LIGHT SCATTERING FROM A CLUSTER CONSISTS OF DIELECTRIC NONCONCENTRIC ENCAPSULATION PARTICLES

Hany L. S. Ibrahim1 and Elsayed Esam M. Khaled2

1Telecom Egypt Company, Qina, Egypt
2Electrical Engineering Department, Faculty of Engineering, Assiut University, Assiut, Egypt

ABSTRACT

Random-orientation scattering properties of a plane wave scattered by a cluster of nonconcentric encapsulated particles, either layered particles form densely packed or linear chains, are presented. The computed results are shown for different spherical offset core in either spherical or nonspherical shell. A technique is based on a method that calculate the cluster T-matrix, and from which the orientation-averaged scattering matrix and total cross sections can be analytically obtained.

Keywords: Light Scattering, Clusters, T-Matrix

1. INTRODUCTION

Many scientific fields require understanding of the radiative properties of cluster particles which relevant to a wide variety of applications, as in pharmaceuticals, nanotechnology, chemistry, astrophysics, and biology and health sciences. So the calculations of electromagnetic scattering by cluster of spherical [1-4] or nonspherical [5] or from aggregated fibres [6] particles are important to realize the interaction between the incident electromagnetic fields and the cluster in such applications.

Micro-encapsulation in material science means the coating of microscopic particles with another material. The reasons for micro-encapsulation are countless. In some cases, improving the handling properties of a material as in a doped zinc sulfide (Zns) particle with a core can enhance the photoluminescence process [7,8]. Therefore the study of a cluster consists of coated spherical and nonspherical particles is the next logical extension. Lars [9] presented multiparticle scattering (MPS) model based on a generalized Lorenz-Mie theory to calculate near- and far-field scattering from arbitrary three-dimensional aggregates of coated spheres using parallel computing. Hany [10] presented scattering from a cluster consists of dielectric coated axisymmetric objects (either coated spherical or spheroidal particles) based on calculation of the $T$-matrix for a cluster.
The crucial advantage of the $T$-matrix method is that in the $T$-matrix all properties of the scattering process are contained. It is also easy to compute multiple scattering by a number of neighboring particles by combining the $T$-matrices of the single constituents of the ensemble to obtain the cluster $T$-matrix.

Most implementations of the $T$-matrix method are restricted to rotationally symmetric scattering objects. In this paper the scattering matrix of a cluster contains a nonhomogeneous coated particle illuminated with a plane wave is calculated, which combine the $T$-matrix of the single nonhomogeneous coated spherical or spheroidal particle using the modified LISA algorithm [11] with cluster $T$-matrix calculation [4]. The cluster $T$-matrix calculation algorithm is modified to fit with the nonconcentric core cases. Different computed results are presented for a cluster consists of coated (either spherical or spheroidal) particle in the form of densely packed clusters or linear chains both with different offset core. The modified code can calculate the efficiency factors and scattering matrix elements of the cluster for either a fixed or random orientation cluster with respect to an incident plane wave or a focused electromagnetic (laser) beam. In addition, the code can calculate either the interior electric field or exterior fields of the coated spheres or spheroids.

2. THEORETICAL ANALYSIS

Figures 1-4 shows a cluster consists of coated spherical and spheroidal particles with an off-centered core. The shell is centered at the origin of a right-handed Cartesian coordinate system $(x, y, z)$. The radius of the shell is $a_s$, and that of the core is $a_c$. The offset distance is measured by the value $L$. The cluster is illuminated with a plane wave propagating along the $z$-direction.

![Fig.1. A linear chain consists of five identical coated spherical particles with off centered spherical cores](image1)

![Fig.2. A packed cluster consists of five identical coated spherical particles with off centered spherical cores](image2)
Fig. 3. A linear chain consists of five identical coated oblate spheroidal particles with off centered spherical cores.

Fig. 4. A packed cluster consists of five identical coated oblate spheroidal particles with off centered spherical cores.

