Light Scattering by Marine Particles: Modeling with Non-spherical Shapes

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LONG-TERM GOALS

The long-term scientific goal of my research is to better understand the distribution of phytoplankton in the world's oceans through remote sensing their influence on the optical properties of the water. An associated goal is the understanding of the absorption and backscattering properties of marine particles in terms of the distributions of their size, shape, and composition.

OBJECTIVES

The inherent optical properties (IOPs) of marine particles are most-often modeled as homogeneous spheres using Mie Theory. Although this approach has been fruitful, the next logical step in modeling marine particles is to abandon the normally-employed spherical approximation and use more realistic approximations to their shape. The advent of computer codes capable of handling more complex shapes, and the increased computational speeds now available, suggest that particle modeling that employs simple non-spherical shapes, e.g., disks, rods, etc., could become routine. However, as such simple shapes are still at best poor approximations to real particles, it is important to ask the following question: how far can the actual shape of a particle deviate from these simple shapes and still be realistically modeled? In other words, will modeling marine particles with these simple shapes be a useful improvement over modeling by spheres? These questions are the focus of the present research.

APPROACH

It is now possible to efficiently compute the absorption and scattering properties of homogeneous particles of many simple shapes using the T-matrix method [Mishchenko et al, 2000]. A less efficient method of computation, the discrete-dipole approximation (DDA), can be used to compute the absorption and scattering properties of particles of *any* shape [Drain, 1988]; however, the computations are time-consuming. Gordon and Du [2001] used the DDA to model the scattering by detach coccoliths from the coccolithophored *E. huxleyi* using disk-like shapes.

Gordon and Du [2001] and Gordon [2004] found that the shape of the backscattering spectrum of detached coccoliths from *E. huxleyi* could be well reproduced using a shape consisting of two parallel disks (diameter ~ 2.75 μm and thickness 0.05 μm) separated by 0.3 μm, but the absolute magnitude of the backscattering cross section of an individual coccolith was significantly smaller than observed (factor of 2 to 3). However, this model structure represents a considerable simplification to the shape of an actual coccolith. SEM images of coccoliths show a complex structure in which two disk-like objects (actually spherical caps) have periodic radial structures resembling the openings between the

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spokes of a wagon wheel. Is the lack of quantitative agreement between the observed and measured backscattering cross sections due to these small scale structures, or does it result from the fact that the measurements of the backscattering were from a small number of stations, WHILE the size, shape, and mass of individual coccoliths were estimates for the same species, but not the actual coccoliths present at the measurement sites?

In what follows, I will use the term "gross morphology" to indicate a smooth homogeneous particle having approximately the same overall shape as the particle in question (e.g., a disk or two parallel disks as a model for a detached coccolith or a spherical shell as a model for an intact cocolithophore cell). The term "fine-scale structure" will be used to indicate deviations from the gross morphology (e.g., the coccolith's periodic radial structures, or the fact that it is a spherical cap as opposed to a flat disk). Our goal is thus, to understand how the fine-scale structure can induce deviations in backscattering from that which are characteristic of a given gross morphology. We use the DDA to compute the scattering by particles with a given gross morphology containing regular and irregular internal structures to try to understand their influence. Since the physical example of interest is a coccolith, we limit our examination to particles with the gross morphology of a disk.

The approach is to compare backscattering by a solid disk with a disk that resembles a wagon wheel to see how a regular (periodic) internal structure will influence the backscattering, and with spherical caps to see how small deviations in the gross shape affect the backscattering. In the process we will try to develop criteria to determine when gross morphology is the determinant of the backscattering. When gross morphology is not sufficient, we will try to understand how computations can be modified to include the presence of fine-scale structures.

WORK COMPLETED

The physical model investigated was a disk of diameter 1.50 μm with a thickness that varies from 0.05 to 0.15 μm. This disk is smaller than the apparent diameter of coccoliths (diameter ~ 2.75 μm) and was chosen as a compromise to make the large number of scattering computations, that are required for a general understanding of the affects of the structure, feasible using the discrete dipole approximation. The refractive index relative to the water in which it is suspended is taken to be 1.20.

