LIGHT SCATTERING BY FRACTAL DUST AGGREGATES. I. ANGULAR DEPENDENCE OF SCATTERING

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ABSTRACT

In protoplanetary disks, micron-sized dust grains coagulate to form highly porous dust aggregates. Because the optical properties of these aggregates are not completely understood, it is important to investigate how porous dust aggregates scatter light. In this study, the light scattering properties of porous dust aggregates were calculated using a rigorous method, the $T$-matrix method, and the results were then compared with those obtained using the Rayleigh–Gans–Debye (RGD) theory and Mie theory with the effective medium approximation (EMT). The RGD theory is applicable to moderately large aggregates made of nearly transparent monomers. This study considered two types of porous dust aggregates—ballistic cluster–cluster agglomerates (BCCAs) and ballistic particle–cluster agglomerates. First, the angular dependence of the scattered intensity was shown to reflect the hierarchical structure of dust aggregates; the large-scale structure of the aggregates is responsible for the intensity at small scattering angles, and their small-scale structure determines the intensity at large scattering angles. Second, it was determined that the EMT underestimates the backward scattering intensity by multiple orders of magnitude, especially in BCCAs, because the EMT averages the structure within the size of the aggregates. It was concluded that the RGD theory is a very useful method for calculating the optical properties of BCCAs.

Key words: methods: analytical – polarization – protoplanetary disks – radiative transfer – scattering

1. INTRODUCTION

Protoplanetary disks form around protostars and are thought to be sites of ongoing planet formation. Planetesimals are formed from dust grains in protoplanetary disks; however, the theory of planetesimal formation involves many problems (e.g., Blum & Wurm 2008; Brauer et al. 2008; Zsom et al. 2010). One serious problem is that once dust grains become an approximately meter-sized body, the grains drift radially toward the central star because of the strong headwind of disk gas (Whipple 1972; Adachi et al. 1976; Weidenschilling 1977). The timescale of this radial drift is much shorter than that of the compact grain growth, and thus the size of the dust grain bodies cannot grow beyond the order of meters. This problem is often referred to as the radial drift barrier. Recent numerical studies have shown that the radial drift barrier and other related problems can be avoided by employing the porous aggregation model of icy particles (Okuzumi et al. 2012; Kataoka et al. 2013). Because of the strong adherence of icy particles to one another due to hydrogen bonding, icy dust aggregates are expected not to suffer severe disruption when they experience high-speed collisions (Wada et al. 2009, 2013; Gundlach et al. 2011). Previous studies have predicted the presence of highly porous dust aggregates in protoplanetary disks, but their presence has not yet been confirmed by observation.

Aggregates in disks are often modeled using one of two limiting aggregation models—the ballistic cluster–cluster agglomerate (BCCA) and ballistic particle–cluster agglomerate (BPCA) models—which have fractal dimensions of $d_f < 2$ (highly porous) and $d_f \approx 3$ (compact), respectively. In the initial stage of the coagulation process, the aggregate tends to have $d_f \lesssim 2$, as in BCCAs (Smirnov 1990; Meakin 1991; Kempf et al. 1999; Blum & Wurm 2000). Highly porous dust aggregates are readily stirred up to the surface layer of the disk because of their strong coupling with the disk gas. Hence, highly porous dust aggregates contribute to the scattering of stellar radiation, and their optical properties govern the appearance of the disks at near-infrared wavelengths, including their surface brightness, brightness asymmetry, and color. As dust aggregates grow larger, they become compressed by mutual collisions, gas compression, and self-gravity (Dominik & Tielens 1997; Blum & Wurm 2000; Suyama et al. 2008, 2012; Paszun & Dominik 2009; Okuzumi et al. 2012; Kataoka et al. 2013), causing them to settle down to the midplane of the disk. Hence, such compressed aggregates can be observed at millimeter wavelengths.

To investigate how the presence of fractal dust aggregates alters the observed image, their optical properties must be known. The opacity and light scattering properties of dust aggregates have been investigated by various authors (e.g., Wright 1987; Kozasa et al. 1992, 1993; Stognienko et al. 1995; Henning & Stognienko 1996; Kimura et al. 2003, 2006, 2008, 2016; Kolokolova et al. 2007; Kolokolova & Kimura 2010; Köhler et al. 2011). More recently, Min et al. (2016) investigated the light scattering properties of compact dust aggregates. In the present study, the light scattering properties of both fluffy and compact dust aggregates have been investigated.

Many previous studies have assumed that dust grains are spherical, which allows the use of the exact Mie solution (Mie 1908; Bohren & Huffman 1983). However, the calculation of the optical properties of nonspherical particles is not an easy task (e.g., Mishchenko et al. 2000) and is generally achieved by utilizing numerical methods, such as the discrete dipole approximation (DDA; Purcell & Pennypacker 1973;
Draine & Flatau 1994 and the T-matrix method (TMM; Mishchenko et al. 1996). Although the radiative transfer calculations that take into account the porosity of the grains in the disks have been performed by several authors (Min et al. 2012; Kirchschlager & Wolf 2014; Murakawa 2014), the high computational demands of such methods restricted these studies to the use of a simple dust model or approximations of the optical properties. Because of the limitations of radiative transfer calculations, methods of modeling observations are also limited. Some near-infrared imaging observations of disks cannot be explained by compact dust grains, and the inconsistencies between the observed properties and the results of Mie theory may be attributable to the presence of dust aggregates (e.g., Pinte et al. 2008; Mulders et al. 2013). These facts motivated us to develop a simple and accurate model of the light scattering properties of dust aggregates.

Because of its simplicity, the effective medium theory (EMT), or Mie theory using the effective medium approximation, is often used (e.g., Cuzzi et al. 2014; Kataoka et al. 2014). The EMT allows the effective dielectric function of an inhomogeneous material to be calculated (e.g., Chýlek et al. 2000). In the EMT, an aggregate is replaced with a single sphere with a characteristic radius and an effective dielectric function. Because the derivation of the effective dielectric function usually assumes the presence of electrostatic fields, the EMT is valid only for Rayleigh inclusions, that is, the inclusions are smaller than the incident wavelength. The validity of EMT has been tested by various authors (e.g., Chýlek et al. 1990; Kozasa et al. 1992, 1993; Voshchinnikov et al. 2005, 2007; Min et al. 2006; Shen et al. 2008, 2009). When the above condition is satisfied and when the volume filling factor of inclusions is small enough, the EMT tends to reproduce general features of integrated properties, such as absorption and scattering opacity. However, it fails to reproduce angle-dependent properties, such as the phase matrix elements, and a subsequent paper in this series will discuss the angle-integrated properties, such as absorption and scattering opacity. This paper is organized as follows. Section 2 summarizes models of light scattering by fractal dust aggregates. In Section 3, the statistical model of fractal dust aggregates, which plays a key role in the RGD theory, is described. Section 4 reports the rigorous results of the phase matrix elements obtained by the TMM and shows that the RGD theory is able to reproduce these rigorous results. The applicability of the RGD theory is discussed in Section 5. Section 6 summarizes the results of this study.

2. LIGHT SCATTERING MODELS

The scattering process can be described by the phase matrix that represents the transition from the vector of the Stokes parameters for the incident light \((I_{\text{inc}}, Q_{\text{inc}}, U_{\text{inc}}, V_{\text{inc}})\) to that for the scattered light \((I_{\text{sca}}, Q_{\text{sca}}, U_{\text{sca}}, V_{\text{sca}})\). This paper focuses on the average optical properties of a distribution of randomly oriented dust aggregates. For example, if the dust aggregates align in the same way owing to some effect, such as a magnetic field, the assumption of random orientation would break down. However, this paper investigates the situation in which the above condition is naturally satisfied in the disks. For a distribution of randomly oriented aggregates, the phase matrix can be reduced to

\[
\begin{pmatrix}
I_{\text{sca}} \\
Q_{\text{sca}} \\
U_{\text{sca}} \\
V_{\text{sca}}
\end{pmatrix} = \frac{1}{k^2 r^2} \begin{pmatrix}
S_{11} & S_{12} & 0 & 0 \\
S_{12} & S_{22} & 0 & 0 \\
0 & 0 & S_{33} & S_{34} \\
0 & 0 & -S_{34} & S_{44}
\end{pmatrix} \begin{pmatrix}
I_{\text{inc}} \\
Q_{\text{inc}} \\
U_{\text{inc}} \\
V_{\text{inc}}
\end{pmatrix}
\]

where \(k\) is the wavenumber, \(r\) is the distance from the scatterer to the observer, and \(S_{ij}\) \((i, j = 1, 2, 3, 4)\) represents the phase matrix elements. In general, a phase matrix contains 16 independent elements. Assuming rotational and mirror symmetry of the aggregates, the phase matrix has eight nonzero elements, six of which are independent (Bohren & Huffman 1983, hereafter BH83). Because of this symmetry, each phase matrix element depends on the scattering angle \(\theta\) but not on the azimuthal angle \(\phi\). Note that the scattering angle is
defined as the angle between the incident wavevector \( \mathbf{k}_i \) and the scattered wavevector \( \mathbf{k}_s \).