The scattered field from a cluster consisting of $N_S$ coated axisymmetric particles is resolved into partial fields scattered from each particle in the cluster [4] i.e.

$$E_s = \sum_{i=1}^{N_S} E_i$$  \hspace{1cm} (1)

where each partial field $E_i$ is represented by an expansion of vector spherical harmonics (VSH) that are manipulated with respect to the origin of the $i$th coated axisymmetric objects,

$$E_i = H \sum_{m,n} D_{mn} \left[ f_m^{e} M_m^{3}(kr) + f_m^{o} M_m^{3}(kr) + g_m^{e} N_m^{3}(kr) + g_m^{o} N_m^{3}(kr) \right]$$  \hspace{1cm} (2)

where $H$, and $D_{mn}$ are normalization factors, are the VSH of the third kind (outgoing wave functions) obtained from the VSH of the first kind. The coefficients $f_m^{e}$, $f_m^{o}$, $g_m^{e}$, and $g_m^{o}$ are the scattered
field expansion coefficients for the \(i\)th coated object. All the parameters and details of the analysis are given in [12-14].

The field arriving at the surface of the \(i\)th coated object consists of the incident field plus the scattered fields that originate from all other coated objects in the cluster. Therefore a system of equations for the scattering coefficients \(f_i, g_i\) of \(i\)th coated particle can be constructed using the centered T-matrix of the cluster as follow [10],

\[
\begin{bmatrix}
    f^{i}_{emn} \\
    f^{i}_{omn} \\
    g^{i}_{emn} \\
    g^{i}_{omn}
\end{bmatrix} = \sum_{j=1}^{N} \sum_{n'=1}^{N_{O,i}} \sum_{m'=-n'}^{n'} T^{ij}_{mn m'n'} \begin{bmatrix}
    a^{j}_{em'n'} \\
    a^{j}_{om'n'} \\
    b^{j}_{em'n'} \\
    b^{j}_{om'n'}
\end{bmatrix}
\]

where \(N_{O,i}\) is the maximum order retained in the individual of coated object scattered field expansions, \(N_{O,i}\) will be proportional to the size parameter \(x_i\) of the individual coated axisymmetric objects, \(N_S\) is the number of the coated axisymmetric particles in the cluster, and \(a_{mn}, b_{mn}\) denote the expansion coefficients for the incident field from the objects \(j\) and it is described in [12], [13], \(e\) and \(o\) refer to even and odd respectively.

The procedure for calculating the \(T\) matrix of a cluster is started with calculating the coated particle-centered matrix \(T^0\) by using the code described in [15] for each coated particle with refractive indices \(m_c\) (core) and \(m_s\) (shell) as,

\[
T^{ij} = -B^*A^{-1} = - \left[ B_s + B_{cs} \left( -B_c A_c^{-1} \right) \right] \left[ A_s + A_{cs} \left( -B_c A_c^{-1} \right) \right]^{-1} \]

where:

- \(T_c = -B_c A_c^{-1}\), is the \(T\)-matrix calculated for any particle in the cluster with refractive index \(m=m_c/m_s\) for the inner layer (core), and the size parameter as \(R/m_s x\). In other words, it is the \(T\)-matrix for the core alone without the shell, where \(R = r_c/r_s\), \(x\) is the size parameter of the outer surface.

- \(B_s\) and \(A_s\), are calculated using the refractive index equal to \(m\), for outer layer and the size parameter equal to \(x\). So the product \(-B_s A_s^{-1}\) would be the \(T\)-matrix for a particle with no core.

- Matrices \(A_{cs}\) and \(B_{cs}\) are calculated in the same way as \(A_s\) and \(B_s\) except that the Bessel functions of the first kind with argument \(kr\) are replaced by Hankel functions with the same argument.

Different shapes can be chosen for core and coating as long as it has a mathematical representation, the only practical limitation, from a logical point of view is that the core should not protrude out of the coating. An offset coated sphere in which the centers of both core and shell are
separated by a distance \( L \) is considered. If the shell is assumed to be centered at the origin of the coordinates and the core of radius \( a_c \) is offset by \( L \). The surface of the core can be described as

\[
r(\theta) = a_c \left[ p \cos (\theta) + (1 - p^2 \sin^2 (\theta))^{\frac{1}{2}} \right]
\]

where \( a_c \) is the radius of the core, and \( p = L/a_s \). By defining the core/particle size ratio \( R = a_c/a_s \), it can be seen that the inner core remains inside the shell as long as the condition \((L/a_s + R) \leq 1\) is fulfilled.