To investigate the influence of periodic fine structure in a disk-like object on backscattering, symmetric portions of the disk were removed. Specifically, the disk was divided into equal angle sectors of angle $\Delta\alpha$ and alternate sectors were removed. The angle $\Delta\alpha$ was given by

$$\Delta\alpha = \frac{2\pi}{2^n},$$

where n is an integer. Figure 1 provides the positions of one layer of dipoles of the resulting structures for as a function of n. I will refer to these objects as "pinwheels." If we let s be the arc length of the open (or closed) regions at the perimeter of the pinwheel, then $s = D_d\Delta\alpha/2$, where D_d is the diameter of the disk. The values of s for the various cases that I examined (D_d = 1.5 μm) were such that at a wavelength (λ) of 400 nm in vacuum (300 nm in water), as n progresses from 4 to 7, s took on the values λ, $\lambda/2$, $\lambda/4$, and $\lambda/8$ in water. One of the goals of this particular study is to determine the relationship between s and λ where the periodic structure becomes important to the backscattering.

In addition, in order to understand the relative importance of fine structure and gross morphology, I computed the scattering by a full disk, but with half of the "atoms" removed from positions selected at random within the disk. Such a disk would have the same number of atoms (mass) and gross morphology (disk) as the pinwheels, but there would be no periodicity to the structure. This is referred to as the "random" disk.

Finally, previous attempts have been made to model the scattering of inhomogeneous particles, i.e., internal variations in the refractive index, by replacing the inhomogeneous particle by a homogeneous particle, having the same gross morphology, with an effective refractive index ($m_{eff.}$) [Chylek, et al., 2000]. The various methods of forming an effective medium, with equal parts by volume of refractive indices 1.00 and 1.20, all yield $m_{eff} \approx 1.10$, so I also examined a homogeneous disk (no missing "atoms") with $m_{eff} = 1.10$. Clearly, when the backscattering from disks with periodic (or random) fine structure can be effectively computed from a full disk with m_{eff}, the gross morphology is more important than the specifics of the fine structure.

In the case of the spherical cap, the dimensions were chosen to be similar in thickness and size to the disks. The projected area of the cap when viewed broadside was the same as the disk (Figure 2). The radius of the sphere R_s was chosen so that the half angle θ_s was 31°. This is approximately the half angle subtended by the individual coccoliths forming the coccosphere. Note that the sagittal distance L_s ($=D_d^2/8R_s$) is approximately 200 nm or approximately half the wavelength of light in the medium (water) corresponding to the middle of the visible spectrum. Thus, one would reasonably expect differences in the scattering by this cap and the associated disk.

RESULTS

Figure 3 provides the results of the computations of the backscattering cross section σ_b carried out for 1.5 μm pinwheels as function of the thickness (t) of the disk divided by the wavelength of the light *in water* (λ_{Water}). Three thickness of the disk are used: 0.05, 0.10, and 0.15 μm. The wavelength λ_{Water} covers the range from 200 nm to over 1000 nm. A striking feature of the computations is that a large number seem to fall on a smooth "universal" curve that is nearly coincident with the computations for the solid disk with $m_{eff} = 1.10$. This suggests that for many (but not all) of the computations the backscattering is governed by the gross morphology of the particle (i.e., the fact that its outer boundary is a disk), not the details of the internal structure. Of more interest perhaps is the condition(s) under which this observation is not satisfied. The cases that deviate from this behavior are indicated in Figure 3 by the solid curves. For these cases, when λ_{Water} is sufficiently large, σ_b still falls close to the universal curve, but as λ_{Water} decreases the backscattering suddenly breaks from the curve and becomes much larger. Choosing the last value of t/λ_{Water} before the computed σ_b departs from the universal curve, I computed the associated value of s/λ_{Water}. The resulting values are all near 0.25, suggesting that for objects that resemble a disk, periodic internal structures with size $\leq \lambda/4$ will influence the scattering only through a reduction of the refractive index from 1.20 to m_{eff}; the gross morphology will still determine the shape-specific aspects of the backscattering.

