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Journal of Quantitative Spectroscopy & Radiative Transfer 70 (2001) 715–723

Journal of Quantitative Spectroscopy & Radiative Transfer

www.elsevier.com/locate/jqsrt

Computer programs for light scattering by particles with inclusions

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Abstract

We present a comparison of computational results from light scattering by spherical particles with inclusions. The different simulation methods like the T-matrix method, multiple multipole method and the method of separation of variables are presented shortly. Exemplary numerical simulations involve scattering by particles with one or two spherical inclusions and scattering by particles with non-spherical inclusions. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: T-matrix method; Multiple multipole method; Multiple inclusions; Non-spherical inclusions

1. Introduction

Light scattering by inhomogeneous particles is a subject of great interest in many fields of science like optical particle sizing, astronomy, optical oceanography, photographic science, coatings technology, meteorology and atmospheric science. For example, in chemical engineering there is a continuing interest to characterize and to measure the size of hollow beads, while in atmospheric science there is an interest to characterize fog droplets with soot or bacteria inclusions.

The diameter of a homogeneous spherical particle can be measured by analyzing the intensity distribution in a given scattering domain [1]. In this case there exists a linear relation between the angular spatial frequency of the scattering pattern and the particle size. In order to apply this technique to spherical particles containing several inclusions it is necessary to accurately simulate the scattering characteristics of an inhomogeneous particle.

By presenting some exemplary simulation results in the present paper we will investigate the numerical efficiency of several scattering methods. Clearly, each light scattering method has its own limitations concerning the size of the host sphere and the size, form and number of

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PII: S0022-4073(01)00040-1

the inclusions. The aim of our comparison is to choose an optimal method for the practical application in optical particle sizing concerning the diameter measurement of an inhomogeneous particle.

2. Simulation methods

The first code for light scattering calculations from a spherical particle containing a concentric inclusion has been developed by Kerker [2]. Later, Toon and Ackerman [3] extended this algorithm to multilayered spheres.

A theory for the scattering by a spherical particle with one non-concentric spherical inclusion has been derived by Borghese et al. [4] and Videen et al. [5]. The optical properties of a spherical particle containing two inclusions are discussed in Borghese et al. [6]. These results are based on the separation of variables method.

The T-matrix method has been used recently by Doicu and Wriedt [7] to compute light scattering for a great variety of particles including the case of inhomogeneous particles. The multiple multipole method has also the capability to treat scatterers with artbitrarily shaped inhomogeneities. For our simulation we choose the separation of variables method by Videen et al. [8], the T-matrix method by Doicu and Wriedt [7] and the multiple multipole method code by Hafner and Bombolt [9]. In the following sections these methods will be introduced briefly.

2.1. T-matrix method

The T-matrix method was originally developed by Waterman and it has become a powerful numerical tool for computing light scattering by non-spherical particles [10]. In the T-matrix method all fields are expanded into spherical vector wave functions. The T-matrix relates the expansion coefficients of the incident field to the expansion coefficients of the scattered field and it depends only on the optical and geometrical properties of the particle.

The T-matrix method has been extended recently by Doicu and Wriedt [7] to scatterers with complex structure, as for instance scatterers containing homogeneous, layered or composite inclusions.

For a system of two neighboring particles the total T-matrix $\mathbf{T}_{12}$ is given by

$$\begin{aligned}\mathbf{T}_{12} = {} & \sigma^1_{OO_1}\mathbf{T}_1[\mathbf{I} - \sigma^3_{O_1O_2}\mathbf{T}_2\sigma^3_{O_2O_1}\mathbf{T}_1]^{-1}[\sigma^3_{O_1O_2}\mathbf{T}_2\sigma^1_{O_2O} + \sigma^1_{O_1O}] \\ & +\sigma^1_{OO_2}\mathbf{T}_2[\mathbf{I} - \sigma^3_{O_2O_1}\mathbf{T}_1\sigma^3_{O_1O_2}\mathbf{T}_2]^{-1}[\sigma^3_{O_2O_1}\mathbf{T}_1\sigma^1_{O_1O} + \sigma^1_{O_2O}], \end{aligned} \tag{1}$$

