UNIVERSITÀ DEGLI STUDI DELL'AQUILA

FACOLTÀ DI INGEGNERIA

Master Thesis
in
Mathematical Modelling in Engineering

MODELLING OF EPSILON-NEAR-ZERO (ENZ) METAL-SEMICONDUCTOR NANOCOMPOSITES

Ayodya Pradhipta Tenggara

MATHMODS MASTER PROGRAM
WITH THE SUPPORT OF THE ERASMUS MUNDUS PROGRAM
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Through zeal, knowledge is gotten; through lack of zeal, knowledge is lost;
let a man who knows the double path of gain and loss thus place himself that knowledge may grow.

Siddharta Gautama (563-623 BCE)

If anyone travels on a road in search of knowledge, God will cause him to travel on one of the roads of Paradise. The angels will lower their wings in their great pleasure with one who seeks knowledge. The inhabitants of the heavens and the earth and (even) the fish in the deep waters will ask forgiveness for the learned man. The superiority of the learned over the devout is like that of the moon, on the night when it is full, over the rest of the stars. The learned are the heirs of the Prophets, and the Prophets leave (no monetary inheritance), they leave only knowledge, and he who takes it takes an abundant portion.

Prophet Muhammad (570-632 CE)

I do not know what I may appear to the world, but to myself I seem to have been only a boy playing on the sea-shore, and diverting myself in now and then finding a smoother pebble or a prettier shell than ordinary, whilst the great ocean of truth lay all undiscovered before me.

Sir Isaac Newton (1642-1727 CE)

Abstract

The novel properties of optical/electromagnetic metamaterials like left-handed-materials and epsilon-near zero metamaterials have been studied and have been implemented in some applications, i.e. superlensing, optical cloaking, nanophotonic circuits, etc. The theoretical study and simulation of metamaterials optical properties are important to determine the physical parameters of metamaterials before they will be implemented or fabricated in real case.

This research aims to design epsilon-near-zero metamaterial by using the composite of core shell nanoparticles (Silver-InAs) and dielectric host medium (PMMA), and studying the properties of the designed epsilon-near-zero metamaterial in a specific interest frequency or wavelength. The studies of the designed metamaterial's optical properties are done based on the Maxwell Garnett Theory. Then, modelling and simulation of the designed epsilon-near-zero are also performed to study the electromagnetic interactions of unit structures of metamaterials by using an electromagnetic finite element solver, i.e. COMSOL Multiphysics.

The developed theoretical and simulation calculations allow us to determine the physical conditions to fabricate nanoparticles in a core/shell geometry in which a semiconductor (core) is surrounded by a thin metal shell. We demonstrated that the epsilon-near-zero condition is completely fulfilled when the induced gain in the semiconductor by external electromagnetic pumping beam (with a photon energy greater than the semiconductor gap) compensates the metal absorption effects.

The simulation results in COMSOL Multiphysics are able to show plasmonic resonance behaviour in the designed metamaterial that can change its electromagnetic response because the full electromagnetic model employed in the Comsol Multiphysics program enabled us to verify the existence of Localized Surface Plasmon Resonances occurring between neighbouring nanoparticles.

Keywords:

Metamaterial, Epsilon-Near-Zero Metamaterial, COMSOL Multiphysics, Maxwell Garnett Theory, Surface Plasmon Resonance

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CHAPTER 1

METAMATERIALS AND THEIR PRINCIPLE USES

1.1- Introduction of Optical Metamaterial

Nowadays, functional electromagnetic devices have developed spectacularly. The devices with novel properties like negative refractive index or zero refractive index, which were unimaginable before, are becoming real now. Those novel properties are able to realize some wonderful applications, for example to make image of small objects like DNA molecules so that it can be seen with eyes directly (superlensing) [1], to make objects become invisible (cloaking) [2] and to develop revolutionary information technology systems based on nanophotonic circuits [3,4]. But, there are still limitations of materials which are available in nature to follow those required novel processes or phenomena, so we need to create new structured composites of materials which are called metamaterials.

Metamaterial is a terminology to describe a man made material which is not available in nature done by some engineering processes. By terminology, 'meta' comes from greek word which means beyond. So, metamaterial means 'beyond conventional material'. The technical meaning of metamaterial, especially in optical field, is *an artificially structured material which attains its properties from the unit structure rather than the constituent materials. Inhomogeneity scale of metamaterial is much smaller than its constituent material, so that the electromagnetic response of metamaterial is expressed in terms of homogenized material parameters* [5]. Although metamaterials commonly are used in optical field, but their applications are not only limited in optics, but also in mechanics, electrical engineering, material science and basic physics.

