

To determine the radius of nano particles using C_{sca} or C_{abs} and this can be finding using Mie Plot Software

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Abstract:

To determine the size of the nano particle Transition electron microscopy (TEM) and Scanning electron microscopy (SEM) are used. But these techniques are very costly for the synthesis of nano particles. To overcome this, Mie Plot software is used to describe the scattering of light by particles.

Key words: scattering cross-sections (C_{ext} , C_{sca} & C_{abs}), scattering efficiencies (Q_{ext} , Q_{sca} & Q_{abs}), Absorption cross section, MiePlotSoftware, Matlab software

❖ Introduction:

Mie Plot software is used to describe the scattering of light by particles. Mie scattering from a sphere – refers to the "Absorption and scattering of light by small particles". In addition to calculations of Mie scattering for single wavelengths, Mie Plot offers calculations for scattering of sunlight - and simulations of atmospheric optical effects (such as rainbows, coronas and glories). Although Mie theory provides an exact mathematical solution to the problem of scattering of electromagnetic waves from a homogeneous sphere, it does not provide any insight into the physical processes involved in scattering.

Mie Plot can plot graphs of scattered intensity as a function of scattering angle, radius, wavelength, refractive index - as well as "Lee diagrams". In addition, it can produce graphs of scattering cross-sections (C_{ext} , C_{sca} & C_{abs}) and scattering efficiencies (Q_{ext} , Q_{sca} & Q_{abs}) as functions of radius of the scattering sphere, size parameter or wavelength.

❖ Nano particle:

A particle is defined as a small object that behaves as a whole unit in terms of its transport and properties.

Particles are further classified according to size: in terms of diameter, fine particles cover a range between 100 and 2500 nanometers. On the other hand, ultrafine particles are sized between 1 and 100

nanometers. Similar to ultrafine particles, nano particles are sized between 1 and 100 nanometers.

❖ Application:

Property	Application
Optical	Anti-reflection coatings. Tailored refractive index of surfaces. Light based sensors for cancer diagnosis.
Magnetic	Increased density storage media. Nano magnetic particles to create improved detail and contrast in MRI images.
Thermal	Enhance heat transfer from solar collectors to storage tanks. Improve efficiency of coolants in transformers.
Mechanical	Improved wear resistance. New anti-corrosion properties. New structural materials, composites, stronger and lighter.
Electronic	High performance and smaller components, e.g., capacitors for small consumer devices such as mobile phones. Displays that is cheaper, larger, brighter, and more efficient. High conductivity materials.
Energy	High energy density and more durable batteries. Hydrogen storage applications using metal nanoclusters. Electrocatalysts for high efficiency fuel cells. Renewable energy, ultra high performance solar cells.

	Catalysts for combustion engines to improve efficiency, hence economy.
Biomedical	Antibacterial silver coatings on wound dressings. Sensors for disease detection (quantum dots). Programmed release drug delivery systems. “Interactive” food and beverages that change color, flavor or nutrients depending on a diner’s taste or health.
Environmental	Clean up of soil contamination and pollution, e.g. oil. Biodegradable polymers. Aids for germination. Treatment of industrial emissions. More efficient and effective water filtration.
Surfaces	Dissolution rates of materials are highly size dependant. Activity of catalysts. Coatings for self cleaning surfaces, Pilkington’s glass for example.
Personal care	Effective clear inorganic sunscreens.

it depends upon the wavelength of light and the permittivity, shape and size of the particle. The total amount of scattering in a sparse medium is determined by the product of the scattering cross-section and the number of particles present. In terms of area, the total cross-section (σ) is the sum of the cross-sections due to absorption, scattering and luminescence

$$\sigma = \sigma_A + \sigma_S + \sigma_L$$

The total cross-section is related to the absorbance of the light intensity through Beer-Lambert’s law, which says absorbance is proportional to concentration:

$$A_\lambda = Cl\sigma,$$

Where C is the concentration as a number density, A_λ is the absorbance at a given wavelength, λ , and l is the path length.

The extinction or absorbance of the radiation is the logarithm of the reciprocal of the transmittance:

$$A_\lambda = -\log T$$

❖ Refractive index:

The refractive index or index of refraction of a substance is a measure of the speed of light in that substance.