where $\mathbf{T}_1$ and $\mathbf{T}_2$ stands for the transition matrices of the scatterers and $\sigma^{1,3}_{OO_1}$ are the roto-translation matrices passing from the origin O to the origin O_1. The most interesting feature of Eq. (1) is that the total T-matrix is expressed in terms of T-matrices of individual scatterers. For three or more scatterers it is difficult to give an explicit expression for the total T-matrix, but the mathematical model involves only the individual T-matrices of each scatterer.

The total transition matrix of a scatterer containing an arbitrarily shaped inclusion is given by

$$\mathbf{T}_{12} = [\mathbf{T}_1 - \mathbf{Q}_1^{1,3}\hat{\mathbf{T}}_2(\mathbf{Q}_1^{3,1})^{-1}][\mathbf{I} - \mathbf{Q}_1^{3,3}\hat{\mathbf{T}}_2(\mathbf{Q}_1^{3,1})^{-1}]^{-1}, \tag{2}$$

where $\hat{\mathbf{T}}_2 = \sigma^1_{O_1O_2}\mathbf{T}_2\sigma^1_{O_2O_1}$. Here, $\mathbf{T}_1$ and $\mathbf{T}_2$ are the transition matrices of the host particle and of the inclusion, and the matrices $\mathbf{Q}_1^{i,j}$ have the same significance as in Peterson and Ström [11].

The case of a host particle containing an arbitrary number of separate inclusions is obtained by inserting the appropriate T-matrix instead of $\hat{\mathbf{T}}_2$. This T-matrix can correspond to an arbitrary number of homogeneous, layered or composite scatterers.

2.2. Multiple multipole method (MMP)

The multiple multipole method was developed by Hafner and Bomhold [9] for general electromagnetic computations. It is a semianalytical method in the sense that the electromagnetic fields are expressed as a linear combination of multiple multipoles, while the amplitudes of the multipoles are obtained by enforcing the boundary conditions in a set of matching points.

Scattering of electromagnetic waves by a dielectric particle with a boundary S and exterior D_s may be formulated as a boundary value problem consisting in Maxwell equations, the Silver Mueller radiation condition at infinity and the boundary conditions on the particle interface.

An approximate solution to the scattering problem can be constructed as a finite linear combination of multipole fields with different origins.

The approximate scattered field $\mathbf{E}_\mathrm{s}^N$, $\mathbf{B}_\mathrm{s}^N$ is represented as a linear combination of radiating functions $\mathscr{M}^3_{mnp}$ and $\mathscr{N}^3_{mnp}$ positioned in D_i, $D_i = \mathbf{R}^3 - D_\mathrm{s}$:

$$\begin{pmatrix} \mathbf{E}_\mathrm{s}^N \\ \mathbf{H}_\mathrm{s}^N \end{pmatrix} = \sum_{p=1}^{P}\sum_{n=1}^{N_p}\sum_{m=-n}^{n} a^N_{mnp} \begin{pmatrix} \mathscr{M}^3_{mnp} \\ -j\sqrt{\frac{\varepsilon_\mathrm{s}}{\mu_\mathrm{s}}}\mathscr{N}^3_{mnp} \end{pmatrix} + b^N_{mnp} \begin{pmatrix} \mathscr{N}^3_{mnp} \\ -j\sqrt{\frac{\varepsilon_\mathrm{s}}{\mu_\mathrm{s}}}\mathscr{M}^3_{mnp} \end{pmatrix}, \tag{3}$$

while the approximated internal field is represented as linear combination of regular functions $\mathscr{M}^1_{mnp}$ and $\mathscr{N}^1_{mnp}$ positioned in D_s:

$$\begin{pmatrix} \mathbf{E}_\mathrm{i}^N \\ \mathbf{H}_\mathrm{i}^N \end{pmatrix} = \sum_{p=1}^{P}\sum_{n=1}^{N_p}\sum_{m=-n}^{n} c^N_{mnp} \begin{pmatrix} \mathscr{M}^1_{mnp} \\ -j\sqrt{\frac{\varepsilon_\mathrm{i}}{\mu_\mathrm{i}}}\mathscr{N}^1_{mnp} \end{pmatrix} + d^N_{mnp} \begin{pmatrix} \mathscr{N}^1_{mnp} \\ -j\sqrt{\frac{\varepsilon_\mathrm{i}}{\mu_\mathrm{i}}}\mathscr{M}^1_{mnp} \end{pmatrix}. \tag{4}$$

Here $\mathscr{M}^{3,1}_{mnp}(\mathbf{x}) = \mathbf{M}^{3,1}_{mn}[k_{\mathrm{s,i}}(\mathbf{x}-\mathbf{x}_{0p})]$, $\mathscr{N}^{3,1}_{mnp}(\mathbf{x}) = \mathbf{N}^{3,1}_{mn}[k_{\mathrm{s,i}}(\mathbf{x}-\mathbf{x}_{0p})]$ are the radiating or the regular spherical vector wave functions with their origin located at $\mathbf{x}_{0p}$.

The expansion coefficients a^N_{mnp}, b^N_{mnp}, c^N_{mnp} and d^N_{mnp} will be obtained by minimizing the residual field on the particle surface:

$$\mathbf{a} = \arg\min\{\|\mathbf{n}\times\mathbf{E}_\mathrm{s}^N + \mathbf{n}\times\mathbf{E}_0 - \mathbf{n}\times\mathbf{E}_\mathrm{i}^N\|^2_{2,S} + \|\mathbf{n}\times\mathbf{H}_\mathrm{s}^N + \mathbf{n}\times\mathbf{H}_0 - \mathbf{n}\times\mathbf{H}_\mathrm{i}^N\|^2_{2,S}\}, \tag{5}$$

where $\mathbf{a}^{\mathbf{T}} = [a^N_{mnp}, b^N_{mnp}, c^N_{mnp}, d^N_{mnp}]$ and $\mathbf{E}_0$, $\mathbf{B}_0$ is an entire solution to Maxwell equations representing an incident electromagnetic field.

In order to reduce the computational effort the surface of the scatterer is divided into a number of cells (matching points) and the surface integrals appearing in (5) are evaluated numerically. The expansion coefficients can then be calculated as the solution of the least squares problem: $\mathbf{a} = \arg\min ||\mathbf{Ax} - \mathbf{f}||^2_{l^2}$, where the matrix $\mathbf{A}$ and the vector $\mathbf{f}$ depend on the values of the basis functions and the incident field at the matching points, respectively. The matrix equation is solved by using the QR decomposition, with an algorithm based on Givens rotations.

2.3. Separation of variables method for a sphere with a non-concentric inclusion

The algorithm of Videen et al. [8] computes the scattering of electromagnetic waves by a sphere with a non-concentric spherical inclusion. The general solution is reached by using the separation of variables method and by satisfying the boundary conditions on both spheres. Since the fields in each homogeneous region are expressed as a linear combination of multipoles with different origins, the method includes the implementation of the translation addition theorem for spherical vector wave functions. The program itself is able to provide the Mueller matrix, the extinction, scattering, absorption efficiencies and the asymmetry parameter.

3. Comparison of simulation results

In this section we present computer simulations for several scatterers that gradually increase in complexity. The incident wave is a linearly polarized plane wave travelling along the z-axis of a global coordinate system. The global coordinate system coincides with the host sphere coordinate system. The scattering characteristics will be evaluated in the azimuthal plane $\varphi = 0$. The refractive index of the host sphere is $n_{\mathrm{H}} = 1.334$, while the refractive index of the inclusions is $n_{\mathrm{I}} = 1.6$.

