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T-matrix method for biaxial anisotropic particles

Vladimir Schmidt^{a,*}, Thomas Wriedt^b^a Universität Bremen, Badgasteiner Str. 3, 28359 Brwemen, Germany^b Institut für Werkstofftechnik, Badgasteiner Str. 3, 28359 Bremen, Germany

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ABSTRACT

Using the T-matrix approach electromagnetic scattering by a biaxial anisotropic non-axisymmetric particle is studied. Electromagnetic fields inside the scatterer are expressed by a system of quasi-spherical vector wave functions which are derived by use of inverse Fourier transform. Using this expansion a solution of the light scattering problem in the framework of the null-field method with discrete sources is obtained.

Numerical scattering results for ellipsoids and cubes are presented. For validation the calculation results obtained are compared with results from other light scattering programs such as DDSCAT and ADDA.

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1. Introduction

Simulation of the optical properties of anisotropic scatterers is important in different scientific and technology applications. Many industrial materials are anisotropic. Such particles can be found for example as white pigments in paper and color pigments in paints.

The T-matrix approach is a modern and effective numerical tool for exactly solving the scattering problem proposed by Waterman [1]. An extensive review of this method have been published by Mishchenko et al. [2]. The method can be used for very accurate scattering calculations and for the determination of the applicability of various approximations, but up to now it has been applied almost exclusively to isotropic scatterers. Light scattering by anisotropic particles can be simulated by different approximate methods: the discrete dipole approximation (DDA) [3], the methods of moments (MoM) [4] and the generalized multipole technique (GMT) [5]. At the present time the solutions for anisotropic scatterers using the T-matrix approach are mostly obtained for simple shapes or for axisymmetric particles such as uniaxial anisotropic spheres [6–8], ellipsoids [9] or bianisotropic spheres [10,11].

For this development we extended the null-field method with discrete sources (NFM-DS) [12]. A review of the capabilities of this method has been published by Wriedt [13]. To solve the scattering problem in the terms of NFM-DS it is necessary to approximate the internal electromagnetic field by a basis of vector wave functions, e.g. in an isotropic medium regular vector spherical wave functions are used. Kiselev et al. [6] solved the scattering problem of radially and uniformly anisotropic spheres by using the so-called quasi-spherical vector wave functions (qSVWF) to represent the electromagnetic fields propagating inside the particle. Doicu [14] obtained the similar (except for a multiplicative constant) set of qSVWF by representing the electromagnetic field propagated in the medium as integrals over plane waves. The particular solution of

* Corresponding author. Tel.: +49 421 218 5418; fax: +49 421 218 3912.

E-mail addresses: vschmidt@iwt.uni-bremen.de, vschmidt@iwt.uni-bremen.de (V. Schmidt).

the light scattering problem using the T-matrix approach for uniaxial anisotropic non-axisymmetric particles is also given by Doicu [14].

Here we extended this approach from uniaxial to biaxial anisotropic scatterers considering homogeneous arbitrary shaped non-axisymmetric particles. For fast computation we developed a parallelized Fortran code using OpenMP technology. Additionally for validation we compare our simulation results with those obtained by other light scattering programs such as DDSCAT [3] and ADDA [15].

2. Quasi-spherical vector wave functions

The electromagnetic fields in the case of anisotropic medium are characterized by the stationary (or reduced) Maxwell equations [12]

$$\begin{aligned}\nabla \times \mathbf{E} &= ik\mathbf{B}, & \nabla \times \mathbf{H} &= -ik\mathbf{D}, \\ \nabla \cdot \mathbf{B} &= 0, & \nabla \cdot \mathbf{D} &= 0,\end{aligned}\quad (1)$$

and the constitutive relations

$$\mathbf{D} = \bar{\epsilon}\mathbf{E}, \quad \mathbf{B} = \bar{\mu}\mathbf{H}, \quad (2)$$

where $\bar{\epsilon}$, $\bar{\mu}$ are the electric permittivity and magnetic permeability tensors, respectively. Some permittivity tensors (particularly a real-valued tensor) can be transformed into the diagonal form (3) by a rotation of the principal coordinate system. Here we consider that the biaxial anisotropic medium consists of the isotropic permeability $\bar{\mu}$ and the anisotropic permittivity $\bar{\epsilon}$, which is described by a tensor with three different complex components

$$\bar{\epsilon} = \begin{pmatrix} \epsilon_x & 0 & 0 \\ 0 & \epsilon_y & 0 \\ 0 & 0 & \epsilon_z \end{pmatrix}, \quad \bar{\mu} = \mu. \quad (3)$$

