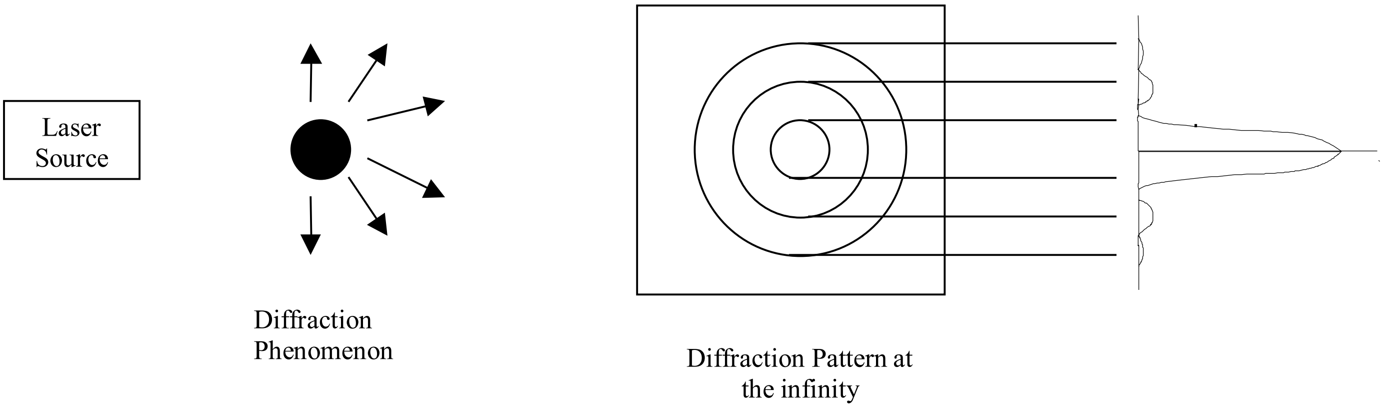
Theory
From the diffraction pattern to the distribution size

1- Principle

This method is based on diffraction and diffusion phenomenon. To obtain the particle size Fraunhofer and Mie theory are used.

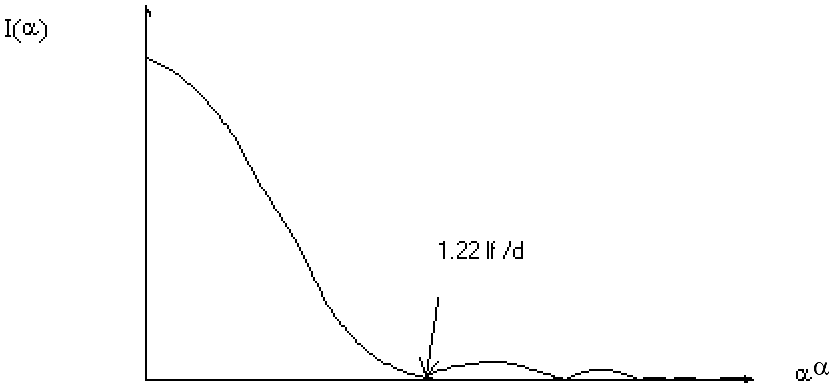
When a particle is lightened by a monochromatic source (laser source) a diffraction pattern, called Airy's pattern, is obtained at the infinity (see document n°1). This diffraction pattern gives the light scattering intensity I, in function of the diffraction angle α. It is composed of concentric rings. The distance between the different rings depends on the particle size.



Document n°1: Diffraction Pattern (called AIRY's Pattern)

1-1 Diffraction pattern characteristics

For a sphere, the diffraction pattern is symmetric (as shown in document n°3). As a consequence we don't need to work with the whole information. Only those contained in a given direction (corresponding to the multicell position) are used for computation. In that case, the diffraction pattern can be plotted in a 2d diagram (see document n°2):



Document n°2: Diffraction Pattern in 2D dimension

The first foot of this pattern is:

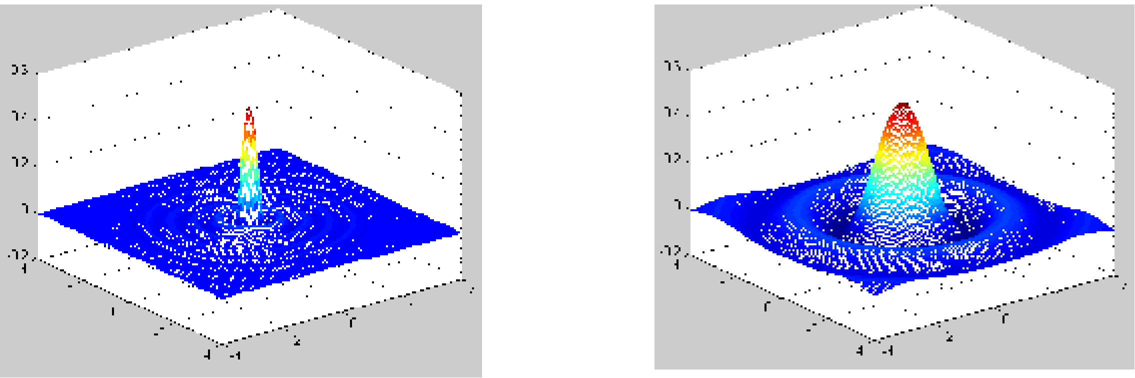
- directly proportional to the wavelength λ
- directly proportional to the the focal length f
- inversely proportional to the diameter d

and equal to: **1.22 λf /d** .

Differences on diffraction pattern between small and big particles:

The first diffraction pattern foot shows that:

The bigger the particle is, the smaller the light distribution is.
At the opposite, the smaller the particle is , the larger the distribution is (see document n°3).



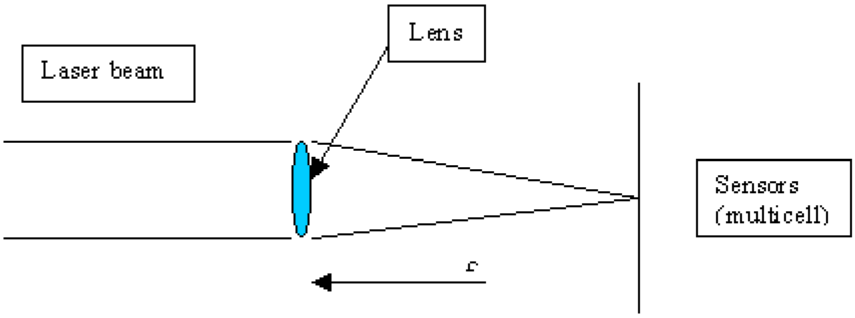
Coarse Particles

Small particles

Document n°3:Diffraction Pattern for coarse and small particles

1-2 How to collect diffraction pattern

To observe this diffraction pattern **at a defined distance**, a convergent lens is applied between the laser beam and the sensors (see document n°4). The sensors (multicell) are placed at the focal length.

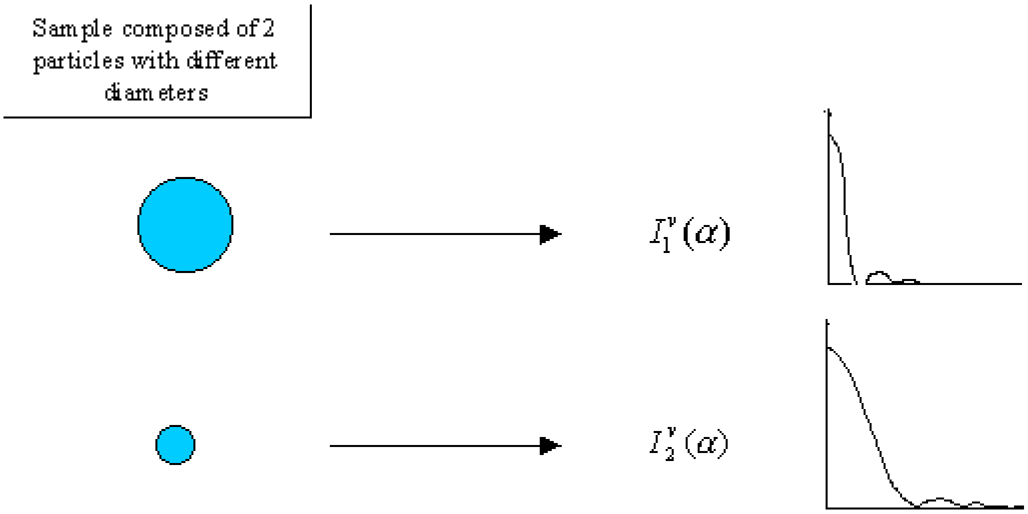


Document n°4 : How to obtain a diffraction pattern at a defined distance.