The computational results comparing σ_b for the spherical cap and the disk (D_d = 1.55 μm) will not be presented in detail as they show little difference between the cap and the disk for $t/\lambda_{Water} \leq 0.25$. For larger thicknesses, the cap and the disk computations follow one another reasonably well, suggesting that the deviations in backscattering moving from a disk to a spherical cap with the same projected area are minimal, at least for D_d = 1.55 μm. Again, the gross morphology appears to be dominant over the finer details of the structure.

For many of the cases examined, I have also computed the backscattering cross section using the Rayleigh-Gans approximation (RGA) to electromagnetic scattering. The RGA is applicable when the relative refractive index of the particle (m) is close to unity, and the "size" is << the wavelength of light divided by $|m - 1|$ (van de Hulst, 1957). Thus the size need not be << the wavelength. It is computationally fast when compared to any other method because analytical formulas are available for many particle shapes. Moreover, extension to particles of any shape is straightforward. In Figure 4 the DDA computations provided in Figure 3 are carried to larger values of $t/\lambda_{\mathrm{Water}}$ and compared with the RGA. They show that the RGA agrees well with the DDA for values of $t/\lambda_{\mathrm{Water}}$ up to, and somewhat beyond the first maximum that occurs in σ_b *after* the departure from the "universal curve." This maximum is near $s/\lambda_{\mathrm{Water}} = ½$. For larger values of $t/\lambda_{\mathrm{Water}}$ the RGA still provides the qualitative nature of the variation of σ_b with $t/\lambda_{\mathrm{Water}}$; however, it no longer quantitatively reproduces the DDA computations.

A more through discussion of the results provided here can be found in Gordon (2006) and Gordon (2007).

IMPACT/APPLICATIONS

These computations show conditions under which the gross morphology (e.g., disk-likeness) of marine particles determines their backscattering, and suggest that backscattering by particles with deviations from simple shapes of the order of a quarter of a wavelength or less can be computed by replacing the deviations by an effective refractive index. In contrast, when the scale of fine-structure exceeds a quarter of a wavelength, the scattering enters a new regime in which the backscattering is significantly higher than expected. Such a behavior may explain the low values of the backscattering cross section determined from models of coccolith scattering based on homogeneous disks. The near validity of the RGA for particles of the size and shape of interest here suggests that it can be used as an exploratory tool in the development of models of backscattering of coccolith-like particles.

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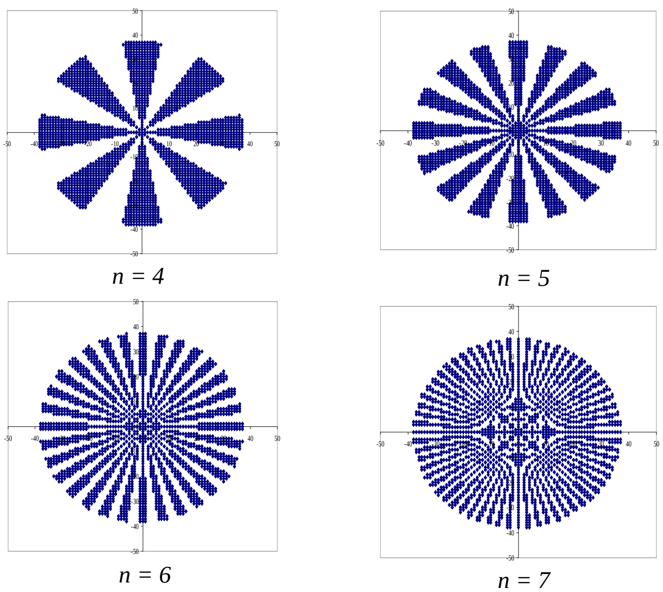

Figure 1. This schematic provides images of the positions of the dipoles in a single layer in the pinwheel model for n = 4, 5, 6, and 7. The pinwheel consists of equal angle sectors of a disk with atoms absent in alternating sectors. The individual dipoles (atoms) are separated by about 20 nm

