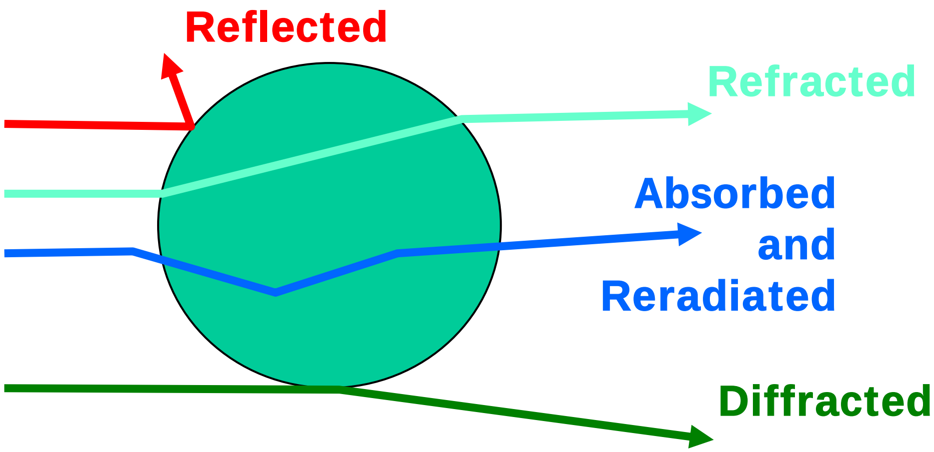
LIGHT SCATTERING THEORY

Laser Diffraction
(Static Light Scattering)

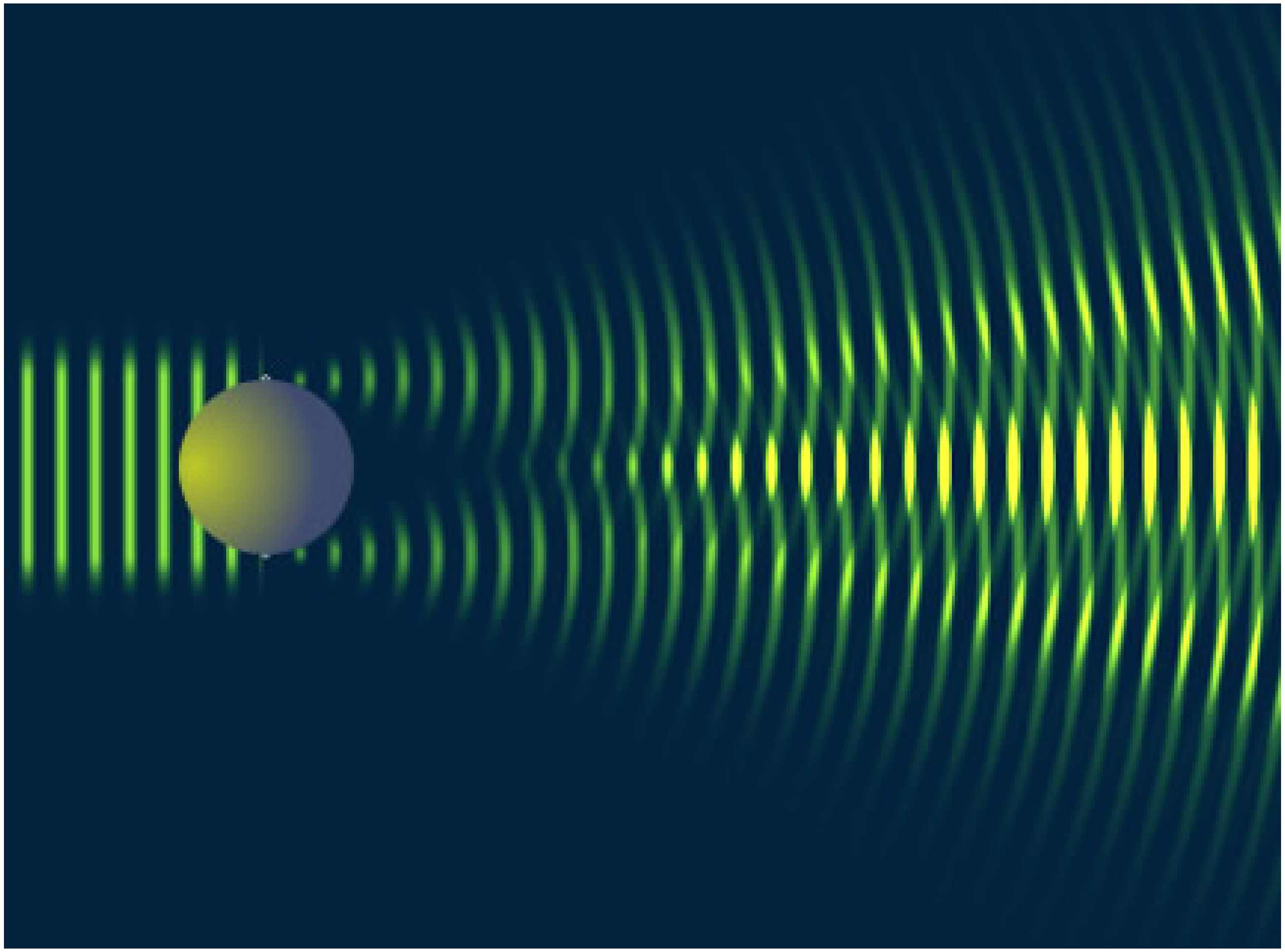
When a Light beam Strikes a Particle

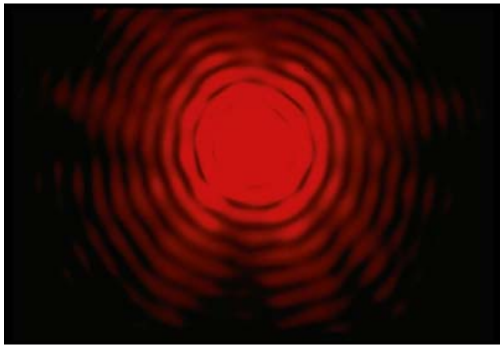
- Some of the light is:
  - Diffracted
  - Reflected
  - Refracted
  - Absorbed and Reradiated



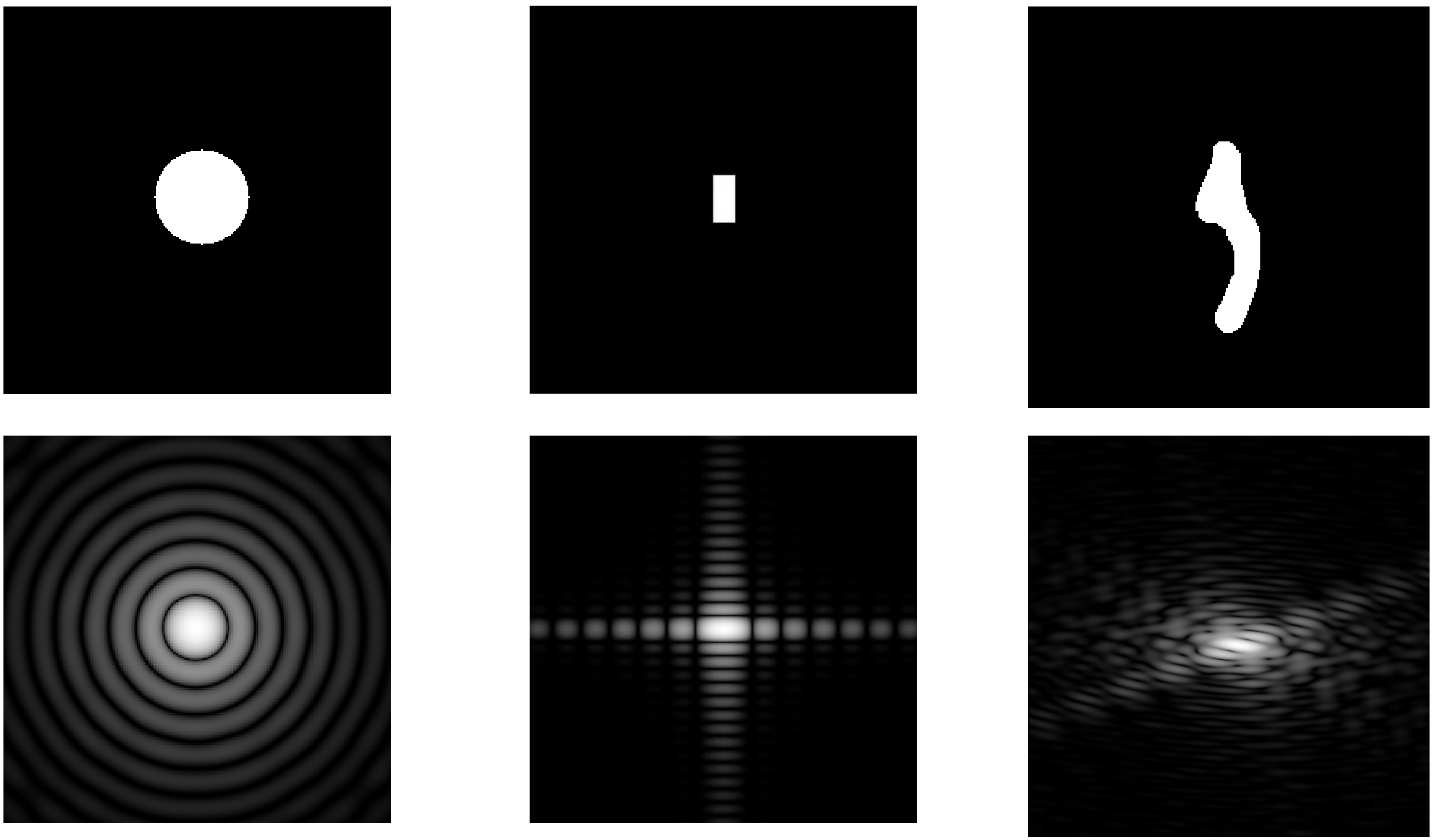
- Small particles require knowledge of optical properties:
  - Real Index (degree of refraction)
  - Imaginary Index (absorption of light within particle)
  - Light must be collected over large range of angles
  - Index values less significant for large particles