1-3 Fraunhofer Hypothesis

To determine the particle size thanks to the diffraction pattern we must use the **Fraunhofer theory**. This theory works if the following criterions are respected:

- Particles are spherical and non porous.
- Particle's diameter " d " must be at least 3 to 5 times bigger than the wavelength. In that case only diffraction phenomenon occurs.
- The distance between 2 particles must be at least 3 to 5 times bigger than their diameter. If it's not the case, the hole between particles will be measured instead of their size.
- Particles must have random positions to avoid speckle.



In that case :

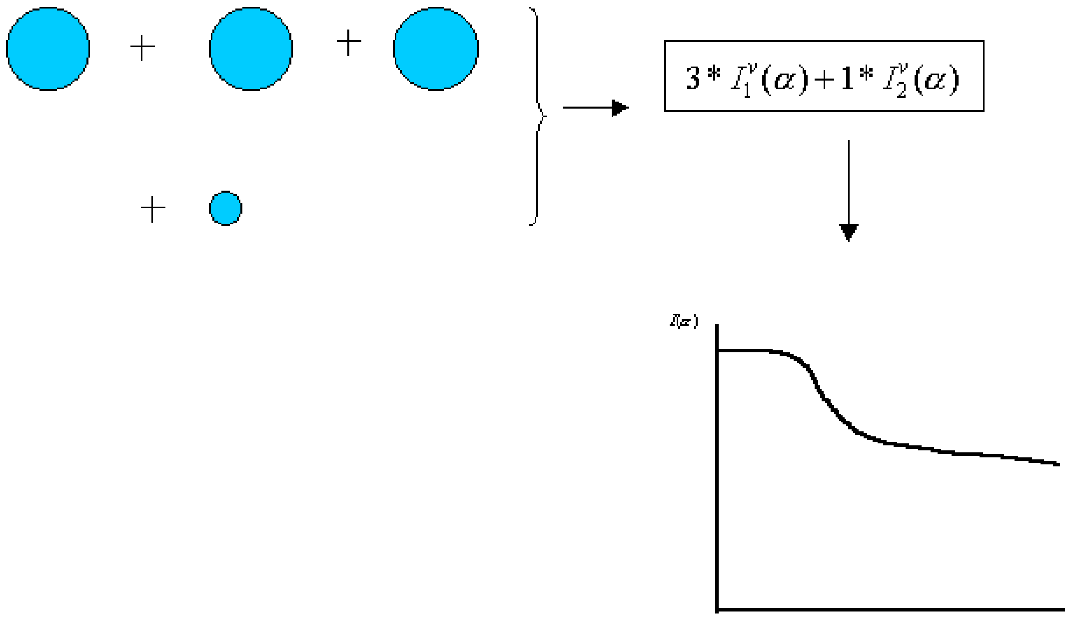
1. **Particles can be considered as isolated.**
2. **Each particle of a sample scatters individually the light and gives its own diffraction pattern (elementary diffraction pattern) noted $I_J^V(\alpha)$.**
3. **The diffraction pattern of several particles with different diameters is given by the sum of each elementary particle's diffraction pattern.**

The whole Intensity ($I(\alpha)$) in function of the angle will be calculated as described below (intensity can be added):

$$I(\alpha)=\sum_{j=1}^{j=n} p_j I_j^V(\alpha) \quad (1)$$

Pj: Number of particles with the diameter dj
$I_J^V(\alpha)$: Intensity diffracted, per volume unit, by one particle of diameter dj at the angle α.
n: number of diameter class.
j: class diameter index

Example:



Document n°5: Diffraction pattern obtained for a sample composed of 4 particles.

