

Application Note

Determining Particle Shape Using Photon Correlation Spectroscopy Technology

By Ren Xu, Ph.D.
Manager Applications Laboratory
Beckman Coulter, Inc

INTRODUCTION

In a PCS measurement, the characteristic correlation decay time of a sample due to the Brownian motion of particles is recorded. Under the assumption that the particles being measured are solid, smooth spheres, the Stokes-Einstein relation is used to convert the translational diffusion coefficient (or its distribution) to diameter (or its distribution) of the particles (or macromolecules). For any particles that are not solid spheres, the resolved diameter is only approximately a solid sphere-equivalent diameter. For many PCS applications, this approximation is sufficient. For synthetic polymers and biopolymers that are coils in solution, the diameter (or its distribution) obtained is the equivalent hydrodynamic diameter (or its distribution). However, in many applications non-spherical particles are measured, such as proteins, cells, and other biological species. With the inclusion of rotational Brownian motions, the deviation from the equivalent spherical diameter to the real particle dimension becomes non-negligible. In addition, when some kind of shape information is needed, equivalent spherical diameters may be less meaningful.

If a PCS instrument measures a sample's Brownian motion at more than one scattering angle, such as that with the Beckman Coulter N5, one can obtain particle dimension information for non-spherical, symmetric particles provided that the axial ratio (x) is presumed. This task is impossible by a single-angle PCS measurement.

PROCEDURE

The following procedure shall be used to obtain the mean particle dimension:

- 1) Make measurements at two or more angles and record the mean diameters $D(\theta)$.
- 2) Plot $\text{Sin}^2(\theta/2)/D(\theta)$ versus $\text{Sin}^2(\theta/2)$ and obtain the slope which is equal to $1/D'$.
- 3) Use the following formulae to convert D' to the dimensions of different shapes:

- a) Prolate ellipsoids (cigar shaped)

$$\frac{1}{D'} = \frac{\ln\left(\frac{1 + \sqrt{1 - x^2}}{x}\right)}{L\sqrt{1 - x^2}}$$

- b) Oblate ellipsoids (discus shaped)

$$\frac{1}{D'} = \frac{\tan^{-1}\sqrt{x^{-2} - 1}}{b\sqrt{x^{-2} - 1}}$$

- c) Thick disks

$$D' = 2L/\pi$$

- d) Thin rods

$$\frac{1}{D'} = \frac{1}{L} \left[6.02 - 4.15 \left(\ln \frac{2}{x} \right)^{-1} + 5.8 \left(\ln \frac{2}{x} \right)^{-2} \right]$$

In the above equations, the axial ratio x ($= b/L$, b is the short axial length and L is the long axial length or disc diameter) needs to be known or assumed.

