Estimating Particle Non-sphericity from the Fourier Spectrum of Its Light-scattering Pattern

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Abstract— Measuring angle-resolved light-scattering patterns (LSPs) of single particles is a powerful approach for their non-invasive characterization. However, most of the practical methods rely on the knowledge of particle shape model, applicability of which can be questionable in real applications. While some methods are resistant to small deviations from the ideal model [1], it is hard to control the smallness of this deviation and, hence, of the incurred error of the retrieved particle characteristics. We consider the simplest scenario — the deviation of particle morphology from a homogeneous sphere. While the brute-force fit of an experimental LSP with the simulated ones can provide estimation of non-sphericity, it is statistically rigorous only if an alternative shape model (e.g., a spheroid) is considered. The latter brings one to the original problem of extra prior assumptions.

Thus, it is fundamentally interesting and practically important to detect and even characterize nonsphericity directly from the LSP. Adhering to a simple ideology of direct calculations in contrast to fitting, we approach this problem through the Fourier spectrum of the LSP. Recently, we developed a "spectral method" to determine size and refractive index of homogeneous spherical particles through the amplitude spectrum [1]. The amplitude spectrum is stable to small shape distortions, which is good for characterization, but bad for detection of non-sphericity. Thus, in present work we additionally considered the phase spectrum. The latter is rarely used in signal processing due to the lack of the reference point, but the LSP does have such point — an exact forward direction.

We developed a direct method to estimate the sphericity of individual particles from their LSPs, measured with the scanning flow cytometer. Specifically, in addition to two previously used parameters of the amplitude spectrum, the location of the non-zero peak and zero-frequency amplitude [1], we introduced two parameters of the phase spectrum: its value at the spectral peak and the complex integral of the main-peak difference between the experimental LSP and that for a sphere with parameters estimated by the standard spectral method. In the framework of the Rayleigh-Gans-Debye approximation, we derived the formulae relating this parameter to the aspect ratio of a spheroid. Due to their direct nature, they can also be used for other shapes to estimate the effective aspect ratio. In generalizing this approach to the Mie theory, we found a pronounced dependence on the refractive index, which have been compensated using the second new parameter. Alternatively, the phase can also be used to determine the refractive index of spheres with better accuracy or in a wider range than that of the standard spectral method.

REFERENCES

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

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