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Computation of various optical properties of a Single Nanowire with up to two shell layers using Mie-Formalism

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Abstract: *In this paper we tried to compute the optical properties of a single nanowire using the Mie-Formalisim methodology on the nanohub open source tool availability. The current version of the tool is limited to only up to two shells and has pre-chosen materials options. Here the total optical properties such as total scattering, absorption and extinction efficiency are computed. Absorption efficiency of individual layers can also be calculated and studied using the same method. The integrated photon flux absorbed and the ideal photocurrent density under AM 1.5 G illumination as a function of layer thickness is used. Different electric and magnetic polarizability under the TE polarization of the E field perpendicular to nanowire axis is computed to study the various optical properties of a single nanowire with two shell layer.The simulations are based on rigorous solutions to the Maxwell's equations using Mie-formalism. Overall absorption as well as properties within each layer can be calculated for given thicknesses of each layer for the CMS (Core multi shell) NW (Nanowires) structures.*

I. Introduction

Tunable optical properties and plasmonic resonances in nanowires (NWs) and nanowire heterostructures have been employed for solar energy harvesting, sensing, metamaterials, and opto-electronics applications. Optimization of NW materials and dimensions will provide a guideline for device design and fabrication for the desirable application. The tool simulates the optical properties of NWs, particularly core-multishell (CMS) NWs, with a focus on absorption properties and plasmonic resonance. The simulations are based on rigorous solutions to the Maxwell's equations using Mie-formalism. Overall absorption as well as properties within each layer can be calculated for given thicknesses of each layer for the CMS NW structures. The simulation tool considers individual 3D CMS NWs in vacuum or medium under arbitrary polarized incidence. It is assumed that the NW is very long (L >> r). The scalar plane wave incidence is determined assuming the nanowire is along the z-axis. The incident light is resolved to two polarizations, the magnetic field is perpendicular to the nanowire axis, and the electric field is perpendicular to the nanowire axis. Mie formalism developed for circular cylinders with and without a shell is used to solve for the Mie coefficients of the system. First, the solutions for the 2D vector wave equation are determined in different spatial regions and the electromagnetic fields are expressed in terms of these solutions. Effectively the vector wave equation is substituting the H field into the E field of Maxwell's equations. In 2D, these solutions take the form of a summation of Bessel functions, whose coefficients are determined from the boundary conditions. Then boundary conditions for continuity at each interface are applied, which results in a system of linear equations. The problem statement can then be presented and experimented in a matrix form and the unknown Mie coefficients can be computed using the Maxwell equations. Using the calculated Mie coefficients, the total scattering, absorption and extinction efficiency, and the absorption efficiency of individual layers are determined. The integrated photon flux absorbed and the ideal photocurrent density under AM 1.5 G illumination as a function of layer thickness can also be obtained. Additionally, the electric and magnetic polarizability under TE polarization can be simulated.

Certain Assumptions are considered such as , 1) Nanowires are infinitely long which is valid as long as the nanowire length is & at 10*diameter. 2) Incident light is a plane-wave whose angle of incidence can be defined. Two polarizations are considered: Case I (H field is perpendicular to the nanowire axis) and Case II (E field is perpendicular to the nanowire axis). Unpolarized response is calculated as an average of Case I and Case II. When the illumination is incident normal to the nanowire axis, Case I corresponds to transverse magnetic (TM) and Case II corresponds to transverse electric (TE). The current version of the tool is limited to only up to two shells and has pre-chosen materials options. The number of shells can be selected from a dropdown menu; the options are core-only, core with a shell (core-shell), and core with 2 shells (core-multishell). Depending on the selection of number shells, the core radius, and shell thicknesses can be input between 1 and 500 nanometers. The material for the core and each of the shells can be selected from dropdown menus. Currently the material options are Ag, Al, Au, CdTe, Cu, Cu2O, Fe2O3, GaP, GaSb, Ge, ITO, Ni, Pt, Si, Si(amorphous), and TiO2. The medium the nanowire is in can be selected from a drop down menu to be air/vacuum, water, glass or other where the dielectric constant of the desired medium can be input (a number between 1 and 50).