In our first example we consider the case of a spherical particle with a non-concentric spherical inclusion. The geometry of the scattering problem is shown in Fig. 1. The size parameter of the host particle is $k_{\mathrm{s}}a_{\mathrm{H}} = 10$ while the size parameter of the inclusion is $k_{\mathrm{s}}a_{\mathrm{I}} = 4$. The inhomogeneity is placed at $k_{\mathrm{s}}x_{\mathrm{I}} = 2$, $k_{\mathrm{s}}y_{\mathrm{I}} = 0$ and $k_{\mathrm{s}}z_{\mathrm{I}} = 0$ with respect to the global coordinate system. The results for the differential scattering cross section computed by the T-matrix method and the separation of variables method are shown in Fig. 2. The results demonstrate a complete agreement between the scattering curves. We mention that the simulations with the multiple multipole method, which we omit here, gave similar results. The time needed for computation lies with a few seconds except for the multiple multipole program, where it takes about 1 h on an AIX RS/6000 workstation. The differences between the computational time are a consequence of the fact that the T-matrix method and the separation of variables method take advantage of the axialsymmetry of the scattering problem.

However, our numerical experiments show that the separation of variables program fails to converge for particles with high size parameters. In contrast, the T-matrix method gives stable and convergent results up to a size parameter of 100. In Fig. 3 we plot the results for an inhomogeneous spherical particle with $k_{\mathrm{s}}a_{\mathrm{H}} = 100$, $k_{\mathrm{s}}a_{\mathrm{I}} = 40$ and $k_{\mathrm{s}}x_{\mathrm{I}} = 40$, $k_{\mathrm{s}}y_{\mathrm{I}} = 0$ and $k_{\mathrm{s}}z_{\mathrm{I}} = 0$.

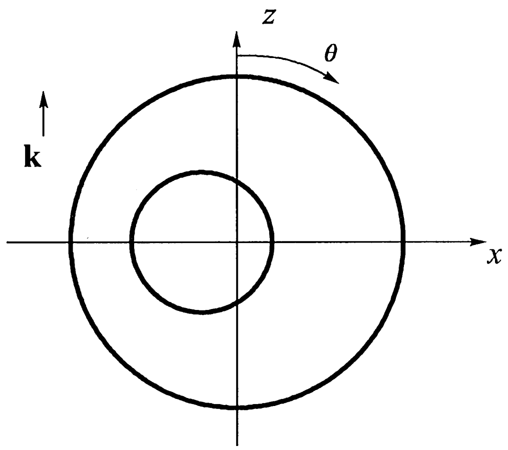

Fig. 1. Model of a sphere (size parameter $k_s a_H = 10$, refractive index $n_H = 1.334$) with one non-concentric spherical inclusion ($k_s a_I = 4, n_H = 1.6$). The particle is tilted 90° against the direction of incident wave. The center–center separation distance is 2 in units of the size parameter.

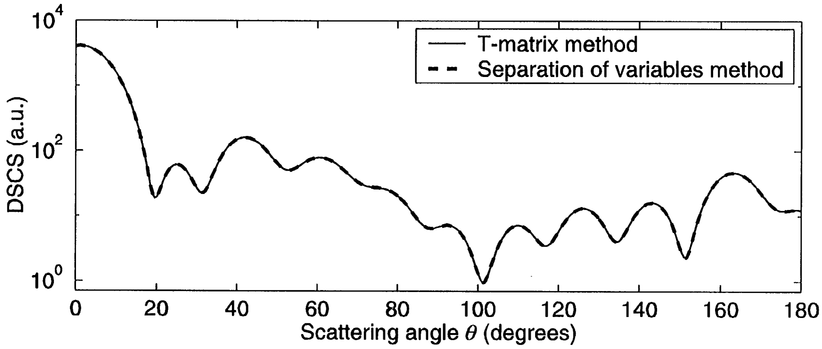

Fig. 2. Computed DSCS (sum of perpendicular and parallel polarization) of a sphere ($k_s a_H = 10, n_H = 1.334$) with one non-concentric spherical inclusion ($k_s a_I = 4, n_H = 1.6$). The particle is tilted 90° against the direction of incident wave.

