Assessing particle non-sphericity from the Fourier spectrum of its light-scattering pattern

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Measuring angle-resolved light-scattering patterns (LSPs) of single particles is a powerful approach for their non-invasive characterization. Because of the lack of a universal approach for solving the inverse light-scattering problem, each developed method adjusts to specific tasks and has its own advantages and disadvantages. Due to the wave nature of the studied physical phenomenon, spectral methods for solving inverse problems occupy a special niche, because they allow obtaining reliable results with minimal computational costs, are more resistant to various signal distortions, and afford an easy control of the solution process [1]. A separate issue for all methods is the potential deviation from the used shape model, incurring error in the retrieved particle characteristics. For example, it is difficult to reliably quantitatively describe deviation even from the simplest model of a homogeneous sphere. A brute-force fit of an experimental LSP with the simulated ones can provide an estimation of non-sphericity only if an alternative shape model (e.g., a spheroid) is considered.

In this work, we enhanced the existing spectral method for solving the inverse light scattering problem for a sphere [1] to estimate the non-sphericity of a particle. As before we used the Fourier transformation of the LSP, but the amplitude spectrum only showed resistance to small deviations from sphericity, which is good for characterization, but bad for non-sphericity detection. Therefore, we used the full complex spectrum for a detailed assessment of non-sphericity. The method is based on quantitative comparison of the complex spectrum around the main peak with that corresponding to the effective sphere. The parameters of the latter are determined by the standard (amplitude) spectral method. Moreover, any other characterization method for spheres can be used, for example, non-linear regression applicable to any size and refractive index, but it might significantly increase the computation time.

We also introduced a quantitative definition of non-sphericity for a particle of arbitrary shape. Extensive simulations of LSPs were carried out for spheroids and red blood cells (RBCs). For the former we chose the non-sphericity parameter based on the analysis in the framework of Rayleigh-Gans-Debye approximation as the effective size times squared eccentricity. For the RBCs we applied geometrical fitting of the real shape by a sphere and defined general non-sphericity parameter as absolute volume discrepancy (residual) multiplied by the effective size.

The developed method was validated experimentally on the LSPs of milk fat globules and the red blood cells during spherization process, measured with the scanning flow cytometer. In particular, the RBCs do not seem to reach the ideal spherical shapes, which is either due to the hydrodynamic tensions in the flow or an artefact of the experimental distortions combined with high sensitivity of the method.

Reference

[1] Romanov, A. V., A. I. Konokhova, E. S. Yastrebova, *et al*., 2017: Spectral solution of the inverse Mie problem. *J. Quant. Spectrosc. Radiat. Transfer* **200**, 280–294.

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