The electromagnetic fields can be expressed as integrals over plane waves by using the inverse Fourier transform (excepting the factor $1/(2\pi)^3$):

$$\mathbf{X}(\mathbf{r}) = \int \mathcal{X}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} dV(\mathbf{k}), \quad (4)$$

where \mathbf{X} stands for \mathbf{E} , \mathbf{H} , \mathbf{D} and \mathbf{B} , \mathcal{X} stands for the Fourier transforms of \mathcal{E} , \mathcal{H} , \mathcal{D} , \mathcal{B} and k is the wave vector. Using the identities

$$\nabla \times \mathbf{X}(\mathbf{r}) = i \int k \times \mathcal{X}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} dV(\mathbf{k}), \quad (5)$$

$$\nabla \cdot \mathbf{X}(\mathbf{r}) = i \int k \cdot \mathcal{X}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} dV(\mathbf{k}), \quad (6)$$

the Maxwell equations (1) and the constitutive relations (2) become

$$\mathbf{k} \times \mathcal{E} = k_0\mathcal{B}, \quad \mathbf{k} \times \mathcal{H} = -k_0\mathcal{D}, \quad (7)$$

$$\mathbf{k} \cdot \mathcal{B} = 0, \quad \mathbf{k} \cdot \mathcal{D} = 0, \quad (8)$$

$$\mathcal{B} = \mu^{-1}\mathcal{H}, \quad \mathcal{E} = \epsilon^{-1}\mathcal{D}. \quad (9)$$

Let us consider a coordinate system with spherical unit vectors (e_k, e_β, e_α), in which the wave vector \mathbf{k} can be represented as the product $\mathbf{k} = k(\mathbf{e}_k \cdot \mathbf{e}_k)$. Denote $(\mathcal{A}_k, \mathcal{A}_\beta, \mathcal{A}_\alpha)$ the spherical coordinates of the vector \mathcal{A} and $\lambda_i = \epsilon_i^{-1}$, $i = \{x, y, z\}$. In this coordinate system Eqs. (7) and (8) become

$$\begin{bmatrix} \mathcal{E}_\beta \\ \mathcal{E}_\alpha \end{bmatrix} = \mu \left(\frac{k_0}{k}\right)^2 \begin{bmatrix} \mathcal{D}_\beta \\ \mathcal{D}_\alpha \end{bmatrix}, \quad \mathcal{D}_k = 0, \quad (10)$$

and Eqs. (9) become

$$\begin{bmatrix} \mathcal{E}_k \\ \mathcal{E}_\beta \\ \mathcal{E}_\alpha \end{bmatrix} = \begin{pmatrix} \lambda_{k\beta} & \lambda_{k\alpha} \\ \lambda_{\beta\beta} & \lambda_{\beta\alpha} \\ \lambda_{\beta\alpha} & \lambda_{\alpha\alpha} \end{pmatrix} \begin{bmatrix} \mathcal{D}_\beta \\ \mathcal{D}_\alpha \end{bmatrix}, \quad (11)$$

where

$$\begin{aligned}\lambda_{\beta\alpha} &= \cos(\beta) \sin(\alpha) \cos(\alpha)(\lambda_y - \lambda_x), & \lambda_{k\alpha} &= \tan(\beta)\lambda_{\beta\alpha}, \\ \lambda_{\alpha\alpha} &= \lambda_x \sin^2(\alpha) + \lambda_y \cos^2(\alpha), & \lambda_{k\beta} &= (\lambda_{\beta\beta} - \lambda_z) \tan(\beta), \\ \lambda_{\beta\beta} &= \cos^2(\beta)(\lambda_x \cos^2(\alpha) + \lambda_y \sin^2(\alpha)) + \sin^2(\beta)\lambda_z.\end{aligned}$$