Diffraction Pattern

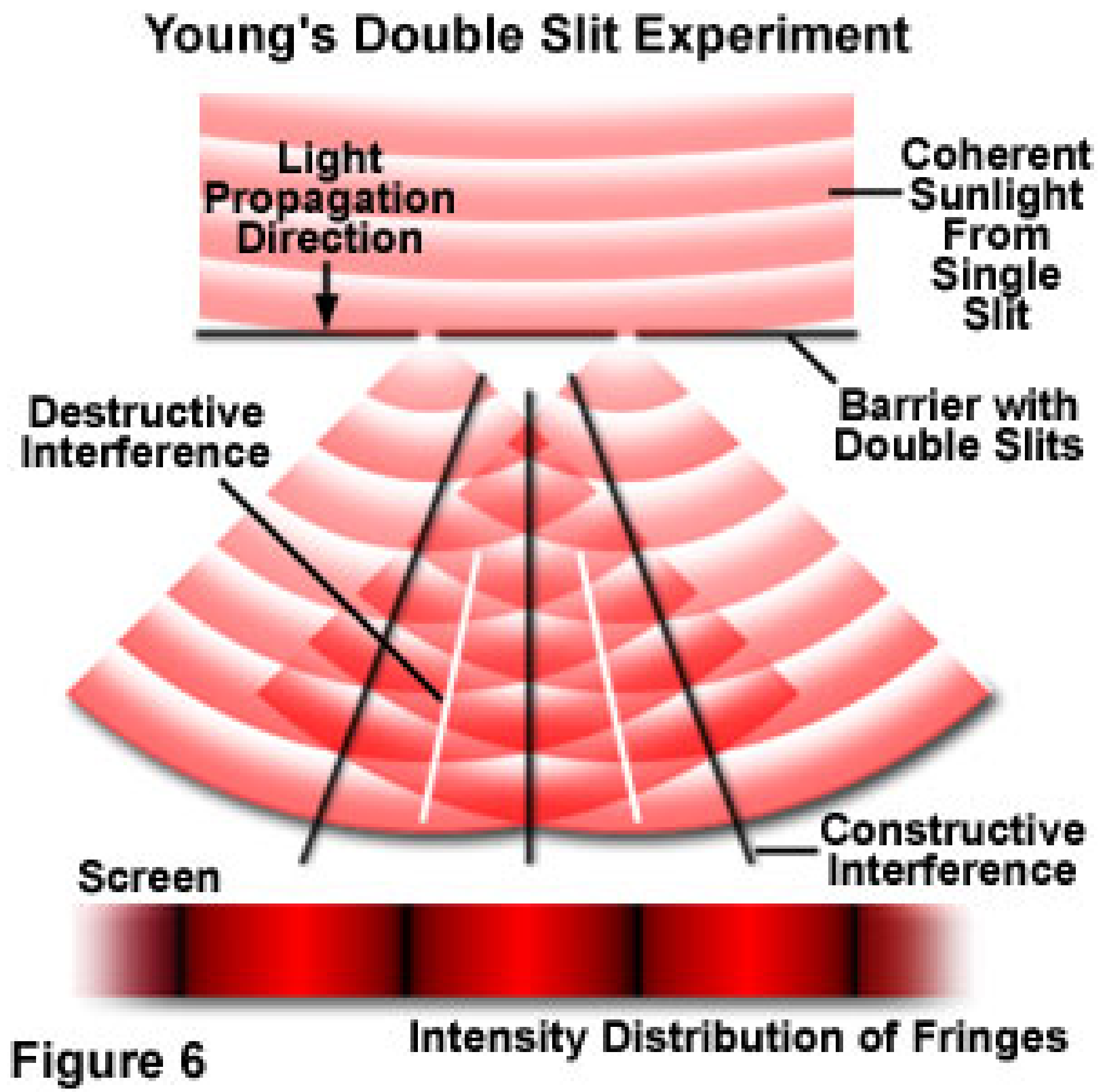


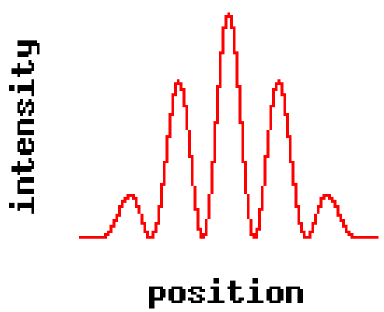


Diffraction Patterns

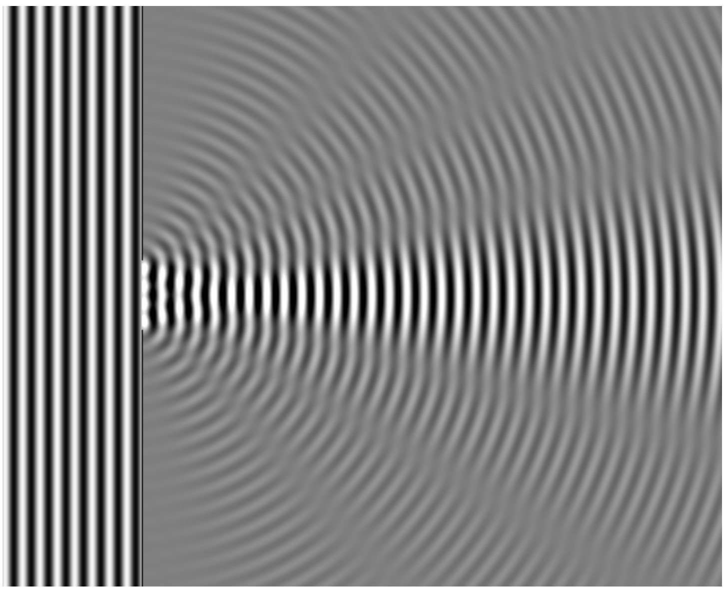


Young's Experiment

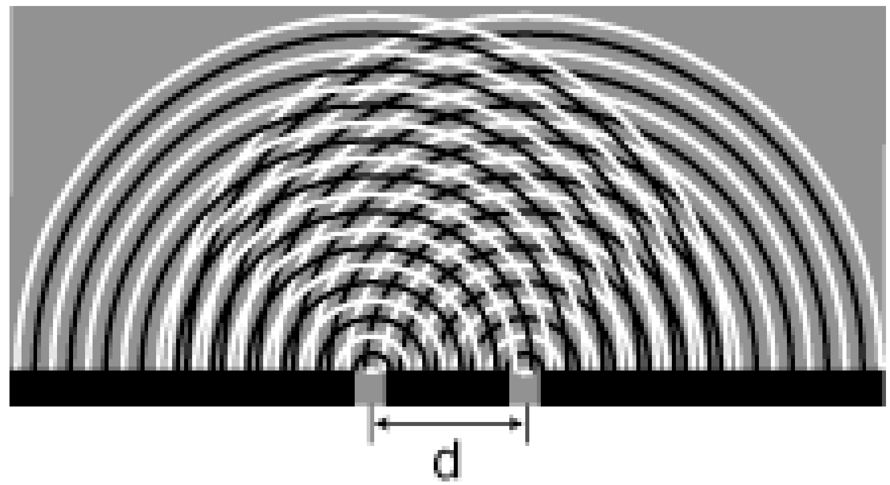




Single vs. Double Slit Patterns



Single slit diffraction pattern

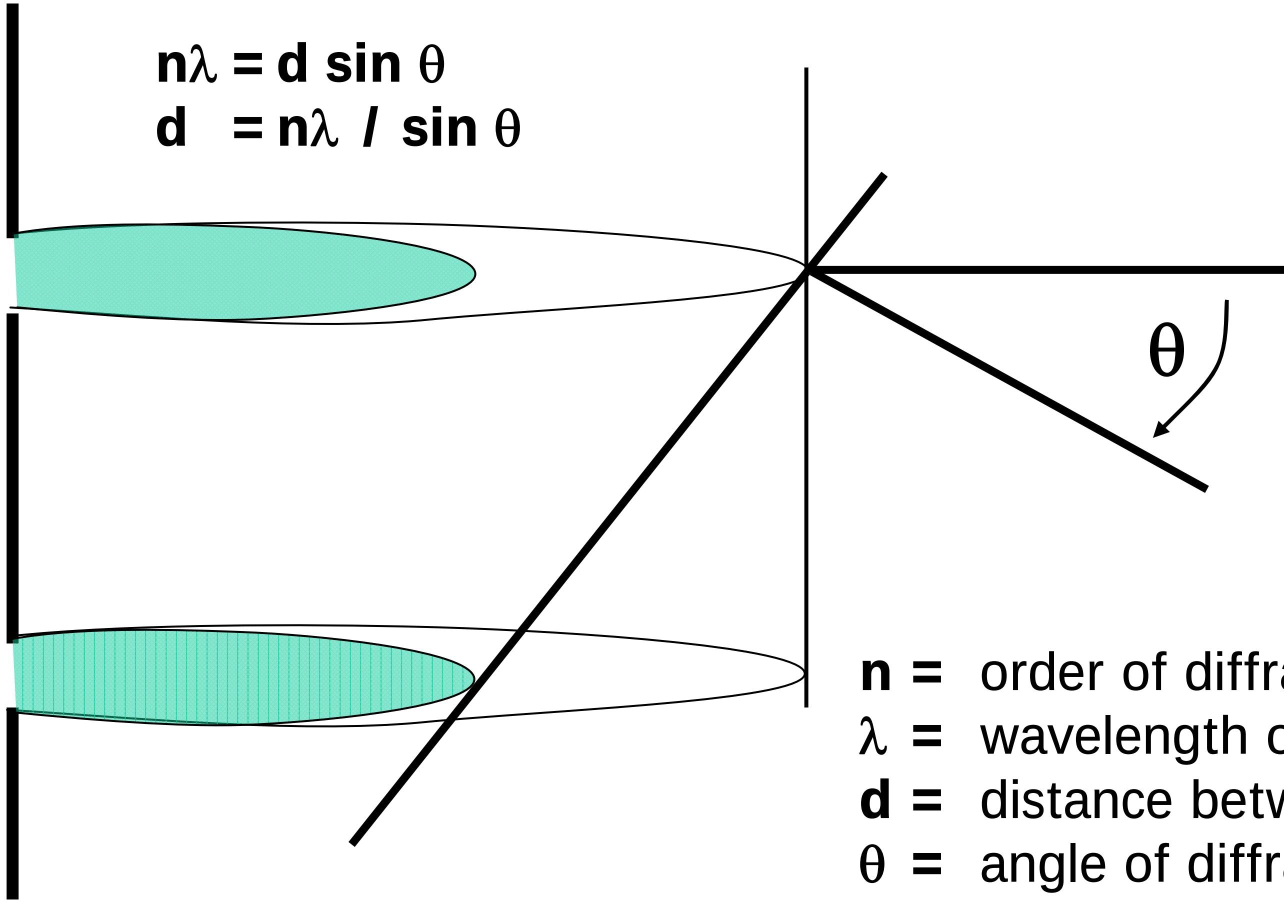


Double slit diffraction pattern

Fraunhofer Diffraction: Young's Double Slit

- **Distance between slits is INVERSELY proportional to angle (θ)**

$$n\lambda = d \sin\theta$$
$$d = n\lambda \,/\, \sin\theta$$



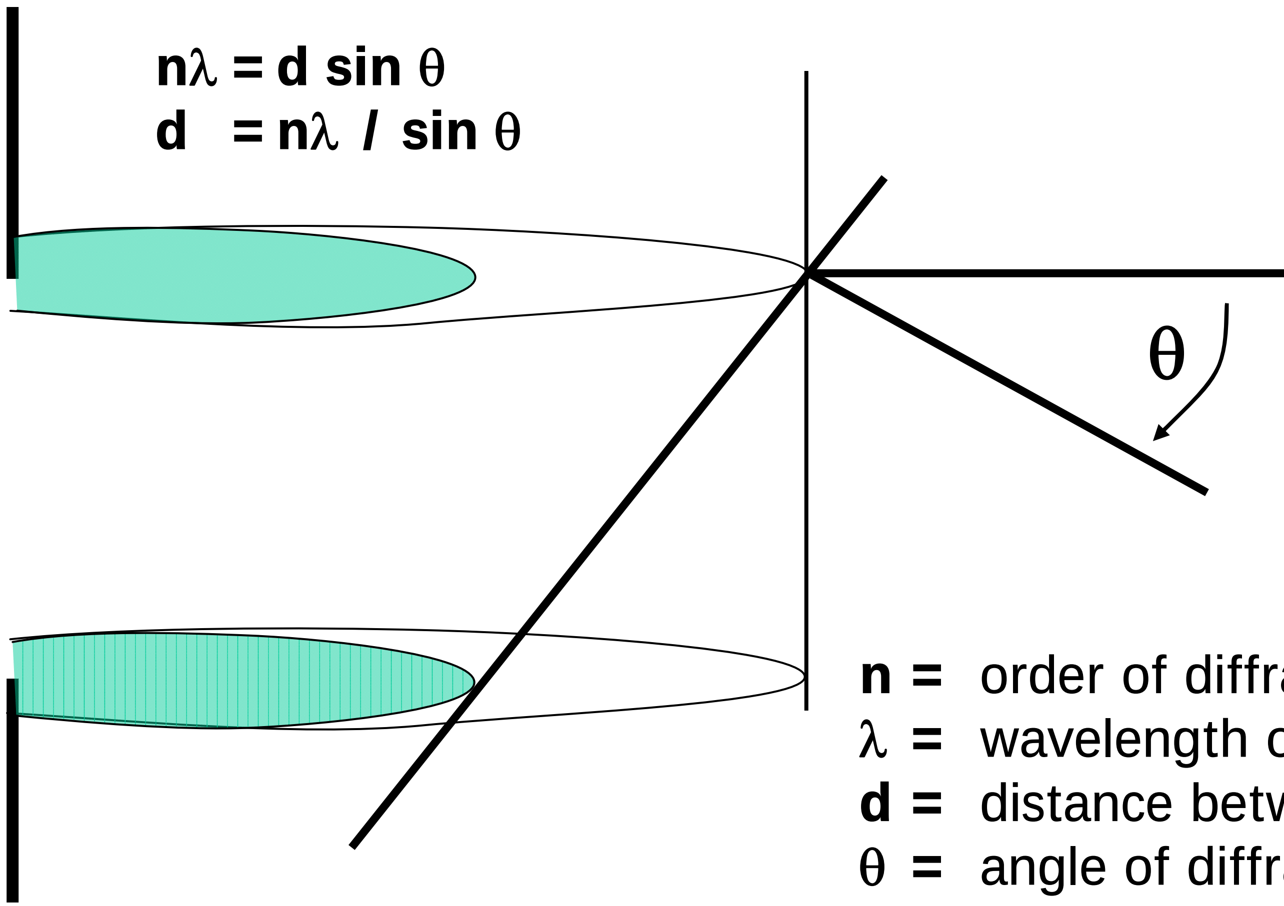
For a given measurement system with a fixed wavelength, the product $n\lambda$ is constant

n = order of diffraction
λ **=** wavelength of light
d = distance between slits
θ **=** angle of diffraction

Fraunhofer Diffraction: Pinhole

- **The diameter of the pinhole is INVERSELY proportional to angle (θ)**

$$n\lambda = d \sin\theta$$
$$d = n\lambda \;/\; \sin\theta$$



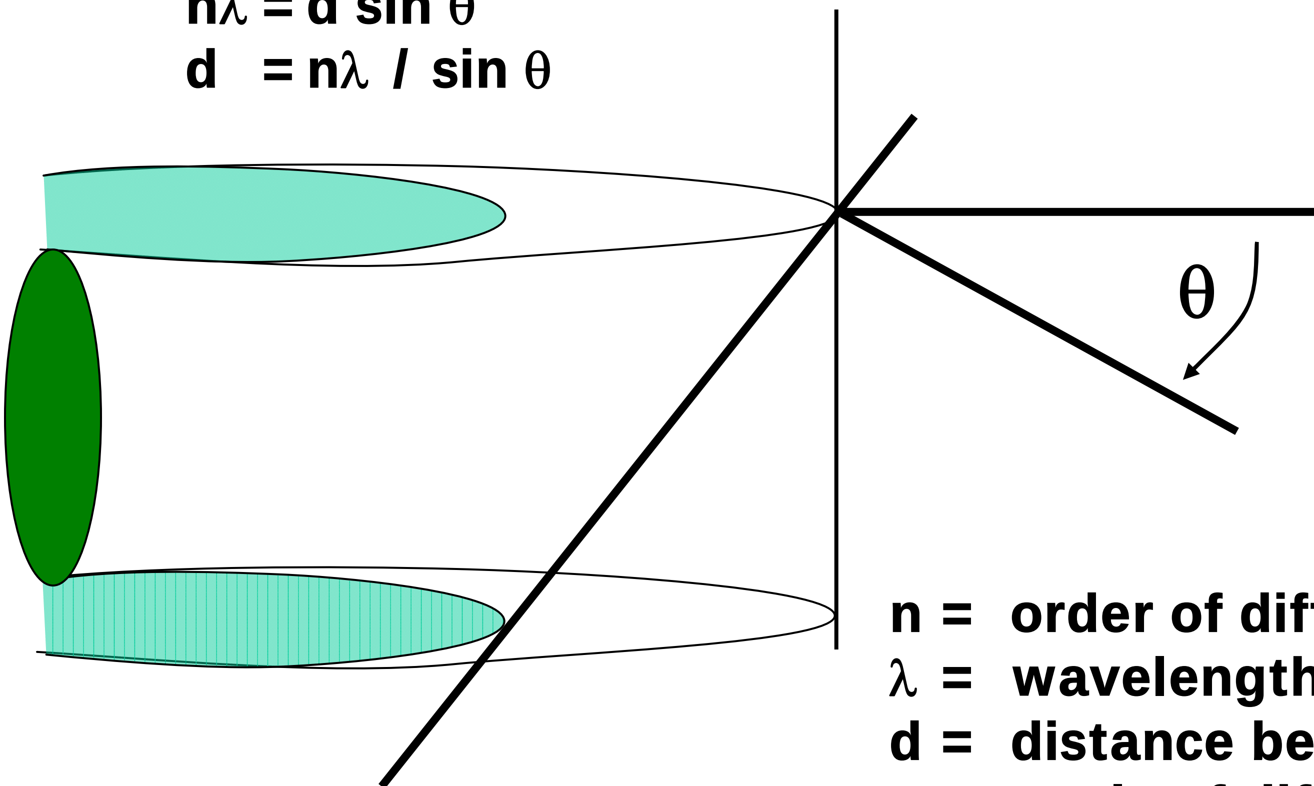
For a given measurement system with a fixed wavelength, the product nλ is constant

n = order of diffraction
λ = wavelength of light
d = distance between slits
θ = angle of diffraction