The detailed analysis for the mathematical and numerical procedures can be found in [15, 16].

Merging the \( T_{ij} \), obtained above, into the cluster matrix through the following equation, the \( T \)-matrix of the cluster can be obtained

\[
T_{nl} = \sum_{i = 1}^{N_s} \sum_{j = 1}^{N_s} \sum_{n = 1}^{N_n} \sum_{l = 1}^{N_l} j_{n l}^{o i} \cdot T_{n l}^{i j} \cdot j_{n l}^{j o}
\]

where \( j_{n l}^{o i} \) and \( j_{n l}^{j o} \) matrices are formed from the addition coefficients based on the spherical Bessel function, the other parameters and details of the analysis are given in [4].

The Stokes parameters \( I, Q, U \) and \( V \) which define the relation between the incident and scattered light are specified with respect to the plane of the scattering direction [12]. The transformation of the Stokes parameters upon scattering is described by the real valued 4×4 Stokes scattering matrix \( S \). Although each element of the scattering matrix depends on the scattering angle \( \Theta_{sca} \), there is no dependence on the azimuthal scattering angle \( \Phi_{sca} \) for the collections of identical randomly oriented particles considered here. For a collection of randomly oriented particles, the scattering matrix reduces to:

\[
\begin{bmatrix}
I_{sca} \\
Q_{sca} \\
U_{sca} \\
V_{sca}
\end{bmatrix} = \begin{bmatrix}
S_{11}(\Theta) & S_{21}(\Theta) & 0 & 0 \\
S_{21}(\Theta) & S_{22}(\Theta) & 0 & 0 \\
0 & 0 & S_{33}(\Theta) & S_{34}(\Theta) \\
0 & 0 & -S_{34}(\Theta) & S_{44}(\Theta)
\end{bmatrix}\begin{bmatrix}
I^{inc} \\
Q^{inc} \\
U^{inc} \\
V^{inc}
\end{bmatrix}
\]

(6)

The elements of the scattering matrix can be used to define specific optical observables corresponding to different types of polarization state of the incoming light. For example, if the incident radiation is unpolarized, then the \((1,1)\) element characterizes the angular distribution of the scattered intensity in the far-field zone of the target, while the ratio \(-S_{21}(\Theta)/S_{11}(\Theta)\) gives the corresponding angular distribution of the degree of linear polarization. If the incident radiation is linearly polarized in the scattering plane, then the angular distribution of the cross-polarized scattered intensity is given by \( \frac{1}{2} [S_{31}(\Theta) - S_{22}(\Theta)] \) as described in [12, 14]. All of the \( S_{ij} \) can be written in terms of \( S_1, S_2, S_3, S_4 \). For example, \( S_{34} = -\text{Im}\left(S_1 S_2^* - S_4 S_3^*\right) \). Where the scattering matrix relating the Stoke's parameter has its basis in the amplitude scattering matrix,

\[
\begin{bmatrix}
\frac{E_1^i}{E_1^\perp} \\
\frac{E_2^i}{E_2^\perp}
\end{bmatrix} = e^{ikr} \begin{bmatrix}
S_2 & S_3 \\
S_4 & S_1
\end{bmatrix}\begin{bmatrix}
\frac{E_1}{E_1^\perp} \\
\frac{E_2}{E_2^\perp}
\end{bmatrix}
\]

(7)
kr is argument of the vector spherical wave function, and \( r \) is the position vector. The incident field has been evaluated at \( z=0 \). \( E_{\parallel} \) is the electric field component polarized parallel to the x-z scattering plane, \( E_{\perp} \) is the electric field component polarized perpendicular to the x-z scattering plane, and

\[
S_1 = \text{the } \perp \text{ scattered field amplitude for } \perp \text{ incident}
\]
\[
S_2 = \text{the } \parallel \text{ scattered field amplitude for } \parallel \text{ incident}
\]
\[
S_3 = \text{the } \parallel \text{ scattered field amplitude for } \perp \text{ incident}
\]
\[
S_4 = \text{the } \perp \text{ scattered field amplitude for } \parallel \text{ incident}
\]

3. NUMERICAL RESULTS

The code used in Ref [10] is modified to handle the elements calculations of the \( T \)-matrix of the ensemble cluster with general case. In case of an axisymmetric object, the \( A \) and \( B \)-matrices in Eq (4) are block diagonal matrices depending on the properties of the scatterer. Each block is a full matrix. In Ref [4], the elements calculations of the \( T \)-matrix restricted to spherical case, which are the calculations of Lorenz/Mie-coefficients for each single sphere. Also the modified code can deal with different shape, size and refractive index for each particle in the cluster. Note that calculating the elements of the \( T \)-matrix for spheroids requires tests for convergence and accuracy. For more details see Ref [15]. Moreover in case of a cluster of coated spheroids with nonconcentric core tests over convergence and accuracy need more attention.

