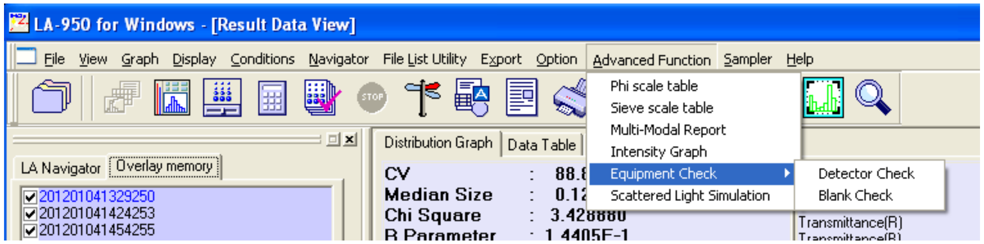
By using blue light source, we double the scattering effect of the particle. This leads to more sensitivity. This plot also tells you that you need to have the background stable to within 1% of the scattered signal to measure small particles accurately.

Why 2 Wavelengths?

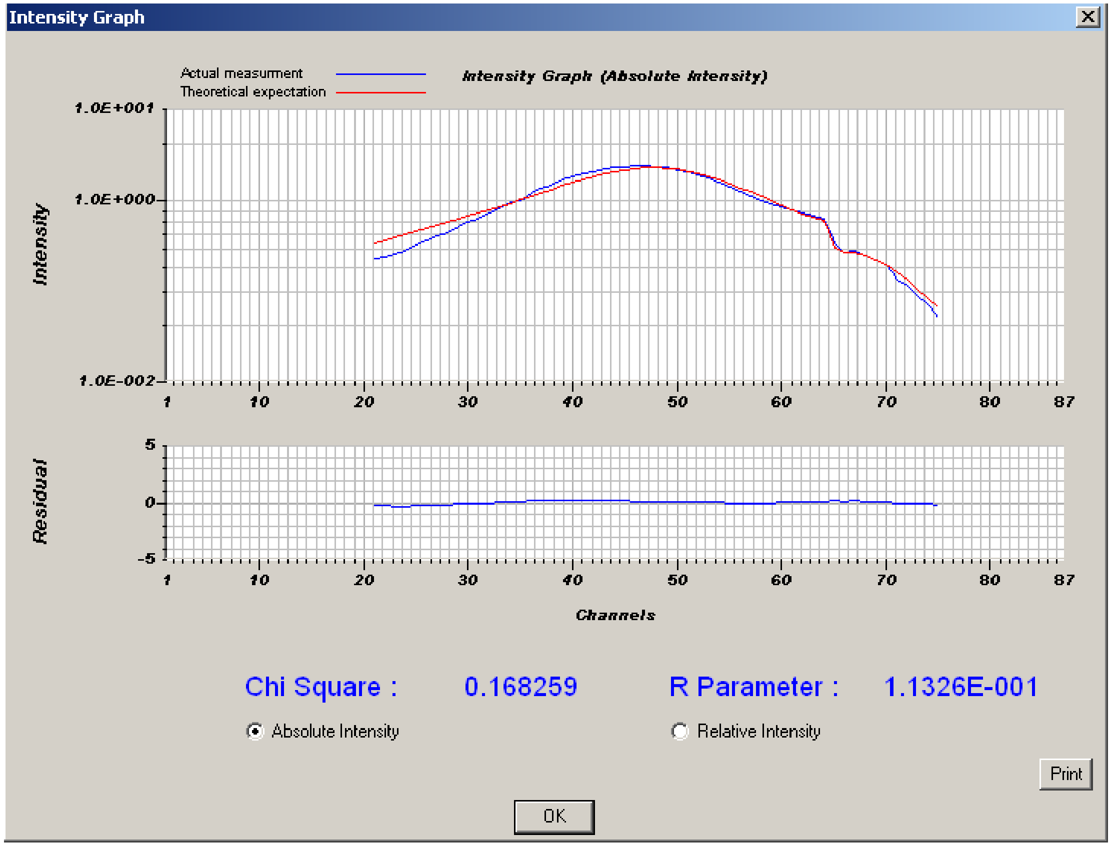


Data from very small particles.