2.1. Scattering by Fractal Dust Aggregates

This section introduces three models for calculating the optical properties of fractal dust aggregates. The term monomer is used to indicate a constituent particle of a dust aggregate, and for the sake of simplicity, all monomers are assumed to be spherical and identical throughout the aggregates.

2.1.1. T-matrix Method

The optical properties of dust aggregates were calculated using the TMM, which is one of the most rigorous methods of calculating the optical properties of an ensemble of spheres (for a review, see, e.g., Mishchenko et al. 1996). By virtue of the exact Mie solution, the optical properties of a collection of spherical particles can theoretically be obtained using the superposition principle. We used the Fortran 77 code SCSMFO1B.FOR developed by Mackowski & Mishchenko (1996), which is designed to calculate the optical properties of multiple spheres. In addition, to reduce the numerical cost, orientation averaging was conducted using the quasi-Monte Carlo method developed by Okada (2008). This averaging was performed with 30 orientations for each dust aggregate. A detailed model of the dust aggregates used in this study is described in Section 3.2.

2.1.2. Mie Theory with Effective Medium Approximation

The EMT allows us to calculate the optical properties of dust aggregates using Mie theory (e.g., Chýlek et al. 2000). Because Mie theory is only applicable to homogeneous spheres, each aggregate is replaced with a single homogeneous pseudosphere with an effective dielectric function. One way to obtain the effective dielectric function is to calculate the average polarizability of the vacuums and monomers weighted by the volume filling factor. The dielectric functions of the monomer (inclusion component) and vacuum (matrix component) are denoted by \( \epsilon_i \) and \( \epsilon_m \), respectively. The single inclusion embedded in the matrix has a polarizability of \( \alpha_0 = 4\pi R_0^3 (\epsilon_i - \epsilon_m)/(\epsilon_i + 2\epsilon_m) \), where \( R_0 \) is the radius of a monomer (see Equation (5.15) in BH83). The total polarizability of an aggregate of \( N \) monomers can be presumed to be

\[
\alpha_{agg} = N\alpha_0 \quad \text{as long as interactions between monomers can be disregarded.}
\]

Equating \( \alpha_{agg} \) with the polarizability of a sphere of radius \( R \) and effective dielectric function \( \epsilon_{eff} \) yields

\[
R_0^3 \epsilon_{eff} - \epsilon_m = N R_0^3 \frac{\epsilon_i - \epsilon_m}{\epsilon_i + 2\epsilon_m},
\]

Solving Equation (2) for \( \epsilon_{eff} \) yields

\[
\epsilon_{eff} = \frac{\epsilon_m + 2\epsilon_m + 2f(\epsilon_i - \epsilon_m)}{\epsilon_i + 2\epsilon_m - f(\epsilon_i - \epsilon_m)},
\]

where \( f \) is the volume fraction of inclusions in the matrix and is given by

\[
f = N \left( \frac{R_0}{R_c} \right)^3.
\]

This effective dielectric function is known as the Maxwell Garnett law (Maxwell Garnett 1904; Bohren & Huffman 1983). Thus, a fractal dust aggregate of \( N \) monomers can be replaced by a single pseudosphere of radius \( R_c \) and effective dielectric function \( \epsilon_{eff} \). Consequently, the optical properties of this pseudosphere can be readily obtained using Mie theory. Because of the symmetry of the phase matrix arising from the spherical symmetry of a particle, the EMT always yields

\[
S_{11} = S_{22} = S_{33} = S_{44}.
\]

Equation (3) is valid only when \( f \lesssim 10\% \) and \( X_0 \lesssim 0.5 \) (Kolokolova & Gustafson 2001). Hence, when at least one of these conditions is not fulfilled, it is necessary to use another mixing rule, such as the Bruggeman rule (Bruggeman 1935) when \( f \gtrsim 10\% \) or the extended EMT theory (Stroud & Pan 1978; Wachniewski & McClung 1986) when \( X_0 \gtrsim 0.5 \). It is worth noting that fluffy dust aggregates have small \( f \), meaning that the EMT yields results similar to the Rayleigh–Gans solutions for a sphere (see Chapter 6 of BH83).

2.1.3. RGD Theory

The basic idea of the RGD theory is as follows. Assuming that multiple scattering inside the aggregates can be ignored, the light scattered by all of the monomers is superposed, taking into account the phase differences between light rays.

The RGD theory assumes that the field inside the particle is approximately the same as the external incident field. This assumption is valid when the following conditions are satisfied:

\[
|m - 1| \ll 1,
\]

\[
2X_0 |m - 1| \ll 1,
\]

\[
2X_c |m_{eff} - 1| \ll 1,
\]

where \( m \) is the complex refractive index of a monomer and \( X_0 \) and \( X_c \) are the size parameters of the monomers and the aggregates of characteristic radius \( R_c \), respectively. The size parameter is defined as

\[
X = kR = \frac{2\pi R}{\lambda},
\]

where \( \lambda \) is the wavelength measured in a vacuum.

The refractive indices are related to the dielectric function as \( m = \sqrt{\epsilon_{eff}} \), and thus \( m_{eff} \) can be calculated using Equation (3). Equation (5) requires the absence of the reflection of light by a monomer. Equations (6) and (7) require the changes in the amplitude and phase of incident light to be negligible within aggregates (Bohren & Huffman 1983). These conditions correspond to the fact that aggregates can be regarded as “almost transparent.”

When the above conditions are satisfied and multiple scattering can be considered negligible, the phase matrix elements of the aggregates reduce to

\[
S_{ij,agg} (\theta) = N^2 S_{ij,mono} (\theta) S(q),
\]

where \( S_{ij,agg} \) and \( S_{ij,mono} \) represent \( S_q \) for the aggregate and monomer, respectively (Botet et al. 1997; Sorensen 2001), and \( S(q) \) is the structure factor. A relation similar to Equation (9) can be obtained by analogy to the theory of scalar wave scattering (see Appendix A). Because multiple scattering is ignored, the phase difference between scattered light rays can be determined from the relative position vector of every pair of monomers in the aggregate. Hence, it is helpful to introduce the
following two-point correlation function:
\[ g(u) = \int n(r)n(r-u)dr, \]
(10)
where \( r \) is the position vector, \( u \) is the relative position vector between two locations inside the scatterer, and \( n(r) \) is the normalized distribution function of monomers. The normalized distribution function \( n(r) \) is defined as
\[ n(r) = N^{-1} \sum_{i=1}^{N} \delta(r-r_i), \]
(11)
\[ \int n(r)dr = 1, \]
(12)
where \( \delta(r) \) is the Dirac delta function, \( r_i \) is the position vector of the \( i \)th monomer, and \( N \) is the number of monomers. The structure factor in Equation (9) can be expressed as the Fourier transform of the following two-point correlation function (Wiener–Khintchin theorem):
\[ S(q) = \int g(u)e^{i\mathbf{q} \cdot \mathbf{u}}du, \]
(13)
where \( q = k_r - k_i \) is the scattering vector. As a result, \( S(q) \) can be understood as the power spectrum that characterizes the configuration of fractal dust aggregates. Because \( n(r) \) is normalized to unity, \( S(q) \) approaches unity when \( q \cdot u \ll 1 \).