II. Use of Mie Coefficients for Simulation

The coefficients obtained from the solution of the linear equation can be utilized to calculate the total scattering, absorption and extinction efficiency. The absorption efficiency of individual layers can also be determined. The total absorption and scattering efficiencies can be calculated from the coefficients as follows:

$$Q_{sca}^{(I)} = \frac{2}{k_0 c}\{\sum_{n=-\infty}^{+\infty}(\left|a_n^{(I)}\right|^2 + \left|b_n^{(I)}\right|^2)\}$$

$$Q_{ext}^{(I)} = \frac{2}{k_0 c}\{\sum_{n=-\infty}^{+\infty} Re(b_n^{(I)})\}$$

$$Q_{abs}^{(I)} = Q_{ext}^{(I)} - Q_{sca}^{(I)}$$

$$Q_{sca}^{(II)} = \frac{2}{k_0 c}\{\sum_{n=-\infty}^{+\infty}(\left|a_n^{(II)}\right|^2 + \left|b_n^{(II)}\right|^2)\}$$

$$Q_{ext}^{(II)} = \frac{2}{k_0 c}\{\sum_{n=-\infty}^{+\infty} Re(b_n^{(II)})\}$$

$$Q_{abs}^{(II)} = Q_{ext}^{(II)} - Q_{sca}^{(II)}$$

The absorption efficiency within individual layers is the ration of the power absorbed over the power incident per unit length of the wire. Thus the absorption efficiency can be calculated for each layer by setting the integration limits appropriately. The integrated photon flux absorbed within each layer is calculated as follows:

$$\Phi_{abs,i} = \int_{\lambda_1=300nm}^{\lambda_2=590nm} \frac{\lambda}{h_{planck}\ c_{light}} I_{AM1.5G}(\lambda)\eta_i \, d\lambda$$

Where I_AM1.5G is the intensity of 1-sun (air mass 1.5 global) illumination, h_planck is Planck's constant, and c_light is the speed of light. The spatial distribution of the integrated photon flux absorbed is the area integral of the spatial distribution with units of photons cm-2 s-1. It can be obtained by multiplying the spatial distribution of absorption with the integrated photon flux over the wavelength. The magnetic and electric polarizability can be obtained from the magnetic moment of the nanowire. Under TE illumination, e^(-iωt), propagating along the x-axis, the polarization of the nanowire.

Currently there are four options for the type of calculation the which can be done, one at a time.

Option 1: Total Scattering, Absorption, And Extinction Efficiency

For this calculation, the wavelength range can be set between 300 and 2000 nanometers. The angle of incidence can be set between 0 and 89 degrees where 0 degrees relates to the incidence being perpendicular to the nanowire axis. The number of multipoles, terms to be considered in the summation can be chosen between 0 and 50. When option 1 is run, three graphs, total scattering efficiency, total extinction efficiency, and total absorption efficiency, will be generated. Each of these graphs contains three curves for the nanowire being under unpolarized light, TM, and TE.

Option 2: Absorption Efficiency Of Individual Layers

For this calculation, the wavelength range can be set between 300 and 2000 nanometers. The angle of incidence can be set between 0 and 89 degrees where 0 degrees relates to the incidence being perpendicular to the nanowire axis. The number of multipoles, terms to be considered in the summation can be chosen between 0 and 50. When option 2 is run, three graphs, core absorption efficiency, shell 1 absorption efficiency, and shell 2 absorption efficiency, will be generated. Similar to option 1, each of these graphs contains three curves for the nanowire being under unpolarized light, TM, and TE. If the input parameters do not include a layer, like shell 2, that graph will simply have a curve at 0.

Option 3: Integrated Photon Flux Absorbed And Ideal Photocurrent Density

When option 3 is chosen in the simulation parameters, a dropdown menu becomes available to decide if the photocurrent and photon flux will be a function of the core, first shell, or second shell for the simulation. Also the dimensions of the nanowire section changes, creating tabs for the core, first shell, and second shell. The tab for the selected parameter allows for the input of a final radius/thickness value that must be larger than the initial radius/thickness between 1 and 500 nm. The increment can also be input as an integer between 1 and 100 nm. The angle of incidence can be set between 0 and 89 degrees where 0 degrees relates to the incidence being perpendicular to the nanowire axis. The number of multipoles, terms to be considered in the summation can be chosen between 0 and 50. When option 3 is run, two graphs are produced: the integrated photon flux absorbed and the ideal photocurrent density under AM 1.5 G illumination as a function of layer thickness. Each graph has three curves for the core, first shell and second shell. Again if the input parameters do not include a layer, like shell 2, that graph will simply have a curve at 0.

