Modelling of Light Scattering by Particles of Extreme Shape Based on the Discrete Sources Method

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Abstract

In this paper the Discrete Sources Method (DSM) is applied to calculate scattering by particles of extreme shape: oblate and prolate spheroids and cylinders with a high aspect ratio. Simulation results for prolate spheroids and cylinders with aspect ratio of 50 are presented. Comparative results corresponding to oblate spheroid and disk-sphere with aspect ratio up to 30 are also given.

Introduction

Light scattering by obstacles of extreme shape is commonly needed in different scientific areas. For example in investigation of scattering and adsorption properties of interstellar dust and ice crystals long finite spheroids and cylinders play a key role, because both ice crystals and dust grains often have a shape like elongated spheroids and cylinders [1]. In optical particle characterization different particles which can cause health problems often also have a very elongated shape. The other case of extreme shape is an oblate particle. Recently interest to such particles increased due to application of light scattering in biology. The red blood cell often is modeled by an oblate spheroid. That is why the interest in methods which can deal with particles of extreme shapes increases. One of the most powerful tools for studying of light scattering by axial symmetric objects is the Discrete Sources Method [2]. In the frame of DSM the idea of quasi-solution is essentially used. The solution of the scattering problem is constructed to satisfy all the conditions of the original scattering problem, except of the boundary condition at the obstacle surface. The field inside and outside the scatterer is represented as a finite linear combination of fields of special sources deposited inside the particle. The unknown amplitudes of DS are defined from the boundary condition at the particle surface. The concept of DSM allows taking into account both the axial symmetry of the object and the polarization of an exciting wave. Besides DSM allows calculating an a-posterior surface residual to estimate an error of the numerical result. In the present paper DSM is applied to calculate scattering from oblate and prolate spheroids and cylinders with a high aspect ratio.

Theory

Let us start with the mathematical statement of the scattering problem. We will consider scattering in an isotropic homogeneous medium in \( \mathbb{R}^3 \) of an electromagnetic wave by a local homogeneous penetrable obstacle \( D \) with the smooth boundary \( \partial D \). We use the cylindrical coordinate system \((z, \theta, \phi)\), and assume the time dependence to be \( \exp(j\omega t) \). Scattering is described by the electromagnetic fields \( \{E_{e,i}, H_{e,i}\} \) satisfying Maxwell equations

\[
\nabla E_{e,i} = jk \varepsilon E_{e,i} \quad \nabla H_{e,i} = -jk \mu H_{e,i} \quad \text{in} \ D_{e,i}, \quad D_{e,i} := \mathbb{R}^3 / \overline{D_i},
\]

the transmission condition enforced on the particle surface
\[ n \times (E_i(p) - E_e(p)) = n \times E_0, \]
\[ n \times (H_i(p) - H_e(p)) = n \times H_0, \quad p \in \partial D, \]

and Silver-Muller radiation condition at infinity.

Here \{E_0, H_0\} is an exciting field, \( n \) is the unit outward normal to \( \partial D \), \( e \) index \( e \) belongs to the external domain \( D_e \) and \( i \) to the domain inside the particle \( D_i \), \( \varepsilon_{e,i} \) is the permittivity, \( \mu_{e,i} \) - permeability, \( \text{Im} \varepsilon_{e}, \mu_{e} = 0 \). The boundary value scattering problem is well known to have an unique solution [3].

The scheme of DSM is shortly described above. We will concentrate only at some principle points. One of the most attractive features of DSM consists in a flexible choice of DS fields that can be used for approximate solution construction. Additionally there are no limitations to a choice of support of DS, which should provide fulfilling Maxwell equations, radiation conditions and yield a complete system of DS fields at the obstacle surface [4]. For oblate obstacles sometimes it is necessary to invent a special DS support. One of the possibilities DSM gives is to dispose DS in a complex plane. Such procedure allows us to limit the sequence of DS's amplitudes when number of DS tends to infinity. The limitation is very important to provide the stability of numerical model based on DSM.

We will consider an axial symmetrical particle. Then the system of lowest order multipoles distributed over the axis of symmetry can be applied to construct an approximation solution. As a consequence the surface approximating problem can be reduced to a number of one dimensional problems enforced at the particle generatrix.

Let the axial symmetry be the z-axis, DS \( \{z_n\}_{n=1}^{\infty} \) distributed over a segment \( \Omega \) of the z-axis, situated inside the particle, which is chosen as a closed multitude with at least one condensing point. Then the following results are valid [2]:

We will construct the approximate solution by taking into account not only the rotational symmetry of the obstacle, but also the polarization of an external excitation as well.

In case of a P-polarized exciting plane wave the exciting field accepts the following form
\[ E_0 = (e_x \cos \theta_o + e_y \sin \theta_o) \gamma, \]
\[ H_0 = -e_y \gamma \cos \theta_o, \]
\[ \gamma = \exp \left\{ -jk_x (x \sin \theta_o - z \cos \theta_o) \right\}; \]
where \( k_x = k \sqrt{\varepsilon_e \mu_e} \).