Equation (9) shows that once the statistical properties \( N \) and \( S(q) \) of the aggregate and those \( S_{ij,\text{mono}} \) of the monomer are specified, \( S_{ij,\text{agg}} \) can be obtained. Because the monomer is assumed to be spherical, \( S_{ij,\text{mono}} \) is calculated using Mie theory.

In the RGD theory (Equation (9)), every phase matrix element is proportional to the structure factor, and thus the ratio \( S_{ij}/S_{11} \) is not dependent on the structure factor. This suggests that the degree of polarization \( P = -S_{11}/S_{12} \) of the aggregates can be determined from that of their constituent particles (monomers). For example, if the monomers show Rayleigh-like scattering, the degree of polarization of the aggregates shows similar behavior. It is worth noting that these characteristics have been observed in both experiments (e.g., Volten et al. 2007) and numerical simulations (e.g., Min et al. 2016).

3. DUST MODEL

As shown in Section 2.1.3, once the statistical quantities of fractal aggregates, such as the two-point correlation function and the structure factor, have been obtained, their light scattering intensity at each angle can be determined. This section first introduces the radius of the aggregate. Second, an analytical expression describing the structure factor for the fractal aggregate is described. Finally, the aggregate models used in the calculation are summarized and compared with the analytic formula of the structure factor.

3.1. Statistical Properties of Fractal Dust Aggregates

Fractal dust aggregates do not have a specific configuration, but their configurations can be characterized statistically; this section describes how.

3.1.1. Radius of Fractal Dust Aggregates

Two frequently used definitions of the radius of a dust aggregate are the radius of gyration \( R_g \) and the characteristic radius \( R_e \). \( R_g \) represents the dispersion of the mass of the monomers with respect to their center of mass, as (e.g., Mukai et al. 1992)
\[ R_g = \left[ \frac{1}{2N^2} \sum_{i=1}^{N} (r_i - r_{\text{cm}})^2 \right]^{1/2}. \]
(14)
Again, all monomers are assumed to be identical. When the radius of gyration is calculated for homogeneous spheres of radius \( a \), it reduces to \( R_g = \sqrt{3/5}a \). When the fractal aggregates are replaced with the pseudospheres used in the EMT calculations, it is convenient to define the characteristic radius, which is given by (e.g., Mukai et al. 1992)
\[ R_e = \sqrt[3]{\frac{5}{3}} R_g. \]
(15)

3.1.2. Analytical Expression of the Structure Factor

A model of the two-point correlation function for fractal dust aggregates is introduced as (e.g., Teixeira 1986)
\[ g(u) = Au^{d_f-3} \exp\left\{-(u/\xi)^\beta\right\} + \frac{1}{N}\delta(u), \]
(16)
where \( A \) is a constant, \( u = |\mathbf{u}| \), \( \xi \) is the cut-off radius or correlation length, and \( \beta \) represents the power of the cut-off. In Equation (16), the power-law function characterizes the fractal structure, where \( d_f \) represents the fractal dimension and the other exponent of 3 comes from the dimension of the space. The meaning of the fractal dimension can be understood as follows. The number of monomers within a distance \( R \) from a monomer is \( N \propto \int_0^R g(u)4\pi u^2du \propto \int_0^R u^{d_f-3}4\pi u^2du \propto R^{d_f} \), where \( R \ll \xi \) is assumed and the second term in Equation (16) is ignored. This yields another expression for the fractal dimension:
\[ N = k_0 \left( \frac{R_e}{R_0} \right)^{d_f}, \]
(17)
where the prefactor \( k_0 \) is a constant. Note that this expression holds when \( N \) is sufficiently large. The fractal dimension describes the dimension of the monomer distribution. For example, when the monomers are distributed with a fractal dimension of two, they are distributed as if they were in a two-dimensional space. BCCAs, which are the product of a series of mutual collisions between aggregates of comparable masses, tend to have \( d_f \approx 1.04 \) and \( d_f \approx 1.9 \) for offset collisions and \( k_0 \approx 1.03 \) and \( d_f \approx 2.0 \) for head-on collisions. BPCAs, which are formed by monomers sticking together one by one, tend to have \( k_0 \approx 0.30 \) and \( d_f \approx 3.0 \). The cut-off function in Equation (16) is intended to take the aggregate size into account. \( \beta \) represents the power of the cut-off, but its value for fractal aggregates is controversial. Owing to its mathematical simplicity, the exponential cut-off model (\( \beta = 1 \)) has been investigated by numerous authors (e.g., Sinha et al. 1984, pp. 87–90; Berry & Percival 1986; Chen & Teixeira 1986; Freltoft et al. 1986; Kozasa et al. 1993; Filippov et al. 2000). However, Sorensen et al. (1992) pointed out that light scattering experiments on fractal dust aggregates support the Gaussian cut-off model (\( \beta = 2 \)). Section 3.2 will demonstrate that the
Gaussian cut-off model more accurately reproduces actual BCCAs and BPCAs than the exponential model; thus, the Gaussian cut-off model ($\beta = 2$) is adopted in the following discussion. The second term in Equation (16) is introduced to ensure this equation is consistent with Equation (10). This term only becomes important when $N$ is small. The calculation of the TMM is confined to small $N$ because of the computational demand; hence, this term cannot be negligible.

The constant $A$ in Equation (16) is determined by the unitary condition

$$\int g(u)du = 1,$$

(18)

and the correlation length $\xi$ is determined from the following relationship (Sorensen 2001):

$$R_g^2 = \frac{1}{2} \int |u|^2 g(u)du.$$

(19)

Equations (16), (18), and (19) yield

$$A = \frac{\beta}{4\pi^2\xi^2 \Gamma(d_f/\beta) \left(1 - \frac{1}{N}\right)},$$

$$\xi^2 = \frac{2\beta}{(d_f - \beta + 2) \Gamma((d_f + 2)/\beta - 1)} \times \left(1 - \frac{1}{N}\right)^{-1} R_g^2,$$

(20)

(21)

where $\Gamma(z)$ is the Gamma function.

Assuming that the monomer distribution is isotropic and $\beta = 2$, it follows from Equations (13) and (16) that

$$S(q) = 4\pi A \int_{0}^{\infty} u^{d_f-1} e^{-\frac{q}{2}u^2} \sin qu \frac{qu}{q} du + \frac{1}{N} \int \delta(u) e^{iq\cdot u} du$$

$$= 4\pi A \sqrt{\frac{\pi}{2q}} \int_{0}^{\infty} u^{d_f-\frac{1}{2}} e^{-\frac{q}{2}u^2} J_{\frac{1}{2}}(qu) du + \frac{1}{N},$$

(22)

where $J_{\frac{1}{2}}(x)$ is a spherical Bessel function of the first kind. Using the integral formula\footnotemark

$$\int_{0}^{\infty} x^\mu e^{-ax} J_{\nu}(\gamma x) dx$$

$$= \frac{\Gamma \left(\frac{\mu + \nu + 1}{2}\right)}{2^{\nu+1} \pi^{\nu+1/2} \Gamma(\nu + 1)}$$

$$\times _{1}F_{1} \left(\frac{\mu + \nu + 1}{2}; \nu + 1; -\frac{\gamma^2}{4\alpha}\right),$$

(23)

finally yields

$$S(q) = \left(1 - \frac{1}{N}\right) _{1}F_{1} \left(\frac{d_f}{2}; \frac{3}{2}; -\frac{(q\xi^2)^2}{4}\right) + \frac{1}{N},$$

(24)

where $\xi$ is the confuent hypergeometric function (see Appendix B) and $q = |q| = 2k \sin(\theta/2)$. Once $R_g$, $N$, and $d_f$ are obtained, the structure factor of the fractal dust aggregates can be determined. It should be noted that Equation (24) in this paper reduces to Equation (9) of Sorensen et al. (1992) in the limit of $N \to \infty$. In the following discussion, $\xi^2 \approx 4R_g^2/d_f$ is assumed for the sake of simplicity, which yields

$$S(q) \approx \left(1 - \frac{1}{N}\right) _{1}F_{1} \left(\frac{d_f}{2}; \frac{3}{2}; -\frac{(q\xi^2)^2}{d_f}\right) + \frac{1}{N}.$$

(25)

Note that the analytic form of $S(q)$ for $\beta = 1$ has been given in previous studies (e.g., Berry & Percival 1986).

