Dynamic Light Scattering: a numerical standard.

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The European community defines a nano material as:
1) nanomaterial means a natural, incidental or manufactured material containing particles, in an unbound state or as an aggregate or as an agglomerate and where, for 50% or more of the particles in the number size distribution, one or more external dimensions is in the size range 1 nm-100 nm.
2) In special cases and where warranted by concerns for the environments, health, safety or competitiveness the number of size distribution threshold of 50% may be replaced by a threshold between 1 and 50%.
Accordingly, the characterization of nanomaterial in air or liquid is a challenge.
Among the various techniques used to measure nano particles, the Dynamic Light Scattering (DLS) technique is particularly attractive as it is a fast, easy to use, popular technique. A good description of DLS can be find in text books as Berne and Pecora (2000). Nevertheless, a standard is needed to quantify measurement quality and to extend the technique towards very low particles concentrations.
Such a numerical standard has been developed and is presented here. It consists in the combination of two modules. The first module is devoted to the simulation of the particles Brownian motion while the second module is devoted to the simulation of the light scattering. In this version the particles are assumed to be perfectly spherical, isotropic and homogeneous hard spheres. The particles are moved according with the Brownian motion laws. Two time steps are defined: the first one for computing the silica particles motion in water (1 nanosecond), the second one to compute the scattered field (2 µs). For a given position of the set of particles the scattered field is computed by using the Lorenz-Mie theory, taking into account the interferences between the light scattered from the different particles. The main behaviour of this module is described by Wu et al (2011). A temporal series of the scattered field on the detector is computed. Examples of such scattered fields are displayed in figure 1 for 10 particles of 20 nm diameter with a time interval of 2 µs. The modification of the scattered field is clearly visible. Then the total intensity of each image is computed by summing the intensities of all its pixels, permitting to observe the evolution of the scattered intensity versus the time. Finally, the time intensity fluctuations have been analysed by calculating the time intensity autocorrelation function (ACF), like in the DLS procedure. The ACF is presented versus the correlation time in figure 2 for few monodisperse samples of 10 spherical particles, with diameters ranging from 15 to 500nm.
Then we have obtained a fully simulation of the DLS diagnostic, from the Brownian motion of fine particles to the ACF curve. In our EAC presentation, this numerical tool will be applied to quantify the effects of the optical configuration, of particles concentrations, or of size distributions, i.e. in order to optimize DLS experiments.

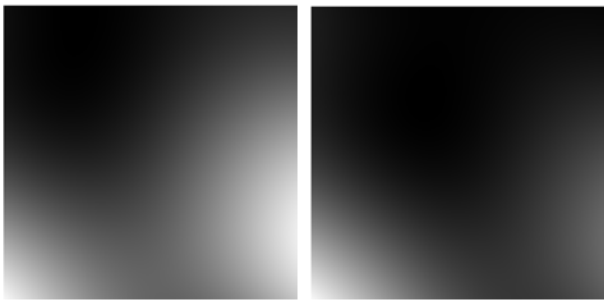

Figure 1. Computed scattered field from 10 particles of diameter 20 nm with a time interval of 2 µs.

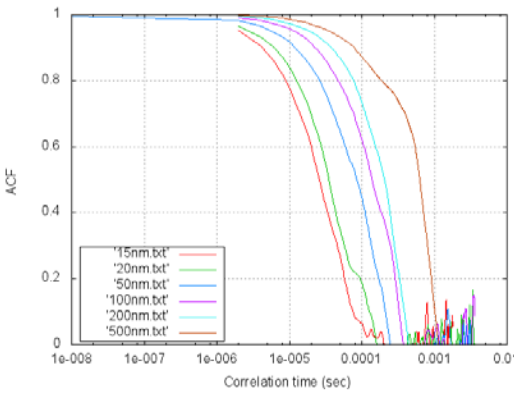

Figure 2. Signal autocorrelation versus time. The parameter is the particle size.

Berne B.J. and Pecora R., *Dynamic light scattering : With applications to chemistry, biology and physics*. (2000), Dover publications, New York.

Wu X.C., Meunier-Guttin-Cluzel S., Wu Y., Saengkaew S., Lebrun D., Brunel M., Chen L.H., Coetmellec S., Cen K.F. and Grehan G., (2011), *Optics Communications*, 285, 3013-3020.