To take the polarization of the external excitation into account we use some linear combination of electrical and magnetic multipoles. For this we need special vector potentials. In case of P-polarization of the plane wave the representation for vector potentials in a cylindrical coordinate system can be represented as
\[ A_{1m}^{1,e,i} = \{ Y_{m}^{e,i} (\rho, z_{n}^{e,i}) \cos (m + 1) \phi; -Y_{m}^{e,i} (\rho, z_{n}^{e,i}) \sin (m + 1) \phi; 0 \} \]
\[ A_{2m}^{2,e,i} = \{ Y_{m}^{e,i} (\rho, z_{n}^{e,i}) \sin (m + 1) \phi; Y_{m}^{e,i} (\rho, z_{n}^{e,i}) \cos (m + 1) \phi; 0 \} \]

Vector potentials for vertical dipoles, which are required to be added to provide completeness of the multipoles’s system, are
\[ A_{3m}^{3,e,i} = \{ 0; 0; Y_{0}^{e,i} (\rho, z_{n}^{e,i}) \} \].
Here:  \( Y_m^i(\eta, z_n') = j_m\left(k, R_{\eta z_n'}\right) \cdot \left(r/R_{\eta z_n'}\right)^m, \quad Y_m^e(\eta, z_n') = h_m^{(2)}\left(k, R_{\eta z_n'}\right) \cdot \left(r/R_{\eta z_n'}\right)^m, \)  where  \( j_m(\cdot) \) is the spherical Bessel function,  \( h_m^{(2)}(\cdot) \) is the spherical Hankel function,  \( R_{\eta z_n'} = r^2 + (z - z_n')^2, \)  \( z_n' \) are the coordinates of the multipoles inside the particle.

So the approximate solution taking into account P-polarization of the plane wave and axial symmetry of the particle can be represented in the form

\[
\left\{ E_x^N, H_z^N \right\} = \sum_{m=0}^{M} \sum_{n=0}^{N} \left\{ p_{mn} D_1 \times A_{mn}^{1,2} + q_{mn} D_2 \times A_{mn}^{2,2} \right\} + \sum_{n=0}^{N} r_n^2 D_1 \times A_{n}^{1,2}, \tag{1}
\]

\[
D_1 = \left( \begin{array}{c} \frac{j}{k\varepsilon_\zeta \mu_\zeta} \nabla \times \nabla \\ \frac{-1}{\mu_\zeta} \nabla \end{array} \right), \quad D_2 = \left( \begin{array}{c} \frac{1}{\varepsilon_\zeta} \nabla \\ \frac{j}{k\varepsilon_\zeta \mu_\zeta} \nabla \times \nabla \end{array} \right).
\]

Then the following result holds: the approximate solution (1) converges to the exact one under  \( M, N_{ie}^m \to \infty. \)

In the case of an S-polarized plane wave the approximation solution is constructed in the same way, see [1].

The numerical algorithm is described in [5]. We will emphasize just the main differences of the extended Discrete Sources Method scheme described above to the conventional Discrete Sources Method [4]:

1. Different numbers of discrete sources  \( N_{ie}^m, N_{e}^m \) are used for the representation of the scattered field outside and total field inside the particle. The numbers of discrete sources are chosen proportionally to the value of refractive index of the corresponding media. For the internal domain (higher refractive index  \( \frac{\varepsilon_\zeta \mu_\zeta}{\sqrt{\varepsilon_\zeta \mu_\zeta}} \)) a higher number of discrete sources then for the scattered field (  \( N_{ie}^m > N_{e}^m \)) is used.

2. The number of discrete sources depends on the rank of Fourier harmonics  \( N_{ie}^m > N_{e}^m \). For higher harmonics a lower number of multipoles  \( N_{ie}^{m+1} \leq N_{e}^m \) is used. This circumstance enables to acquire a more accurate simulation result, provides a monotone decrease of the surface residual and reduces the demand on computer resources up to 30% for larger particles compared to the conventional Discrete Sources Method model. Besides it allows extending the range of validity of the Discrete Sources Method for the particles of larger size.

Results

We will mostly study the Differential Scattering Crosssection (DSC)

\[
DSC = \left| F_{\theta}^{P,S} (\Theta, \Phi) \right|^2 + \left| F_{\phi}^{P,S} (\Theta, \Phi) \right|^2,
\]

here  \( F_{\theta,\phi}^{P,S} (\Theta, \Phi) \) are the components of the far field pattern [1] for P and S polarized excitation, which can be calculated analytically. We will represent just some of results obtained with the extended DSM scheme described above. The wavelength of  \( \lambda = 488\text{nm} \) was chosen because lasers with such
wavelength are usually used in particle characterization. As material we have chosen $\text{SiO}_2$ ($n=1.46-0.00i$). To compare scattering by different shapes we took cylinder and prolate spheroid of aspect ratio of 50:1, length of particles is $l=20\,\mu m$ and diameter $D=0.4\,\mu m$ and disk-sphere and oblate spheroid of aspect ratio 1:30, $l=0.1\,\mu m$, $D=3.0\,\mu m$. The dependence of DSC from scattering angle for elongated particles for different shapes for P-polarized excitation one can see at Fig. 1. In Fig. 2 DSC versus scattering angle for oblate particles of different shapes also for P-polarized light is given. In both examples the incident angle $\theta =90^\circ$. More results will be presented in oral presentation.

![Figure 1](image1.png)  
![Figure 2](image2.png)

**Conclusion**

The renewed algorithm of DSM was applied to light scattering by particles of extreme shapes. The main differences of the extended DSM scheme to the conventional one [4] are: firstly different numbers of DS are used for the representation of the scattered field outside and total field inside the particle, and secondly the number of DS depends on the rank of Fourier harmonics. This means that for higher harmonics the lower numbers of multipoles are used. Such circumstance enables to acquire more accurate simulation results, provides a monotone decrease of the surface residual and reduces the demand on computer resources for larger particles compared to the conventional DSM model.

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**REFERENCES**