3.1.3. Simplistic Form of the Structure Factor for Large $qR_g$

For $qR_g \gg 1$, using the asymptotic form of the hypergeometric function yields

$$\left(1 + \frac{1}{N}\right) _{1}F_{1} \left(\frac{d_f}{2}; \frac{3}{2}; -\frac{(q\xi^2)^2}{d_f}\right) \approx \left\{ C(qR_g)^{-d_f} \exp\left[-(q\xi^2)^2/d_f\right] \right\}$$

(26)

where $C$ is a function of the fractal dimension and $C = 1$ when $d_f = 2$ (see Appendix B). In the case of BCCAs, using Equation (17) with $d_f = 2$ and $k_0 = 1$ for simplicity yields

$$S(q) \approx \left(1 - \frac{1}{N}\right)(qR_0)^{-2}\frac{1}{N} + \frac{1}{N},$$

(27)

$$\approx \frac{1}{N} \{(qR_0)^{-2} + 1\},$$

(28)

where higher orders of $(1/N)^2$ are ignored. As a result,

$$S_{ij,agg}(\theta) \approx NS_{ij,mono}(\theta)\{(qR_0)^{-2} + 1\}.$$

(29)

The expression $(qR_0)^{-2} + 1$ inside the square brackets in Equation (29) indicates the enhancement of the scattered intensity due to interference of the scattered waves of each monomer. This term may be important to distinguish between light scattered by separately distributed monomers and that scattered by fluffy dust aggregates with $d_f = 2$. Because such aggregates are thought to be present in the surface layer of protoplanetary disks owing to their strong dynamical coupling to disk gas, Equation (29) might be useful to model the scattered light of the disks. Note that this expression holds for large-angle scattering, defined as $\theta_{\min} < \theta < \pi$, where $\theta_{\min} \propto X_{\text{agg}}^{-1}$ (see Section 4.1.3 for more detail). Thus, as the size of the aggregate increases, this expression becomes accurate for most scattering angles.

3.2. Proposed Particle Models

This paper considers two types of dust aggregates, BCCAs and BPCAs. BCCAs are generated by a series of mutual collisions of aggregates of comparable masses, whereas BPCAs are generated by monomers sticking together one by one. BCCAs have a highly porous structure, whereas BPCAs have a more compact structure. BCCAs and BPCAs typically have fractal dimensions of $d_f \lesssim 2.0$ and $d_f \simeq 3.0$, respectively. Simulations were performed to model these aggregates numerically. The number of monomers was set to $N = 128, 256, 512, 1024,$ and 8192. Figure 1 shows examples of the two types of aggregate models generated with 1024 monomers.

\footnotetext{See, e.g., Equation (6.133.1) of Gradshteyn et al. (2007).}
Figure 1. Models of (a) BCCA and (b) BPCA. The number of monomers in each model is 1024, and the BCCA and BPCA models have radii $R_c/R_0$ of approximately 46.2 and 19.6, respectively. The gray shaded regions illustrate the characteristic radii of the aggregates.

Even for models with the same number of monomers and agglomerate type, the aggregate configuration can vary widely because of the randomness of the collisional parameters, such as the impact parameter and the orientation of the aggregates. To remove the effect of the randomness, $N_a$ aggregates were produced for $N = 128, 256, 512, 1024$, and $8192$, where $N_a$ is the number of statistically independent aggregates. $N_a = 10$ and 4 were adopted for the BCCA and BPCA models, respectively, for all values of $N$ except $N = 8192$, where $N_a = 100$ and 10 were adopted respectively.

First, the radii of gyration of our generated aggregates are described. These were calculated using Equation (14), and the arithmetic mean value among $N_a$ aggregates is given in Table 1. For comparison, the radii of gyration were also calculated using Equation (17), which gives their asymptotic values for large $N_a$. In Equation (17), the fractal dimensions of BCCAs and BPCAs are assumed to be $d_f = 1.9$ and $3.0$, respectively, and the prefactors adopted for the BCCA and BPCA models are $k_0 = 1.04$ and 0.30, respectively. The generated aggregates have radii of gyration that are almost equal to their asymptotic values for large $N_a$. It should be noted that the small values of $N_a$ are likely responsible for the slight discrepancy between the radii of the aggregates and their asymptotic values. The following discussion adopts the radius of gyration calculated using Equation (14).

Second, the fractal dimensions of the aggregates were determined by employing two different models of correlation functions. The fractal dimension can be determined from the chi-square fitting of the measured correlation function using Equation (16). The results of the fits are summarized in Table 1. Table 1 shows that the Gaussian cut-off model ($\beta = 2$) is consistent with the typical fractal dimensions of BCCAs and BPCAs, whereas the exponential cut-off model ($\beta = 1$) is not. Indeed, the reduced chi-square values for $\beta = 1$ and 2 for the BCCA model containing 8192 monomers are $\chi^2_\nu = 3.98$ and 2.20, respectively, and therefore the Gaussian cut-off model ($\beta = 2$) exhibits a better fit. A suitable $d_f$ could not be found within the range $1.5 < d_f < 4.0$ for BPCAs when the exponential cut-off model ($\beta = 1$) was adopted. As a result, the Gaussian cut-off model was adopted in Equation (16). It should be noted that the reduced chi-square obtained for $\beta = 2$ is slightly larger than 1.0 because of a strong peak at $u = 2R_0$ and a discontinuity at $u = 4R_0$ (see, e.g., Figure 2 of Hasmy et al. 1993).

Figure 2 shows a plot of the structure factor calculated using the proposed particle model and statistical model. Small $qR_g$ values indicate large-scale structures, whereas large $qR_g$ values represent small-scale structures. Figure 2 indicates that the modeled structure factor reproduces the measured statistical properties of fractal dust aggregates in most $qR_g$ regimes. Although Equation (25) yields nearly correct results for the BCCA model, it fails for the BPCA model at small scales.

The slope of the actual structure factor for BPCAs is similar to the slope for BCCAs at $4 \lesssim qR_g \lesssim 20$. The main reason is that BCCAs and BPCAs are hardly distinguishable at small scales for $u \lesssim 8R_0$.

4. RESULTS

In this study, the chemical composition of the monomers was assumed to be the same as that of astronomical silicate (Draine & Lee 1984; Laor & Draine 1993), and the monomer radius was set to $R_0 = 0.1 \mu m$. Figure 3 shows a plot of the optical constants of astronomical silicate. The phase matrix elements of fractal dust aggregates were calculated using the TMM, the RGD theory, and the EMT.

4.1. Scattered Intensity $S_{11}$

This section discusses the scattered intensity $S_{11}$ of unpolarized incident light scattered by fractal dust aggregates.

4.1.1. Dependence on Wavelength

The wavelength dependence of the scattering is discussed first. In Figure 4, the scattered intensity normalized by $S_{11}(\theta = 0)$ is plotted against the scattering angle $\theta$. The dust model is the BCCA model with $N = 1024$, which means the radius of gyration is $R_g \simeq 3.73 \mu m$ (see Table 1). If the size parameter $X_{agg} = 2\pi R_g/\lambda$ is much smaller than unity, the scattering can be understood in terms of Rayleigh or isotropic scattering. If the size parameter is larger than unity, the forward scattering dominates the backward scattering even though each monomer scatters isotropically. As will be discussed in Section 4.1.2, the underlying physics of the wavelength dependence can be clearly understood in terms of the interference between the light rays scattered by different monomers.

Figure 4 also shows that the RGD theory is consistent with the wavelength dependence of the scattering results obtained using the TMM. Conversely, the EMT yielded accurate results for $X_{agg} \ll 1$ but not for $X_{agg} > 1$.