As shown here-above, the diffraction pattern of a single particle is composed of concentric rings well separated whereas the global diffraction pattern of several particles is monotone (without any ring). The difficulty is to determine from a monotone diffraction pattern the proportion of each diameter class in order to give a distribution size.

This problem is solved thanks to **matrix**.

2 Determination of the distribution size

Diffraction intensity for particles of same diameters dj

$$I_j(\alpha) = A_j(d_j)V_j\left[\frac{J_1(kd_j \sin\alpha)}{kd_j \sin\alpha}\right]^2 \quad \mathbf{(2)}$$

α :	Diffraction angle
J1	Bessel function at the order 1
k	$2\Pi/\lambda$
Aj(dj)	Proportionality constant
Vj	Volume of Nj particles
Nj	Number of particle of diameter dj
Dj	class j diameter

Diffraction intensity for particles of different diameters dj

$$I(\alpha) = \sum_{j=1}^{j=n} \frac{V_j}{V} I_j^v(\alpha) \quad (3)$$

j	class size index.
V	Total volume of sample:
Vj	Volume of class dj particles.
$I_j^v(\alpha)$	Light intensity per volume of a particle of diameter dj in the α direction.

I (α) is known, and corresponds to the sensors measured signals.
I_j^v (α) is determined theoretically thanks to the Bessel function, described here-above (1) .

The distribution size searched is given by the serie Pj:

$$p_j = \frac{V_j}{V} \quad (4)$$

$$I(\alpha) = \sum_{j=1}^{j=n} p_j I_j^v(\alpha) \quad (5)$$

2-1 Computation

Measured signals I(α)

The signal observed by sensors I(α) is analogical. To increase computation speed, a sampling is performed. We obtain for each sampling angle α, the total scattered light intensity for the whole particles.

Information are stored in column vector noted **S**.

Example: 4 angles sampling,

$$I(\alpha)\ \text{(analogic signal)} \longrightarrow I(\alpha)\ \text{(numerical)} \quad \mathbf{S=} \begin{pmatrix} I(\alpha 1) \\ I(\alpha 2) \\ I(\alpha 3) \\ I(\alpha 4) \end{pmatrix}$$

Theorical Matrix $I_j^v(\alpha)$

Thanks to the Bessel function, we are able to determine the scattering light intensity, per volume, $I_j^v(\alpha)$ for each diameter class dj.

A theoretical matrix is constructed, **noted M**.

We define a series of diameters dj (computation diameters).
Angles are fixed by the sampling.

$$M=\begin{array}{c|cccc|} & d1 & d2 & d3 & d4 \\ \alpha 1 & I(\alpha_1,d_1) & I(\alpha_1,d_2) & I(\alpha_1,d_3) & I(\alpha_1,d_4) \\ \alpha 2 & I(\alpha_2,d_1) & I(\alpha_2,d_2) & I(\alpha_2,d_3) & I(\alpha_2,d_4) \\ \alpha 3 & I(\alpha_3,d_1) & I(\alpha_3,d_2) & I(\alpha_3,d_3) & I(\alpha_3,d_4) \\ \alpha 4 & I(\alpha_4,d_1) & I(\alpha_4,d_2) & I(\alpha_4,d_3) & I(\alpha_4,d_4) \end{array}$$

Each column corresponds to the elementary scattering light Ijv(α) of 1 particle of diameter dj per volume unit

For each diameter dj, we determine the intensity values for the sampling angles.

This matrix is noted M and is proper to each type of particle size analyser. 920, 1064, 1180.
Their sampling angle or computation diameters are different.

Resolution: Determination of pj

In theory, S is a linear combinaison of M matrix column.
We search each size class proportion contained in a column vector P such as the following equation is solved:

$$S=M*P$$

This can be obtained by inversion of M matrix.

$$P=M^{-1}*S$$

Specific cases:

If M has more lines than columns, M can't be inverted.
P is deduced of mean squared method

$$P=((M)^{\dagger}.(M))^{-1}*(M)^{\dagger}.(S)$$

$(M)^{\dagger}$: M matrix transposed.

