Physics Simulation Project

Absorption and scattering of light by nanoparticles

Part II: Field plots (Project 7)

Project 7

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1. Introduction

The objective of our work is to interpret and explain the experimental results given by Figure 2 (the extinction cross section of a polydisperse distribution of aluminum spheres) thanks to the Mie Theory Algorithm we coded.

Our code is run on Matlab (https://ch.mathworks.com/fr/products/matlab.html). It allows us for example to calculate absorption and scattering cross sections of a sphere of a given radius and refractive index thanks to Mie Theory.

In order to interpret Figure 2, we will need to figure out:

- The size of the objects (diameter a)
- The nanoparticle concentration (our Mie code works for a single particle)
- The optical behaviour of aluminum

To find the optical index of aluminum at wavelength difference (or photon energy) we used the data from https://refractiveindex.info/ (Figure 1).

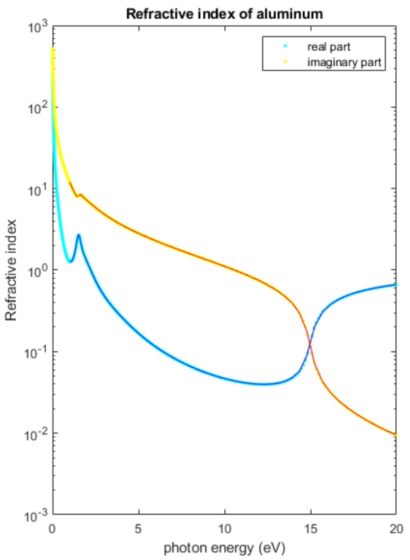

Figure 1: Refractive index of aluminium

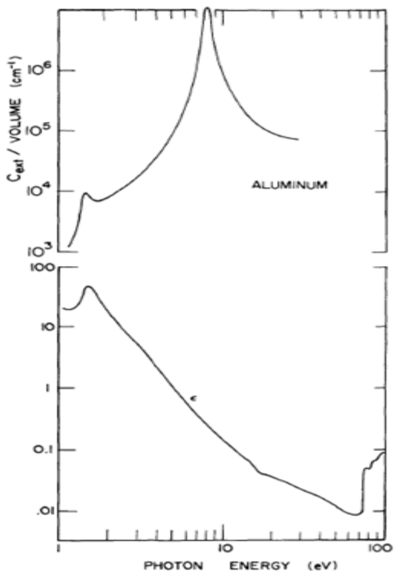

Figure 2 : The top graph is the extinction cross section of a polydisperse distribution of aluminium spheres The bottom graph is a comparison with the bulk absorption of aluminium

2. Interpretation of the experience (*Why are the spectra so different?*)

The shape of an object has a considerable impact on its absorption, extinction and scattering spectrum.

The properties of the objects (spheres in our example) are extremely different when its typical size is in the order of magnitude of the exciting field wavelength. Mie Theory is the one correctly describing this behaviour in this regime. One can explain this particular behaviour by considering that the cavity acts as a resonator for some wavelength because of the multiple interferences between the coming fields.

3. What is the typical size of the aluminium particles?

In order to answer to this question, we are going to find what sphere radius best fit the extinction curve of the polydisperse distribution of spheres (we managed to recover the data from the plot given in the subject using point-by-point data extraction tool software: https://plotdigitizer.com/) . We will be able to conclude that the polydisperse distribution mainly acts as a collection of spheres of diameter "a" so the typical size of the aluminium particles should be "a".

To find the size of the spheres, we will carry out an algorithm to search for the global minimum of a performance criterion. Our performance criteria to compare the spectrum is the sum of the squared errors (Euclidean norm). The error is the difference between the experimental result and the result of Mie's theory.

We can run our algorithm (Figure 4). It gives us a graph of our performance criteria. We can conclude that the typical size of aluminium corresponds to spheres of diameter $a = 10.48\ nm$.

We still have one unknown which is the concentration of aluminum nanoparticles. We will assume that the concentration is low enough not to use the Beer-Lambert law. It is assumed that the extinction efficiencies of the ensembles are proportional to the concentration. In order to find the concentration, we will increase or decrease it so that our performance criteria is as weak as possible. And we find: $C = 2 \times 10^{17}$ number of particles in a cubic centimeter.

Finally, we know all the features to put in our Mie Theory code. The result is given by Figure 3. Our result seems to correctly describe the experiment.