We want to point out that the T-matrix method and the separation of variables method are equivalent for one spherical inclusion. The limitations of the separation of variables program to a size parameter of about 50 is perhaps a consequence of some internal constraints of the computer code available via internet [8,12].

In our next examples we consider scattering geometries without axial symmetry. Firstly, we consider the case of a spherical particle with two spherical inclusions. The geometry of the scattering problem is shown in Fig. 4. The scattering characteristics are computed with the T-matrix method and the multiple multipole method. The results corresponding to the case $k_s a_H = 10$, $k_s a_{I_1} = k_s a_{I_2} = 2$, $k_s x_{I_1} = 4$, $k_s y_{I_1} = -4$, $k_s z_{I_1} = 4$ and $k_s x_{I_2} = 2$, $k_s y_{I_2} = 2$, $k_s z_{I_2} = -2$ are shown in Fig. 5. These results clearly demonstrated that no significant differences exist between the scattering diagrams.

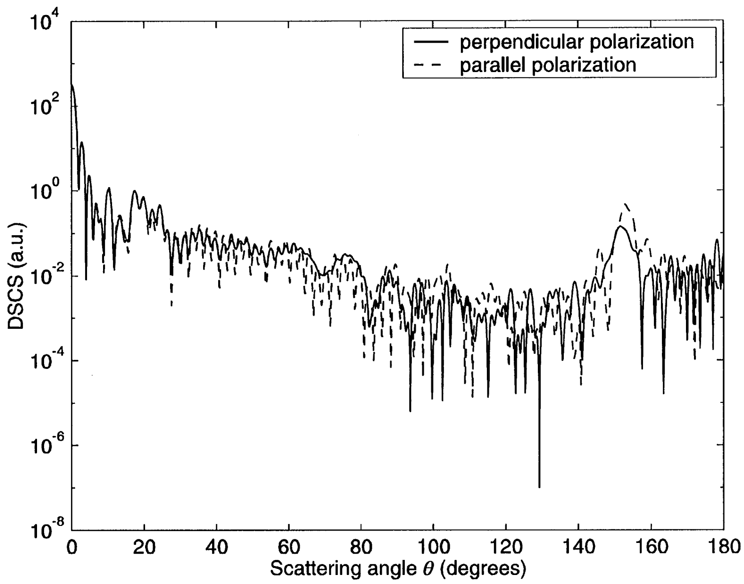

Fig. 3. Computed DSCS of a sphere ($k_s a_H = 100$, $n_H = 1.334$) with one non-concentric spherical inclusion ($k_s a_I = 40$, $n_H = 1.6$). The particle is tilted 90° against the direction of incident wave. The center–center separation distance is 40 in units of the size parameter.

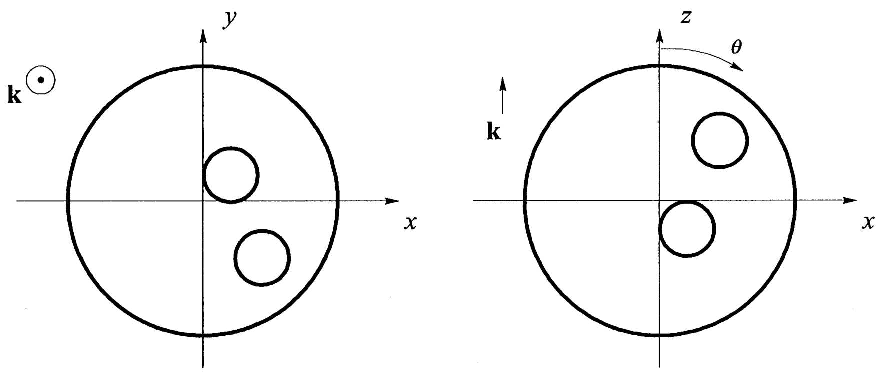

Fig. 4. Model of a sphere ($k_s a_H = 10$, $n_H = 1.334$) with two spherical inclusions ($k_s a_I = 2$, $n_I = 1.6$, $\mathbf{r}_1 = (4; -4; 4)$, $\mathbf{r}_2 = (2; 2; -2)$). The position coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ of the inclusions are given in units of the size parameter.

