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Optical Properties of Nano-circuits for Metallic and Non-Metallic Nanoparticles

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Abstract

Optical properties of the nanoparticles can be studied theoretically by using the lumped electronic components. The particles having ε >0 behaved as capacitor whereas for ε <0 had inductor properties on the other hand the electric field perpendicular to the components then the properties of series combinations dominates and vice versa. A first principles electronic structure-based method is presented to determine the equivalent circuit representations of nanostructured physical systems at optical frequencies, via a mapping of the effective permittivity calculated for a lattice of physical nano-elements using density functional theory to that calculated for a lattice of impedances using circuit theory. Specifically, it is shown that silicon nanowires and carbon nanotubes can be represented as series combinations of inductance, capacitance and resistance. It is anticipated that the generality of this approach will allow for an alternate description of physical systems at optical frequencies, and in the realization of novel opto and nanoelectronic devices, including negative refractive index materials.

Keywords:
Metallic Nanoparticles, Nanocircuit elements, Refractive Index, Circuit Theory

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Introduction:

Light-matter interaction concept revolutionized the great era of science and technology. By Photon interaction with light the macro and nanotechnology developed and open the new horizon of different filed. Surface Plasmon Resonance (SPR) and Localized Surface Plasmon Resonance (LSPR) are the is of great interest and significance for the study of nanoparticle. Scientist working on them to inlovove it into detection of Covid-19 parallel to PCR tests in the world. Noble metals like Au, Ag in optical frequency like plamonic materials which has either negative real permittivity or positive. The size of the particles of metal is very small compared to optical wavelength therefore the metal behaves either like metallic or non-metallic naturally and it produces strong plasmon resonance effect to fabricate biosensor by producing strong optical response at micro/nanoscale. To improve the performance of SPR and LSPR, the refractive index and the size of the nanoparticle is of great importance, as scattering and absorption cross sections are size dependent and is proportional to the radius (r3) of nanoparticle (NP) in Quisi static approximation. Frohilich condition (equation 1) is the basic principle of LSPR working,

$$\varepsilon_r = -2\varepsilon_m$$

Where εr is complex permittivity of NP and its real part is negative and imaginary will be positive which can be negligible. Because of these conditions nobel matels that is Gold and silver are the commonly used metals for this purpose . The size of the particle can be smaller than 10nm and therefore they can treated as lumped nano-elements that is nano-capaciotor, nano-inductor and nano-resistors. Circuit theory can be in approximation of Maxwell equations in this situation and the particles in lower frequency range can be studied theoretically to optimize the size, optical and thermal properties of nanoparticles for the applications in biomedical, nano-opticas and optical information storage.