It is expressed as a ratio of the speed of light in vacuum relative to that in the considered medium. The velocity at which light travels in vacuum is a physical constant, and the fastest speed at which energy or information can be transferred. However, light travels slower through any given material, or medium, that is not vacuum. A simple mathematical description of the refractive index is as follows:

$$n = \text{velocity of light in a vacuum} / \text{velocity of light in medium}$$

For example, the refractive index of water is 1.33, meaning that in a vacuum; light travels 1.33 times as fast as it does in water.

❖ Scattering cross-section:

The scattering cross-section, σ_{scat} , is a hypothetical area which describes the likelihood of light (or other radiation) being scattered by a particle. In general, the scattering cross-section is different from the geometrical cross-section of a particle, and

❖ Absorbance:

The absorbance of an object quantifies how much of the incident light is absorbed by it (not all photons get absorbed; some are reflected or refracted instead). This may be related to other properties of the object through the Beer-Lambert law.

❖ Absorption cross section:

Absorption cross section is a measure for the probability of an absorption process. More generally, the term cross section is used in physics to quantify the probability of a certain particle-particle interaction, e.g., scattering, photo absorption, etc. (Note that light in this context is described as consisting of particles, i.e., photons.)

It can be finding by Mie plot software.



In the laboratory, the radius is found from the scattering angle. But Mie plot give the relation Between nano particle and absorption.

Procedure of the getting the necessary data from the Mie plot:

NanoLab(Phys4970) Mie Theory &Extinction Spectra [ver 1.1.0] L.A. BUMM

Part B) Model your results in MiePlot.

Step 0) Download MiePlot from the Nanolab www site. Install this on your computer. It is a small program and should not present any difficulty.

Step 1) Start MiePlot and set it up to model the extinction spectra of gold Nanoparticles.

1A) Set up for gold spheres in water:

From the Advanced drop down menu select refractive index, sphere, gold. Then again from the Advanced drop down menu select refractive index, surrounding medium, water, segelstein, then a box will pop up, check complex.

1B) Set up to calculate and to plot the extinction, Scattering, and absorption cross sections versus wavelength: On the top right from the drop box (initially: intensity v. scattering angle) select Cext/ Csca/Cabs v. wavelength.

1c) Set up the wavelength range to correspond to the 400nm to 1000nm range that you measured with the Cary 50.

1D) Select the size of the Sphere. NOTE MiePlot uses RADIUS in units of MICROMETERS. Start with a radius of $0.005\mu\text{m}$.

1E) Calculate the values and make the plot. Click New Plot. A progress bar will appear on the upper right. When it is finished your plot will be

displayed .Note the three cross sections are displayed in different colors. We are specifically interested in C_{ext} .

Step 2) Perform the modeling. Mie theory calculations are a complex. They can be used to calculate the spectra of nanoparticles give their size and refractive index. However the mathematics cannot be easily inverted. You cannot put a spectrum into the calculation and get a practice out! To determine the particle size we perform several calculations and then compare them to our experiment data. The particle size of the best-fit spectrum will be the particle size we determine from Mie Theory.

See the examples that follow. Note that as you increase the particle size, the peak moves to longer wavelength and becomes broader. This peak is the dipole Plasmon resonance.

Dipole means that the wave set up on the surface of the particles has one node. On further increase in particle size, a second peak begins to emerge where the dipole resonance occurred for small particles. This is the quadrupole Plasmon resonance.

Quadrupole means that the wave set up on the surface of the particles has two nodes.

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Exporting and working with data from MiePlot.

From the file menu, select save numerical results as text file.

This file can be improved into excel as a **TAB** delimited text file.

From the file drop down menu select open. From the open window, select files of type: text files (*.prn, *.txt, *.csv). Now navigate to your file and select open. The text import wizard will start. Note tab delimited text is the default, so pressing finish on this screen often will give you the desired result.

Here for a data taken from the Mie plot software with following setting.