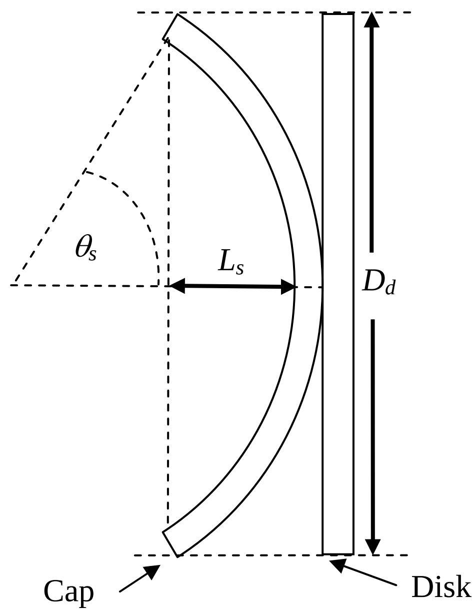

***Figure 2.** Schematic showing the relationship between the disk and the associated spherical cap. The cap and disk have the same projected area when viewed normal to their axis. The radius of curvature of the cap is about 1.5 μm and the diameter of the disk is 1.55 μm.*

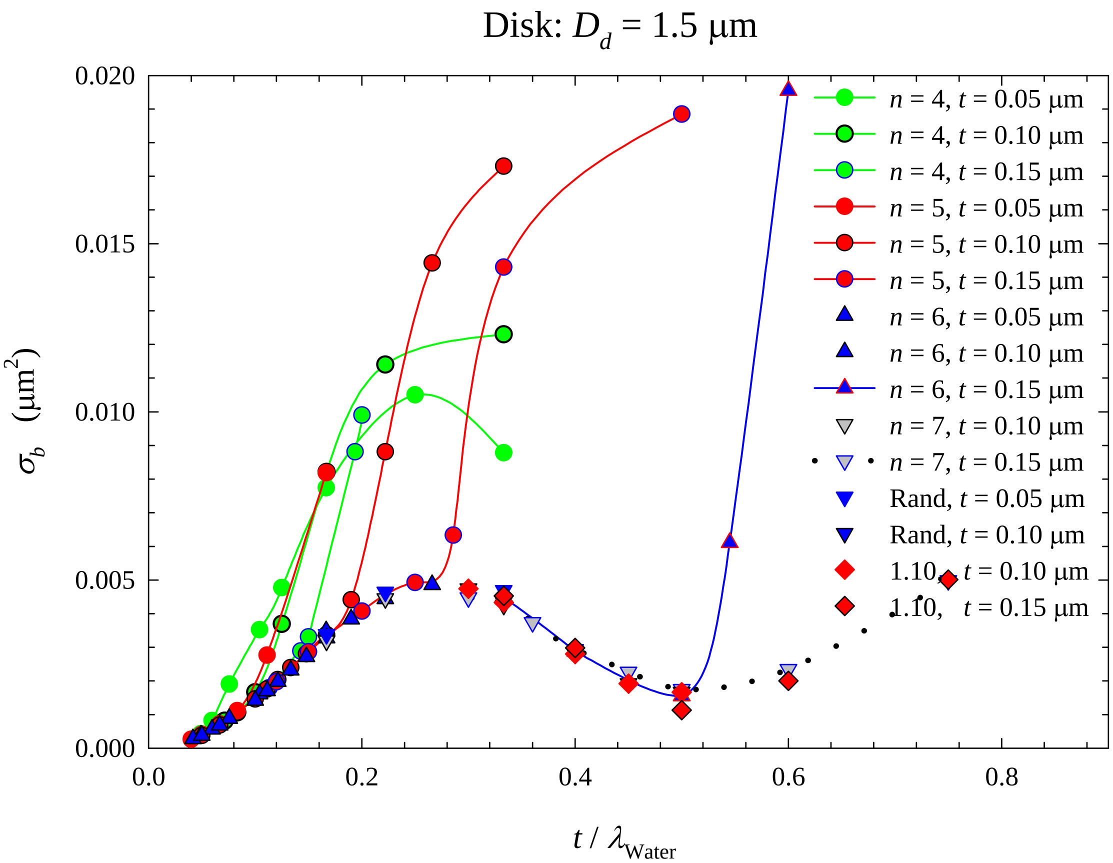

Figure 3.* *Computations of the backscattering cross section of randomly oriented disk-like particles with D_d = 1.5 µm, and various thicknesses t. The pinwheel models are described by the value of n and the thickness. The models for which half of the dipoles have been removed from random positions are indicated by "Rand," and the homogeneous models with m_{eff} = 1.10 are indicated by "1.10." Note that the backscattering for many cases appears to fall on a universal curve that is close to the homogeneous model. The solid curves for various values of n deviate from the universal curve at a position where s ≈ λ/4.