FRAUNHOFER DIFFRACTION - PARTICLE

- **Angle of scatter from a particle is INVERSELY proportional to angle (θ)**

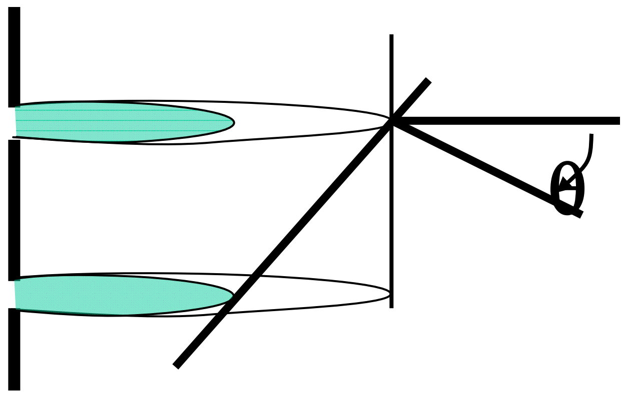
$n\lambda = d \sin\theta$
$d = n\lambda / \sin\theta$



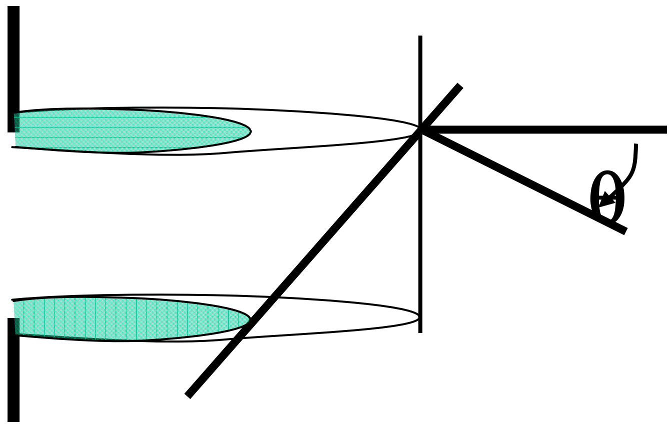
For a given measurement system with a fixed wavelength, the product $n\lambda$ is constant

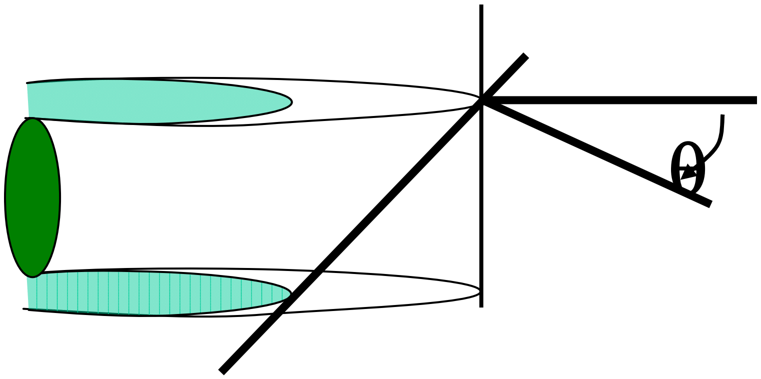
n = order of diffraction
λ = wavelength of light
d = distance between slits
θ = angle of diffraction

Edge Scattering Phenomenon



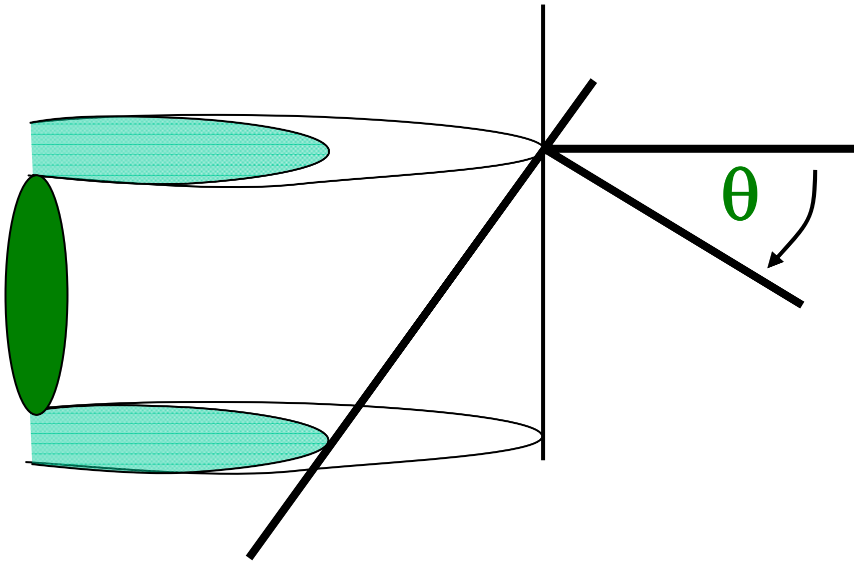
- Light Scatter occurs whether from a slit, a pinhole or a particle. It occurs at the edge of an object. A SLIT and PARTICLE of the same size produce the same diffraction pattern





Fraunhofer Diffraction: Particles

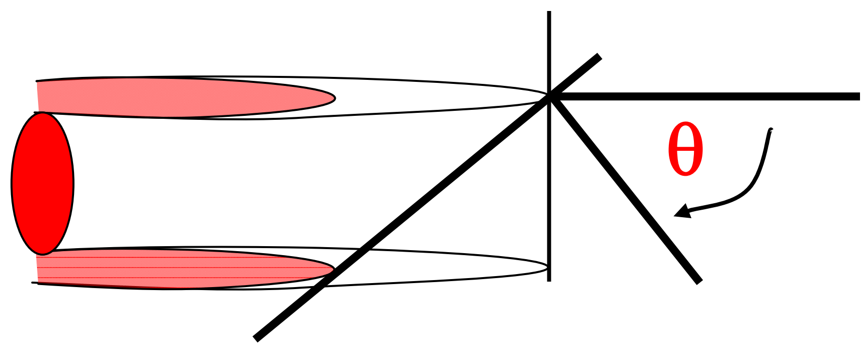
- Large particles scatter light through SMALLER angles



- Small particles scatter light through LARGER angles

Large Particle

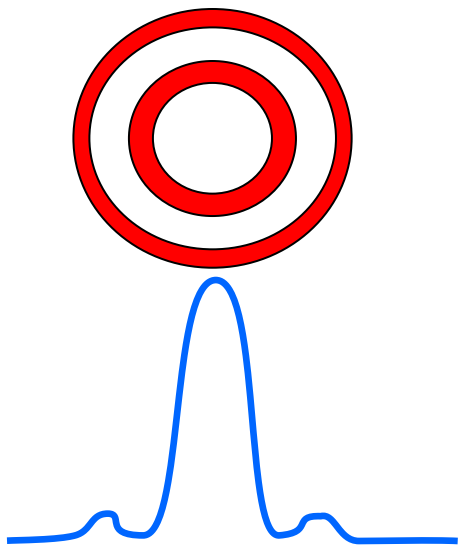
Small Particle



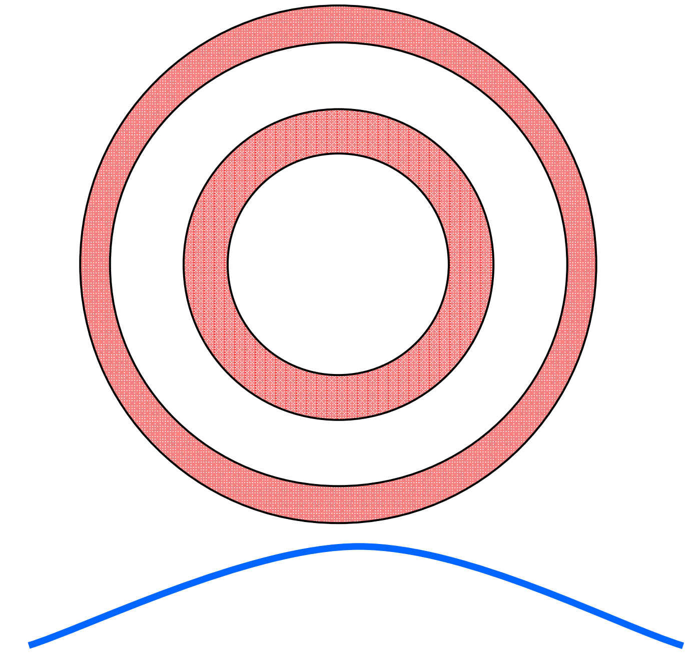
Diffraction Pattern: Large vs. Small Particles

LARGE PARTICLE:

- Low angle scatter
- Large signal



Narrow Pattern - High intensity



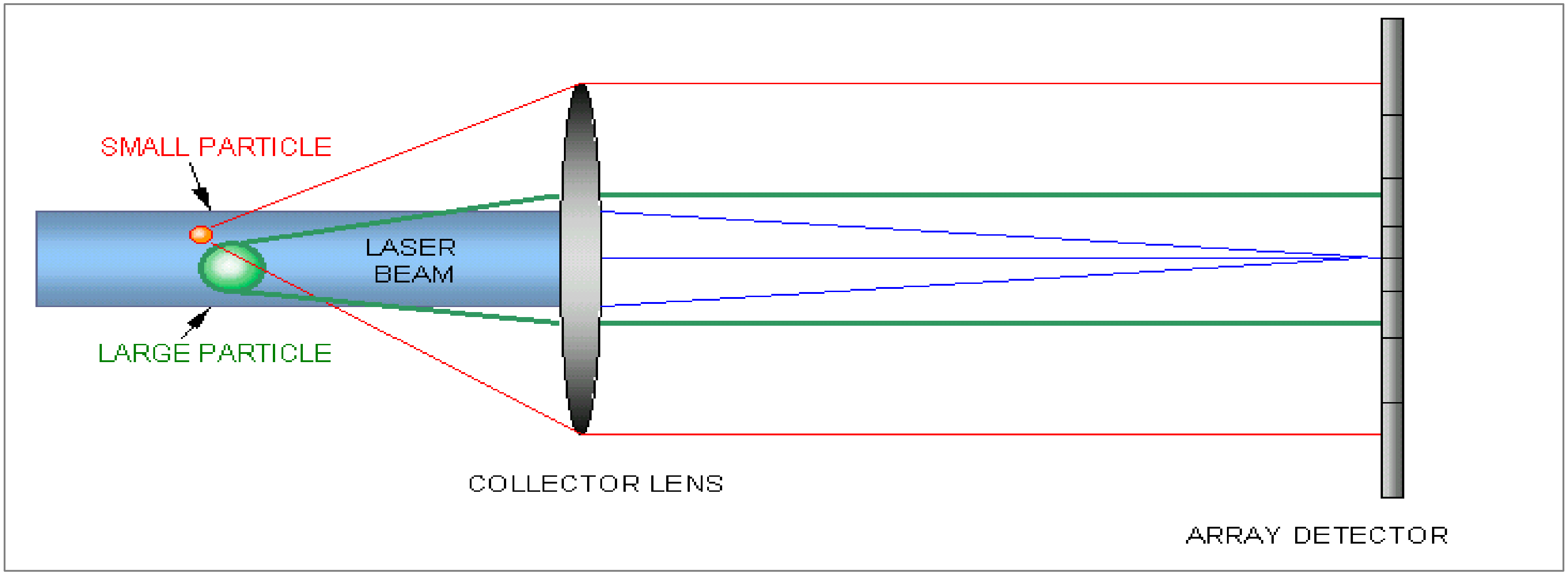
Wide Pattern - Low intensity

SMALL PARTICLE:

- High Angle Scatter
- Small Signal

Angle of Scatter vs. Particle Size

- Fraunhofer Diffraction describes forward scatter technology. Scatter angles are relatively small, less than 30°



- **<u>ANGLE OF SCATTER</u> is INVERSELY proportional to particle size. SMALL particles scatter at larger angles than large particles.**

- **The <u>AMOUNT OF LIGHT</u> scattered is DIRECTLY proportional to particle size. LARGE particles scatter MORE light than small particles.**

Light Scattering

$$I(\Theta) = \frac{I_0}{2k^2 a^2} \left\{ \left[S_1(\Theta) \right]^2 + \left[S_2(\Theta) \right]^2 \right\}$$

$I(\Theta)$ is the total scattered intensity as a function of angle Θ;

I_0 is the intensity of the incident light;

