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Discrimination between spheres and spheroids in a detection system for single particles based on polarization characteristics

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ABSTRACT

The polarization characteristics of light scattered by particles are sensitive to the morphology of the scatterers. In this study, we employed the finite element method (FEM) with a finite element software (COMSOL multiphysics) to retain the potentiality to extend the theoretical study of scattering in this work to single particles with more complex morphology and arbitrary orientation. The angular distribution profiles of the scattering field components perpendicular and parallel to the incident polarization direction are obtained for spherical and spheroidal particles. By comparison with the spheres' preservation of the polarization, cross-polarization effects for differently oriented spheroidal particles are revealed. The question how to experimentally discriminate the particles with smooth surface moving freely in the detected area at single-particle level according to polarization is addressed. To this end, polarizing devices are inserted into an interference particle imaging (IPI) system. By detecting the orthogonally polarized components of the light, the preservation of the polarization state after scattering by spheres and the occurrence of cross-polarization effects after scattering by spheroids are verified experimentally with the fringes in the IPI system as a reference. A feasible method for distinguishing a spheroidal from a spherical shape at the single-particle level based on the existence of a cross-polarized component of the scattered light is proposed.

1. Introduction

Particles in nature always exhibit varied morphology, which is one of their most important properties. The characterization of the particles' morphology provides strong and firm support to atmospheric monitoring, microbial studies, and industrial production. The methods for morphological discrimination mainly include microscopic imaging [1–4], digital holography [5–10], speckle pattern evaluation [11–16], and polarization measurements. Out of all of these methods, polarization measurements attract active research interest because of their sensitivity to the particle morphology, the convenient operation, and the minimal disturbance by other factors.

There are numerous studies devoted to the polarization of light scattered by an ensemble of particles [17–24]. Quantities of numerical simulations and measurements

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from polarimetric lidars revealed the particle shape by analysis of the polarization characteristics of the scattered light, i.e., based on the fact that the spherical scatterers preserve the polarization, whereas the non-spherical ones generate a nonzero cross-polarized component [23,25–27]. However, research works aiming at single particles are rare.

Researchers theoretically established the solution coordinate system for the morphology of scatterers with perfect symmetry. The exact solutions of the classical electromagnetic functions were subsequently derived. The pioneering efforts were used to obtain the solution for electromagnetic scattering by a homogeneous spheroid, and the cross-polarized components of light scattered from a spheroidal particle were analyzed in the spheroidal coordinate system [28]. Recently, the problem of electromagnetic scattering by spheroidal-spherical and spherical-spheroidal particles was solved [29]. Nevertheless, for particles with a complex morphology, the method of solving Maxwell's equation under given boundary conditions is insufficient. Besides, it is impractical to establish the corresponding solution coordinate systems for each particle one by one in an ensemble of particles. To avoid the electromagnetic boundary-value problem, geometric optics approximation (GOA) [30] was adopted and two different types of cross-polarization effects were found. However, the caustic problem for transmission through an arbitrarily oriented spheroid is not yet fully solved, i.e., only the problem of a spheroidal particle with special orientations could be solved. The scattering properties of triaxial ellipsoids were characterized [31], which enabled the adoption of ellipsoid models instead of spheroid ones to simulate particles in nature. However, the calculation methods applicable to the particles with more complex morphology are still missing. The present problem that needs to be solved urgently is how to calculate the theoretical scattering field of particles with complex morphology.

Experimentally, Wyatt et al. [32] first evaluated the lack of a spherical symmetry in some bacteria by studying the depolarization of the signal light. Unfortunately, the measurement for a single bacterium takes substantially large time because a continuous scattering function is required in a large angle range. The measurement efficiency increased dramatically when Strokotov et al. [33] used an innovative instrument to simultaneously measure the polarized light-scattering profile after scattering of individual particles at several fixed positions. The characteristics of each sphere composing a bi-sphere were retrieved from the solution of the inverse light-scattering problem, but multi-angle detection was in this case inevitable. Recently, Ran Pan and Wang et al. [34,35] extracted information on the scatterer's morphology by simultaneous s- and p-polarized diffraction imaging. Nevertheless, a mechanical structure had to be employed to ensure that the particles passed through a flow chamber one by one. A rapid detection method at the single-particle level without the limitation of the particles' movement should be further studied.

Study of scattering particles problem by classical electromagnetic theory, GOA, T-matrix were only applicable to particles with specific types of symmetrical geometry and orientation. In this paper, in order to retain the potentiality to reveal the relation between morphology and polarization characteristics of the particles with more complex morphology and arbitrary orientation, the finite element method (FEM) is adopted with a finite element software (COMSOL multiphysics). The distributions of the scattering field components for a spheroid with different orientations and their equivalent spheres are obtained. As in the case of spheres, the components perpendicular (named cross-polarized components) and parallel to the incident polarization (named co-polarized components) of light scattered by spheroidal particles are analyzed. The significant differences in the polarization characteristics are investigated. With the fringes that occur in the interference particle imaging (IPI) system used as a reference, the existence of cross-polarization states of light scattered by a single particle moving freely in a particle field is evaluated experimentally. Based on spheres' preservation of the polarization and cross-polarization effects of spheroids, a method to discriminate between the morphology of particles with smooth surface at the single-particle level is proposed.

2. Simulation and analysis

For the FEM calculation, we use wave optics module in the scattering formulation to find the normalized cross-polarized and co-polarized field components in far field. Fig. 1 defines the orientation of an arbitrarily oriented spheroidal particle. Θ is the angle between the major axis of the particle and the z-axis. Φ represents the angle between the projection of the major axis in the xOy-plane and the x-axis. The incident beam propagates along the x-axis. The xOy-plane is the observation plane.

Fig. 2 shows the COMSOL simulation domain, with the speroid particle as the inner layer, perfectly matched layer (PML) as the outer one and the medium surrounding the particle in the middle. The medium/PML interface and the outer boundary of PML are concentric spherical shells sharing same center with the speroid. Supposing an incident linearly polarized plane wave with an initial electric field intensity E_0, a wavelength of $\lambda=532$ nm, and a polarization direction perpendicular or parallel to the observation plane is scattered by a prolate spheroidal, the scattering electric field components perpendicular and parallel to the observation plane are expressed as ${}^{(s)}\boldsymbol{E}_1$ and ${}^{(s)}\boldsymbol{E}_2$, respectively. The thickness of the PML and the medium layer are both $\lambda/2$, which is enough to simulate the infinite space around and to satisfy the condition of far-field. The semifocal distance and the major and minor axes of the spheroidal particle are l, a, and b, respectively. c is the dimensionless particle size parameter, where $c=2\pi l/\lambda$. The electromagnetic wave propagating in the particles and the surrounding medium satisfies the Helmholtz equation,

$$\nabla \times \mu_{I,\text{II}}^{-1}(\nabla \times \boldsymbol{E}_{I,\text{II}}) - k_0^2\left(\varepsilon_{I,\text{II}} + \frac{i\sigma_{I,\text{II}}}{\omega\varepsilon_0}\right)\boldsymbol{E}_{I,\text{II}} = 0 \tag{1}$$

where, k_0 and ε_0 are the wave number and the dielectric constant in vacuum, ω is the angular frequency of the