IARPA MORGOTH'S CROWN: Overview of Particle and Thin Film Models

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Summary Overview of Exemplar Surface-Particle Models

A standard goal in remote sensing is to identify materials based on their chemical composition. This is difficult for solid materials because the spectrum of a single chemical can change dramatically as a result of variations in morphological aspects such as particle size and packing density.

The related (and simpler) problem of free-standing particles in air (or other medium) has been extensively modeled since it is of great interest to environmental and climate science (soot and other aerosols) as well as astronomy (space dust). Understanding the variables and solutions for this problem are a good starting point for the more complex case of particles on surfaces. Mie scattering theory was initially developed for free-standing, isolated spheres, and has been adapted for a variety of other particles shapes.

The Mie solution to Maxwell's equations (also known as the Lorenz–Mie solution, the Lorenz–Mie–Debye solution or Mie scattering, and named after Gustav Mie) describes the scattering of an electromagnetic plane wave by a homogeneous sphere. The solution takes the form of an infinite series of spherical multipole partial waves.

The term "Mie solution" is also used for solutions of Maxwell's equations for scattering by stratified spheres or by infinite cylinders, or other geometries where one can write separate equations for the radial and angular dependence of solutions. The term Mie theory is sometimes used for this collection of solutions and methods; it does not refer to an independent physical theory or law. More broadly, "Mie scattering" suggests situations where the size of the scattering particles is comparable to the wavelength of the light, rather than much smaller or much larger.

Mie solutions are implemented in a number of programs written in different computer languages such as Fortran, MATLAB, Mathematica. These solutions are in terms of infinite series and include calculation of scattering phase function, extinction, scattering, and absorption efficiencies, and other parameters such as asymmetry parameter or radiation torque. Current usage of a "Mie solution" indicates a series approximation to a solution of Maxwell's equations. There are several known objects which allow such a solution: spheres, concentric spheres, infinite cylinders, cluster of spheres and cluster of cylinders. There are also known series solutions for scattering on ellipsoidal particles. For a list of these specialized codes, examine these articles:

- Codes for electromagnetic scattering by spheres — solutions for single sphere, coated spheres, multilayer sphere, cluster of spheres: https://en.wikipedia.org/wiki/Codes_for_electromagnetic_scattering_by_spheres

- Codes for electromagnetic scattering by cylinders — solutions for single cylinder, multilayer cylinders, cluster of cylinders: https://en.wikipedia.org/wiki/Codes_for_electromagnetic_scattering_by_cylinders

In 1986, P.A. Bobbert and J. Vlieger extended the Mie model to calculate scattering by a sphere in a homogeneous medium placed on flat surface. Like Mie model, the extended model can be applied to spheres with a radius close to the wavelength of the incident light. There is a C++ code implementing Bobbert - Vlieger (BV) model. Basic Mie theory can also be modified to include substrate interaction. However, this still involves treating the particle as a perfect sphere, which may not be adequate for non-spherical particles.

A generalization that allows for a treatment of more general shaped particles is the T-matrix method, which also relies on the series approximation to solutions of Maxwell's equations. The T-matrix method is a computational technique of light scattering by nonspherical particles originally formulated by P. C. Waterman in 1965. The technique is also known as null field method and extended boundary technique method (EBCM). In the method, matrix elements are obtained by matching boundary conditions for solutions of Maxwell equations.

To deal with the general problem of reflectance from complex surfaces, reflectance models have been generated for particulate layers – often combining the computation of scattering/extinction properties for the particle population(s) with solutions of the radiative transfer equation – with advanced open-source computational tools available as well.

These numerical modeling approaches, while producing exact results, can be very computationally costly. General examples of such techniques are the finite-difference time-domain (FDTD) and discrete-dipole approximation3 (DDA). Most DDA code applies to isolated particles only, but recently a code was made available that includes surface interactions. The main problem with existing numerical methods is that the computation time diverges with particle size. While modeling a particle with a diameter close to the wavelength of light may be feasible, modeling of much larger particles requires dramatically more memory and computation power.

In all of the above techniques, it is assumed that the particle coverage is sparse, so that any scattering between particles can be neglected. In this case, the infrared signal from an ensemble of particles can be approximated by a (linear) sum of individual contributions from each of the particles in the ensemble. The portions of the target area not covered by particles will contribute a signal equivalent to a blank substrate.

A collection of relevant open-source computational tools is available at:
https://scattport.org/index.php/light-scattering-software/particle-on-surface