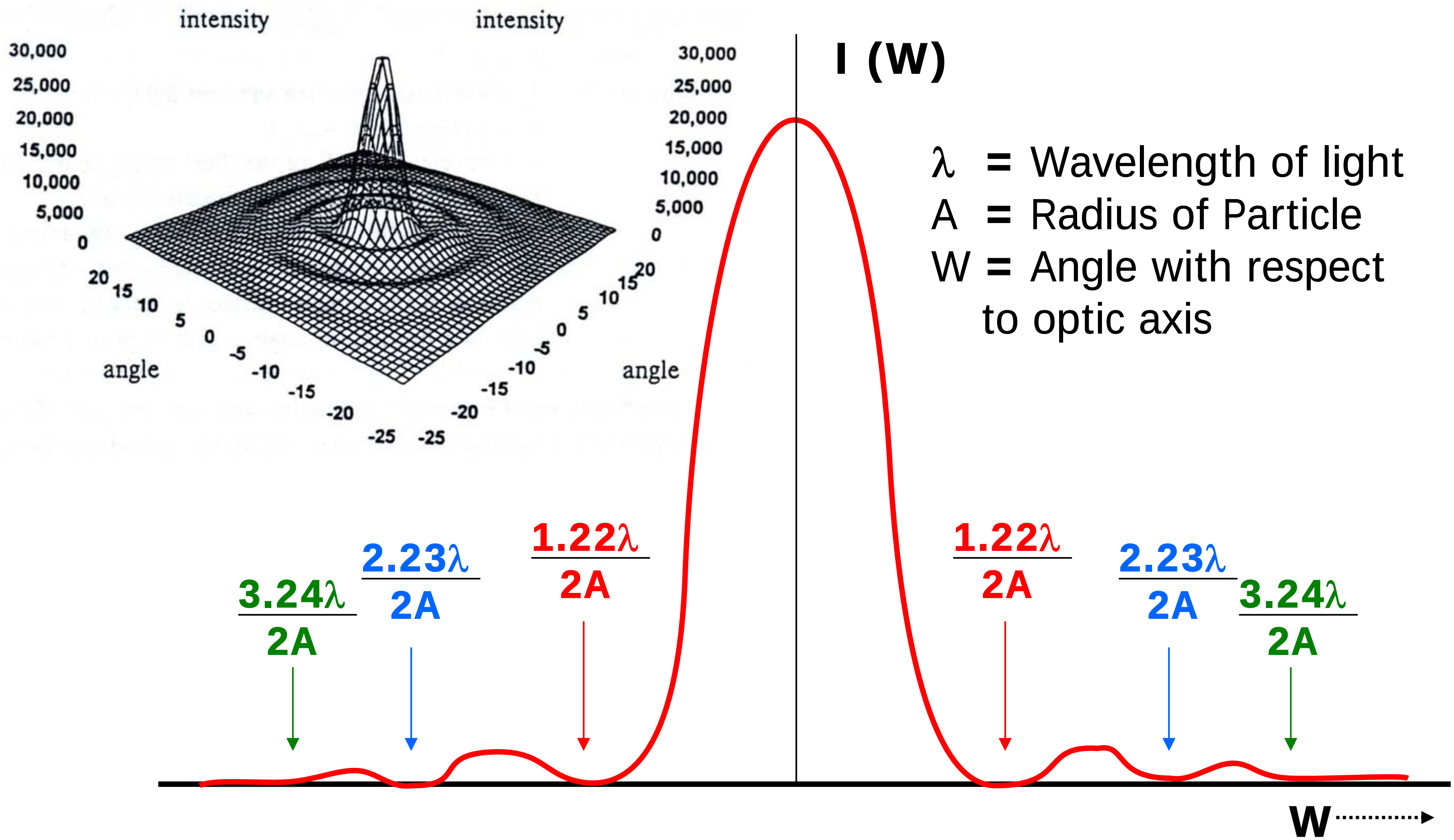
k is the wavenumber = $2\pi/\lambda$;

λ is the wavelength of I_0 of the illuminating source in air;

a is the distance from scatterer to detector;

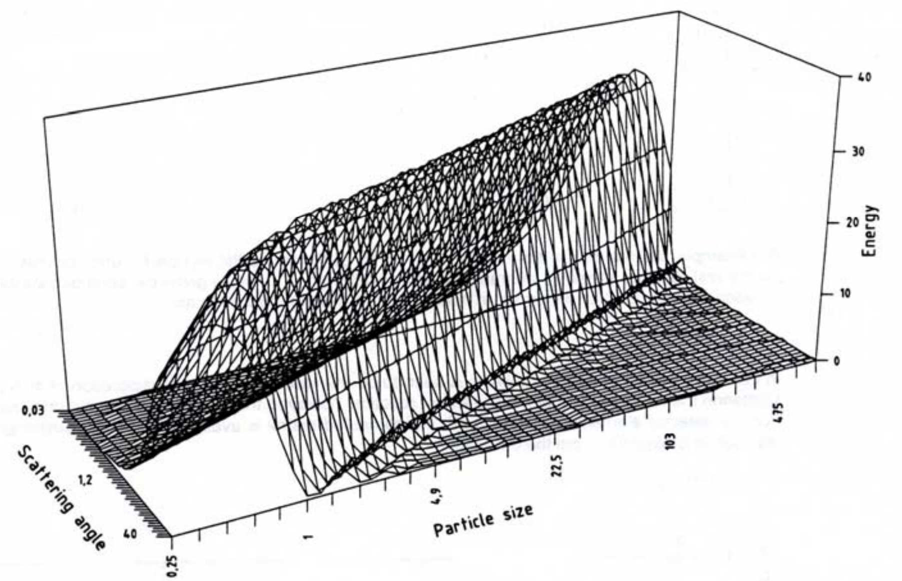
$S1(\Theta)$ and $S2(\Theta)$ are dimensionless, complex functions defined in general scattering theory, describing the change of amplitude in respectively the perpendicular and the parallel polarized light as a function of angle Θ with respect to the forward direction. Computer algorithms have been developed in order to allow computation of these functions and, thus, of $I(\Theta)$.

Plot of Airy Function

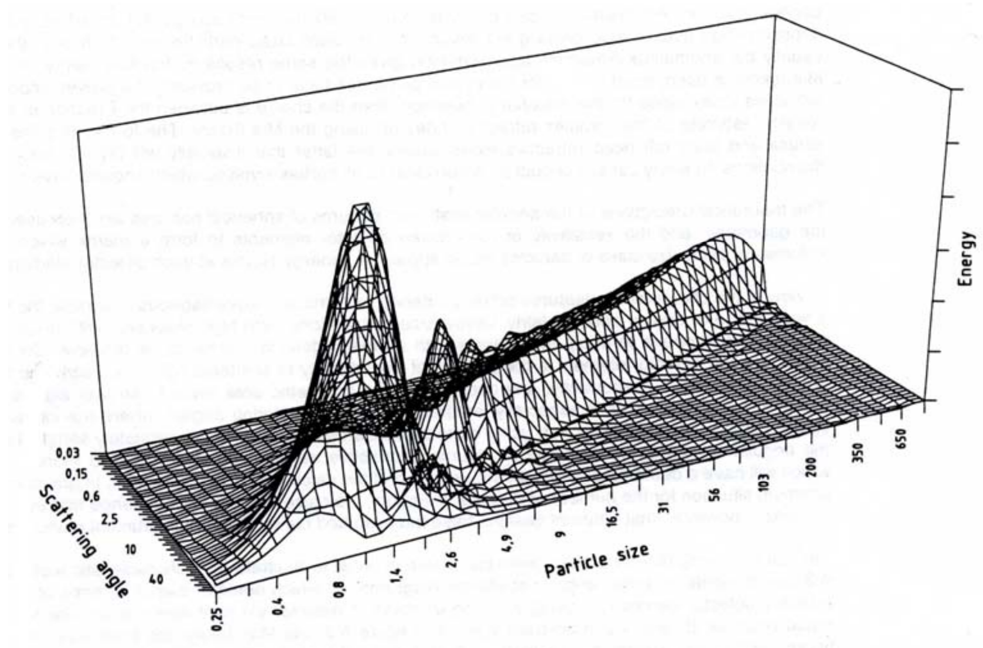


λ = Wavelength of light
A = Radius of Particle
W = Angle with respect to optic axis

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)

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 $\alpha = \pi x / \lambda$;

$J1$ 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)

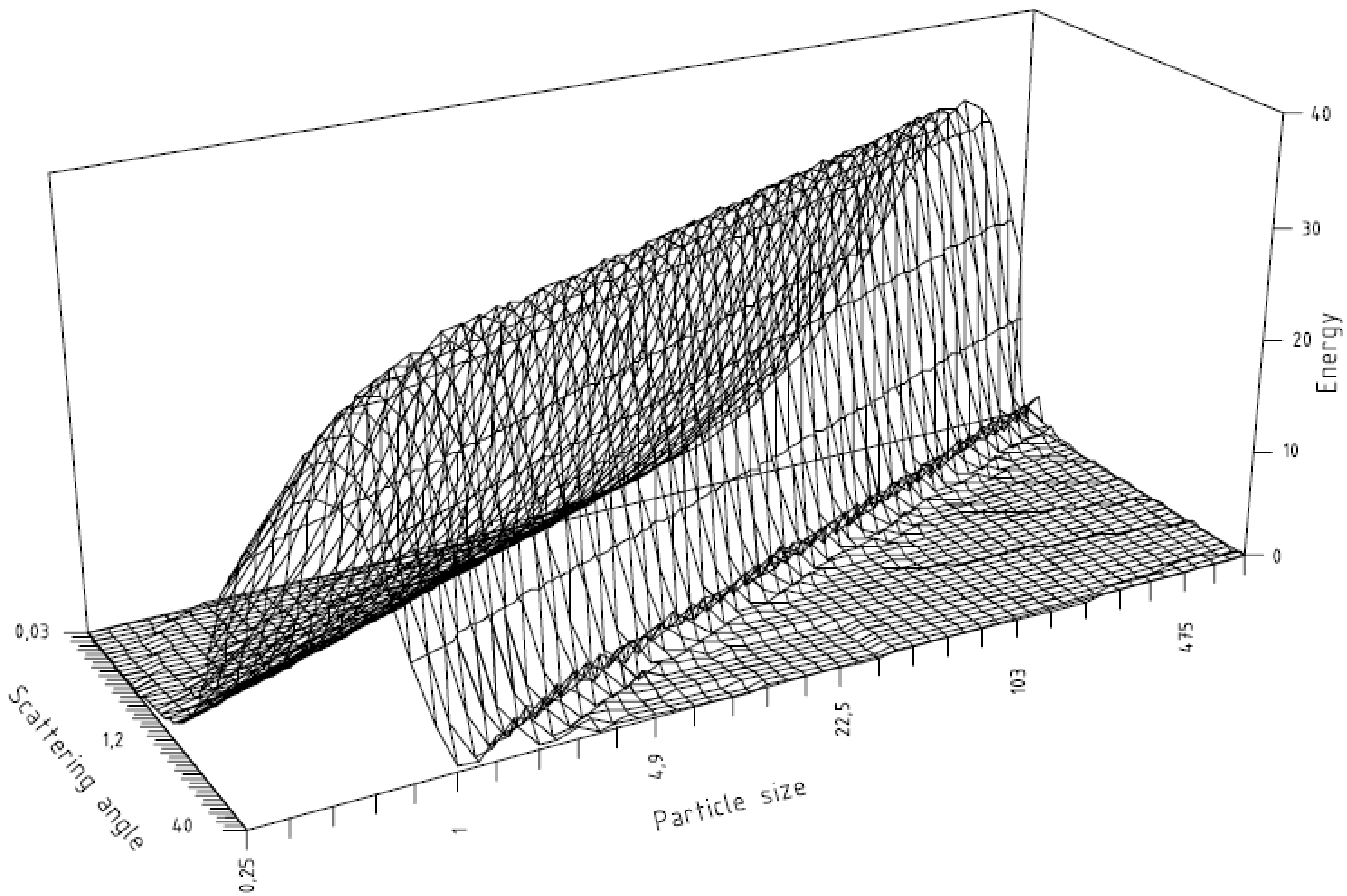
b) only scattering in the near-forward direction is considered (Q is small).

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

If λ=680nm (.68 μm), then 40 x .68 = 27 μm

If the particle size is larger than about 50 μm, then the Fraunhofer approximation gives good results.

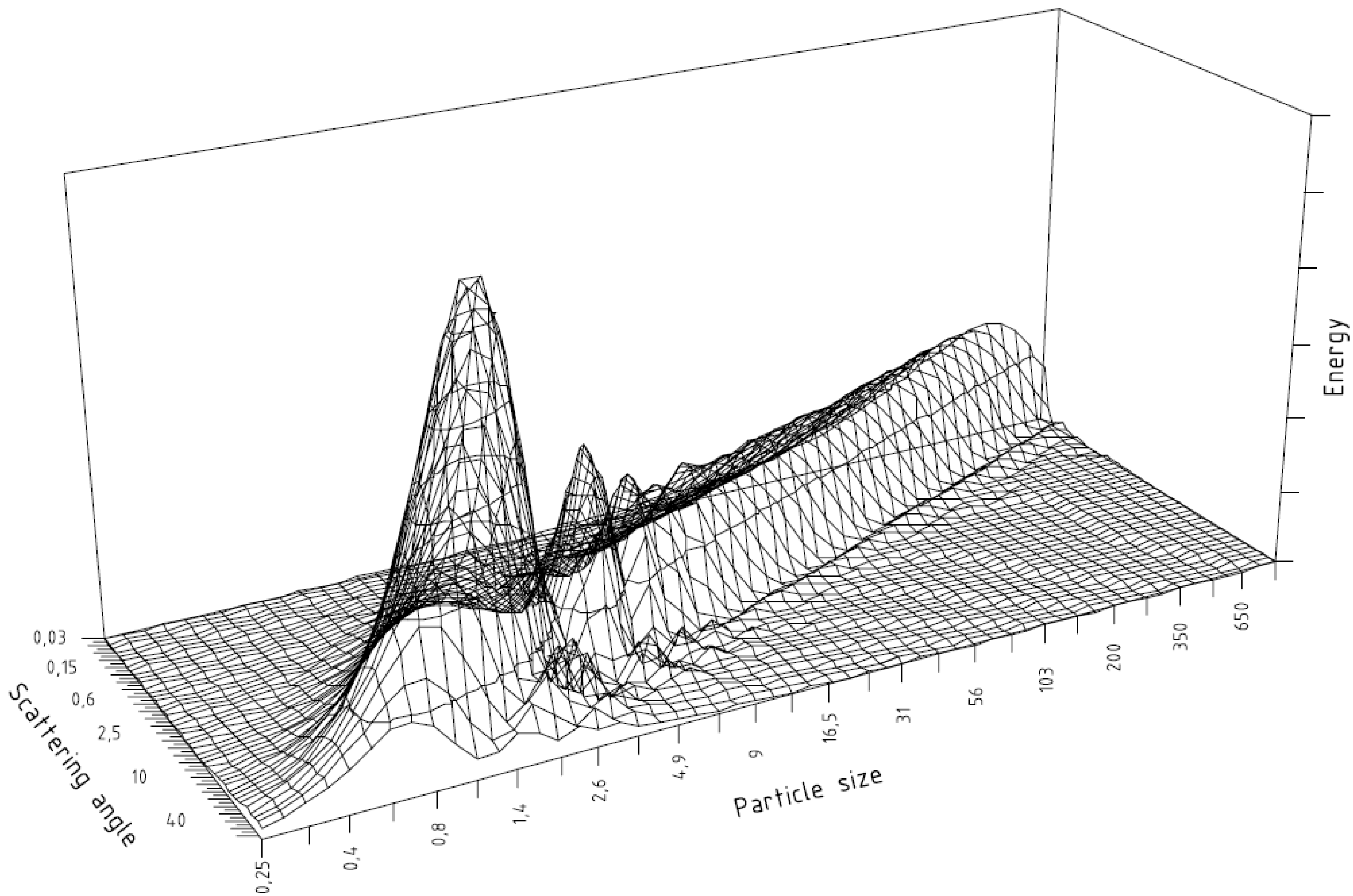
Fraunhofer Approximation



Explore the future

HORIBA

Mie Theory



Energy
0,03
0,15
0,6
2,5
10
40
Scattering angle
0,25
0,4
0,8
1,4
2,6
4,9
9
16,5
31
56
103
200
350
650
Particle size