Like another solid state materials, metamaterials also have structured atoms or molecules called 'meta-atoms or meta-molecules'. A metamaterial is arranged by atoms/molecules of constituent materials which form a united and homogeneous material. The distance between meta-molecules is called inhomogeneities and the inhomogeneities of metamaterials should be less than the scale of interest wavelength (in optical context or, in general, electromagnetic context). Macroscopically, metamaterials are homogeny like another materials because the inhomogeneity of their unit structure is less than wavelength scale. If an electromagnetic wave is applied in metamaterial, the response is a representation of whole metamaterials as a homogeny material.

Although metamaterial terminology was started to be used around year 2000 in Smith's paper [6], actually metamaterial itself has existed since a long time ago. Lycurgus Cup, the Roman Cup done at 4AD (Figure 1.1) is one example of metamaterial. It is a glass material with gold nanoparticles embedded. The cup has a unique and beautiful characteristic such that it will reflect green light and will transmit red light when the light scatters the crystal [5]. But, the application of that crystal was still limited in art without sufficient knowledge of its physical structure. The application of metamaterials specifically in optics also have been found before metamaterial terminology is used, like artificially dielectric, 'twisted jute' material to produce artificially chiral effect, split ring resonator, etc.

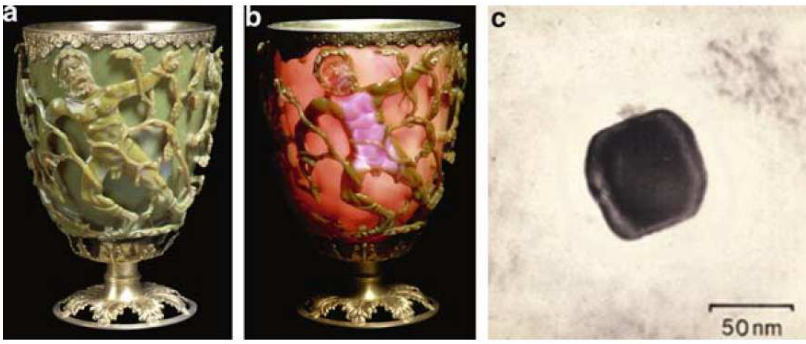

Figure 1.1 The Lycurgus Cup viewed (a) in reflected light and (b) in transmitted light. The cup is formed by many (c) gold nanoparticles [5]

Researches in metamaterial were started in left-handed material, or negative-index material (NIM). According to Cai in Optical Metamaterial [5], there are 3 important papers that open horizons and cornerstones of metamaterial research in optics, i.e. Vaselago's paper [7], Simth's observation [6], and Pendry's work [8]. Those 3 papers are mostly related to left-handed materials. Left-handed material is material whose electromagnetic properties, i.e. electric field **E**, magnetic field **H** and wave vector **k**, are represented by left hand, instead by right hand like conventional material. Left-handed materials are called negative-index materials (NIM) because their left handed property is resulted by negative refractive index n. Initially left-handed materials were the most important topics in metamaterial research, indeed left-handed material is used interchangeably with metamaterial.

Now, metamaterial research is not only limited in left-handed material, but also expands its area to another fields. In optical areas, there are many unusual electromagnetic properties that can be explored by arranging structural unit of materials, like nonlinear optics, optical magnetism, giant artificial chirality, super resolutions of metamaterial, electromagnetic cloaks of invisibility, perfect reflector, and so on [5]. Structural units arrangement can be done by modifying their size, shape, composition and morphology. The fabrication method of metamaterial's arrangement has evolved and is able to tailor unit structure in nanoscale. It is also coupled by electromagnetic simulation solvers that are able to perform good computations of metamaterials model design, like CST Microstudio, COMSOL Multiphysics and many other solvers. Nanofabrication process and simulation process cannot be separated and support each other in metamaterial research and production.

Homogeneity and isotropics are very important in designing optical devices. Homogeneity means that the structure of device is uniform macroscopically. Isotropic optical device responds scattered electromagnetic waves uniformly in all orientation and direction. To obtain a homogeneous and isotropic metamaterial, microscopic architectural strategy and exhaustive nanofabrication processes are required because metamaterial is arranged in its unit structure. Every single point of metamaterial's unit structure has to be controlled precisely.

Research in metamaterial area is still growing to design and fabricate homogeneous and isotropic metamaterials with low dissipation and high efficiency. Although many metamaterials have been produced and applied, but they are still far from ideal requirements. Recently, most produced metamaterials, not to say all, are still anisotropic, high dissipative and dispersive. So that the improvements have to be done simultaneously, from design, computation, fabrication until experimental examination.