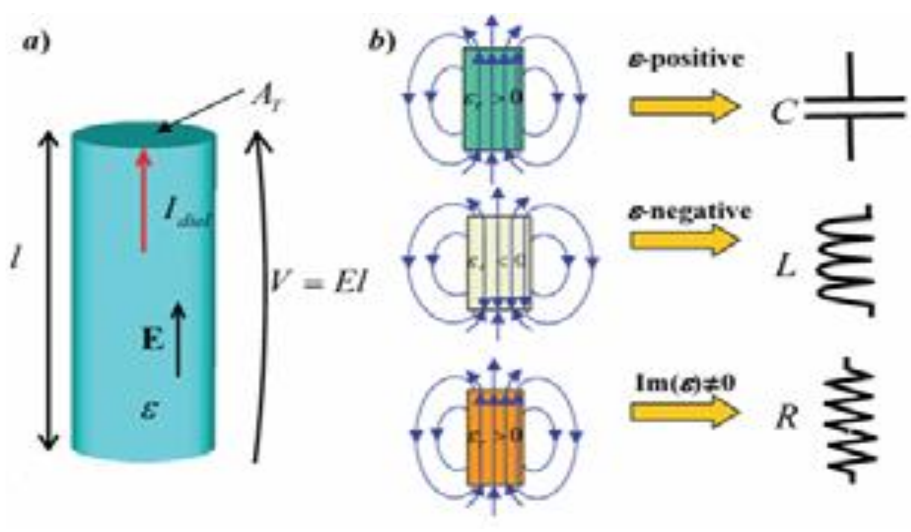

Fig. 1: Lumped Elements

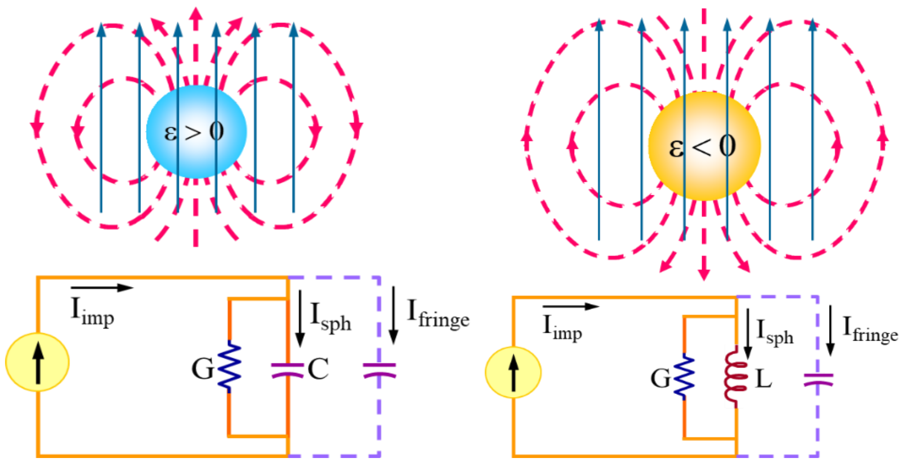

Fig. 2: Combination of Components with Respect to Propagation of Radiations.

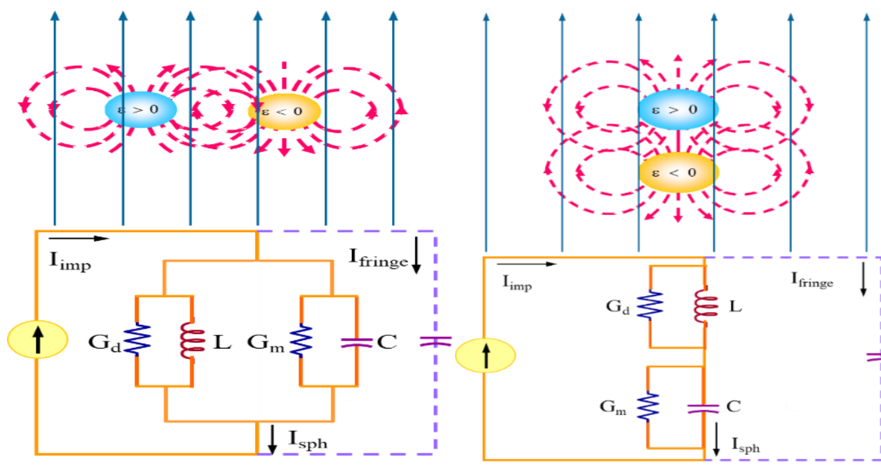

Fig. 3: More than on NP in Device.

In standard optical circuits, the lumped elements connected by the wire instead of direct combination and optical displacement current passing through out the circuit and the electric field can be calculated using the equations given below.

$$\mathbf{J}_D = -i\omega\mathbf{D}_n$$

$$\mathbf{E}_{res} = \mathbf{E}_{\text{int}} - \mathbf{E}_o$$

$$\mathbf{E}_{in} = \frac{3\varepsilon_d}{\varepsilon_m + 2\varepsilon_d}\mathbf{E}_o$$

$$\mathbf{E}_{out} = \mathbf{E}_o + \left(\frac{3\mathbf{n}(\mathbf{n} \cdot \mathbf{p}) - \mathbf{p}}{4\pi\varepsilon_o\varepsilon_m} \right) \frac{1}{r^3}$$

This current leakage, which can lead to coupling among various tightly packed nano-elements, can be accounted for as dependent sources in the circuit paradigm (1). To strengthen optical circuits, use of additional thin layers of materials with proper values of permittivity around the nanoparticles is required as mentioned before that the components cannot directly connected. For these layers to act as "insulators" for the optical displacement current, that is, to allow negligibly small displacement current and to stop the leakage, the real part of their relative permittivity needs to be very small. If "epsilon-near-zero" (ENZ) materials, designed properly, should prevent leakage of the optical electric displacement current, because inside such materials the displacement vector D should be negligibly small for a finite electric field. On the other hand, if one wants layers of materials that allow an easy flow of displacement current without introducing a noticeable optical electric field, materials with high relative real part of permittivity should be considered, because in such high permittivity media a very small electric field can produce a high amount of displacement current . Such "epsilon-very-large" (EVL) materials can play the role of nanoscale "conduit" for the optical displacement current, analogous to the role that metallic wires play for the conduction current in the RF domains.

Now let us consider a subwavelength nanoparticle that has a thin layer of an ENZ material around its sides and thin layers of EVL materials on its two ends (Fig. 1B). Such a composite nanoparticle can allow the flow of the optical displacement current in and out of its two EVL terminals and yet confine this current within it without any leakage from its ENZ side. Depending on the permittivity of the main material in the particle, this composite nanostructure can indeed act approximately as a modularized lumped nano element at optical frequencies. Thus, the addition of the ENZ and EVL materials for shielding and connecting the nanoparticle, although not always necessary, provide us with closer analogy between the RF and the optical circuit concepts and can also lead to lumped impedance values that would effectively be independent of the orientation of this Nano module with respect to the impressed optical electric field.