Next, we consider the case of a spherical particle with a non-spherical inclusion. The geometry of the scattering problem is shown in Fig. 6. In Fig. 7, we plot the differential scattering cross section computed with the T-matrix method and the multiple multipole method. The results correspond to a scattering geometry with $k_s a_H = 10$. The inhomogeneity is a prolate spheroid with $k_s a_I = 5$ and $k_s b_I = 2.5$ placed at $k_s x_I = 2$, $k_s y_I = 4$ and $k_s z_I = 2$ with respect to the global coordinate system. The orientation of the spheroid is given by the Euler angles $\alpha_I = 0$ and $\beta_I = 90°$.

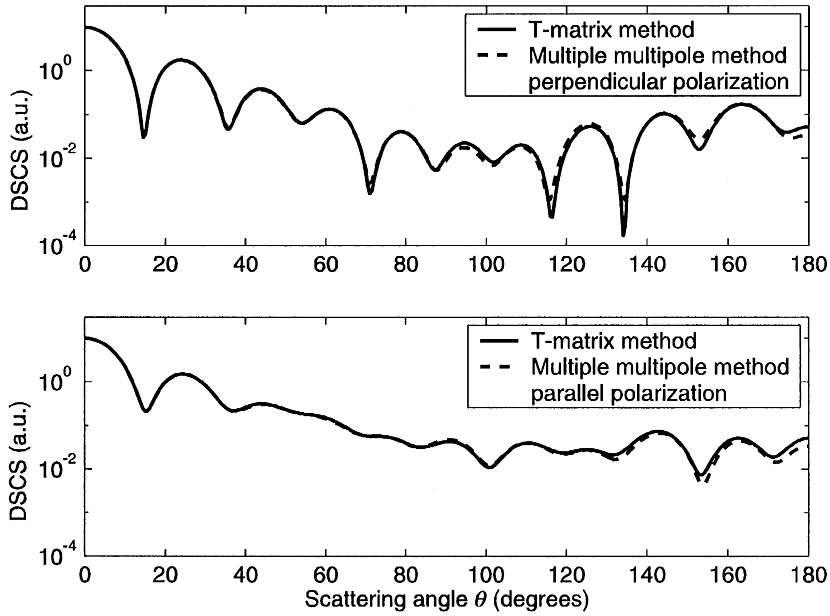

Fig. 5. Simulation of the scattering by a sphere $(k_S a_H = 10, n_H = 1.334)$ with two spherical inclusions $(k_S a_{I_1} = k_S a_{I_1} = 2,\ n = 1.6)$ with two different methods. The graphs show the perpendicular and parallel polarization, respectively.