Mie vs. Fraunhofer

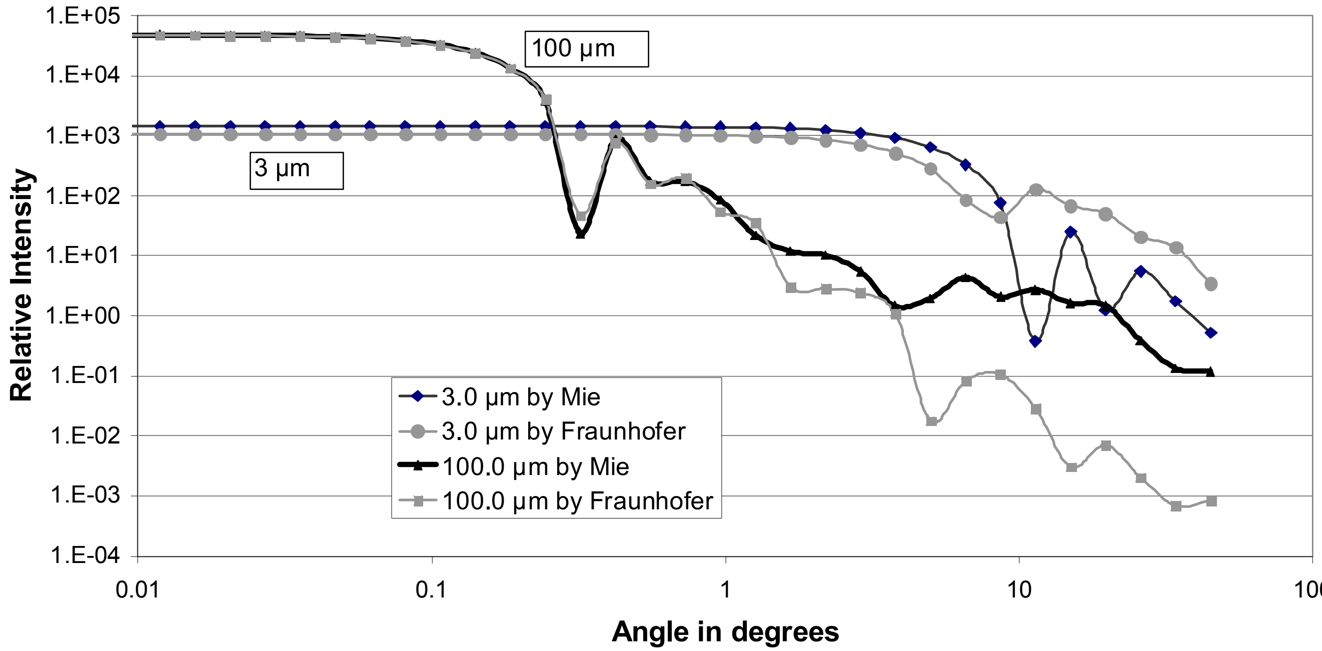
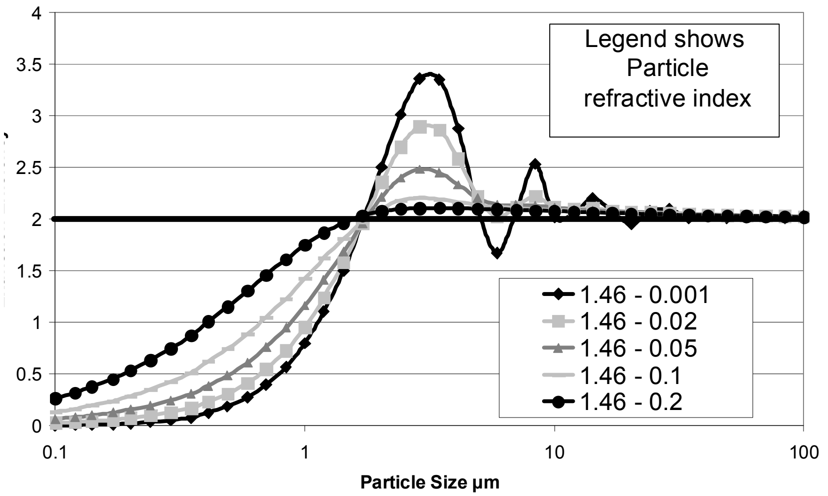


Figure A.3 -- Comparison of scattering patterns of non-absorbing particles according to Fraunhofer and Mie calculations (N_p = 1,59 – 0,0; n_{water} = 1,33; wavelength = 633 nm)

Extinction Efficiencies



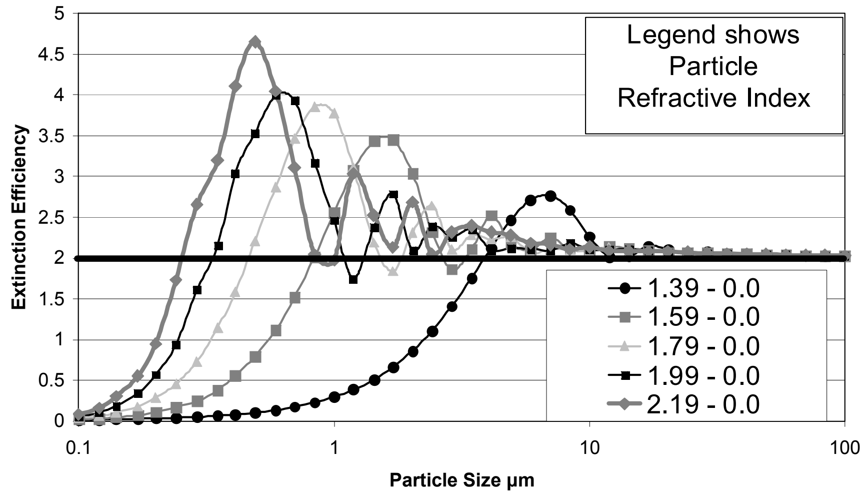


Figure A.2 -- Extinction efficiencies in relation to particle size and refractive index (Mie prediction). (n_p and k_p as indicated; n_{water} = 1,33; wavelength = 633 nm) (Fraunhofer assumes an extinction efficiency of 2 for all particle sizes)

Good agreement for transparent particles >50 μm
" " " opaque particles > 2 μm

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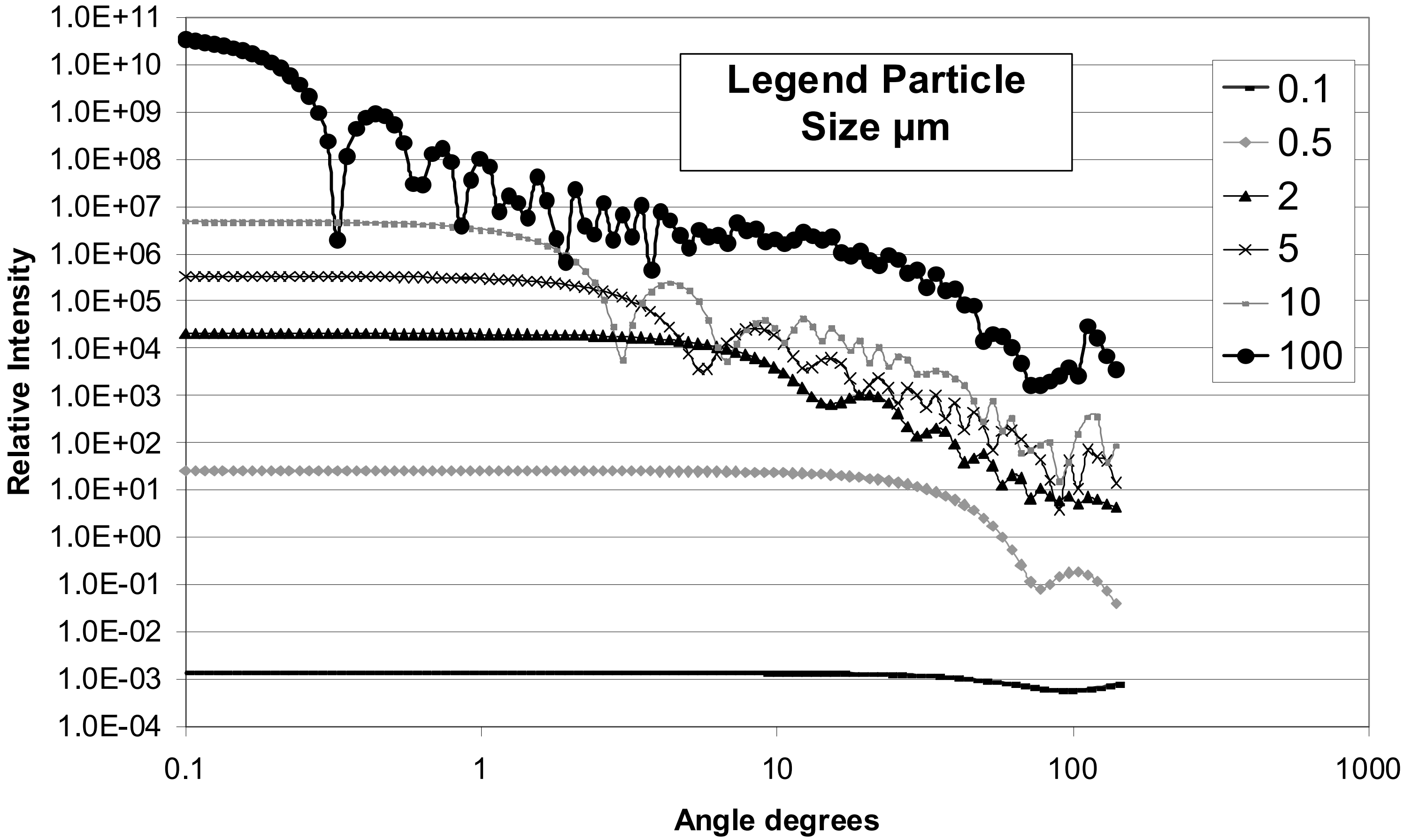
Scattering intensity pattern for single particles in relation to size