4.1.2. Forward and Backward Scattering Intensity

This section investigates the reason for the intense forward scattering by an aggregate with $X_{agg} > 1$. Figure 5(a) shows the scattered intensity of the BCCA model with $N = 1024$ for incident radiation of $\lambda = 1 \mu m$. This plot demonstrates that the RGD theory is in good agreement with the rigorous TMM results. For this reason, it is helpful to use Equation (9) to investigate the origin of the intense forward scattering. By definition, forward scattering always gives rise to $q = 0$, and then $S = 1$ (see Equations (13) and (18)). Thus, Equation (9) gives $S_{11,agg}(\theta = 0^\circ) = N^2S_{11,mono}(\theta = 0^\circ)$. The reason the forward scattered intensity is proportional to $N^2$ is because of the coherent scattering. This can be intuitively understood as follows. In the forward scattering region, where $q \cdot u \ll 1$, the
waves scattered by each monomer are in phase and are thus added constructively. This means that the forward scattering amplitude is proportional to $N$; thus, the intensity is proportional to $N^2$. In the backward scattering region, where $q \cdot u \gg 1$, Equation (9) reduces to $S_{11,ag} (\theta = 180^\circ) = N S_{11,mono} (\theta = 180^\circ)$ because $S \to 1/N$ for $X_{agg} \gg 1$. In this case, the backward scattered intensity is proportional to $N$ because of the incoherent scattering. For backward scattering angles, the phases of the waves scattered by each monomer are random, meaning that the waves are added destructively. For this reason, the amplitude is proportional to $\sqrt{N}$, and thus the intensity is proportional to $N$.

Figure 5(b) shows a plot of the scattered intensity for the BPCA model with $N = 1024$. As with BCCAs, BPCAs show intense forward scattering; however, they exhibit a slightly smaller forward scattered intensity than predicted by the RGD theory. This is related to the breakdown of the assumption of the RGD theory, which is discussed in more detail in Section 5. The RGD theory also fails to reproduce accurately results at angles in the range of $20^\circ \lesssim \theta \lesssim 100^\circ$. This inaccuracy comes from the error in the structure factor (see Figure 2).

**4.1.3. Dependence on Scattering Angle**

Next, the angular distribution of the scattered intensity is discussed. Figure 6 shows the scattered intensity plotted against the magnitude $q$ of the scattering vector. Figure 6 shows that...
the angular distribution of the scattering can be scaled using $q$. This is because the structure factor or the power spectrum governs the scattering phenomenon. Equation (9) indicates that the angular distribution of the scattered light is determined from a combination of the phase matrix elements of a single monomer and the structure factor. The angular distribution of scattering is classified into three regimes—the aggregate, fractal, and monomer scales—according to the structure factor, as illustrated in Figure 7(a).

The region in which $q < R_g^{-1}$ corresponds to the large-scale structure of aggregates and is termed the aggregate scale. In this regime, the detailed structure of the aggregate is not important, and the size of the aggregate plays a significant role. Because the radius of a pseudosphere is intended to be equal to that of the aggregate in the EMT calculation, this calculation can produce accurate results in this regime. In other words, in this regime, the aggregate scatters light as if it were a single sphere with radius $R_g$. The value of $q$ decreases with decreasing scattering angle, and $q = 0$ when $\theta = 0$; hence, small-angle scattering is characterized by the large-scale structure of dust aggregates. Physically, this behavior is the result of the fact that small-angle scattering is coherent scattering. It is worth noting that the aperture angle of the forward scattering, or primary, lobe can be characterized by $qR_g = 1$, which yields $\theta_c \propto X^{-1}$, where $\theta_c$ is the aperture angle of intense forward scattering. As the size parameter increases, the forward scattering is focused into a narrower region.

In the regime where $R_g^{-1} < q < R_0^{-1}$, the arrangement of monomers comes into play because the scattering is no longer coherent. Because the arrangement of monomers can be described by the fractal dimension, the angular dependence of the scattered intensity can also be characterized by the characteristics of the fractal dimension. In this regard, this regime is denoted the fractal scale. In this regime, the scattered intensity is proportional to $q^{-d_f}$ (see Equation (26)), as demonstrated by Figure 6. In general, the slope is determined by the surface fractal dimension $d_s$ and the mass fractal dimension $d_m$ as $- (2d_m - d_s)$ (e.g., Sorensen 2001). In the case of fractal aggregates, $d_f = d_m = d_s$, and thus the slope is simply $-d_f$. In the case of a solid sphere composed of almost transparent material (Rayleigh–Gans sphere), the slope in the fractal regime equals $-4.0$ because $d_m = 3$ and $d_s = 2$. This is known as Porod’s law (Porod 1951). Because the pseudosphere of the EMT for the BCCA model is almost the same as the Rayleigh–Gans sphere, it obeys Porod’s law, as shown in Figure 6. As a result, the EMT for the BCCA model cannot yield the angular dependence of fractal dust aggregates in this regime.

Increasing $q$ such that $q > R_0^{-1}$, the scattering becomes dominated by the small-scale structure, that is, monomers. Because of this, this regime is named the monomer scale. In this regime, the structure factor again has a constant value, and the optical properties of the monomer determine the scattering.

Figure 6. $S_{11}$ of the BCCA model containing $N = 1024$ monomers plotted against $q = 2k \sin(\theta/2)$. The red solid lines represent the rigorous results obtained using the TMM, and the blue dotted and green dashed lines represent the results obtained by the RGD theory and the EMT, respectively. The incident wavelength was set to $\lambda = 1 \mu m$. The thick gray solid line indicates the slope of the scattering for fractal aggregates with $d_f = 1.91$ and solid spheres. The vertical gray dotted lines on the left and right indicate where $qR_g = 1$ and $qR_0 = 1$, respectively.
Because the EMT calculation assumes an infinitesimally small monomer radius or infinitely large monomer number, at a fixed $R_g$, it fails to reproduce the angular dependence in this regime.

The smallest scale appearing in the scattering pattern is roughly comparable to the wavelength of the incident light. If $\lambda \lesssim R_0$, the monomer scale is not relevant to the scattering pattern, and the backward scattering can be interpreted as Rayleigh scattering from the volume within a radius of $\lambda$ (see Figure 7(b)). Therefore, the incident wavelength $\lambda$ functions as the spatial resolution of the structure.

The angular dependence of the scattering reveals the hierarchical structure of fractal aggregates from large-scale structures in the forward direction to small-scale structures in the backward direction. The reason the EMT calculation fails to reproduce the backscattering regime (fractal and monomer scales) is because small-scale structures, such as the arrangement of the monomers and the structure of the monomer itself, are ignored. It is worth noting that a BPCA model containing a large number of monomers may not show a hierarchical scattering structure, because the hierarchy is based on the RGD theory, which is not applicable to large BPCA models because of the inaccuracy of the assumptions (see Section 5 for more detail).

4.1.4. Dependence on Monomer Number

Figure 8 shows the dependence of the scattered intensity on the number of monomers in the BCCA and BPCA models. Again, the incident wavelength was set to $1.0 \mu m$. For both dust models, as the monomer number increases, the forward and backward scattering intensities also increase as a consequence of the interference. For the BCCA model, even
for high numbers of monomers, the RGD theory still achieves high accuracy. This is because the phase shift of the incident light within BCCAs remains nearly constant with increasing \( N \), whereas it varies in BPCAs. In addition, multiple scattering is not relevant to the aggregates if \( d_f < 2 \) (Berry & Percival 1986; Botet et al. 1997); therefore, the condition for the RGD is still satisfied as \( N \) increases. However, for large \( N \), the effect of multiple scattering cannot be ignored for \( d_f > 2 \), as is the case in BPCAs.