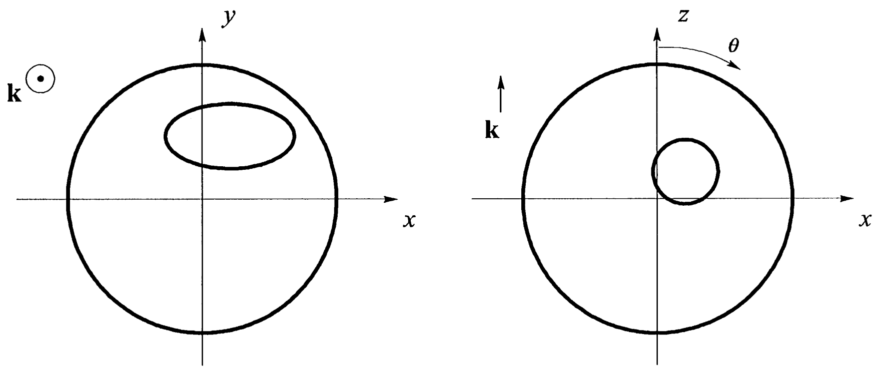

Fig. 6. Model of a sphere $(k_S a_H = 10,\ n_H = 1.334)$ with a prolate spheroid inclusion $(k_S a_I = 5,\ k_S b\mathrm{I} = 2.5,\ n_I = 1.6,\ \mathbf{r} = (2;4;2))$. The position coordinates $\mathbf{r}$ of the inclusion are given in units of the size parameter.

Complete agreement between the results serves as an evidence of the accuracy of both methods. In Table 1 we show the CPU-time for the T-matrix method and the multiple multipole method for the scattering geometries given in Figs. 5 and 7. Clearly, the T-matrix method needs less computational time than the multiple multipole method.

From our numerical analysis we may conclude that the T-matrix method can efficiently be used to compute the scattering characteristics of inhomogeneous spherical particles.

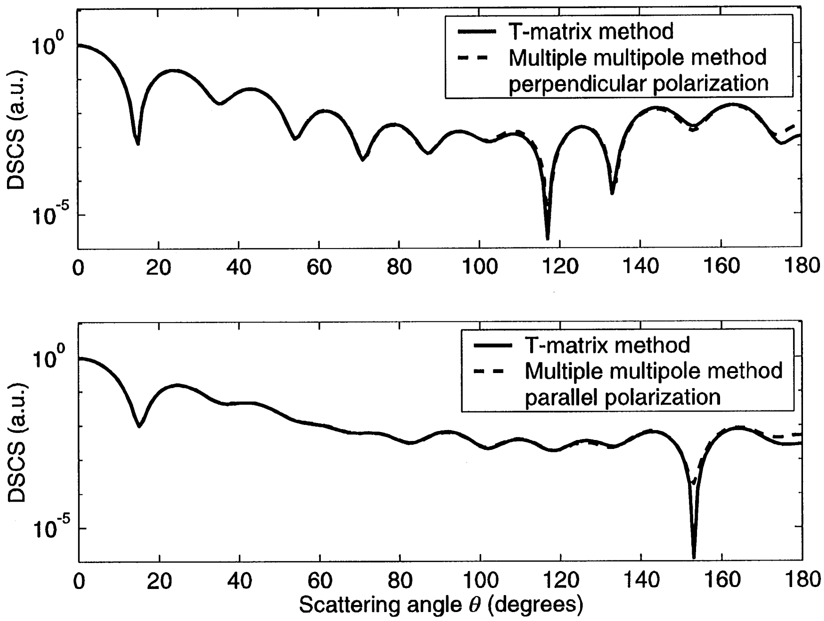

Fig. 7. Simulation of the scattering by a sphere ($k_s a_H = 10$, $n_H = 1.334$) with a prolate spheroid inclusion ($k_s a_I = 5$, $k_s b_I = 2.5$, $n_I = 1.6$, $\mathbf{r} = (2; 4; 2)$). The graphs show the perpendicular and parallel polarization, respectively.

Table 1

CPU-time for $k_s a_H = 10$	Spherical inclusion	Two inclusions	Prolate inclusion
Separation of variables method	~2 s	—	—
T-matrix method	~1 s	18 min	11 min
Multiple multipole method	50 min	175 min	155 min

4. Conclusion

Simulation of light scattering by inhomogeneous particles has been demonstrated for inhomogeneous spherical particles. Exemplary simulations have been done with three different methods: the T-matrix method, the multiple multipole method and the separation of variables method. Our computer simulations show that both the T-matrix program and the multiple multipole program demonstrated high flexibility for scattering by spheres with various types of inclusions. The computational demand is one order lower for the T-matrix program.

Acknowledgements

The authors acknowledge the support of this research project by the Deutsche Forschungsgemeinschaft (DFG).

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