Option 4: Electric And Magnetic Polarizability

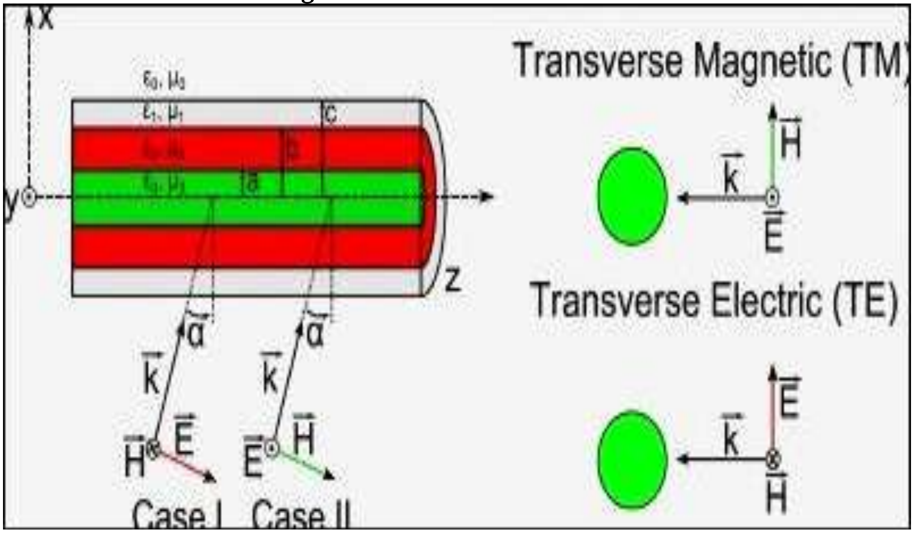
For this calculation, the wavelength range can be set between 300 and 2000 nanometers. There is no setting of the angle of incidence, since it is calculated under TE polarization. The number of multipoles, terms to be considered in the summation can be chosen between 0 and 50. When option 4 is run two graphs are produced: the electric polarizability and the magnetic polarizability. Each graph has two curves for the real and imaginary polarizability.

III. III.Result and Simulations

Optical response of the single NWs coated with multiple shells under plane-wave incidence can be Computed precisely using Mie formalism where Maxwell's equations shown and discussed above are solved in cylindrical coordinates and the NWs are assumed to be infinitely long. The total scattering, absorption and extinction efficiency can be expressed as infinite summations of contributions from each angular momentum channel depicting oblique plane-wave incidence on a CMS NW. Unpolarized light incident on the NW can be resolved into Case I and Case II where the magnetic and electric fields are perpendicular to the NW axis, respectively as shown in Figure1. When the incidence is normal to the NW axis, Case I and Case II correspond to transverse magnetic (TM) and transverse electric (TE) polarizations, respectively.

The nanowire schematic is shown in Figure 1 below. The Transverse Magnetic (TM) and Transverse Electric (TE) for case I and case II is also explained in the schematic. For the simulation the initial wavelength used is 300nm and the final wavelength is 1000 nm with20 number of multipoles used. The nanowire paramenters are as, number of shells are Core with 10 nm as diameter in Air / Vaccum medium. The core material used is Si with dielectric constant of the medium is 1.77.

Figure 1. Nanowire Schematic:



The Electric and Magnetic polarizability simulation graphs are shown in the figure 3. The number of multipoles, terms to be considered in the summation can be chosen between 0 and 50. When option 4 is run two graphs are produced: the electric polarizability and the magnetic polarizability. The figure 2 gives the graph of total absorbtion and Extenction efficiency computations. As we discussed in the Mie formulization that how the angle of incidence can be set between 0 and 89 degrees where 0 degrees relates to the incidence being perpendicular to the nanowire axis and is utilized. The number of multipoles, terms to be considered in the summation can be chosen between 0 and 50.