### 4.2. Degree of Linear Polarization

This section discusses the degree of polarization of the aggregates. The degree of linear polarization \( P \) is defined as \( P = -S_{12}/S_{11} \). The bottom left graphs in Figures 9 and 10 show plots of the degrees of linear polarization as functions of the scattering angle for the BCCA and BPCA models, respectively, with \( N = 1024 \). The rigorous calculation using the TMM shows that the maximum \( P \) is achieved for \( \theta \approx 90^\circ \) and that the angular distribution is almost symmetric about \( \theta \approx 90^\circ \). As predicted by the RGD theory (see Section 2.1.3), the degrees of linear polarization for both BCCAs and BPCAs exhibit angular distributions similar to that of a monomer, which is a Rayleigh scatterer. However, the maximum \( P \) obtained in the rigorous TMM results was slightly smaller than 100%. In the case of a spherical grain, depolarization occurs when the size parameter exceeds unity. However, the mechanism of depolarization for the aggregate is essentially different from that for a spherical grain. This aggregate...
depolarization is due to the occurrence of cross-polarization. Appendix C discusses depolarization by cross-polarization in more detail.

Thus, the RGD theory can achieve a symmetric angular distribution of the degree of linear polarization of fractal aggregates with respect to $\theta = 90^\circ$ but fails to reproduce its magnitude by a small margin. In the case of the EMT for the BCCA model, the solution is similar to the Rayleigh–Gans solution (see Chapter 6 in BH83), and the polarization is equal to the Rayleigh scattering. Note that the EMT results show some spiky features at certain angles; these originate from the small but non-negligible phase shift of the incident light by a pseudosphere. When the phase shift is negligible, this spiky feature does not appear in $P$; however, this feature arises as the phase shift approaches unity. This spiky feature develops a more wavy pattern with increasing phase shift, as shown in the bottom left plot in Figure 10.

4.3. Other Phase Matrix Elements

The phase matrix elements $S_{12}$, $S_{22}$, $S_{33}$, $S_{34}$, and $S_{44}$ normalized by $S_{11}$ are shown in Figures 9 and 10 for the BCCA and BPCA models, respectively. This section discusses elements $S_{33}$, $S_{34}$, and $S_{44}$ of the phase matrix, and Appendix C discusses $S_{22}$. In the case of Rayleigh scattering, that is, in the Rayleigh–Gans solution, $S_{34}$ vanishes (see Chapter 13 of BH83), and thus $S_{34}$ in the RGD theory also vanishes.

Although some spikes can be observed in the polarization pattern because of the non-negligible amount of phase shift, $S_{34}$ in the EMT for the BCCA model is almost zero. $S_{34}$ in the EMT for the BPCA model shows more complex behavior because the BPCA model is not transparent. $S_{33}$ and $S_{44}$ are the same as those of a monomer in the absence of cross-polarization, and the angle dependence becomes $S_{33}/S_{11} = S_{44}/S_{11} = 2 \cos \theta/(1 + \cos^2 \theta)$ (see Equation (5.5) of BH83). The results obtained using the RGD theory follow this formula. As shown in Figures 9 and 10, at large scattering angles, the rigorous TMM results deviate from those obtained using the RGD theory. This inconsistency may be attributable to the occurrence of cross-polarization (Appendix C).

5. APPLICABILITY OF RGD THEORY

Section 4 demonstrated that the RGD theory can achieve results that are in fairly good agreement with the rigorous TMM results for most phase matrix elements and that this is true especially for BCCA models. As described in Section 2.1.3, the conditions for the RGD theory are given by Equations (5)–(7). This section discusses the applicability of the RGD theory to fractal dust aggregates.

5.1. Relative Error in Scattered Intensity

To estimate the relative error between the RGD theory and TMM results, the relative error $\Delta$ was defined as

$$\Delta = \frac{S_{11}(\text{RGD}) - S_{11}(\text{TMM})}{S_{11}(\text{TMM})},$$

where $S_{11}$ is evaluated at $\theta = 0$.

Figure 11. Relative error $\Delta$ between forward scattered intensities obtained using the RGD theory and the TMM plotted against refractive index. The red squares indicate the dust aggregate with $R_g = 3.61 \mu m$ and $R_o = 0.1 \mu m$, and a BCCA model with $N = 1024$ is assumed; in this model, all monomers are in contact with each other. The green squares represent the tentative dust model; in this model, each monomer is separated from its nearest neighbor(s) by a distance of $2R_0$. The considered refractive indices range from $|m - 1| = 0.01$ to 3. The incident wavelength was set to $\lambda = 1000 \mu m$. The upper and lower horizontal lines represent errors of 10% and $-10\%$, respectively.

5.1.1. Relative Error Due to Refractive Indices

Figure 3 shows that astronomical silicate violates or only marginally satisfies Equation (5). To investigate the error arising from large $|m - 1|$ values, the relative error is shown as a function of the refractive index $|m - 1|$ in Figure 11. The incident wavelength was set to $\lambda = 1000 \mu m$; hence, the angular dependence of every scattering matrix element is equal to that of Rayleigh scattering (see Figure 4). Figure 11 shows that the error increases with increasing $|m - 1|$ and that the RGD theory slightly underestimates the scattered intensity. For example, when $|m - 1| \approx 0.5$, the results of RGD theory agree with the TMM results to an accuracy of $\leq 1\%$, whereas when $|m - 1| = 3$, the relative error increases to $\Delta \approx 15\%$. The enhancement observed in the TMM calculation at large $|m - 1|$ has been reported when using the DDA (see, e.g., Figures 3 and 4 of Kozasa et al. 1992), noting that in their paper, enhancement was observed in the absorption and scattering cross sections. A possible explanation for this behavior is the monomer–monomer interactions. To test this possibility, all monomers were tentatively separated from each other by an interval of $2R_0$ in the BCCA model with $N = 1024$; hence, the monomers were not in contact with each other in this tentative dust model. The error for the tentative dust model is plotted as green squares in Figure 11. The enhancement did not appear in the tentative dust model, and the results of RGD theory were shown to agree with the TMM results to an accuracy of $\leq 10\%$. Therefore, the enhancement of the scattered intensity at large $|m - 1|$ could be interpreted as being a result of monomer–monomer interactions.

5.1.2. Relative Error Due to Phase Shift

The phase shift induced by a single monomer is plotted as a function of incident wavelength in Figure 12. The phase shift
for a monomer with \( R_0 = 0.1 \mu m \) at \( \lambda = 1 \mu m \) is \( 2X_0 |m - 1| \approx 0.8 \). Thus, the condition given by Equation (6) is marginally satisfied, although the left-hand side approaches unity as the wavelength decreases. Figure 12 shows that the condition given by Equation (6) is only marginally satisfied for large monomers at short wavelengths. Note that the phase shift depends on the composition of the monomers. For example, this condition is only marginally satisfied for opaque materials, such as graphite.

Figure 13 shows the relative error \( \Delta \) plotted against the phase shift for different aggregate models and incident light with \( \lambda = 1 \mu m \). The dependence of the phase shift of the BCCA model on \( N \) is weak. Because \( |m_{\text{eff}} - 1| \approx |f|m - 1| \), the phase shift is proportional to \( R_f \). Equation (17) can be used to demonstrate that the phase shift by the aggregates is proportional to \( N^{d_f - 2d_f} \). Thus, in the case of \( d_f = 2 \), as in BCCAs, the phase shift by aggregates does not depend on the number of monomers. Therefore, the relative error of the BCCA model is expected to be independent of \( N \). However, as shown in Figure 13, the relative error in the BCCA model grows gradually with increasing \( N \). This increasing error may be attributable to the overlapping of monomers along the line of slight. This argument assumes that the prefactor \( k_0 \) does not depend on \( N \), but this is not generally true. Minato et al. (2006) studied the projected area in BCCAs and BPCAs and found an empirical formula for this. If an empirical formula can be extrapolated to large \( N \), the degree of overlap in BCCAs would be saturated. This suggests that the relative error \( \Delta \) would also become saturated with increasing \( N \). In the case of \( d_f = 3 \), as in BPCAs, the phase shift increases with increasing \( N \); thus, the RGD theory is not applicable to BPCAs at sufficiently large \( N \). If the phase shift due to the aggregates cannot be considered negligible, the forward scattered light rays are not in phase, and thus the forward scattered intensity might be slightly smaller than that of coherent scattering. As a result, the relative error in the forward scattering for the BPCA model increases with increasing \( N \), as shown in Figure 13.