Unusual optical properties of metamaterial like negative-index-metamaterial (NIM) and epsilon-near-zero metamaterial (ENZ) are very useful in many applications like electronics, control systems, signal processing and telecommunication. Optical sensings, miniature antennas, novel waveguides, subwavelength imaging devices, nanoscale photolithography are some examples. They show some prospects of metamaterial to be developed in future, not only in research area but also in massive industrial process. It is not impossible that applications of metamaterials can penetrate in renewable energy, agriculture, medics, and many other technological fields.

1.2- Macroscopic Properties of Optical Metamaterial

Metamaterial macroscopically responses scattered electromagnetic waves as a homogeneous media, although there are many complicated electromagnetic processes in its unit structure, like reflection, refraction, transmission, absorption, emission, Surface Plasmon Polariton (SPP) excitation, etc. Homogeneity in macroscopic structure is occurred due to inhomogeneity of metamaterial's unit structure is less than wavelength scale of interest. Then, macroscopic response of metamaterial (reflection, refraction, transmission, polarization, etc) is the 'average' response of unit structures and represents homogeneity of metamaterial in macroscopic structure.

Although metamaterials have unusual electromagnetic responses, but those responses must be satisfied Maxwell Equations. Maxwell Equations are equations describing electromagnetic interactions between source, field and material properties. Electromagnetic field can influence the configuration of electrons and magnetic dipoles in material so that polarization and magnetization in material happen. Degree of polarization and magnetization depends on material properties and also the incident field itself as function of electromagnetic source. Another electromagnetic responses of incident field due to material properties which are known commonly are reflection, refraction, diffraction, transmission, absorption and emission.

There are two important dimensionless parameters that represent macroscopic material properties, i.e. relative permittivity ε and relative permeability μ . For later passage, they will be shortly called permittivity ε and permeability μ . In isotropic media, both permittivity and permeability are constant for all spatial directions and it responds polarization and magnetization of incident field uniformly. On the contrary, anisotropic media does not respond polarization and/or magnetization uniformly for every direction so that there happen retardation (delay) for polarization and/or magnetization field. For non-magnetic material, permeability μ is always equal to 1 so that magnetization process inside material does not exist. There are also another two macroscopic material properties which are derived from permittivity and permeability, i.e. refractive index $n = \sqrt{\varepsilon\mu}$ and impedance $Z = \sqrt{\frac{\mu}{\varepsilon}}$.

It is shown in figure 1.2 the classification of material properties respect to the real part of permittivity and permeability. That classification is based on Maxwell Equations so that all materials properties, both constituent and engineered material (metamaterial), has to be satisfied by Maxwell Equations. Common transparent material like glass and polymer whose permittivity and permeability are positive is described in the first quadrant. Its electromagnetic fields, i.e. electric field **E**, magnetic field **H** and wave vector **k** are represented by right hand. In contrary, when both permittivity and permeability of material are negative, material will respond to transmit electromagnetic fields in opposite behavior such that electric field **E**, magnetic field **H** and wave vector **k** are represented by left hand. Moreover, positive permittivity material propagates electromagnetic waves whereas negative permittivity material cannot support propagation. Example of natural materials with negative permittivity and positive permeability (as described in the second quadrant) are metals when they respond electromagnetic waves for visible light (optical frequencies). Having negative permittivity, metals are not transparent and always reflect light. As a note, materials used in optical domain are usually non magnetic with permittivity equal to 1.

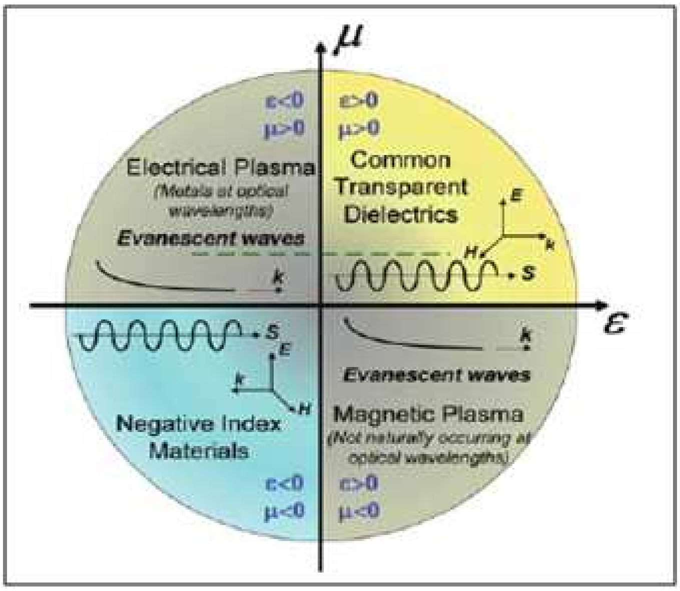

Figure 1.2 The parameter space of (relative) permittivity and permeability in real values. Dashed green lines represent non-magnetic material with permittivity μ=1. [5]