Eqs. (10) and (11) yield a homogeneous system of equations for \mathcal{D}_β and \mathcal{D}_α

$$\begin{bmatrix} \lambda_{\beta\beta} - x & \lambda_{\beta\alpha} \\ \lambda_{\beta\alpha} & \lambda_{\alpha\alpha} - x \end{bmatrix} \begin{bmatrix} \mathcal{D}_\beta \\ \mathcal{D}_\alpha \end{bmatrix} = 0, \quad x = \mu \left(\frac{k_0}{k} \right)^2. \quad (12)$$

The solution of the eigenvalue problem (12) gives two eigenvalues (the wave numbers $k_{1,2}$) and two eigenvectors (the orthogonal plane waves $\mathbf{v}_{1,2}$)

$$\mathbf{v}_1 = f\mathbf{e}_\beta + \mathbf{e}_\alpha, \quad \mathbf{v}_2 = -\mathbf{e}_\beta + f\mathbf{e}_\alpha, \quad (13)$$

$$k_{1,2} = k_0 \sqrt{\mu/x_{1,2}}, \quad x_{1,2} = \frac{1}{2}(\lambda_{\beta\beta} + \lambda_{\alpha\alpha} \pm D), \quad (14)$$

$$D = \sqrt{(\lambda_{\beta\beta} - \lambda_{\alpha\alpha})^2 + 4\lambda_{\beta\alpha}^2}, \quad f = -2\lambda_{\beta\alpha}/(\lambda_{\beta\beta} - \lambda_{\alpha\alpha} - D). \quad (15)$$

Each solution \mathcal{D} of Eq. (12) can be presented as a linear combination of two orthogonal plane waves $\mathbf{v}_1, \mathbf{v}_2$ with two in general different wave number k_1, k_2 . Taking into account that $\mathbf{k}_{1,2} = k_{1,2}(\mathbf{e}_k) \cdot \mathbf{e}_k$ we find the integral representation of the electric displacement in the terms of unknown scalar functions

$$\mathbf{D}(\mathbf{r}) = \int_{\Omega} [\mathcal{D}_1(\mathbf{e}_k)\mathbf{v}_1(\mathbf{e}_k)e^{ik_1(\mathbf{e}_k)\mathbf{e}_k\cdot\mathbf{r}} + \mathcal{D}_2(\mathbf{e}_k)\mathbf{v}_2(\mathbf{e}_k)e^{ik_2(\mathbf{e}_k)\mathbf{e}_k\cdot\mathbf{r}}] d\Omega(\mathbf{e}_k), \quad (16)$$

where Ω is the unit sphere, \mathcal{D}_1 and \mathcal{D}_2 are the unknown scalar functions of spherical coordinates β and α .

Let us expand the tangential vector function $\mathcal{D}_1(\beta, \alpha)\mathbf{v}_1(\beta, \alpha) + \mathcal{D}_2(\beta, \alpha)\mathbf{v}_2(\beta, \alpha)$ on the unit sphere by the vector spherical harmonics $\mathbf{m}_{mn}(\beta, \alpha)$ and $\mathbf{n}_{mn}(\beta, \alpha)$ [16] as follows:

$$\mathcal{D}_1(\beta, \alpha)\mathbf{v}_1(\beta, \alpha) + \mathcal{D}_2(\beta, \alpha)\mathbf{v}_2(\beta, \alpha) = -\varepsilon_{xy} \sum_{n=1}^{\infty} \sum_{m=-n}^n \frac{1}{4\pi i^{n+1}} [-ic_{mn}\mathbf{m}_{mn}(\beta, \alpha) + d_{mn}\mathbf{n}_{mn}(\beta, \alpha)], \quad (17)$$