### 6. CONCLUDING REMARKS

We investigated the angular dependence of scattering by two types of fractal dust aggregates, BCCAs and BPCAs, which have fractal dimensions of 2 and 3, respectively. Three methods were used to calculate the light scattering: the TMM, Mie theory with the EMT, and the RGD theory. In the formulation of the RGD theory, each phase matrix element of the fractal dust aggregates can be expressed as the product of the corresponding phase matrix element of the monomer and the structure factor. For the two-point correlation function of fractal aggregates, the Gaussian cut-off model was adopted (Equation (16) with \( \beta = 2 \)). Employing this model, the structure factor is expressed analytically as a function of the aggregate radius \( R_g \), the monomer radius \( R_0 \), and the fractal dimension \( d_f \) (Equation (24) or (25)).

Our results show that the RGD theory is a useful tool for calculating the phase function of fractal dust aggregates with \( d_f \leq 2 \). The main conclusions of this study are summarized as follows.

1. The RGD theory is consistent with both the wavelength and angle dependence of the scattered intensity (Section 4.1). The RGD theory agrees with the TMM with an accuracy of \( \lesssim 10\% \) for the BCCA model with \( N \leq 1024 \) (Section 5.1).
2. The angular distribution of scattered light can be understood to be dependent on the hierarchical structure of dust aggregates. The scattered intensity at small angles where all scattered light rays are in phase is determined by the large-scale structure of the aggregates. In the case of large-angle scattering, the intensity depends on the degree of coherence of the scattered light; hence, the relative position of monomers comes into play. Therefore, the internal structure is responsible for the intensity at large scattering angles (Section 4.1.3).
3. The effective medium theory underestimates the backward scattering intensity by multiple orders of magnitude when \( X_{\text{agg}} > 1 \). This is because the EMT ignores the internal structure of dust aggregates (Section 4.1.3).

4. Although the RGD theory tends to slightly overestimate the degree of linear polarization, it exhibits results that are qualitatively similar to the rigorous results from TMM calculation (Section 4.2). The occurrence of cross-polarization may be responsible for this overestimation (Appendix C).

The applicability of the RGD theory to BCCAs is determined by whether the phase shift of the monomer is negligible. In addition, for \( X_m \gtrsim 1 \), monomer–monomer interactions are induced, which causes slight depolarization at \( \theta = 90^\circ \). The quantitative modeling of polarization by fractal aggregates and phase matrix elements by opaque BCCAs (e.g., Kimura et al. 2006) is a goal for future work, whereas transparent BCCAs were investigated in this paper. In addition, the conditions of the RGD theory (Equations (5)–(7)) should be tested over a wide range in parameter space. This is also a future objective. Because of the large phase shift or the occurrence of multiple scattering, the light scattering properties of BPCAs containing a large number of monomers cannot be calculated using the RGD theory.

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**APPENDIX A**

**RGD THEORY**

Because electromagnetic waves are vector quantities, Equation (9) should be derived by vector analysis. However, the nature of Equation (9) can be easily understood by analogy with the scalar wave scattering theory. In this appendix, the derivation of Equation (9) is summarized by analogy with scalar wave scattering.

The propagation of a scalar wave \( \psi \) in a medium obeys the Helmholtz equation, which is given by

\[
\nabla^2 \psi + k^2 \psi = U(\mathbf{r}) \psi, \tag{31}
\]

where \( U(\mathbf{r}) \) is the perturbing potential. If \( U = 0 \), the solution \( \psi \) to this equation is a plane wave. It can be written in the following form:

\[
\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \int d\mathbf{r}' U(\mathbf{r}') G(\mathbf{r} - \mathbf{r}') \psi_{\text{inc}}(\mathbf{r}'), \tag{32}
\]

where \( G(\mathbf{r}) \) is an outgoing-wave Green function, \( \psi_0 \) is an incident plane wave, and \( \psi_{\text{inc}} \) is the sum of \( \psi_0 \) and multiply scattered light. If the multiple scattering can be disregarded, \( \psi_{\text{inc}} \approx \psi_0 \) (first-order Born approximation). Now, the scatterer is a collection of monomers, and the perturbing potential \( U(\mathbf{r}) \) can thus be expressed as the sum of the perturbing potentials of all monomers, \( U(\mathbf{r}) = \sum_{j=1}^{N} U_j(\mathbf{r}) \), where \( U_j(\mathbf{r}) \) is the potential of the \( j \)-th monomer. Assuming a spherical potential for all monomers yields

\[
U_j(\mathbf{r}) = k^2 (1 - \epsilon_0) W(|\mathbf{r} - \mathbf{r}_j|, \alpha), \tag{33}
\]

where \( \mathbf{r}_j \) is the position vector of the \( j \)-th monomer, \( W(|\mathbf{r} - \mathbf{r}_j|, \alpha) \) is a window function in which \( \alpha \) represents the monomer radius, and \( \epsilon_0 \) is the dielectric function of the monomer. \( W \) is unity when \(|\mathbf{r} - \mathbf{r}_j| \leq \alpha\) and 0 when \(|\mathbf{r} - \mathbf{r}_j| > \alpha\).

The second term of Equation (32) has the form \( f(\theta, \phi) e^{iqr/r} \) at large distances, and \( f(\theta, \phi) \) is referred to as the scattering amplitude. Because a spherically symmetric potential is assumed, the scattering amplitude is reduced to \( f(\theta) \). From Equations (32) and (33), the scattering amplitude of the aggregates can be described as

\[
f(\theta) = -\frac{1}{4\pi} k^2 (1 - \epsilon_0) \int d\mathbf{r}' W(|\mathbf{r}' - \mathbf{r}_j|, \alpha) \times e^{-(1 - \delta) iqr/r}, \tag{34}
\]

By substituting \( \mathbf{R} = \mathbf{r}' - \mathbf{r}_j \) and \( \mathbf{q} = \mathbf{k}_s - \mathbf{k}_i \), the variables can be separated as

\[
f(\theta) = -\frac{1}{4\pi} k^2 (1 - \epsilon_0) \int d\mathbf{R} W(\mathbf{R}, \alpha) e^{-i\mathbf{q} \cdot \mathbf{R}}, \tag{35}
\]

where \( \mathbf{R} = |\mathbf{R}| \). Because the differential scattering cross section \( dC_{\text{sca}}/d\Omega \) equals the square of the scattering amplitude,

\[
dC_{\text{sca}}/d\Omega = \frac{1}{4\pi} \frac{k^4 |\epsilon - 1|^2 v^2}{16\pi^3} \times \left| \frac{1}{v} \int d\mathbf{R} W(\mathbf{R}, \alpha) e^{-i\mathbf{q} \cdot \mathbf{R}} \right|^2 \sum_{j=1}^{N} e^{-iqr_j} \right|^2, \tag{36}
\]

where \( v = 4\pi a^3/3 \) is the volume of the monomer. The Gans form factor is defined as (Gans 1925; Bohren & Huffman 1983)

\[
F(q) = \sum_{j=1}^{N} e^{-iqr_j} \right|^2. \tag{37}
\]

From Equations (36) and (37), the following relationship can be obtained:

\[
dC_{\text{sca}}/d\Omega = \frac{1}{9} \frac{k^4 a^6 |\epsilon - 1|^2 F(q)^2}{16\pi^3} \sum_{j=1}^{N} e^{-iqr_j} \right|^2. \tag{38}
\]

The scattering amplitude for the monomer can be described as \( f_i = \sin \delta_i \exp(i\delta_i)/k \), where \( \delta_i \) is the phase shift of an \( l \)-wave. Assuming \( ka \ll 1 \), the phase shift of the lowest order of a partial wave (\( l = 0 \) or \( s \)-wave) becomes approximately \( \delta_0 \approx \frac{1}{3} (ka)^2 |\epsilon - 1| \) (e.g., Landau & Lifshitz 1965). Thus,

\[
dC_{\text{sca}}/d\Omega = \left[ \frac{dC_{\text{sca}}/d\Omega}{d\Omega} \right]_{\text{Rayleigh}} F(q)^2 \sum_{j=1}^{N} e^{-iqr_j} \right|^2, \tag{39}
\]

where \( [dC_{\text{sca}}/d\Omega]_{\text{Rayleigh}} = |f_0|^2 \). The last summation term is called the Debye factor. Using Equations (10) and (11), we
obtain
\[ N^{-2} \left| \sum_{j=1}^{N} e^{-iq r_j} \right|^2 = \int g(u) e^{iq u} du, \] (40)