For single particles range from 0.1 to 100 µm is 10^{13}

Reduce by weighting to volume

Mie calculation; wavelength 633 nm; *N*p = 1,59 – 0,0 i; *n*m = 1,33

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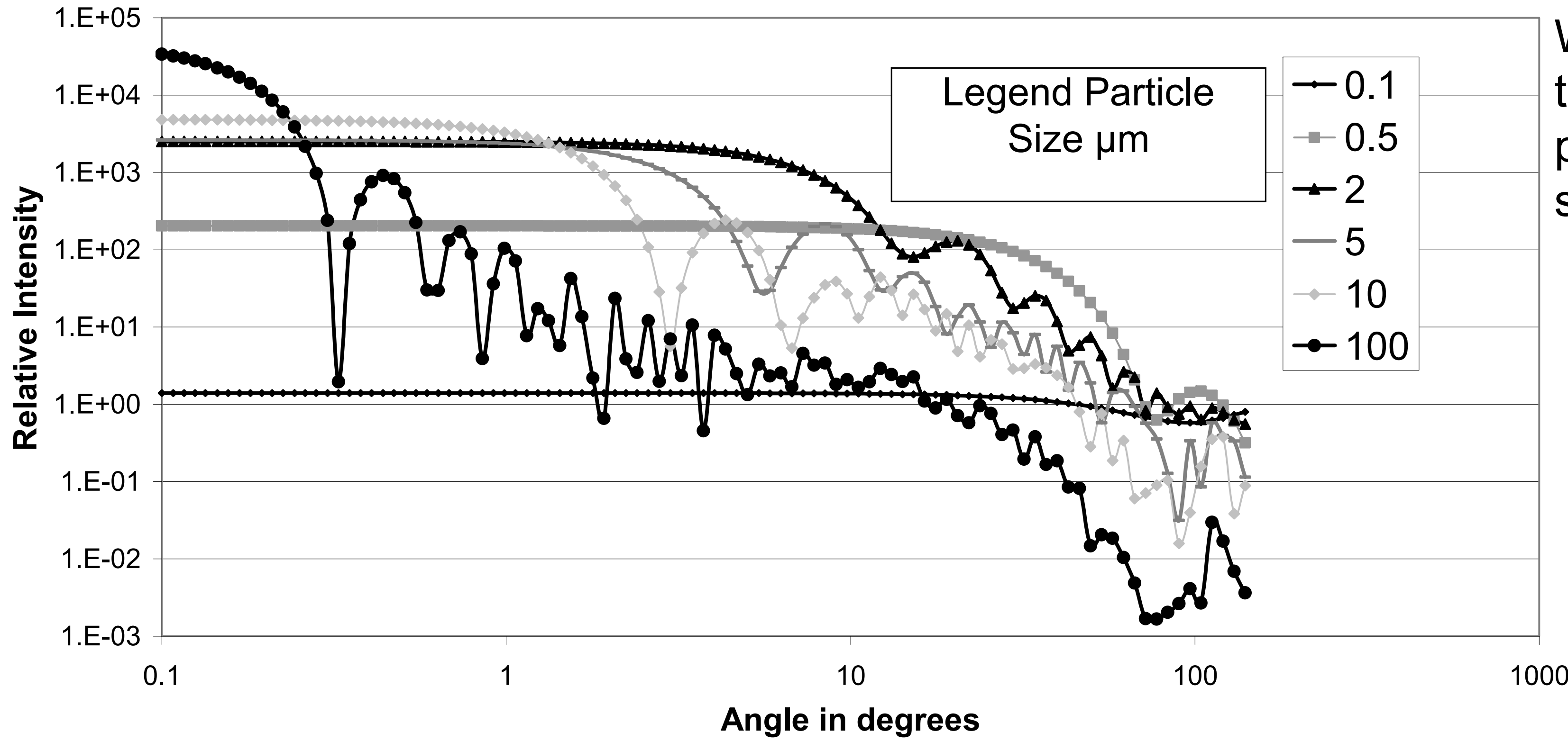
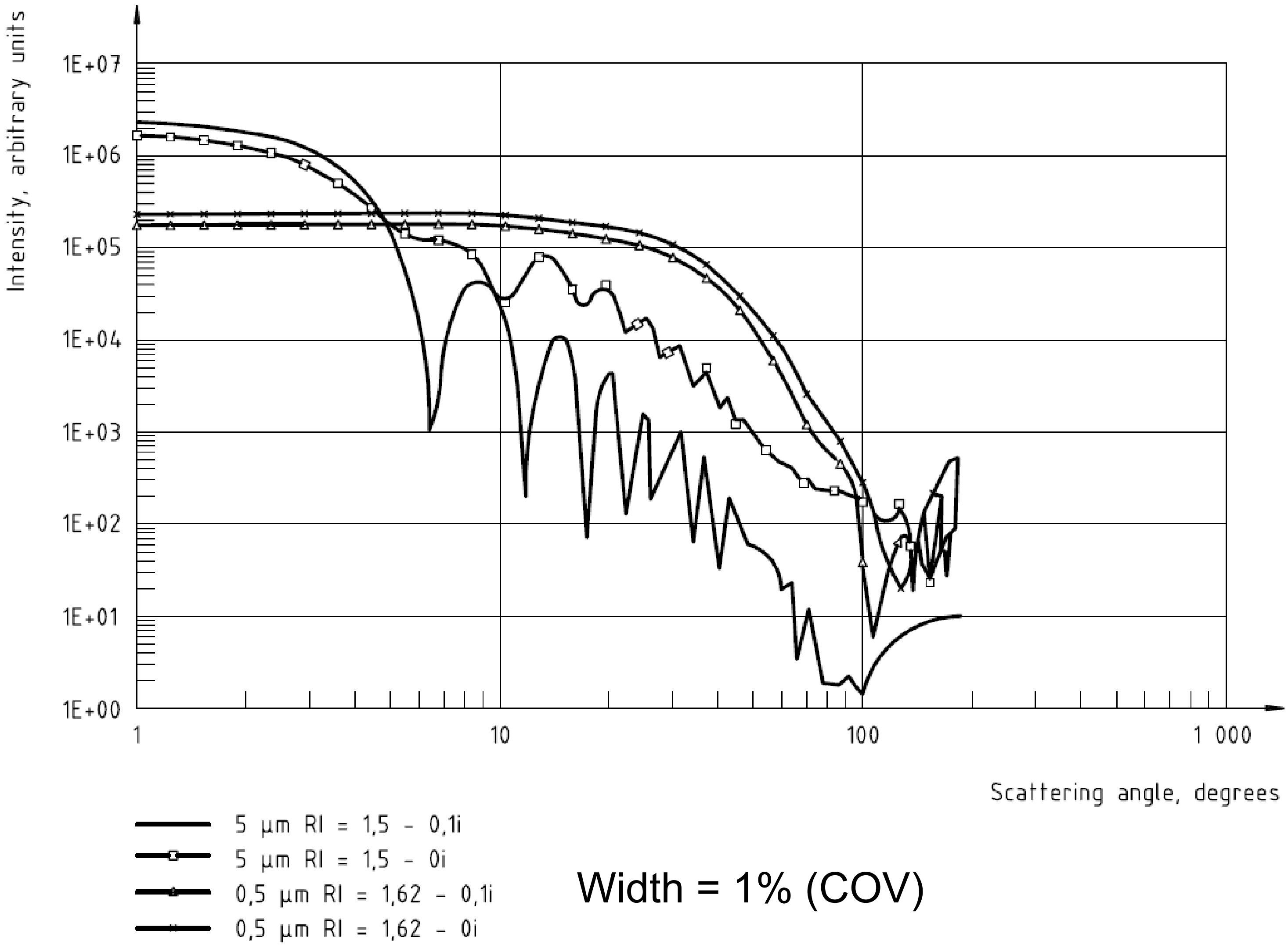
Light intensity scattering patterns for equal particle volumes in relation to size



Weighting to third power of size

Mie calculation; wavelength 633 nm; *N*p = 1,59 – 0,0 ; *n*m = 1,33

Influence of particle size on angular light intensity scattering patterns



Width = 1% (COV)

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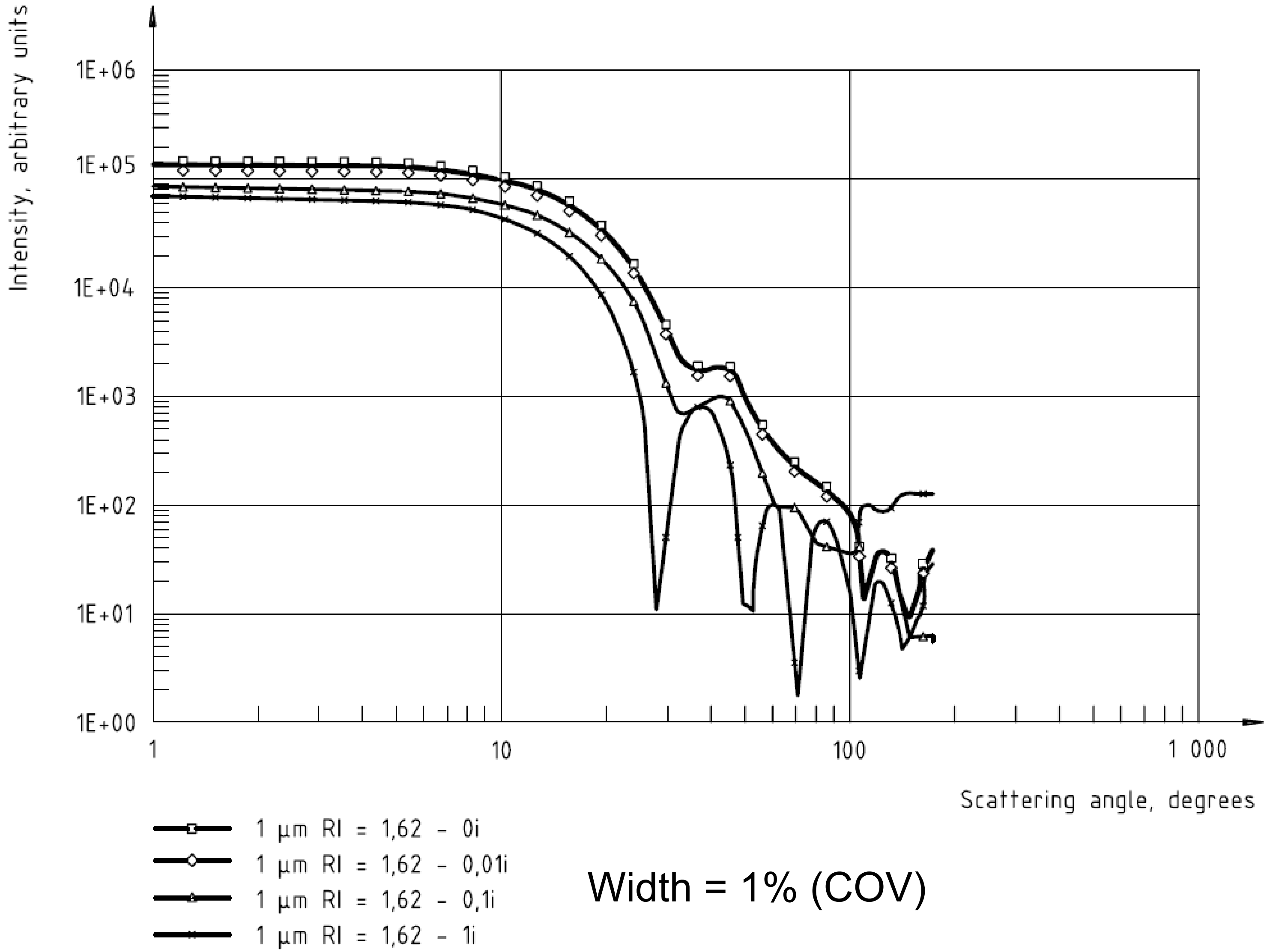
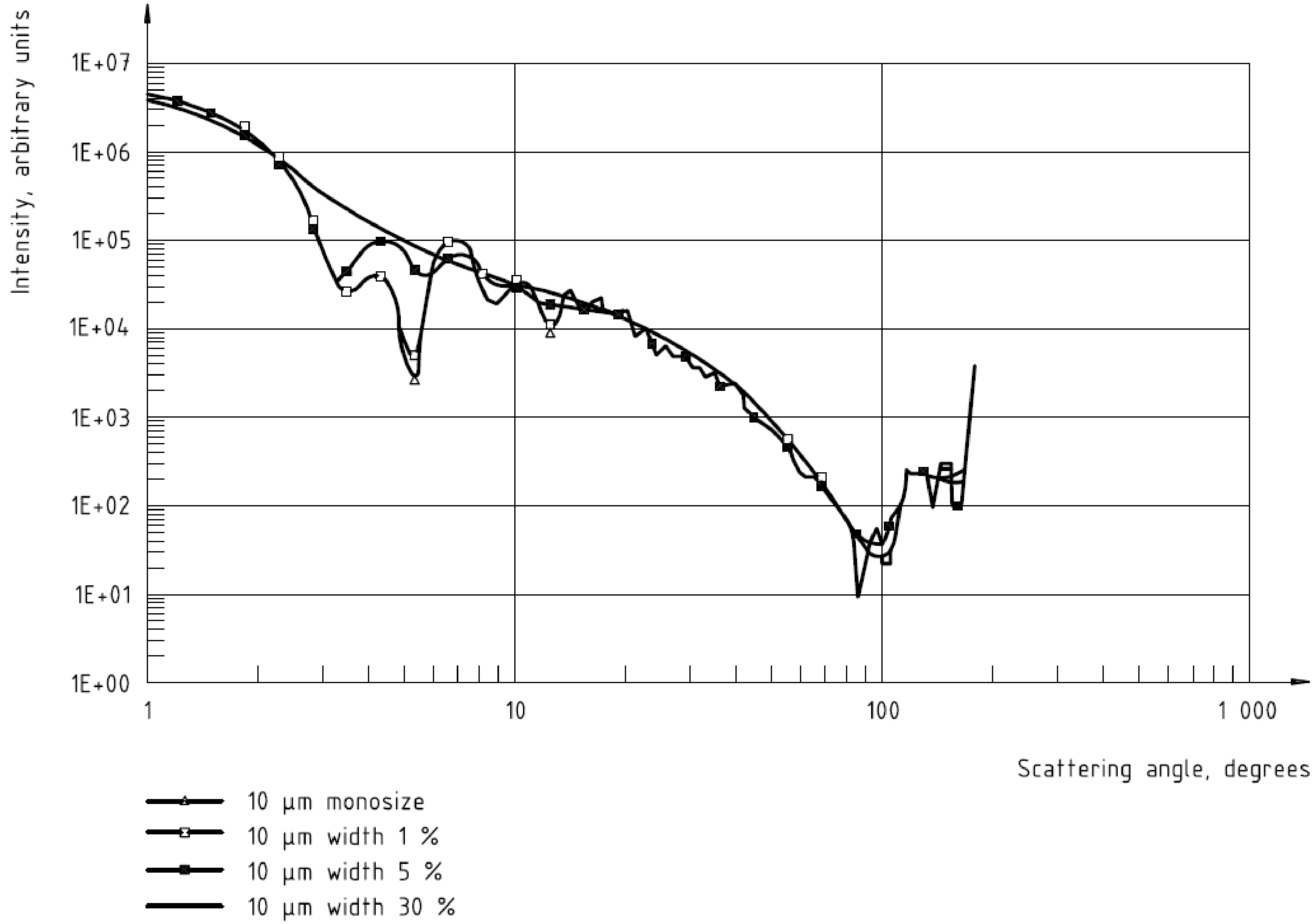
Influence of imaginary parts of RI (absorbancies)