where

$$\begin{aligned} \mathbf{m}_{mn}(\beta, \alpha) &= [im\pi_n^{|m|}(\beta)\mathbf{e}_\beta - \tau_n^{|m|}(\beta)\mathbf{e}_\alpha]e^{im\alpha}, \\ \mathbf{n}_{mn}(\beta, \alpha) &= [\tau_n^{|m|}(\beta)\mathbf{e}_\beta + im\pi_n^{|m|}(\beta)\mathbf{e}_\alpha]e^{im\alpha}, \\ \varepsilon_{xy} &= (\varepsilon_x + \varepsilon_y)/2. \end{aligned} \quad (18)$$

This series representation is valid because the system of vector spherical harmonics is orthogonal and complete in $L_2(\Omega)$ [16]. Taking into account (10), (11) and (16)–(18) yields the series representations for the electric and magnetic fields

$$\mathbf{E}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^n c_{mn}\mathbf{X}_{mn}^e(\mathbf{r}) + d_{mn}\mathbf{Y}_{mn}^e(\mathbf{r}), \quad (19)$$

$$\mathbf{H}(\mathbf{r}) = -i\sqrt{\frac{\varepsilon_{xy}}{\mu}} \sum_{n=1}^{\infty} \sum_{m=-n}^n c_{mn}\mathbf{X}_{mn}^h(\mathbf{r}) + d_{mn}\mathbf{Y}_{mn}^h(\mathbf{r}), \quad (20)$$

where $\mathbf{X}_{mn}^{e,h}, \mathbf{Y}_{mn}^{e,h}$ are the basis vector functions

$$\begin{aligned} \mathbf{X}_{mn}^{e,h}(\mathbf{r}) &= \int_{\Omega} [A_{mn}\mathbf{w}_1^{e,h}e^{ik_1(\mathbf{e}_k)\mathbf{e}_k\cdot\mathbf{r}} + B_{mn}\mathbf{w}_2^{e,h}e^{ik_2(\mathbf{e}_k)\mathbf{e}_k\cdot\mathbf{r}}] dS(\Omega), \\ \mathbf{Y}_{mn}^{e,h}(\mathbf{r}) &= \int_{\Omega} [B_{mn}\mathbf{w}_1^{e,h}e^{ik_1(\mathbf{e}_k)\mathbf{e}_k\cdot\mathbf{r}} + A_{mn}\mathbf{w}_2^{e,h}e^{ik_2(\mathbf{e}_k)\mathbf{e}_k\cdot\mathbf{r}}] dS(\Omega), \\ A_{mn} &= [fm\pi_n^{|m|}(\beta) + i\tau_n^{|m|}(\beta)]e^{im\alpha}d_n/(1+f^2), \\ B_{mn} &= [im\pi_n^{|m|}(\beta) + f\tau_n^{|m|}(\beta)]e^{im\alpha}d_n/(1+f^2), \\ \mathbf{w}_{1,2}^e &= -\varepsilon_{xy}\mathbf{A} \cdot \mathbf{v}_{1,2}, \quad \mathbf{w}_{1,2}^h = \mp i\sqrt{\varepsilon_{xy}\mu}k_0/k_{1,2} \cdot \mathbf{v}_{1,2}. \end{aligned} \quad (21)$$

In (21) the electromagnetic fields are expressed in terms of the unknown coefficients c_{mn}, d_{mn} , which can be determined from the boundary conditions for each specific scattering problem. The vector functions $\mathbf{X}_{mn}^{e,h}$ and $\mathbf{Y}_{mn}^{e,h}$ can be regarded as a generalization of the regular vector spherical wave functions \mathbf{RgM}_{mn} and \mathbf{RgN}_{mn} , because they are equal to regular spherical vector wave functions in the isotropic case. According to Doicu [12] this system of vector functions will be referred to as the system of qSVWF.

3. Null-field method

Let us denote the homogeneous biaxial anisotropic interior of a particle as D_i and the homogeneous isotropic exterior as D_s . The transmission boundary-value problem has the following formulation.