If M has more columns than lines, M can't be inverted.
P is deduced of mean squared method added with smoothing function

$$P=((M)^{\dagger}.(M)+\sigma^{2}(R)^{\dagger}(R))^{-1}*(M)^{\dagger}.(S)$$

R filtering matrix
σ Smoothing parameter

3 Application of diffraction theory for the 1180 (Fine and coarse particles)

3-1 How to measure both fine and coarse particles

The previous method is reliable and accurate for normal or small particles (0.04μm to 500μm) where the diffraction pattern spreads over a large angle range.

For bigger particles, most of the information is contained in the first diffraction pattern foot. This foot tends to small angle with the increase of particle size. Above a given size, those information are mixed or closed to the non diffracted laser beam (angle:0°). Results can't be correct.

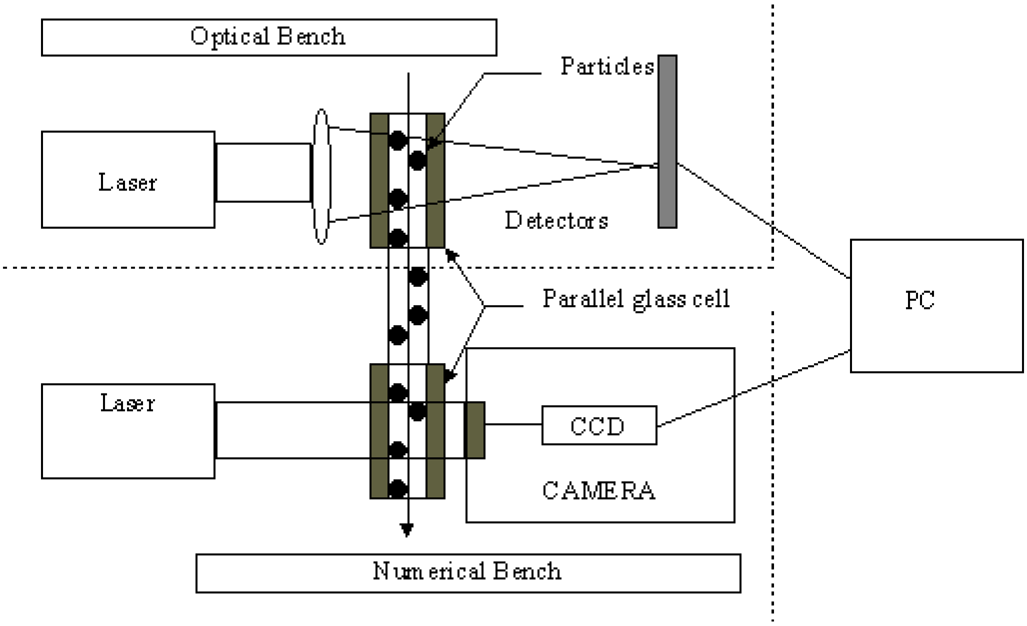
To improve the particle size analyser's range size and measure both fine and coarse particles, several possibilities are available:

1-change the lens, and use a higher focal length f (first foot: **$1.22\ \lambda f\ /d$**). Increasing f will move the foot far from the optical axis, setting the useful information for coarse particle in a readable area. However, the foot of fine particles will also move away. This implies the use of a long bench compatible with the use of two lens.
Disadvantage: In optics the best system is the one that doesn't move. A system which has to be realigned even with an automatic realignment feature is less stable and reliable.

2-use of two methods such as sieves / diffraction, sedimentation / diffraction laser. This solution is impossible because theories used are different.

3-use image analysis with a numerical fourier transformation. In that case, information are the same and can be mixed. This system has been used for the 1180 and is described hereafter.

3-2 System used



Document n°6: 1180 working diagram

Case of a standard diffraction particle size analyser:

In a regular laser diffraction system, the sensor is placed at a focal convergent lens and allows to measure the diffraction pattern at the infinity.

The intensity of the particle's diffraction pattern corresponds to the Fourier Transform's square module of the image in front of the lens (particles shadows).

Case of camera sensors:

The particle is lighted by a parallel beam, and creates a projected image (particles shadows), which is acquired by a CCD camera.
This numerical image can be very easily computed (dsp) to give its numerical Fourier Transform. The square module of the numerical fourier transform gives the numerical diffraction pattern.

These two techniques describe the same physical phenomenon.