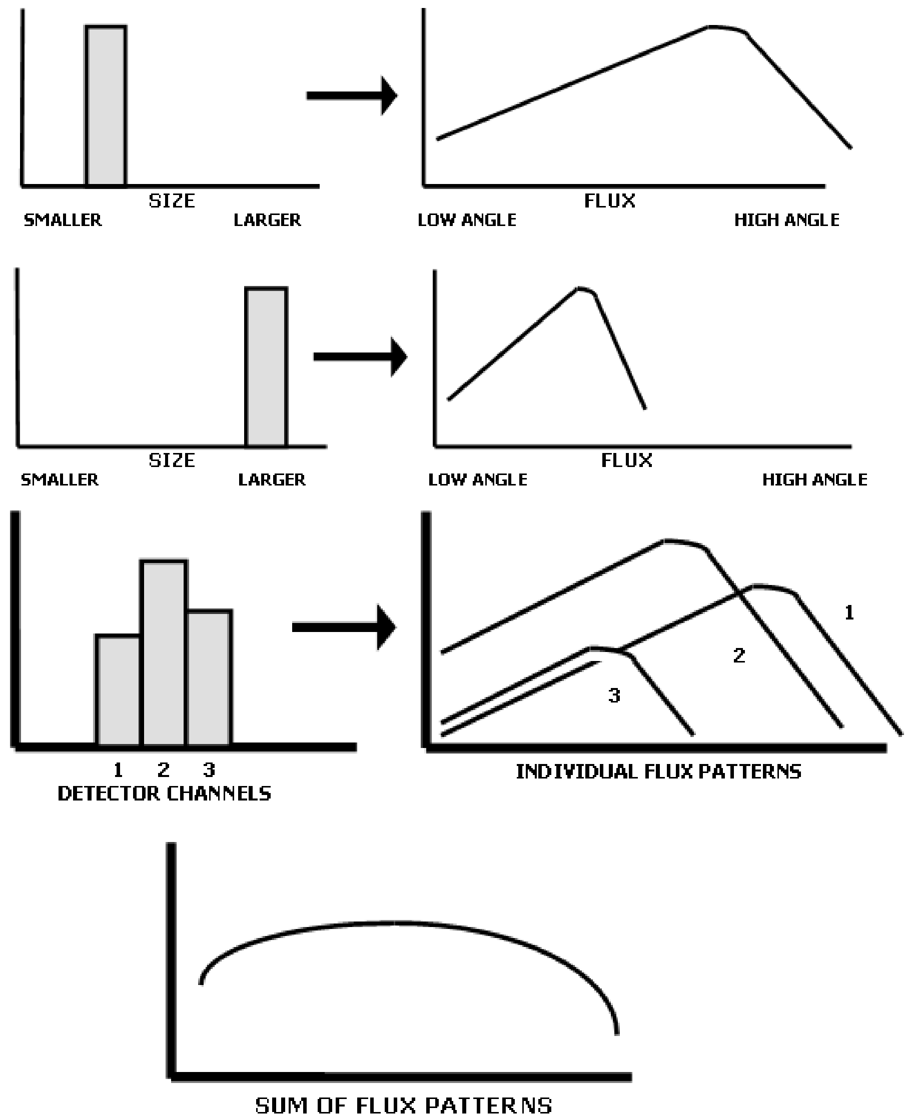


Width = 1% (COV)

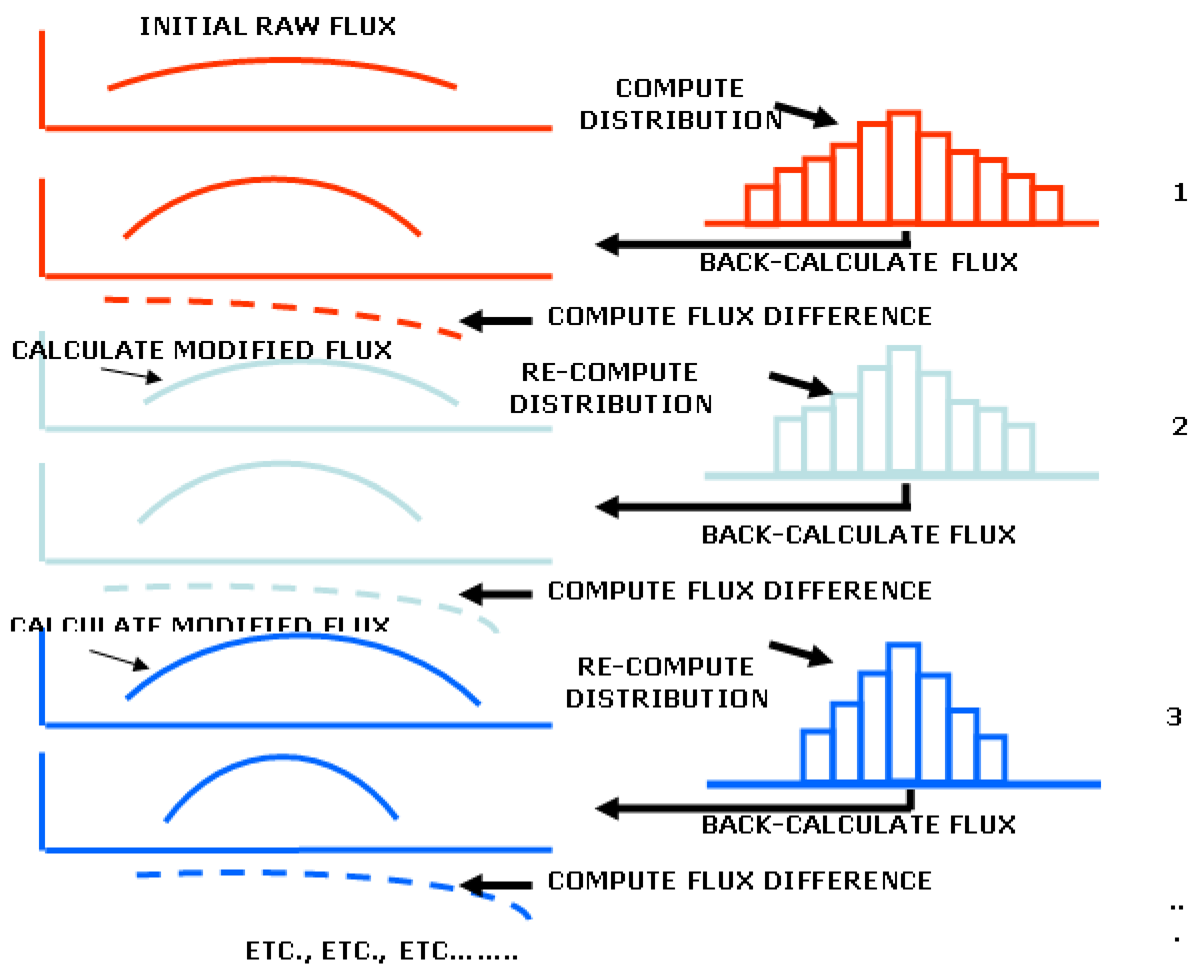
Influence of distribution width on angular light intensity scattering patterns



Result Calculation

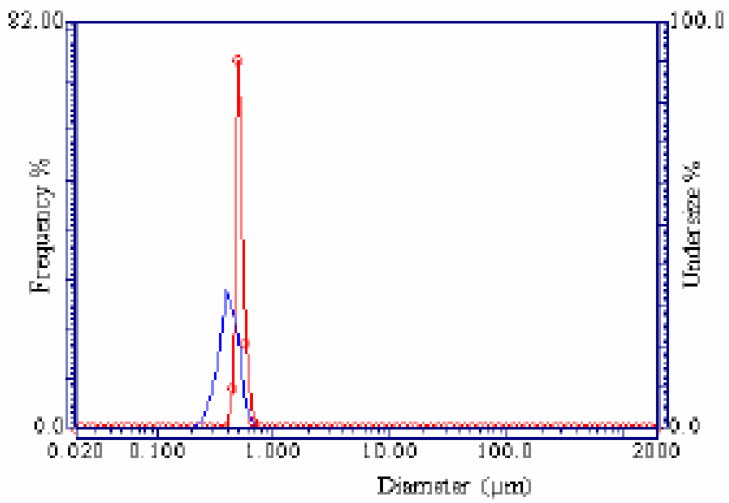


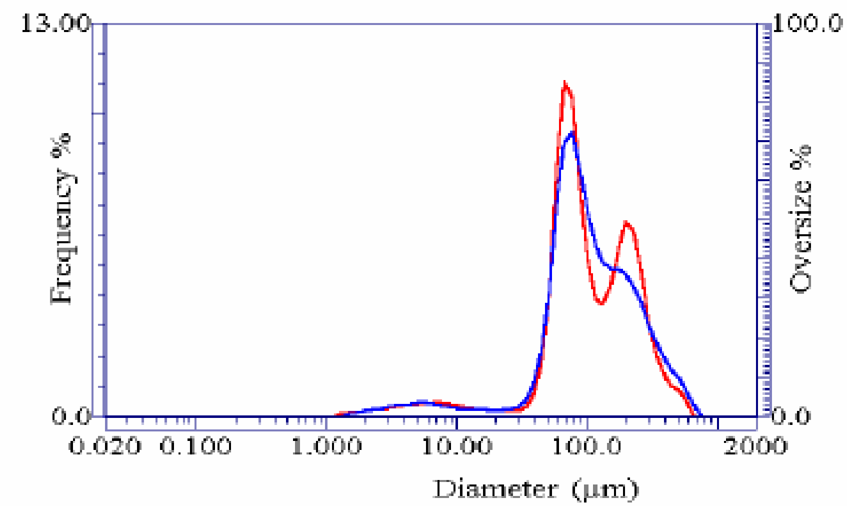
Iterations


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.……

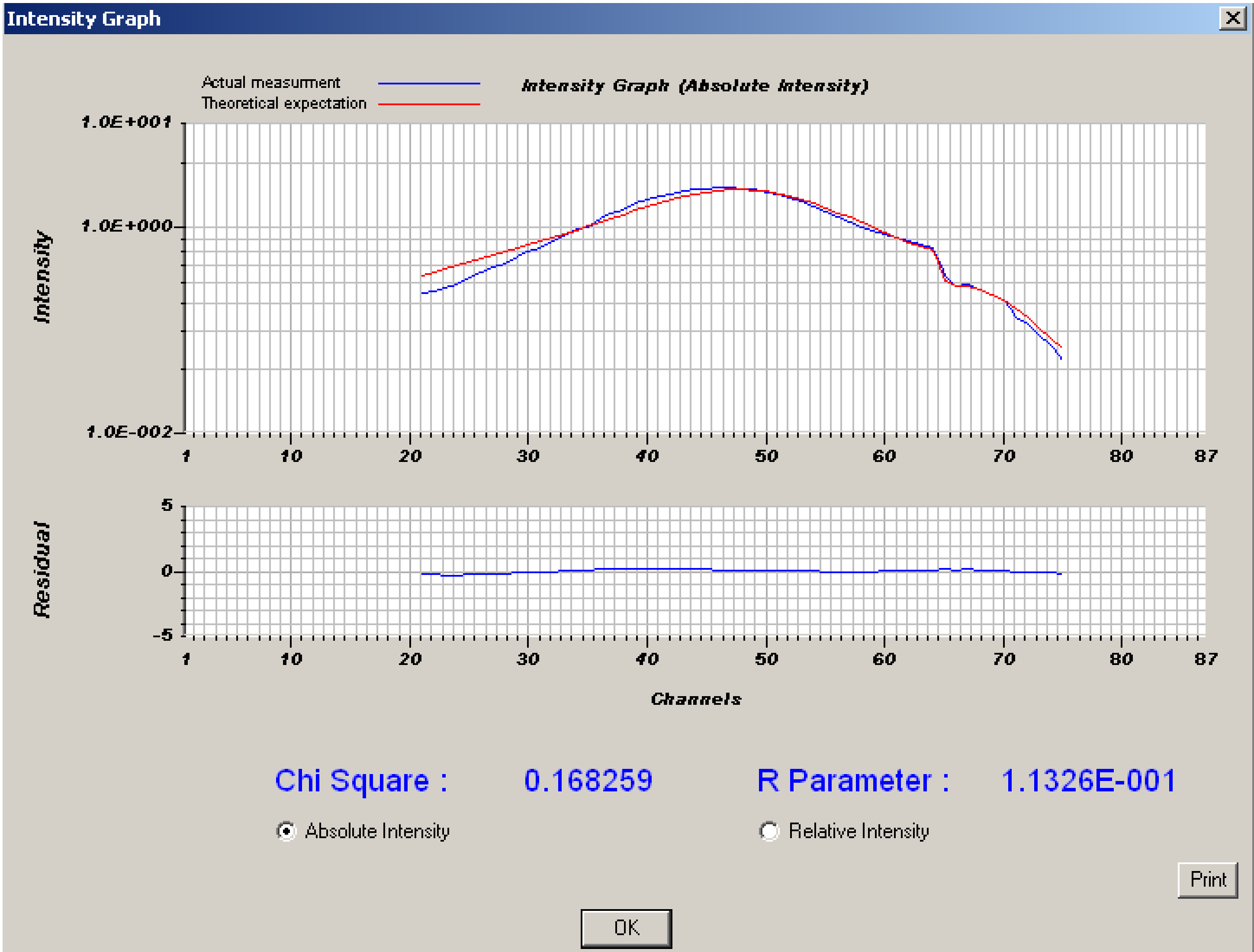
Iterations

- How many times to calculate new (better) results before reporting final result?
- For LA-930 standard = 30, sharp = 150
- For LA-950 standard = 15, sharp = 1000
- Fewer iterations = broader peak
- More iterations = narrow peak
- Too many iterations = fit to noise, over-resolved