From given $\mathbf{E}_e, \mathbf{H}_e$ as an entire solution of Maxwell equations representing the external excitation, find the vector fields $\mathbf{E}_s, \mathbf{H}_s$ and $\mathbf{E}_i, \mathbf{H}_i$ satisfying the Maxwell equations

$$\nabla \times \mathbf{E}_s = ik_0\mu_s\mathbf{H}_s, \quad \nabla \times \mathbf{H}_s = -ik_0\mu_s\mathbf{E}_s, \quad \mathbf{r} \in D_s \quad (22)$$

and

$$\nabla \times \mathbf{E}_i = ik_0\mu\mathbf{H}_i, \quad \nabla \times \mathbf{H}_s = -ik_0\bar{\epsilon}\mathbf{E}_i, \quad \mathbf{r} \in D_i. \quad (23)$$

In addition, the vector fields must satisfy the transmission conditions on S

$$\begin{aligned} \mathbf{n} \times \mathbf{E}_i - \mathbf{n} \times \mathbf{E}_s &= \mathbf{n} \times \mathbf{E}_e, \\ \mathbf{n} \times \mathbf{H}_i - \mathbf{n} \times \mathbf{H}_s &= \mathbf{n} \times \mathbf{H}_e \end{aligned} \quad (24)$$

and the Silver–Müller radiation condition

$$\frac{\mathbf{r}}{r} \times \sqrt{\mu_s}\mathbf{H}_s + \sqrt{\epsilon_s}\mathbf{E}_s = o\left(\frac{1}{r}\right) \quad \text{as } r \rightarrow \infty, \quad (25)$$

uniformly for all directions \mathbf{r}/r .

Following the null-field method the electromagnetic fields outside the circumscribed sphere are expanded into series of spherical vector wave functions

$$\mathbf{E}_e(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^n [a_{mn}\mathbf{M}(k_s\mathbf{r}) + b_{mn}\mathbf{N}(k_s\mathbf{r})], \quad (26)$$

$$\mathbf{E}_s(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^n [f_{mn}\mathbf{RgM}_i(k_s\mathbf{r}) + g_{mn}\mathbf{RgN}_i(k_s\mathbf{r})], \quad (27)$$

where $k_s = \sqrt{\epsilon_s\mu_s}$ is the wave number of isotropic surrounding medium, a_{mn} , b_{mn} and f_{mn} , g_{mn} are the expansion coefficients of the incident and scattered fields, respectively. Inside the inscribed sphere the electromagnetic fields are expressed in the terms of qSVWF (19).

Considering the null-field equations [12] and the expansions (19), (26), (27), the transition matrix of a biaxial anisotropic particle becomes

$$\mathbf{T} = -\mathbf{Q}_{biax}^{11}(\mathbf{Q}_{biax}^{31})^{-1}, \quad (28)$$

where the elements of the \mathbf{Q}_{biax}^{31} matrix for $\mu = \mu_s = \mu_0$ are given by

$$\begin{aligned} (Q_{anix}^{31})_{mm'n'}^{11} &= i\frac{k_s^2}{\pi} \int_S \left[(\mathbf{n} \times \mathbf{X}_{m'n'}^e) \cdot \mathbf{N}_{mn} + \sqrt{\frac{\epsilon_{xy}}{\epsilon_z}} (\mathbf{n} \times \mathbf{X}_{m'n'}^h) \cdot \mathbf{M}_{mn} \right] dS, \\ (Q_{anix}^{31})_{mm'n'}^{12} &= i\frac{k_s^2}{\pi} \int_S \left[(\mathbf{n} \times \mathbf{Y}_{m'n'}^e) \cdot \mathbf{N}_{mn} + \sqrt{\frac{\epsilon_{xy}}{\epsilon_z}} (\mathbf{n} \times \mathbf{Y}_{m'n'}^h) \cdot \mathbf{M}_{mn} \right] dS, \\ (Q_{anix}^{31})_{mm'n'}^{21} &= i\frac{k_s^2}{\pi} \int_S \left[(\mathbf{n} \times \mathbf{X}_{m'n'}^e) \cdot \mathbf{M}_{mn} + \sqrt{\frac{\epsilon_{xy}}{\epsilon_z}} (\mathbf{n} \times \mathbf{X}_{m'n'}^h) \cdot \mathbf{N}_{mn} \right] dS, \\ (Q_{anix}^{31})_{mm'n'}^{22} &= i\frac{k_s^2}{\pi} \int_S \left[(\mathbf{n} \times \mathbf{Y}_{m'n'}^e) \cdot \mathbf{M}_{mn} + \sqrt{\frac{\epsilon_{xy}}{\epsilon_z}} (\mathbf{n} \times \mathbf{Y}_{m'n'}^h) \cdot \mathbf{N}_{mn} \right] dS. \end{aligned}$$