Calculation Method: Mie (plane wave)

Sphere: Silver

Medium: water

Refractive index (sphere)

Real part: 0.0522441

Imaginary part: 4.4087207

Refractive index (medium)

Real part: 1.3311805

Wavelength: 0.65 um

Graph type: Cext/Csca/Cabs v. radius

Matlab code for finding the radius of the nano particles from the given absorption. (We are taking the 3000 data from the Mie plot software)

```
% c_f_all.m (calculating radius and
plotting original data and creating the higher
order equation. )
```

```
clc
clearall
formatlonge
x=input('Abs=');
```

```
if x<9.90187045446282*10^(-18)
loadcf18
rad=cf18(x)
```

In detail:

- 1) Step 1) under delimited, click next;
- 2) Step 2) in the delimiters box select tab, click next;
- 3) Step 3) in the column data format box select general, now click finish.

```
elseif x>1.0001578841758*10^(-17) &&
x<9.9707375458999*10^(-17)
loadcf17
rad=cf17(x)
elseif x>1.00869238640966*10^(-16) &&
x<9.94372828105649*10^(-16)
loadcf16
rad=cf16(x)
elseif x>1.00047991205235*10^(-15) &&
x<9.98186215553783*10^(-15)
loadcf15
rad=cf15(x)
elseif x>1.00090116386398*10^(-14) &&
x<9.98788751928449*10^(-14)
loadcf14
rad=cf14(x)
elseif x>1.00126184694218*10^(-13) &&
x<9.93277417194823*10^(-13)
loadcf13
rad=cf13(x)
elseif x>1.01407741654687*10^(-12) &&
x<9.97248870027865*10^(-11)
loadcf1112
rad=cf1112(x)
else x>1.00326338927701*10^(-10)
loadcf10
rad=cf10(x)
end
```

```
-----
---
plot(DATA(:,4),DATA(:,1));
```

```
title('all DATA');
xlabel('ABS'); ylabel('Radius');
```

```
figure, plot( DATA(1:186,4),DATA(1:186,1) );
title('10 ^ (-18) DATA');
xlabel('ABS'); ylabel('Radius');
```

```
figure, plot(
DATA(187:402,4),DATA(187:402,1) );
title('10 ^ (-17) DATA');
```

```

xlabel('ABS'); Ylabel('Radius');
figure, plot(
DATA(403:610,4),DATA(403:610,1) );
title('10 ^ (-16) DATA');
xlabel('ABS'); Ylabel('Radius');

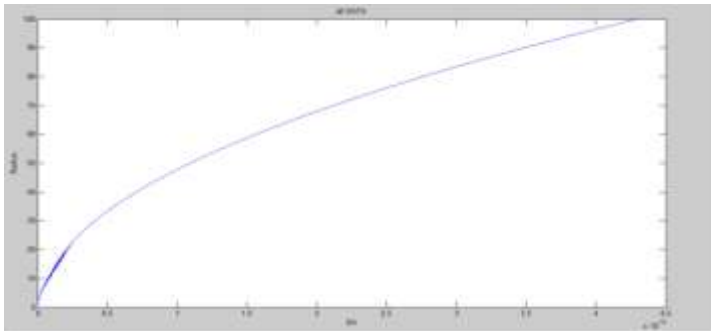
figure, plot(
DATA(611:1104,4),DATA(611:1104,1) );
figure, plot( DATA(1504:1890,4),DATA(1504:1890,1) );
title('10 ^ (-13) DATA');
xlabel('ABS'); Ylabel('Radius');

figure, plot( DATA(1891:2760,4),DATA(1891:2760,1) );
title('10 ^ (-11,12) DATA');
xlabel('ABS'); Ylabel('Radius');

figure, plot( DATA(2761:3001,4),DATA(2761:3001,1) );
title('10 ^ (-10) DATA');
xlabel('ABS'); Ylabel('Radius');
%output-----
rad =

2.734920914845263e-001
%-----

```



With the help of data from the Mie plot and using Matlab coding we have shown the graph of nanoparticle radius verses absorption.

Conclusion:

The size of the nano particle Transition electron microscopy (TEM) and Scanning electron microscopy (SEM) are used. But these techniques are very costly for the synthesis of nano particles. To overcome this, Mie Plot software is used to describe the scattering of light by particles. Here we have calculated the radius of the nano particle using matlab coding in a very easy way and in a very less

time and along with that graph Cext/Csca/Cabs v. radius.

Other new features include graphs of scattering cross-sections (Cext, Csca& Cabs) and scattering efficiencies (Qext, Qsca&Qabs) as functions of radius of the scattering sphere, size parameter or wavelength.

MiePlot offers the following additional methods of modelling the scattering of light by a sphere: Ray tracing (based on geometrical optics), Ray tracing including the effects of interference between rays, Airy theory Rayleigh scattering Diffraction.

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