Experiment:

To get the ENZ and EVL material, the optical NP depends on the radius of the particles therefore different properties of NP are theoretically predicted by using mathematical models as well as the Mie theory of scattering and the NP of enhanced properties can be generated.

$$R := \frac{1}{\pi \cdot r \cdot \omega \cdot \varepsilon_i}$$

$$C := 2 \cdot \pi \cdot r \cdot \omega \cdot \varepsilon_0$$

$$L := \frac{-1}{\pi \cdot \omega^2 \cdot \varepsilon_r r \cdot \varepsilon_0}$$

$$R_{abso} := \frac{1}{\pi \cdot r \cdot \omega \cdot \varepsilon_i}$$

$$\text{Impedance} := \frac{1}{\sqrt{\left(\frac{1}{R}\right)^2 + \left[\omega \cdot \left(C - \frac{1}{\omega^2 \cdot L} + \frac{1}{\pi \cdot r \cdot \omega^2 \cdot \varepsilon_i}\right)\right]^2}}$$

$$Z_{abs} := \frac{1}{(\omega \cdot L)} + \frac{1}{\pi \cdot r \cdot \omega \cdot \varepsilon_i}$$

The equations help to calculate the optical properties of the lumped elements, and the impedance as well as the absorbance of the nanocircuits to accurate the values of components with respect to the radius of the NP.

Results and Discussions:

In this work, the optical properties of gold nanospheres were analyzed numerically. The optical properties of nanospheres were tuned by changing the size and the surrounding medium. Gold nanospheres are good absorbers as shown in the graph below, Under certain conditions, silver nanospheres can be more effective for the treatment of tumor cells. Gold nanospheres can also be used to prepare other complex structures. The resonance peak shifted toward larger wavelengths with an increase in the size of the nanosphere.

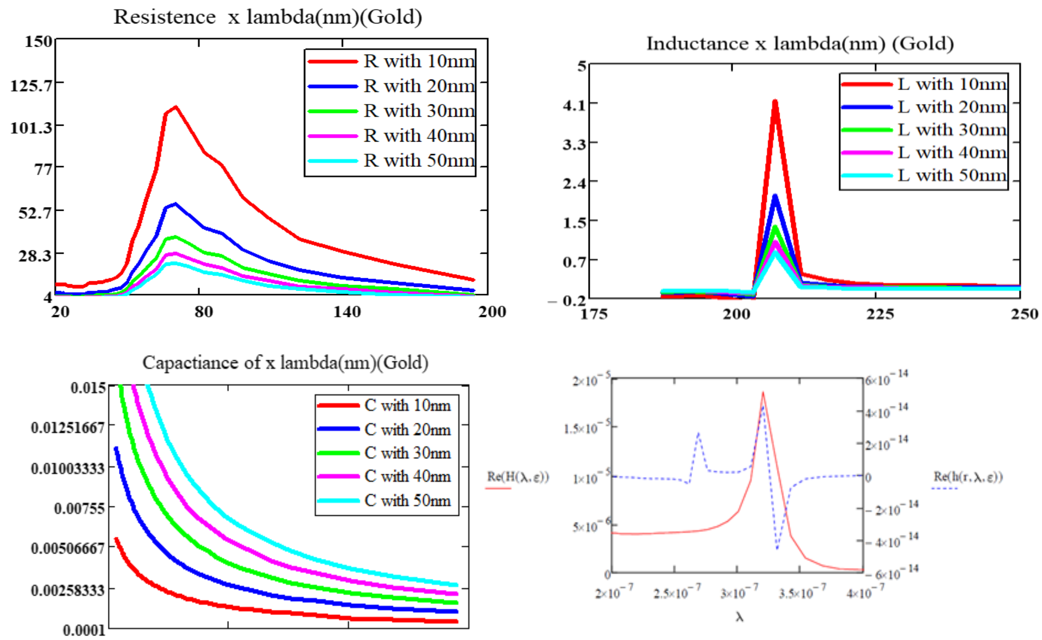

Fig. 4: The component values of Gold NP with different Radius

The resonance peak shifted with an increase in size from 10 to 50 nm. The effect of the scattering and absorption cross section on the extinction cross section changed with a change in the size of nanospheres. The uniform distribution of electric field inside the nanospheres is useful in applications where heating of nanoparticles is required. The experimental and numerical results showed close agreement in all cases. The calculated values of the resistor, inductor, and capacitor were very small as compared to the values used for electronics, indicating that the reported nanospheres can be used to design complex circuits for nanodevices. Resistance of the nanocircuit will behave as dissipation of displacement current through the fringes of the circuit, last graph in figure shows the impedance of the circuit.

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