Some published cases in literature are recomputed using the modified new codes to confirm the performance, capabilities, and truthful results that can be obtained using the presented modified technique. The first test case is that the cluster shown in Figs 1-4. is considered but with the refractive indices for the cores be unity, i.e. the cluster becomes a linear chain or packed cluster consists of five identical homogenous spherical or spheroidal particles as the cases presented in [4,17] with size parameter \( x=2\pi a_s/\lambda=5 \) for each particle. The obtained results for these cases are typical with results in Refs [4, 17]. The second test case is that the offsets of the cores in cases presented in Figs.1-4 are zero, i.e. the cluster becomes chain or packed cluster consists of five identical homogenous coated spherical or spheroidal particles as the cases presented in [10]. The obtained results for each case are typical with corresponding results in Ref [10] for the same parameters. Finally the last test case is that assigning the relative refractive indices of the nonhomogeneous coated particles presented in Figs.1, 2 to one except the centered particle, i.e. the cluster becomes a centered nonhomogeneous coated spherical particle alone. The results of the angular scattering intensities are identical with the corresponding results published in the literature [16].

The modified codes are then used for different cases as illustrated in Figs. 1-4. First consider a cluster consists of nonhomogeneous coated spherical particles form a linear chain or a packed hexagonal lattice illuminated with a plane wave as in Figs 1, 2. Different computed results of the scattering matrix elements as a function of scattering angle \( \Theta \) are presented for different offsets of the core \( p=L/a_c=0, p=0.1 \text{ and } p=0.5 \), and the size parameter of the individual coated spheres are 5. The ratio \( R= a_c/a_s \) is 0.5 and the refractive indices \( m_s=1.36 \text{ and } m_c=1.5+0.005i \) for the shell and the core respectively. The computed results are shown in Figs 5, 6.
Fig. 5. Orientation-averaged scattering matrix elements for a linear chain cluster consist of five identical coated spherical particles each with an off centered spherical core as illustrated in Fig. 1. The ratio \( R = \frac{a_c}{a_s} = 0.5 \) for each case, the size parameter is \( x = \frac{2\pi a_s}{\lambda} = 5 \), and \( m_s = 1.36 \), \( m_c = 1.5 + 0.005i \). The cluster is illuminated with a plane wave propagating in the z-direction.

The offset parameter for the core is \( p = \frac{L}{a_c} = 0, p = 0.1, p = 0.5 \).
Fig. 6. Orientation-averaged scattering matrix element for a packed cluster consists of five identical coated spherical particles each with an off centered spherical core as illustrated in Fig.2.. The ratio $R=ac/as=0.5$ for each case, the size parameter is $x=2\pi as/\lambda=5$, and $m_s=1.36$, $m_c=1.5+0.005i$. The cluster is illuminated with a plane wave propagation in the z-direction. The offset parameter for the core is $p=L/ac=0$, $p=0.1$, $p=0.5$. 
P=0 means concentric core, P=0.1 means the separated distance L between the centers of the core and the shell equal to p*a_c=0.0397887μm and P=0.5 is corresponding to an offset distance equal to p*a_c=0.1989436μm.

A quick glance at the results illustrated in Fig. 5, reveals that the configuration of the nonhomogeneous coated spheres can have a significant effect on the scattering properties of the cluster. The results of each case having successive values p=0.0, 0.1, 0.5 are changed gradually which gives logical interpretation. The values of the element S_{11} vary with the parameter p=L/a_c around the backward direction. In the forward direction S_{11} is nearly independent of the ratio p. Increasing the offset in this case the effect becomes more evidence. The locations of the oscillations of the scattering elements for the linear chain and packed cluster are nearly the same, which means the movement of the core have no effect in locations of the oscillations but has effect in the amplitude of the oscillations. Note that the only difference between the two configurations is the placement of the nonhomogeneous coated spheres in the cluster.