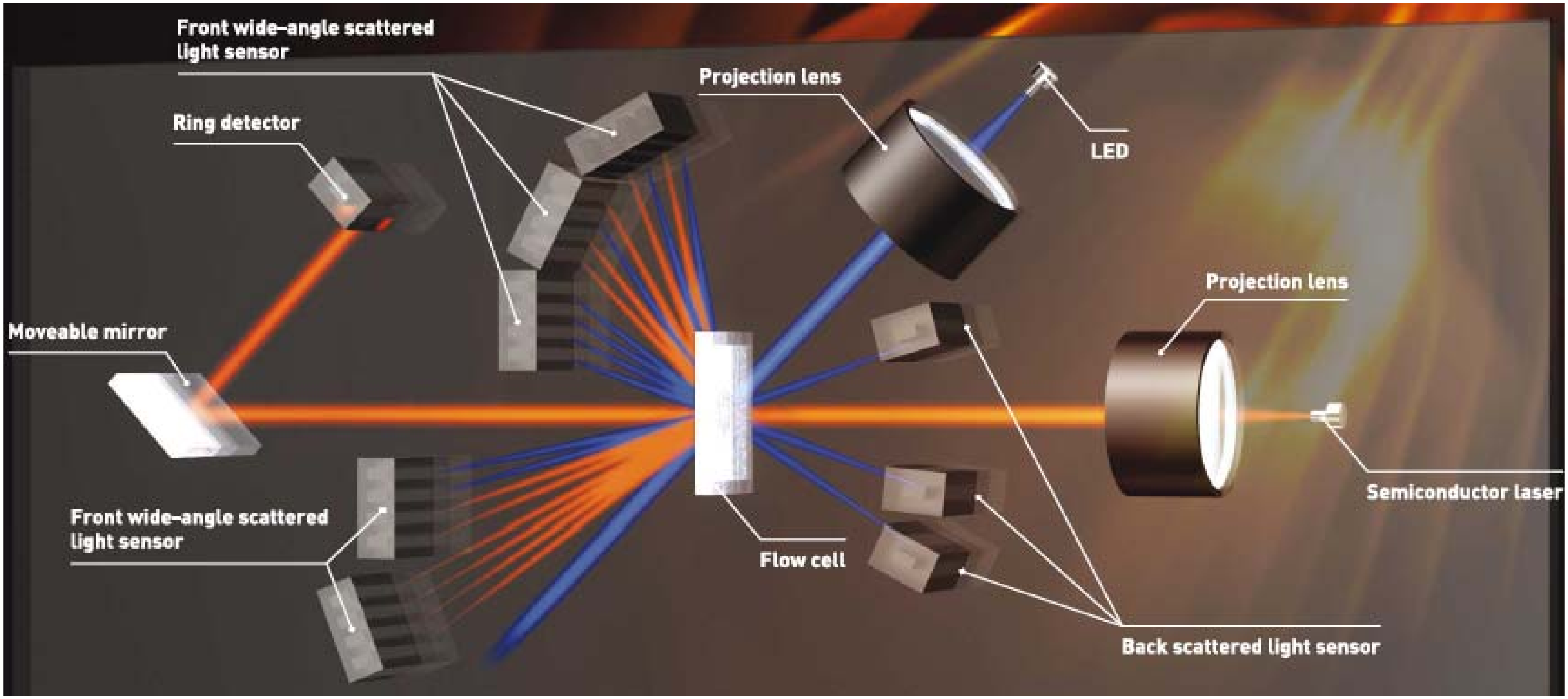




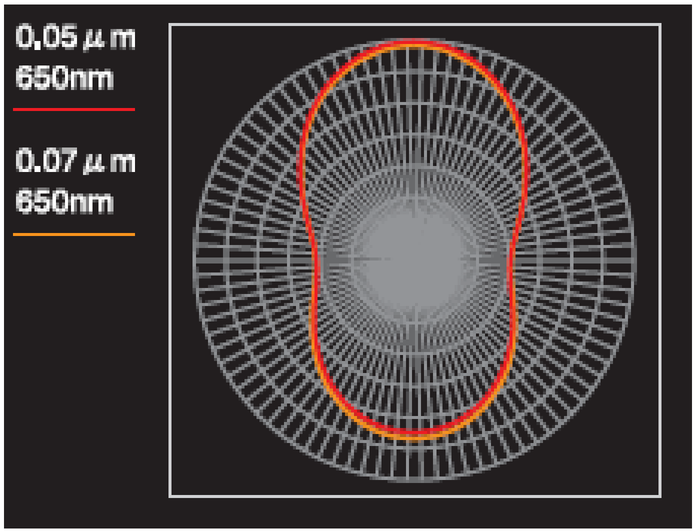
Viewing Raw Data

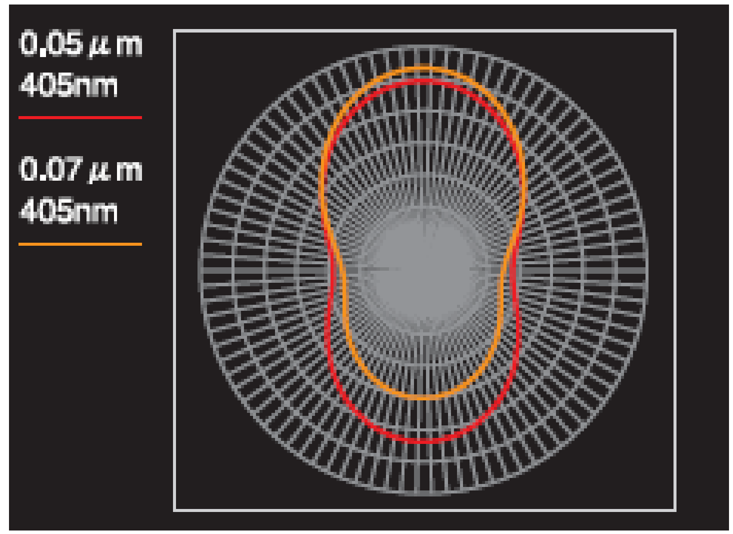


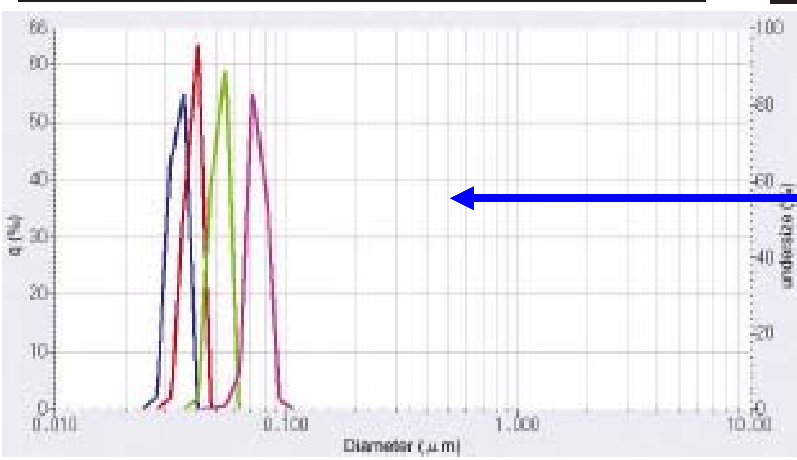
LA-950 Optics



Why 2 Wavelengths?



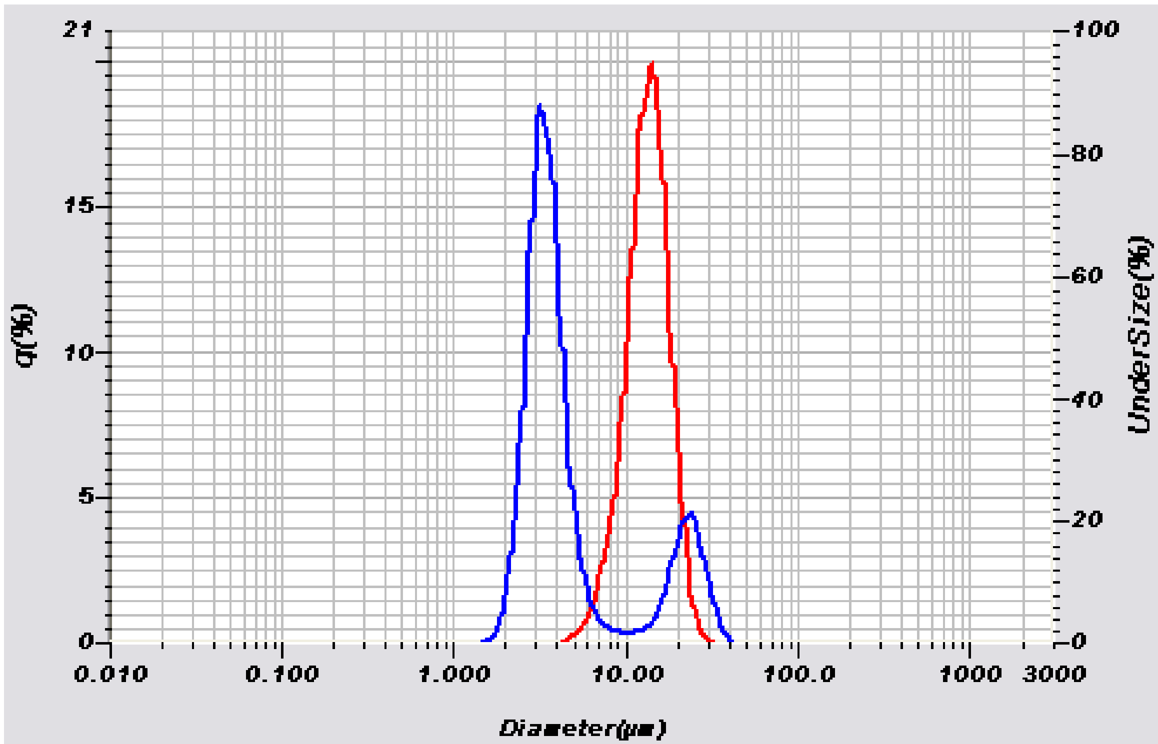




30, 40, 50, 70 nm
latex standards

Practical Application of Theory:
Mie vs. Fraunhofer for Glass Beads

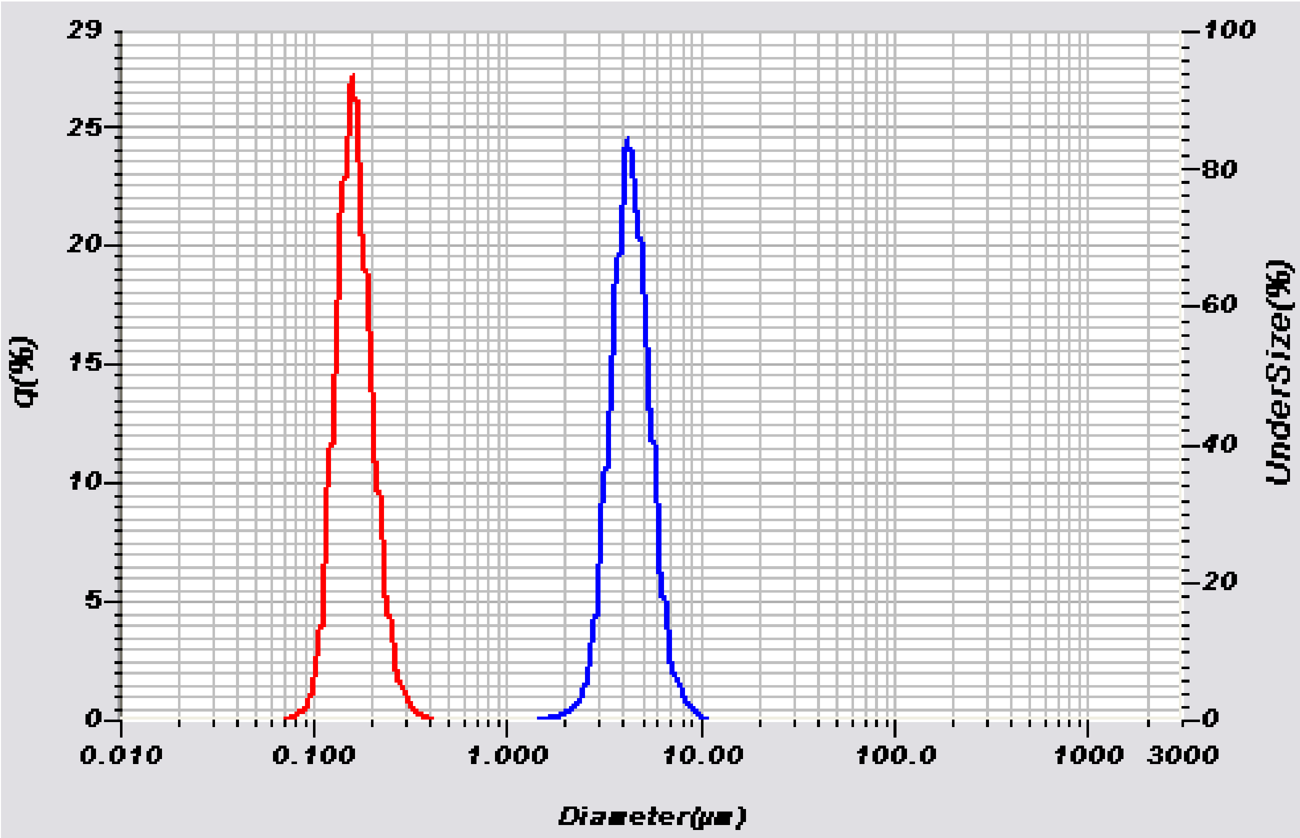
Data Name	Graph Type	Refractive Index (R)
Standard Glass Beads Mie	——	STD-GLASSBEADS[STD-GLASSBEADS(1.510 - 0.000i),'
Standard Glass Beads Fraunhofer	——	Fraunhofer Kernel[Fraunhofer Kernel(0.000 - 0.000i]



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

Practical Application of Theory: Mie vs. Fraunhofer for CMP Slurry

Data Name	Graph Type	Refractive Index (R)
CMP Slurry Mie	red	2.20-0.0i[2.20-0.0i(2.200 - 0.000i),Water(1.333)]
CMP Slurry Fraunhofer	blue	Fraunhofer Kernel[Fraunhofer Kernel(0.000 - 0.000i)



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, R parameter & Chi square calculations
- Use Mie theory at all times (default whenever choosing an RI kernel other than Fraunhofer)