Using Equations (39), (40), and (13) yields
\[ \frac{dC_{\text{sca}}}{d\Omega} = N^2 \left[ \frac{dC_{\text{sca}}}{d\Omega} \right]_{\text{Rayleigh}} F(q^2 S(q)). \] (41)

Thus, the differential cross section of the aggregates can be given in terms of the differential Rayleigh cross section, the Gans form factor, and the Debye, or structure, factor. In this regard, this approach is called the RGD theory. Replacing the Rayleigh–Gans term with the exact Mie solution for a spherical monomer and using \( S_{11}/k^2 = dC_{\text{sca}}/d\Omega \) yields
\[ S_{11,\text{agg}} = N^2 S_{11,\text{monos}} S(q). \] (42)

A1

APPENDIX B
CONFLUENT HYPERGEOMETRIC FUNCTION

The confluent hypergeometric function is defined as
\[ _1F_1(\alpha; \beta; z) = \sum_{n=0}^{\infty} \frac{(\alpha)_n z^n}{n!}, \] (43)

where \((\alpha)_n (x = \alpha, \beta)\) is the Pochhammer symbol given by
\[ (\alpha)_0 = 1 \]
\[ (\alpha)_n = \prod_{k=0}^{n-1} (x + k). \] (45)

If \( \alpha = \beta \), \[ _1F_1(\alpha; \beta; z) = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} = \exp(z). \]

It is quite useful to use the asymptotic form of the confluent hypergeometric function for \(|z| \gg 1\); hence,
\[ _1F_1(\alpha; \beta; z) \approx \frac{\Gamma(\beta)}{\Gamma(\beta - \alpha)} (-z)^{\alpha} \sum_{n=0}^{\infty} (-1)^n \frac{\alpha_n (\beta - \alpha)_n}{n! z^n} + \frac{\Gamma(\beta)}{\Gamma(\alpha)} e^{z} \sum_{n=0}^{\infty} \frac{(1 - \alpha)_n (\beta - \alpha)_n}{n! z^n}. \] (46)

When \( z \) has a large negative value, Equation (46) reduces to
\[ _1F_1(\alpha; \beta; -|z|) \approx \frac{\Gamma(\beta)}{\Gamma(\beta - \alpha)} |z|^{\alpha} \sum_{n=0}^{\infty} \frac{(\alpha)_n (\beta - \alpha)_n}{n! |z|^n}. \] (47)

Equation (47) shows that for \( z \gg 1 \), the summation decreases to approximately unity so that the asymptotic form of the confluent hypergeometric function gives rise to a simple power-law function. Substituting \( \alpha = d_f/2, \beta = 3/2, \) and \( |z| = (qR_g)^2/d_f \) yields
\[ _1F_1 \left( \frac{d_f}{2}, \frac{3}{2}, -\frac{(qR_g)^2}{d_f} \right) \approx C(d_f)(qR_g)^{-d_f}, \] (48)

\[ C(d_f) = \frac{\sqrt{\pi}}{2} \frac{d_f^{d_f/2}}{\Gamma\left(\frac{3 - d_f}{2}\right)}. \] (49)

Consequently, \( d_f = 2 \) gives \( C = 1 \) because \( \Gamma(1/2) = \sqrt{\pi}. \)

Figure 14 shows the degree of linear polarization occurring at small scattering angles. The reason for this depolarization is the monomer–monomer interaction. Because Rayleigh scattering shows completely polarized scattered light at \( \theta = 90^\circ \), the light scattered by the aggregates is completely polarized as long as the interaction between monomers is disregarded. Therefore, the depolarization can be interpreted as a consequence of

Figure 14. Confluent hypergeometric function for various fractal dimensions \( d_f. \)

APPENDIX C
DEPOLARIZATION EFFECT OF AGGREGATES

As discussed in Section 4.2, despite the fact that monomers are Rayleigh scatterers, the degree of linear polarization from the aggregates is slightly reduced at \( \theta = 90^\circ \). This appendix discusses the depolarization effect of aggregates. The depolarization is found to be caused by the occurrence of cross-polarization, which may increase \( S_{11} \) and decrease \( S_{12} \), thereby reducing the degree of polarization. In this regard, the depolarization of dust aggregates is essentially different from the case of a single sphere in which cross-polarization does not occur. When cross-polarization occurs, scattered light has a component that is perpendicular to the scattering plane even if the incident light has only a parallel component, and vice versa. In other words, \( S_3 \) and \( S_4 \) of the scattering amplitude matrix elements are not zero (see Chapter 3 of BH83). The occurrence of cross-polarization can be determined based on the ratio \( S_{22}/S_{11} \) because \( S_{22}/S_{11} \) is less than unity whenever cross-polarization occurs. Figure 15 shows the degree of linear polarization \( P \) and \( S_{22}/S_{11} \) for BCCA and BPCA models with \( N = 1024 \). Figure 15 demonstrates that \( S_{22}/S_{11} \) equals unity at small scattering angles, whereas it is less than unity at large scattering angles. The reason \( S_{22}/S_{11} = 1 \) at small scattering angles is because the aggregate can be regarded as a single sphere owing to the coherent scattering (see Section 4.1.3). The maximum value of the degree of linear polarization correlates with \( S_{22}/S_{11} \). Therefore, to determine the maximum degree of polarization of the aggregates, cross-polarization should be considered, which is not the case in the RGD theory.

Next, the origin of the cross-polarization is discussed. A possible mechanism for this depolarization is the monomer–monomer interaction. Because Rayleigh scattering shows completely polarized scattered light at \( \theta = 90^\circ \), the light scattered by the aggregates is also completely polarized as long as the interaction between monomers is disregarded. Therefore, the depolarization can be interpreted as a consequence of

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monomer–monomer dipole interactions (Lu & Sorensen 1994; Mishchenko et al. 1995; Kimura & Mann 2004; Kolokolova & Kimura 2010). Berry & Percival (1986) argued the importance of the multiple scattering of fractal aggregates by means of the mean-field approximation and concluded that multiple scattering can be negligible for fractal aggregates of small monomers with \( d_f \lesssim 2 \), like BCCAs. However, even if \( d_f \lesssim 2 \), monomer–monomer interactions cannot be considered negligible for large monomers, Okada & Kokhanovsky (2009) and Mishchenko et al. (2013) found that the linear depolarization ratio can be used as a diagnostic tool for the density of the aggregates. A monomer in a dense aggregate, like a BPCA, tends to interact with many nearby monomers; therefore, it is expected that the depolarization effect is more prominent for dense aggregates than for fluffy aggregates. Indeed, Figure 15 shows that BPCAs tend to show more depolarized scattering than BCCAs.

Because of the monomer–monomer interaction, the polarized vector excited by each monomer is not always parallel to the external incident field. Hence, these interacting monomers might be treated approximately as anisotropic Rayleigh spheres with different polarizabilities with respect to the three different axes. Mishchenko et al. (2013) investigated the modeling of linear depolarization by aggregates using the formula for an anisotropic Rayleigh sphere:

\[
P = \frac{1 - \cos^2 \theta}{y + \cos^2 \theta},
\]

where \( y \) is the anisotropy parameter, and it varies from 1 to 13 (see Equations (5.53) and (5.54) of BH83). In the case of an isotropic sphere, \( y = 1 \) so that the polarizability in \( \theta = 90^\circ \) is 100%. Note that the anisotropic sphere shows a symmetric profile with respect to \( \theta = 90^\circ \), whereas aggregates show slightly asymmetric profiles. Our results for BCCA and BPCA models with \( \lambda = 1 \mu \text{m} \) are \( y \simeq 1.1 \) and \( y \simeq 1.2 \), respectively.

To model the depolarization of the fractal aggregates, it is important to investigate how \( y \) varies as a function of the number \( N \) of monomers, the monomer radius \( R_0 \), the aggregate composition, and the fractal dimension \( d_f \). This remains as an objective for a future study.

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