Another kind of metamaterials which also can be created are epsilon-near zero (ENZ) material. ENZ material is a material whose relative permittivity is close to zero for its corresponding frequency or wavelength of electromagnetic wave. In figure 1.2, the position of this material is in the green dashed line (with relative permeability is equal to 1) between the first and the second quadrant. By some theoretical and experimental researches, there are some electromagnetic properties and applications that can be implemented or generated by designing suitable epsilon-near zero (ENZ) materials, i.e. supercoupling effect [4], nonlinear optics [9,10] and multi-beam antennas [12].

This research aims to design and to make a model of metamaterial which can reach ENZ property with metal-semiconductor nanocomposites as the nanoparticles and a polymer as the host medium. The structure of the model is explained below. The modeling and simulation of metamaterial structure and its optical response is not less important than its fabrication, because metamaterial structure has a small dimension and has complicated physical behaviors. Doing simulation can substitute expensive experimental studies to predict the responses before fabrication is done.

1.3-Optoelectronic Materials

Electronic materials are classified into 3 kinds, i.e. dielectric, metal and semiconductor. Dielectric has a large energy gap (>5eV) between valence band and conduction bands so that it is required relatively high photon energies applied to dielectric to make electrons moving from valence band to conduction band. In contrary, energy gap in metal is very close (approaching zero) so electron can easily move from valence band to conduction band with small energy applied to metal. In electronics dielectric and metal are usually used as insulator and conductor, respectively. The third category of electronic material is semiconductor whose energy gap is between metal and dielectric. Electrons in semiconductor can excite from valence band to conduction band with several amount of energy which is more or equal to its energy gap.

The properties of electronic materials, i.e. insulator, conductor and semiconductor also have implication in optics. As it is known, light as electromagnetic wave always brings photon energy which is proportional to its frequency as it was discovered by Einstein. The photon energy of visible light is between 1.5 eV and 3 eV. Because photon energy of visible light cannot make excitation of electrons in dielectric, light can propagate inside dielectric and it looks as transparent medium. That phenomena also exists in semiconductors whose energy gap are higher than photon energy of light so that some semiconductors are considered as transparent medium in optics.

In optics, every material has the variable called critical wavelength λ_c, which is the minimum wavelength required to make excitation of electron in the material. The critical wavelength of material depends on its energy gap and the relation between them are expressed in equation (1.1)

$$\lambda_c = \frac{hc}{E_g} \tag{1.1}$$

λ_c : critical wavelength [m]

h : Planck constant ($= 6.626 \cdot 10^{-34}\ Js$)

c : speed of light in vacuum ($= 3 \cdot 10^{8}\ m/s$)

E_g : energy gap between conduction band and valence band [J, eV]

1.3.1 - Optical Properties of Dielectric

Dielectrics are very important media to propagate light because of their transparent behavior, as explained in the previous passages. Most of dielectrics used in optics are media in crystalline or amorphous form like glasses or quartz and sapphire. Some semiconductors also behave as dielectrics in optics and have transparent appearances. Transparent media are very suitable to propagate light because their critical absorbing band wavelengths are higher than electromagnetic wavelength in the visible range. In optics, refractive index n is usually used as the parameter to see 'transparency degree' of the medium. The value of refractive index should be equal or greater than 1 and complex values of the refractive index means that the medium is absorbing one for certain band of wavelengths, while for n=1 is equivalent to free space in vacuum.

The relationship between electrical properties of dielectric and the refractive index can be explained by Maxwell Equations. As written before, Maxwell equations are set of differential equations describing electromagnetic interaction between source and matter. The constitutive interactions between dielectrics and electromagnetic fields (electric and magnetic fields) are given in equations (1.2a) and (1.2b)

$$\boldsymbol{D} = \varepsilon_0\mathbf{E} + \mathbf{P} = \varepsilon_0\mathbf{E} + \varepsilon_0\chi_e\mathbf{E} = \varepsilon_0(1+\chi_e)\mathbf{E} = \varepsilon_0\varepsilon\mathbf{E} \tag{1.2a}$$

$$\boldsymbol{B} = \mu_0(\mathbf{H} + \mathbf{M}) = \mu_0(\mathbf{H} + \chi_m\mathbf{H}) = \mu_0(1+\chi_m)\mathbf{H} = \mu_0\mu\mathbf{H} \tag{1.2b}$$

where:

D : electric displacement

P : polarization

ε_0 : permittivity in vacuum ($= 8.85 \cdot 10^{-12} F$)

ε : relative permittivity, or shortly called 'permittivity'

χ_e : electric susceptibility

B : magnetic field

M : magnetization

μ_0 : permeability in vacuum ($= 4\pi \cdot 10^{-7}$H/m)

μ : relative permeability, or shortly called 'permeability'

χ_m : magnetic susceptibility

It has to be noticed that dielectrics commonly are not magnetic materials, so relative permeability, or shortly called 'permeability', is equal to 1. Then, relative permittivity, or 'permittivity', is dimensionless number and might be a complex number. For isotropic dielectrics, permittivity is always similar in all direction and is manifested in scalar form. In other hand, if a dielectric is anisotropic it has different permittivity for every coordinate spatial direction. Thus, permittivity is manifested as a tensor matrix. The expression of permittivity which has complex is shown in equation 1.3a such that ε' and ε'' are the real and imaginary part of permittivity, respectively.

Equation 1.3b shows the relationship between the medium permittivity and its refractive index n. If permittivity is a complex number, refractive index is also complex. The real part of refractive index represents the refractive and dispersion properties of the medium to transmitted light. In optical study, negative values of n''represent absorption of light by the medium, whereas for positive values of ε'' the medium admits energy to the light, i.e. represents a gain for the incident light.

$$\varepsilon = \varepsilon' \pm i\varepsilon'' \qquad (1.3a)$$

$$n = n' \pm in'' = \sqrt{\varepsilon} \qquad (1.3b)$$

The other important thing is that dielectrics are dispersive materials, especially when they responds visible light. So that dielectrics have different permittivity for different frequency of light coming to the medium. The permittivity of medium also corresponds to the refractive index, since the refractive index is square root of permittivity as written in equation (1.3b). The relation between the refractive index and the frequency of light what is called dispersion relation, is expressed by the Drude-Helmholtz model as written in equation (1.4). A typical example of dispersion relation ranging from ultraviolet to infrared is reported in the figure 1.2

$$\varepsilon(\omega) = 1 + \sum_j \frac{S_j \omega_j^2}{\omega_j^2 - \omega^2 - i\omega\gamma_j} \tag{1.4}$$

where:

S_j : the strength of component j

ω_j : the resonance frequency of component j

γ_j : the damping ratio of component j

In the example of Figure 1.3 shows the fact that in the visible range, the real part of permittivity is positive and the imaginary part of dielectric is close to zero. It means that dielectric behaves as transparent medium without absorption/emission when it interacts with visible light. The resonance frequencies exist in the infrared and ultraviolet ranges. When the dielectric interacts with the light in the resonance frequencies, ε' changes from positive to negative or vice versa and ε'' becomes positive. It should be noticed that refractive index is not independent respect to light frequency since permittivity depends on light frequency and refractive index is nothing else but the square root of permittivity.

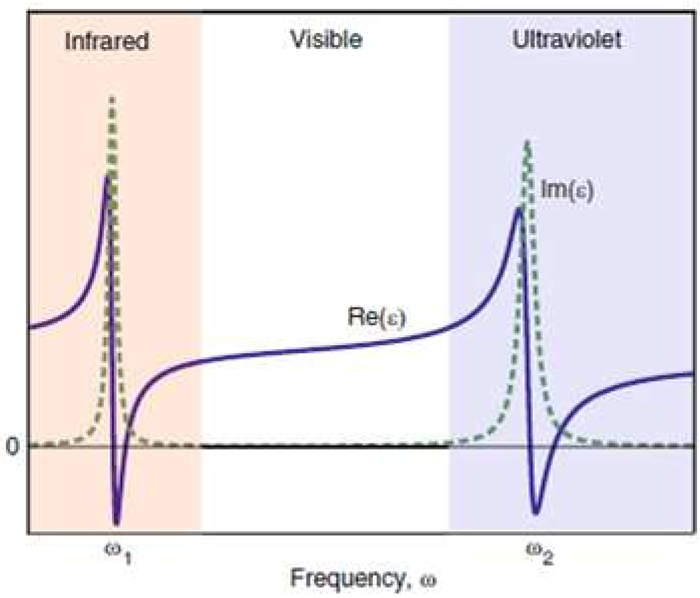

Figure 1.3 The dispersion relation of permittivity function ε(ω) for typical dielectric material with resonance frequencies ω_1 and ω_2