Viewing Raw Data

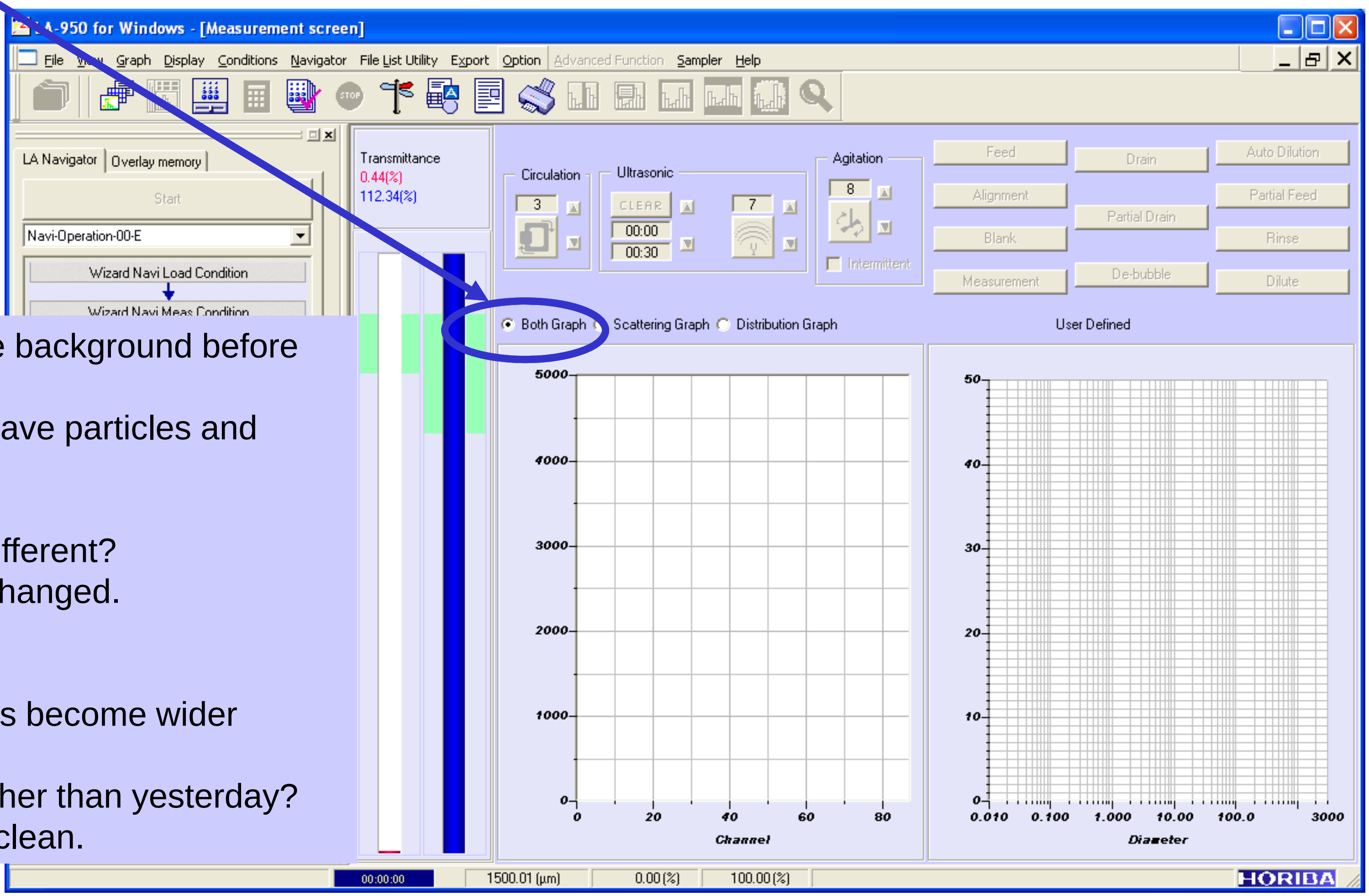


Advanced Function
->Intensity Graph



During Data Collection

Choose “Both Graphs”



Are there peaks in the background before adding sample?
You may already have particles and need to clean.

Is the peak position different?
The average size changed.

Is the peak wider?
The distribution has become wider

Is the background higher than yesterday?
Then you need to clean.

Conclusions

- It helps to know some of the theory to best use a laser diffraction particle size analyzer
  - Small particles – wide angles
  - Large particles – low angles
- Look at Intensity curves
- Big peaks in your background (blank) mean particles or bubbles
- Use Mie theory at all times (default whenever choosing an RI kernel other than Fraunhofer)

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Q&A

Ask a question at labinfo@horiba.com

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Visit the Download Center to find the video and slides from this webinar.

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Thank-you