The elements of the \mathbf{Q}_{biax}^{11} matrix are equivalent but with \mathbf{RgM}_{mn} and \mathbf{RgN}_{mn} in place of \mathbf{M}_{mn} and \mathbf{N}_{mn} , respectively.

4. Numerical results

The formulation presented in Sections 2 and 3 has been implemented into a Fortran program. The calculation of surface integrals within the matrixes Q^{11} and Q^{31} was parallelized using OpenMP technology. We divide the particle surface on a computer with N processors into N areas, provide integration for each area on each processor separately and then collect the results. Thereby the program can be effectively used on multi-processor computers.

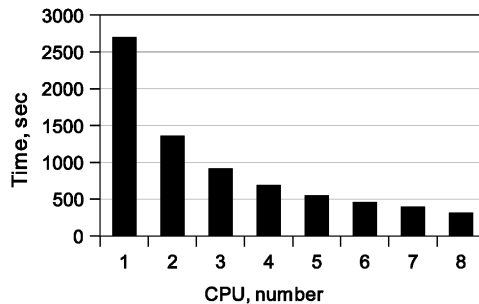


Fig. 1. Calculation time on computers with different number of processors computing scattering by a cube with the size parameters $k_s a = 4$, $k_s c = 4$ and the refractive index $m_r = (1.1, 1.5, 1.1)$.

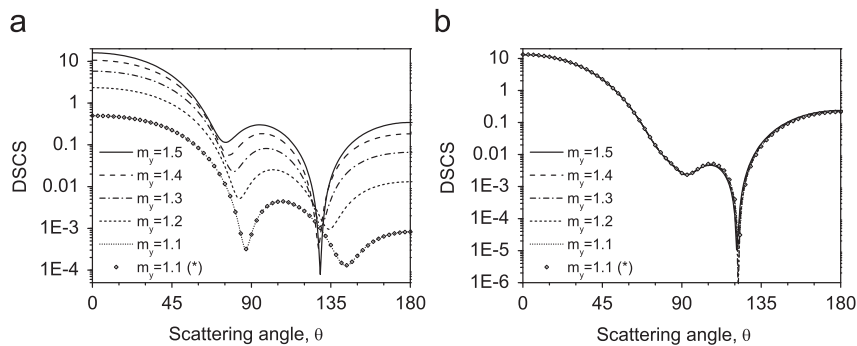


Fig. 2. Parallel (a) and perpendicular (b) components of the normalized differential scattering cross sections for an ellipsoidal particle with size parameters $k_s a = 2$, $k_s b = 3$, $k_s c = 4$ and the biaxial anisotropic refractive index $m_x = 1.5$, $m_z = 1.1$, $m_y \in \{1.1, 1.2, 1.3, 1.4, 1.5\}$ calculated with T-matrix and DDA program (*). The orientation of the particle is $\alpha = 0^\circ$, $\beta = 0^\circ$, $\gamma = 0^\circ$. The maximum number of azimuthal modes and expansion order are $M_{max} = 20$, $N_{max} = 20$. The number of integration points on the particle surface is 10 000 ($N_\theta = 100, N_\phi = 100$).