As it was mentioned above, the imaginary part of refractive index manifests degree of absorption of light intensity inside the dielectric medium. Equation 1.5a shows the relation between the absorption coefficient α and the imaginary part of the refractive index n′′. It can be concluded that absorption coefficient's sign is similar with the sign of n''. By using the Beer's law in equation 1.5b which describes the intensity of light inside the medium at any position z, light intensity will decrease (is absorbed) when α is negative and it will increase (light is emitted) when α is positive. I_0 and λ_0 are the light intensity and the wavelength of light in the first interface between air and dielectric medium, respectively. Light intensity I is proportional to electric field's square E^2.

$$\alpha = \frac{4\pi n''}{\lambda_0} \tag{1.5a}$$

$$I = I_0\, e^{-\alpha z} \tag{1.5b}$$

1.3.2- Optical Properties of Metal

As It has been explained above, metals have small energy gap between valence and conduction bands to the extent that electrons will move from valence band to conduction band although the energy applied to metal is so small (almost no gap). In optical point of view, visible light cannot propagate inside metals because the photon energy of the light makes electron excitation in metal. Because the only possible way for light to propagate is being reflected from the surface, metal looks bright and shiny.

Interaction between metal and electromagnetic field (light) is also satisfied by the constitutive relation of Maxwell Equation in equation 1.2a and 1.2b. So that metals have permittivity, permeability, displacement and magnetic field. The relations with refraction index and absorption coefficient are also similar, although metal is not transparent. But, the different between metal and dielectric when they interact with light is in the electron displacement. In metals, electrons can move freely along the crystalline structure and do not need force to move. In contrary, electrons in dielectrics are subject to a restoring force so that dielectrics show resonance frequencies as a direct consequence of the effect of restoring force. The permittivity of metals as a function of the light frequency is modeled by the Drude Model as written in equation 1.6a and 1.6b. The magnitudes of the Drude Model parameters to obtain permittivity in some noble metals are given on table 1.1

$$\varepsilon(\omega) = 1 - \frac{{\omega_p}^2}{\omega^2 + i\Gamma\omega} + i\,\frac{{\omega_p}^2\Gamma}{\omega(\omega^2+\Gamma^2)} \tag{1.6a}$$

$$\omega_p = \sqrt{\frac{n_e e^2}{\varepsilon_0 m}} \tag{1.6b}$$

where:

ω_p : plasma frequency [rad/s]

Γ : damping frequency [rad/s]

n_e : electron density in metal
e : electron charge ($= 1.6 \cdot 10^{-19}$)

Because electrons can move freely along the crystal, the polarization density $\vec{P}$ becomes an important parameter in the interaction between the metal and the electromagnetic field. By definition, polarization density P is the total dipole moment (vector) per unit volume and it depends on the electron density inside the metal, electron charge and displacement. Polarization density vector $\vec{P}$ and electron displacement vector $\vec{r}(t)$ as the function of time are expressed in equation 1.7a.

$$\vec{P} = n_e e\vec{r} \tag{1.7a}$$

$$\vec{r}(t) = \frac{e}{m}\frac{\vec{E}_0\, e^{-i\omega t}}{(\omega^2 + i\Gamma\omega)} \tag{1.7b}$$

where:
$\vec{P}$: the polarization density
n_e : the electron density
$\vec{r}(t)$: the electron displacement vector
$\vec{E}_0$: the initial electric field [V/m]

Equation 1.6a shows that the damping frequency or damping constant Γ contributes the imaginary part of permittivity. It is nothing else but the collision rate of electron inside metal crystalline. The inverse of damping constant is the collision time which is the average time needed when electrons collide each others. In the Drude Model, the damping constant Γ depends on the Fermi velocity v_f and the electron mean free path l as written in equation 1.8.

$$\Gamma = \frac{v_f}{l} \tag{1.8}$$

Table 1.1 Drude Parameters in Metals

Metal	ω_p (eV)	ω_p ($10^{15}\,s^{-1}$)	Γ (eV)	Γ ($10^{15}\,s^{-1}$)	v_F ($10^6\,ms^{-1}$)
Silver	9.2	14.0	0.021	0.032	1.4
Gold	9.1	13.8	0.072	0.11	1.4
Copper	8.8	13.4	0.092	0.14	1.6
Aluminum	15.1	22.9	0.605	0.92	2.0

Although the Drude Model for metal permittivity is quite good, but it also has weakness. Interband transitions, i.e. transitions of electrons from one energy state to others energy states when light scatters to metal happen and it are not predicted or calculated by the Drude Model. Interband transitions in metals influence many other things, for example the appearance color of metals and of course the permittivity. So that the Drude Model should be improved or modified to get a better model that considers also interband transitions of electrons in metals. The modified Drude Model is given in equation 1.9. The constant offset ε_∞ is an additional parameter to represent interband transitions of electrons in metal and it is experimentally observed.

