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An exact solution to Maxwell's equation for a Sphere applied to Silver Nanoparticles

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Abstract*— *With in this work the exact solution to Maxwell's equation for a sphere, sometimes called Mie theory, is applied to silver nanoparticles embedded in various constant index materials. The albedo, or fraction of the incident light which is scattered away from the particle is calculated and plotted as a function of the size of the particles relative to the incident wavelength.

Keywords*— *Maxwell's equations, organic light emitting diodes (OLEDs), scattering, silver nanoparticles.

I. INTRODUCTION

In a Mie theory description for scattering from spheroids, the scattering and absorptions are described by an exact solution of Maxwell's equations. The term "Mie theory" is a misnomer because it is not so much of a theory as an exact, analytic solution to one of several equivalent partial differential equations. These differential equations are Maxwell's equations and are solved exactly for a sphere for the cases of polarized and unpolarized uniform incidences. A full alternative derivation of this solution is performed in Feldheim and Foss[1] and Van de Hulst[2]. A key assumption is that the media is non-magnetic and that the complex refractive index is not dispersive. The real part is approximately .2 throughout the visible; however the imaginary portion varies mildly. One possible method to account for this is a particle size-dependent correction factor; however, such a derivation is outside of the scope of this work. This solution does not make the long wavelength (quasi-static) approximation that simplifies to the Laplace equation. The derived results give the scattering and extinction cross sections.

Methods: The infinite series was terminated after 13 terms. This is more terms than the author has seen used in any application of this Mie theory. Other applications of Mie theory consider non-uniform incident fields[3]. In the a and b coefficients, they quickly drop to 10^{-13} in less than ten terms for the refractive indices picked and each successive term (value of l) drops off by a factor of 10^3, therefore numerical precision should not be a concern. The albedo, R, is the ratio of scattered light to extincted light:

$$R[a] = \frac{C_{Scat}[a]}{C_{Ext}[a]} \quad (1)$$

This is not to be confused with the ratio of scattered to absorb. The size parameters are a product of the wave vector, $\frac{2\pi}{\lambda}$, and particle size. The entire Fourier series is evaluated at the size parameter which is a rather simple solution. In a single evaluation of the series weighting coefficients for a given internal and external refractive index, the scattering behavior can be determined throughout the entire visible for particle sizes from 10-200 nm. These size parameters were initially defined in Fu and Sun[7] as: q is the size parameter associated with vacuum wave number, q_1 is the size parameter associated with the external media wave number, q_2 is the size parameter associated with the wave number in silver.

For the wavelength and particle size specified: C_{Scat} = 0.126 microns^2, C_{Abs} = 0.011 microns^2, and C_{Ext} = 0.138 microns^2.

Now, define the scattering, absorption and extinction efficiency as $Q_{Scat} = \frac{C_{Scat}}{\pi * r^2}$, $Q_{abs} = \frac{C_{Abs}}{\pi * r^2}$, and $Q_{Ext} = \frac{C_{Ext}}{\pi * r^2}$. The truncated series for C_{Scat}, C_{Abs}, C_{Ext}, Q_{Scat}, Q_{Abs}, Q_{Ext}, asymmetry factor (g) and albedo are too long to post in this work. A single term written with the size parameter as a variable can be over four pages long. This is the same reason that these plots are made as a function of size parameter. It is much more time efficient to plot the size parameter, for a given refractive index ratio and have a plot that explains many cases than to generate a plot for each particle size.

Results: When the complex index of the silver particle is held constant and the refractive index of the external media, n_1, is altered from 1.0 to 2.0, the following data are obtained and are plotted on the same axes:

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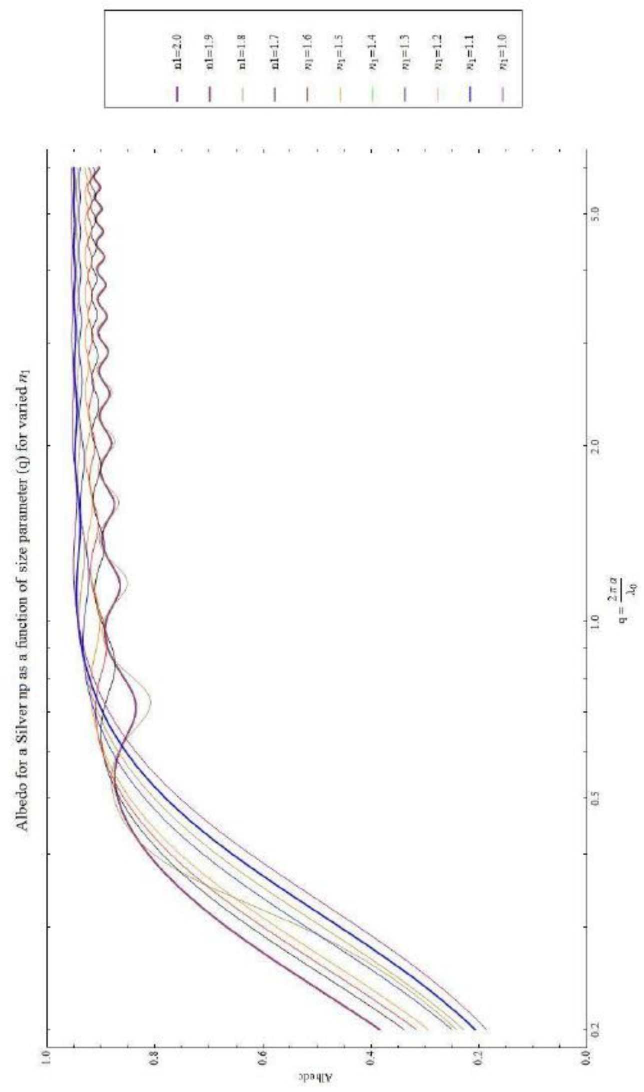

Fig.1: Albedo as a function of size parameter for a silver nanoparticle embedded in media with refractive index from 1.0 to 2.0. Fu and sun[4] have plotted only six terms of the scattering series, however that was for a different material than this study.

Interacting with a certain number of particles, Ξ, will reduce the light to Λ%. This will determine the equivalent particle interactions, denoted Ξ. This value is equal to:

$$\Xi = \left\lfloor \frac{-1}{R(\lambda)} * \log_{10}\left(\frac{\Lambda}{100}\right) \right\rfloor \quad (2)$$

where ⌊ ⌋ denotes the "round down" function.

II. DISCUSSION

The solution to Maxwell's equations for a non-dispersive sphere is known exactly and was evaluated for silver in combination with various ambient dielectric media. For a given refractive index ratio, the scattering, absorption and extinction properties were completely determined by the size parameter. The size parameter is a dimensionless number that is the product of the wave number of the light and the particle size. Mie theory indicates that the scattering cross-section is larger than the particles actual cross-section and that the absorption cross-section is smaller than its actual cross-section. The scattering efficiency is not monotonic as a function of particle size because the particle is acting as a microcavity. As the size is increased, there is constructive and destructive interference taking place within the particle. The reflection of a light wave on the exiting side of the particle interacts with the next trough of the incident wave. The largest scattering efficiencies correlate to the maximum constructive interference for a given wavelength at a specific particle size.

The scattering to absorption ratio, known as albedo, quickly approaches .85 and above regime for size parameters larger than .5. It is a significant result that the albedo remains high throughout the entire visible spectrum for particles greater than 50 nm radius. The scattering cross-section is larger for larger external indices and the absorption cross-section is larger in small indices. The efficiency, asymmetry factor and albedo are similar in varying the external refractive index as a function of size parameter. This theory tells that backscattering dominates throughout the visible for particles less than 100 nm in radius. Also, as the real part of the external refractive index increases, there is a slight decrease in the albedo for the same size parameter. However, this is countermanded by the benefit of high extraction from the organic layer into the scattering layer. In other words, there will be no critical angle or TIR limitation on how much of the light generated interacts with the particles.

In the scattering layer, the nanoparticles are unlikely to be in a periodic or organized structure such that there will be passes where the ray does not intersect a particle. In these cases, the angle of the light will remain within the critical angle as it bounces throughout the device until it does interact with a particle. It is, therefore, important that the concentration of nanoparticles within the scattering layer are high enough such as to scatter light before it interacts with the edges of the device but not so high that light must interact with more than Ξ particles; otherwise the probability of absorption with become dominant.

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REFERENCES

[1] D.L. Feldheim, C.A. Foss; “Metal Nanoparticles: Synthesis, Characterization and Applications” Marcel Dekker Inc., New York, NY (2002).

[2] H.C. Van de Hulst, “Light Scattering by Small Particles” John Wiley and Sons, New York (1957).

[3] N.J. Moore, M.A. Alonso “Closed form formula for Mie scattering of nonparaxial analogues of Gaussian beams” Optics Express Vol. 16. No. 8 (2008) p. 5926.

[4] Fu and Sun, Applied Optics, Vol. 40, No. 9, 2001,pp. 1354-1361.