Figure 2. Absorption Efficiency and Extinction Efficiency Graph:

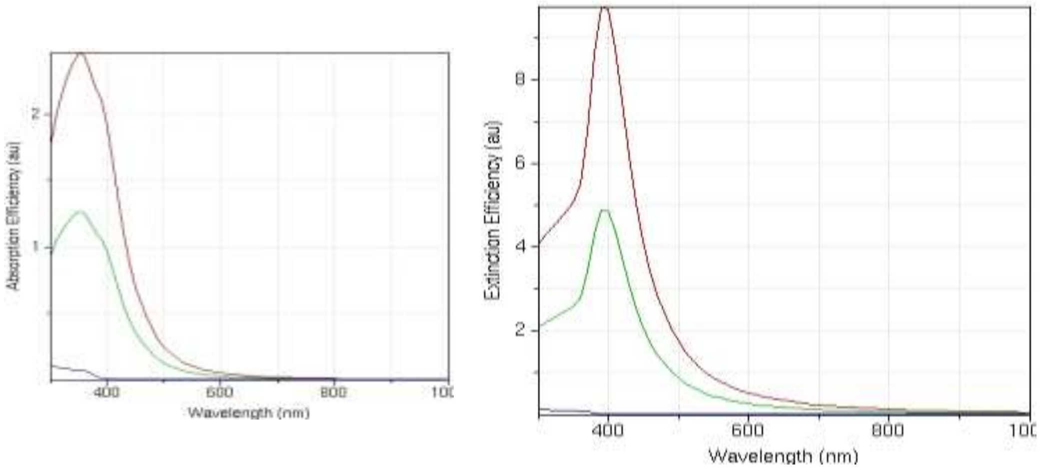
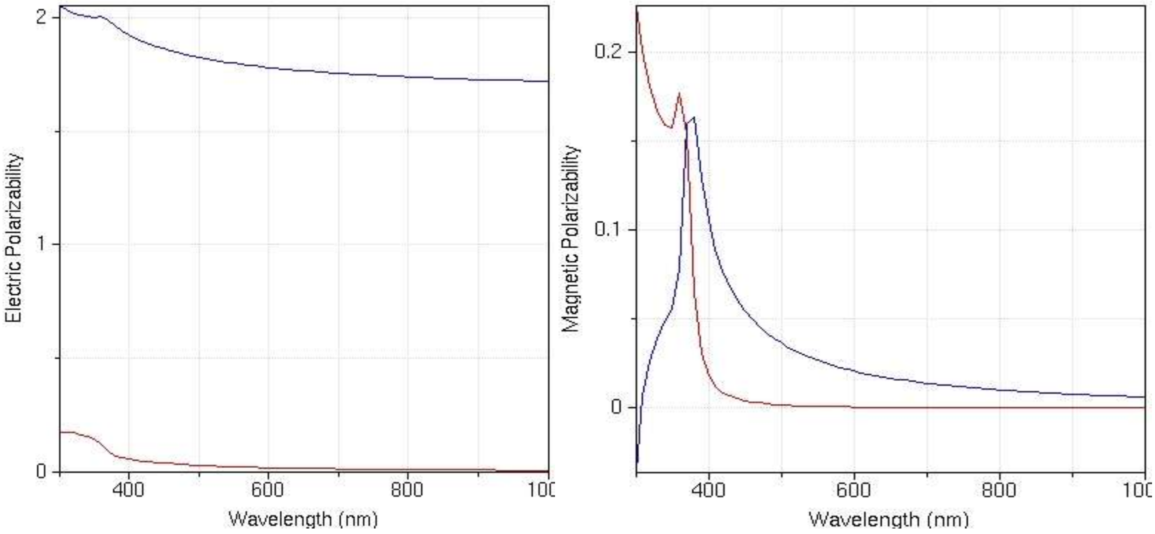


Figure 3. Electric and Magnetic Polarizability Graph:



IV. .Conclusion

In conclusion, our recent Computational studies on metal and semiconductor based Si materials CMS NWs as modular components for nano photonics application have been reviewed. Such structures demonstrate size dependent, highly tunable optical (Mie) and surface plasmon resonances in the visible range. This unique optical response can be used to achieve negative refraction and efficient light harvesting. In particular, plasmon hybridization in semiconductor metal semiconductor CMS NWs is an effective route to achieve visible range double resonance without the need for large changes in the size of the NW meta-atoms. For future scope instead on Si or other then the material we used aluminum and copper are excellent alternatives to silver and gold respectively for plasmon enhanced light harvesting in such NWs which enables the design of scalable plasmonic photoelectrodes. This are studied to to show high photocurrent . Application of such nanowires are such as photovoltaics, sensors, lasers and optical switches. Amongst the various possible applications, we believe, such coaxial nanostructures have a tremendous and immediate role in solar energy harvesting devices.

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