$$\varepsilon(\omega) = \varepsilon'^{(\omega)} + i\varepsilon''^{(\omega)} = \varepsilon_\infty - \frac{{\omega_p}^2}{\omega^2 + i\Gamma\omega} = \varepsilon_\infty - \frac{{\omega_p}^2}{\omega^2 + \Gamma^2} + i\frac{{\omega_p}^2\Gamma}{\omega(\omega^2 + \Gamma^2)} \quad (1.9)$$

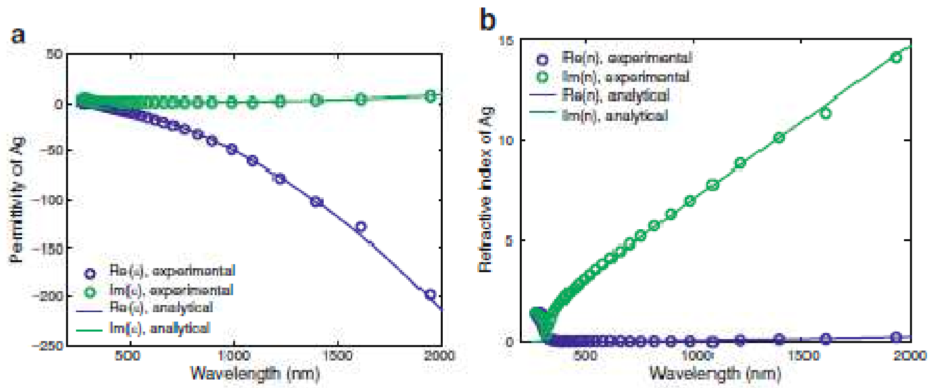

Figure 1.4 (a)permittivity and (b)refractive index of silver obtained by modified Drude Model and experiment data

Figure 1.4 shows the permittivity ε and the refractive index n of silver (Ag) obtained by analytical calculation of the Drude Model and experimental results. The real part of the permittivity in metals is always negative because free electrons move out of phase respect to the driving electric field of light and most of incident light coming to the interface between air and metal are reflected. It is the reason why noble metals look shiny.

1.3.3- Metal-Dielectric Composites

As it was described, metamaterials are engineered materials which attain their properties in unit structure rather than the constituent material and the inhomogeneity of metamaterials is less than their interest wavelength scale. As an engineered material, metamaterial is a kind of composite whose unit structures are 'created'. The unit structures must be arranged such that it can have special optical properties. The components of metamaterial composites are optical materials available in nature that are divided into two kinds, i.e. metal and dielectric (electronic dielectric and semiconductor). So that metamaterials are also called metal-dielectric composites.

The interaction between the metal-dielectric and electromagnetic field in unit structure of material is very complicated to be described by Maxwell Equations because its inhomogeneity scale is very small, less than a wavelength. Also there are special properties of metals when their dimensions are so small and they make more complicated problems. Therefore, in a macroscopic scale, the metamaterial structures are homogenous and they can be analyzed by the Maxwell Equations to study their interaction with electromagnetic fields. The Maxwell-Garnett theory (MGT) and the Bruggemann effective medium theory (EMT) are usually used to homogenize the unit structures' inhomogeneity and calculate the effective metamaterial properties in the macroscopic scale [5].

1.4- Objectives of the Research

The main goal of this research is to model epsilon-near-zero (ENZ) metamaterials. The metamaterial which is studied in this thesis is the composite of dielectric/insulator and metal/semiconductor nanoparticles. The investigation has been divided in two parts: a theoretical study and a simulation study.

The specific objectives of the research are shown below:

1. Studying the properties of the metamaterials (i.e. the composite of dielectric host medium and metal-semiconductor nanoparticles) which attain epsilon-near-zero (ENZ) by theoretical calculations in MATLAB. The constituent materials which are used in this research are InAs, Ag and polymethyl methacrylate (PMMA) [12] for the semiconductor, the metal and the dielectric host medium, respectively.
2. Performing the simple geometry models of the composite of dielectric insulator and metal-semiconductor nanoparticles' structures that represent the inhomogeinity of unit structures and simulating their electromagnetic response by COMSOL Multiphysics.
3. Conducting comparative study based on the obtained results of theoretical computation and model simulation.