3-3 How to obtain a diffraction pattern on a whole range

The silicon sensors acquire a spectrum corresponding to an intensity in function of an angular frequency α, $I=f(\alpha)$.
The ccd sensors after FFT computation, give a spectrum corresponding to an intensity in function of a linear frequency i, $I=f(i)$.

This linear frequency "i" is directly proportional to an angular frequency α, meaning to a diameter.
The ccd spectrum $I=f(i)$ is transformed to an angular frequency spectrum $I=f(\alpha)$. This spectrum covers the range size 300-2500µm.
The silicon sensors spectrum covers the range size 0.04-500µm.

Information of both silicon and ccd sensors can be mixed to obtain a whole range spectrum (0.04-2500µm). Information between 300-500µm are used for overlapping.
The way to obtain distribution size is the same as the one described in the first chapter 1.2.

3-4 Conversion between numerical and analogical fourier transform

Analogical FFT (acquired by multicell sensors)

In case of Fraunhofer diffraction, the analogical FFT (continuous) is given by:

$$A(\alpha,\beta) = \frac{1}{S}\iint_D f(x,y).e^{-j\frac{2.\pi}{\lambda}(x.\sin(\alpha)+y.\sin(\beta))}.dx.dy \qquad (6)$$

λ	wavelength
α	Diffraction angle in x axis
β	Diffraction angle in y axis
f(x,y)	Image function in front of the focal lens
S	Laser beam surface
x,y	Spatial parameters
D	Integration field (= laser beam surface passing through the focal lens).

The square module of the analogical FFT corresponds to the spectrum acquired by silicon sensors, I= f(α).

$$I = f(\alpha,\beta) = \left|A(\alpha,\beta)\right|^2$$

Numerical FFT (acquired by multicell sensors)

The numerical FFT (non continuous) is given by:

$$A(i,k) = \frac{1}{M.N} \iint_{p,q} f(p,q).e^{-j\left(\frac{2.\pi}{M}i.p+\frac{2.\pi}{N}k.q\right)}.dp.dq \qquad (7)$$

M	Number of points in a line.
N	Number of lines in the image.
p	Point order number of a line.
q	Order number of a line.
i	Horizontal order number of the FFT amplitude.
k	Horizontal order number of the FFT amplitude.

The square module of the numerical FFT is given by:

$$I = f(i,k) = \left|A(i,k)\right|^2$$

If we define:

a	horizontal ccd sensor length.
b	Vertical ccd sensor length.
S' = a.b	Ccd sensor surface.
D'	Integration field for ccd sensor

The link between the order number i and the length x can be written as follows:

$$p = \frac{M.x}{a} \qquad et \qquad q = \frac{N.y}{b}$$

$$dp = \frac{M.dx}{a} \qquad et \qquad dq = \frac{N.dy}{b}$$

By changing these parameters in the numerical FFT , we obtain:

$$A(i,k) = \frac{1}{S'} \iint_{D'} f(x,y).e^{-j\left(\frac{2.\pi}{a}.i.x+\frac{2.\pi}{b}.k.y\right)}.dx.dy \qquad (8)$$

By comparison with the analogical FFT:

$$\frac{2.\pi.x.i}{a} = \frac{2.\pi.x.\sin(\alpha)}{\lambda} \qquad \text{and} \qquad \frac{2.\pi.y.k}{b} = \frac{2.\pi.y.\sin(\beta)}{\lambda}$$

The relation-ship between analogical and numerical FFT is given by :

$$\sin(\alpha) = \frac{\lambda}{a}.i \qquad (9) \qquad\qquad \sin(\beta) = \frac{\lambda}{b}.k \qquad (10)$$

In fact we are only working in one direction x. Only the equation (9) is used to convert ccd spectrum I=f(i) to I=f(α).
When this spectrum is modified in an angular frequency, it can be mixed with the one issued of silicon sensors. The whole spectrum obtained is treated as described in chapter 1.2 to deduce the distribution size.

Remark:

The ccd sensors acquire several images during a measurement. For each of them a FFT computation is done. The sum of the FFT gives a monotone spectrum I=f(i). The transformation from i to α is applied on it to obtain an angular frequency spectrum I=f(α).