The modified code deals with not only cluster consists of spherical particles of nonconcentric cores but also it deals with cluster consists of spheroidal particles with nonconcentric spherical core as shown in Figs. 3, 4. In the first case the cluster consists of five particles of an oblate spheroidal particles form a linear chain (Fig.3) or a packed of a hexagonal lattice (Fig.4). The refractive index of the particle is m_s=2.2, size parameter x_s=4, and the ratio a/b=0.8 for each particle. Each particle is doped by a spherical core of a size parameter x_c=2 and refractive index m_c=2.43. The cluster is arranged with respect to a Cartesian coordinate system x,y,z as shown in Figs.3, 4. The cluster is illuminated with a plane wave propagating in the z-direction. Different computed results of scattering matrix elements as a function of scattering angle θ are presented for different offsets of the cores p=L/a_c =0, p=0.1 and p=0.5. The computed results are shown in Figs.7, 8. The parameters m_c, m_s, x_c, x_c which are considered in this case are coincident with a particle case in which the shell is a zinc sulfide (ZnS) doped by a core of spherical copper (CU). This construct illuminate light for longer time when illuminated with picosecond pulsed light due to low order resonant modes excited in the particle [7, 8].

The results of S_{11} show that when a cluster of ZnS oblate particles of ρ=0.8 doped by CU core sat p=0, the scattered field is smaller than that for the cluster of homogeneous ZnS particles of the same axial ratio as shown for the chain and packed cluster in Figs 7 and 8 respectively. It means that the field intensity distribution inside and outside the cluster depend on the value of the ratio ρ=a/b of the coated particle [8] and on the position of the doping. Also the illustrated results reveal that doping the copper cores in position p=0.1 to 0.5 provide gradually changes from p=0 doping position. Increasing the offset of the copper cores in the ZnS coated particle, increase the changes in the scattering matrix as shown in Figs.7, 8. The results show that the amplitude of the oscillations in this case is greater than those for a similar cluster consists of homogeneous spheroidal particles. This finding helps to calculate maps of the electric field distribution in and out of the cluster to enhance the photoluminescence criteria. Note that the only difference between the two configurations is the placement of the nonhomogeneous coated particles in the cluster as illustrated in Figs.3, 4.

Maximum number of particles (either homogeneous or coated) included in a cluster depends on how much memory the code will use. Calculations of the T-matrix of a cluster consists of five nonhomogeneous coated particles by the present modified code required 10 min of CPU time computer of 4GB RAM and CPU i5, 2.4GHz.
Fig. 7. Orientation-averaged scattering matrix element for a linear chain cluster consists of five identical oblate spheroidal particles as shown in Fig. 3 with refractive index $m=2.2$, size parameter $x=4$, and the ratio $a/b=0.8$ for each particle, doped by a spherical copper (CU) core. The size parameter of the core is 2 and refractive index 2.43. The cluster is illuminated with a plane wave propagating in the $z$-direction. The offset parameter for the core is $p=L/\lambda c = 0, p=0.1, p=0.5$.
Fig. 8. Orientation-averaged scattering matrix element for a packed cluster consists of five identical oblate spheroidal particles as shown in Fig. 4 with refractive index $m=2.2$, size parameter $x=4$, and the ratio $a/b=0.8$ for each particle, doped by a spherical copper (CU) core. The size parameter of the core is 2 and refractive index 2.43. The cluster is illuminated with a plane wave propagating in the $z$-direction. The offset parameter for the core is $p=L/ac=0$, $p=0.1$, $p=0.5$. 
4. CONCLUSIONS

A technique is modified and developed in this paper based on calculations of a cluster $T$-matrix to determine the random-orientation scattering properties. The cluster consists of nonhomogeneous coated spherical and spheroidal particles in the form of densely linear chains and packed clusters. The feature of the presented code is that it deals with a cluster of spherical particles as well as with a cluster consists of spherical or nonspherical particles doped with concentric or nonconcentric spherical cores. Different computed results are presented with different offsets of the cores.

REFERENCES


