

Exercises taken from the Nano-Optics Module, 2015 BioNanotechnology Summer Institute
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Part 1:

Size Dependence

Repeat the above procedure with Au spheres of sizes 20, 30, 40, 50 and 60 nm. Plot the resonance maximum, peak absorption, and peak scattering cross-section (m^2) as a function of size. How does the absolute and relative magnitude of absorption and scattering change as a function of size? What is the physical reason for this dependence? What are the implications for biomedical applications? (Hint: Imaging vs photothermal therapy).

(see J. Phys. Chem. B, 2006, 110 (14), pp 7238–7248).

Plasmon Modes of Anisotropic Nanoparticles

In the first tab of the DDA tool, (see above part 3) change the shape of the ellipsoid such that it is anisotropic. Namely, set SHPAR 1 and 2 = 5 nm and SHPAR 3 = 20 nm. This will elongate the shape along one axis (x in this case). Repeat the same calculation with all of the same parameters, except change the spectral window to 500-1000 nm in 10 steps. Save the scattering, absorbance and extinction spectra. Look at the E-field cut plane visualization to see what the field distribution looks like. Which axis is the field localized to? Next repeat the calculation with the same shape, but (on the first tab) change the target rotation to 90° in x. Rerun the calculation. Save the scattering, absorbance and extinction spectra. Now which axis have we excited? How do the spectra of the long and short axis differ in terms of their resonance peak? Which one has higher extinction? Now change SHPAR 3 to make the aspect ratio larger. How do the long-axis and short-axis peaks differ depending on aspect ratio of the rod? Discuss these observations. (see J. Phys. Chem. B, 2001, 105 (19), pp 4065–4067).

Dielectric Sensing

In the first tab of the DDA tool, reset the shape to “concentric ellipsoids”. This will generate an ellipsoid of one dielectric material with a shell of another dielectric material. Set the SHPAR 4, 5, and 6 = 70 nm and set the dielectric of this material to SiO₂ to make a silica nanoparticle core 70 nm in diameter. Next, set the SHPAR 1, 2, and 3 to either 74, 80, or 90 nm to make a symmetric shell around the silica nanoparticle of 4, 10, or 20 nm. Set the dielectric of this material to Au. For the spectrum, choose 500 to 700 nm, in 10 divisions. Set the refractive index of the medium to $n=1$. Run the simulation, save, and plot the extinction spectra. Now change the refractive index of the medium to $n=1.2$ and run the simulation again. Increase the refractive index of the medium another time to $n=1.4$ and run the simulation again. Plot the peak maximum of the extinction as a function of medium refractive index. Now compare with another person or group who used a different shell thickness. How does the sensitivity of the peak maximum with respect to medium refractive index change based on the thickness of the gold shell? (See J. Phys. Chem. C, 2007, 111, (47), 17451-17454.)

Part 2:

Simulations of New Geometries of Metal Nanoparticles

Try to generate a few custom objects of different shapes, put a couple of objects of different types in close proximity, rotate the light around the object, whatever your heart desires. Some questions you may want to keep in mind as you work through this:

What does the spectra look like?

Is my object primarily scattering or absorbing light?

Where are the positions of high field located?

If you have multiple objects how is the light localized?

How sensitive is my objects to changes in the environment dielectric constant?

How do objects of different composition vary in sensitivity and field strength?