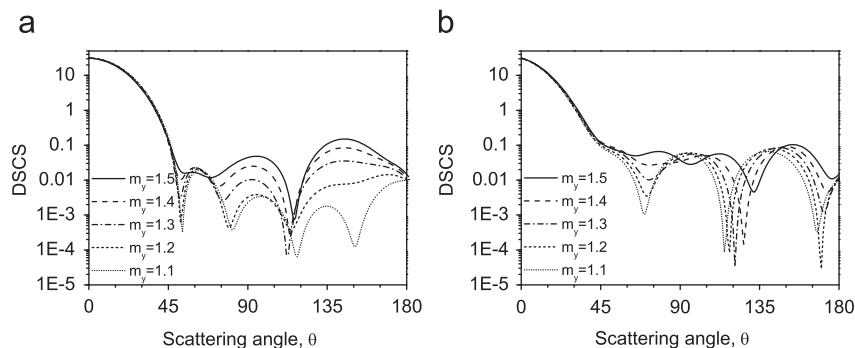


Fig. 3. Parallel (a) and perpendicular (b) components of the normalized differential scattering cross sections for a cube with size parameters $k_s a = 4$, $k_s b = 4$, $k_s c = 4$ and the biaxial anisotropic refractive index $m_x = 1.1$, $m_z = 1.1$, $m_y \in \{1.1, 1.2, 1.3, 1.4, 1.5\}$. The orientation of the particle is $\alpha = 45^\circ$, $\beta = 30^\circ$, $\gamma = 0^\circ$. The maximum number of azimuthal modes and expansion order are $M_{max} = 18$, $N_{max} = 18$. The number of integration points on each of the six facets is 625 ($N_\theta = 25, N_\phi = 25$).

The exemplary calculation times of computing scattering by cubes with the size parameters $k_s a = 4$, $k_s c = 4$ and the refractive index $m_r = (1.1, 1.5, 1.1)$ for different numbers of cores using the developed program are presented in Fig. 1. The simulations were produced on a Linux Workstation with double Quad Core Intel(R) Xeon(R) 2.33 GHz and 16 Gb RAM. One can see that the calculation time on eight cores is reduced to the factor about $\frac{1}{7}$.

In Figs. 2 and 3 we present the simulation results for a biaxial anisotropic ellipsoid and a cube, respectively. In both cases the incident wave is a plane wave travelling along the Z-axis of a global coordinate system OXYZ. The orientation of the particle with respect to the global coordinate system is given by the Euler angles α , β and γ . The differential scattering cross section (DSCS) normalised by πa_{eff}^2 is computed in the azimuthal plane $\phi = 0^\circ$ of the global coordinate system. Here we varied the m_y component of the refractive index, which is different from m_x and m_z giving biaxial anisotropy. In Fig. 2 the perpendicular component of DSCS is practically independent from this effect because in this case the electrical field oscillates in a plane, that is perpendicular to the y-axis, whose component of the refractive index is being varied.

To check our program we compared the simulation results in Fig. 2 with those obtained from other light scattering programs DDSCAT [3] and ADDA [15]. There is perfect agreement. Further comparisons show good congruence for non-imaginary anisotropic refractive indices as well for imaginary anisotropic refractive indices. Small differences in the case of a complex refractive index and for a non-cubic shape can be explained by approximation errors for the scatterer volume in the DDA approach.

5. Conclusion

The electromagnetic fields propagating in a biaxial anisotropic media have been expressed in terms of qSVWF, which can be considered a generalization of the system of regular spherical vector wave functions in the isotropic case. Using this expansion the T-matrix method has been extended from uniaxial to biaxial anisotropic scatterers of arbitrary shape. The comparison of simulation results to those using scattering programs based on the DDA approach shows good congruence, which confirms the correctness of the obtained results.

A parallelized Fortran code with high efficiency coefficient using OpenMP technology for calculating the T-matrix for such particles was developed. Thus a fast program to compute the T-matrix and in this way scattering for biaxial anisotropic as well as isotropic particles on modern multi-processor computers is available.

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