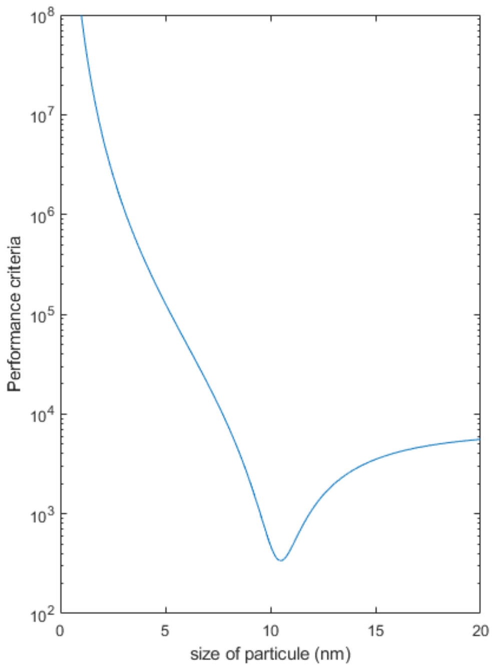

Figure 4: performance criterion between the Mie theory simulation and the experimental result.

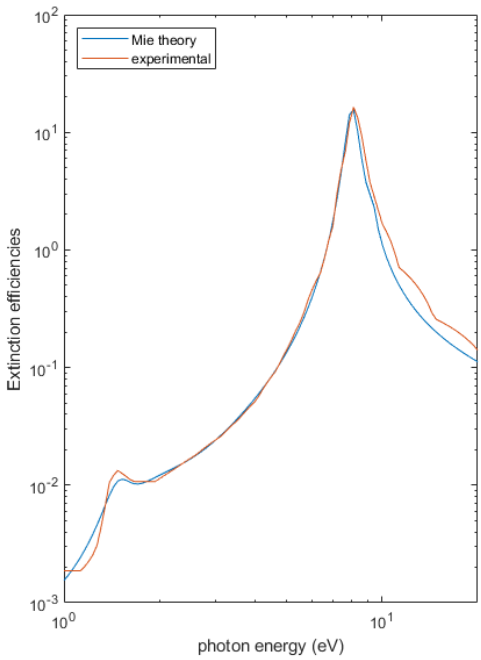

Figure 3 : Blue color corresponds to what Mie Theory predicts for a sphere of diameter a. Red color corresponds to the plot given at the beginning of the subject.

4. What is the multipolar content of the polydisperse distribution?

Now, we can carry out a study on the mode convergence given by the Mie theory. To use Mie theory, we need to calculate several coefficients which have a physical interpretation: Electric Dipoles a_1, Electric Quadrupoles a_2, Magnetic Dipoles b_1, Magnetic Quadrupoles b_2...

We can therefore plot the modulus of these coefficients. we notice that our sphere behaves mainly like an electric dipole. the other modes decrease very quickly and become negligible.

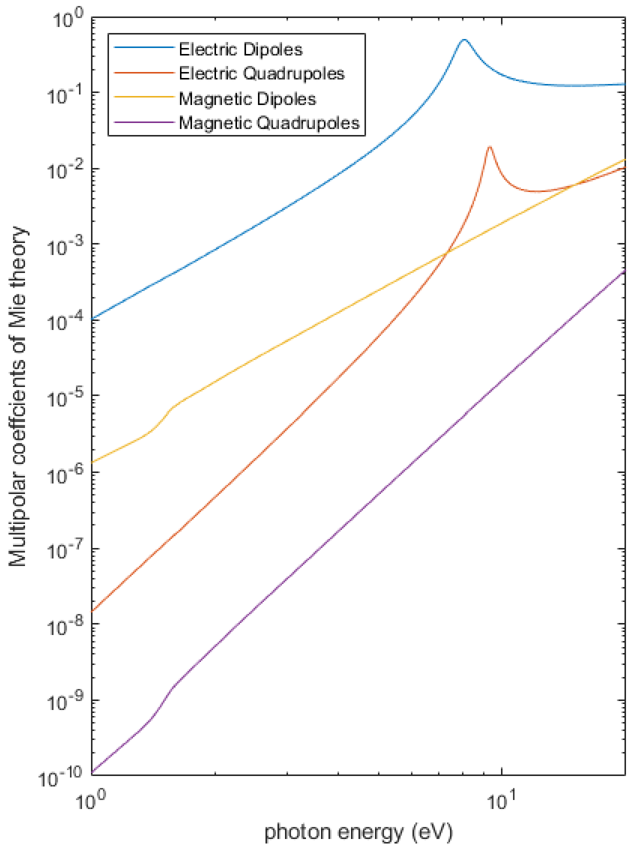

Figure 5: modulates the crumb coefficients of the external electric and magnetic fields for the first 2 modes.

Note : We believe the remaining error between the two graphs of Figure 3 comes from the plot digitizer tool that is not meant to be very precise.