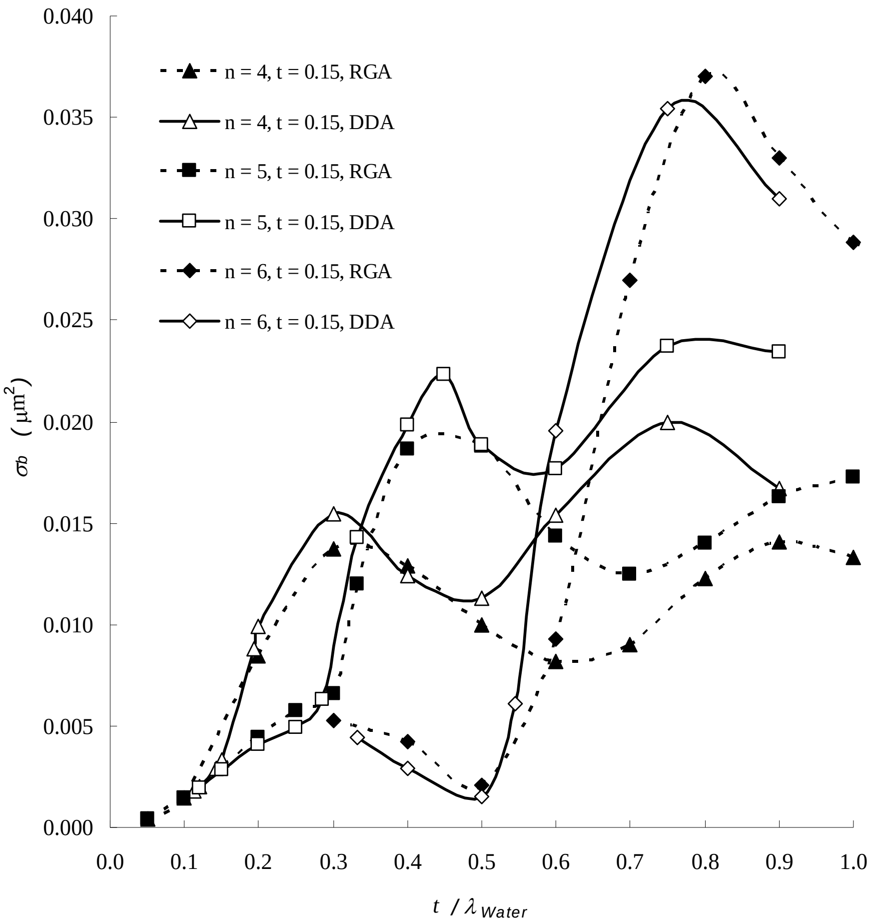

Figure 4. Computations for the backscattering coefficients of a pinwheel (D_d = 1.5 μm) for some of the cases provided in Figure 3, but extended to larger values of t/λ_{Water}. Also provided are the RGA results for the same cases. The results show that the RGA agrees well with the DDA for values of t/λ_{Water} up to, and somewhat beyond the first maximum that occurs in σ_b after the departure from the "universal curve." This maximum is near s/λ_{Water} = ½. For larger values of t/λ_{Water} the RGA still provides the qualitative nature of the variation of σ_b with t/λ_{Water} (i.e., an oscillatory behavior with period in s of approximately a half of a wavelength); however, it no longer quantitatively reproduces the DDA computations.