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CHAPTER 2

THE DESCRIPTION OF THE NANOPARTICLE (METAL-SEMICONDUCTOR NANOCOMPOSITE) AND ANALYTICAL FORMULA

As discussed in the previous chapter, the designed metamaterial in this research is a composite of metal-semiconductor nanoparticles and dielectric. Metal semiconductor nanoparticles, or shortly called 'nanoparticles', are set of sphere nanoparticles which are distributed randomly in a dielectric medium. Each nanoparticle contains two main elements, i.e. semiconductor in the shell and metal in the core The constituent materials which are used in this research are InAs, Ag and polymethyl methacrylate (PMMA) for the semiconductor, the metal and the dielectric host medium, respectively. Based on Y. Zeng, et al [1] and P. Holmstrom, et al [2], the Drude Model, the Quantum Dot (QD) and the formula from the Maxwell Garnett Theory can be used to model the metal-semiconductor nanoparticles. Then, to calculate the effective permittivity of the metamaterial (i.e. the composite of nanoparticles and dielectric host medium), the formula from the Maxwell Garnett Theory (MGT) can be used too. The objective of the metamaterial is to get the special material property, that is epsilon near zero (ENZ) when it interacts with the frequency of interest of the electromagnetic field.

2.1–The Model of the Metal-Semiconductor Nanoparticle

The nanoparticle which is used to be implemented in this research is a composite of metal and semiconductor such that the semiconductor (InAs) and the metal (Ag) are placed as the core with radius R1 and the shell with the radius R2, respectively (see Figure 2.1). The Drude Model, the Quantum Dot (QD) approach and the Maxwell Garnett Theory (MGT) are used to study the average optical properties and the interaction of components in the nanoparticle.

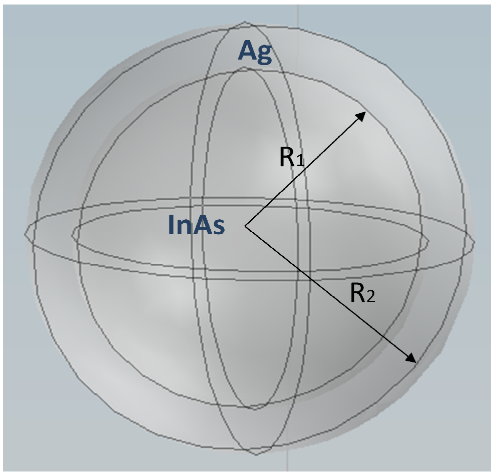


Figure 2.1 Model of the Nanoparticle

The Drude Model generally is used to model the optical properties of metal. In chapter 1, it has been explained that metals are a conductive materials such that electrons along the crystal can be excited from valence band to conduction band easily with a small energy applied to it. The consequence of that property makes metals tend to reflect the light and their real part of permittivity is negative. Silver (Ag) is used for metal as the shell in the metal-semiconductor nanoparticle. Based on P. Holmstrom, et al [2], the Drude model for permittivity of silver ε_{Ag} respect to the frequency ω is expressed in equation 2.1.

$$\varepsilon_{Ag}(\omega) = 1 - \frac{{\omega_p}^2}{\omega^2 - i\omega\Gamma_{Ag}} \quad (2.1)$$

where:

ω_p : the plasma angular frequency

Γ_{Ag}: the collision rate of silver

with the parameter values for Ag [3]:

$\Gamma_{Ag} = 3.00 \cdot 10^{14}/s$

$\omega_p = 1.38 \cdot 10^{16}/s$

InAs which is used as the core in the nanoparticle is able to compensate the negative permittivity of silver in the shell. Its permittivity is modelled by Quantum Dot (QD) model whose function has been formulated by P. Holmstrom et al [3] as it is written in equation 2.2a and 2.2b. The parameter A is related to the gain factor of semiconductor and can be activated by exposing the semiconductor nanoparticles to an external pumping light having a frequency inside its absorption band. If the parameter A is positive, it indicates a positive gain and the electromagnetic wave passing through the semiconductor is amplified. On the other hand, if the value of A is negative, the semiconductor will absorb part of the energy of electromagnetic wave passing inside the semiconductor.

$$\varepsilon_{InAs}(\omega) = \varepsilon_b + A \frac{{\omega_0}^2}{(\omega^2 - {\omega_0}^2) - 2i\omega\gamma_{QD}} \tag{2.2a}$$

$$A = \frac{2}{V_{QD}} [f_c(E_e) - f_v(E_h)] \frac{e^2 f / m_0 \varepsilon_0}{{\omega_0}^2} \tag{2.2b}$$

where:

A : the gain factor

f : the oscillator strength for the QD interband transition

f_c : the carrier of the carrier distribution functions in the QD conduction band

f_v : the carrier of the carrier distribution functions in the QD valence band

V_{QD}: the QD core volume ($V_{QD} = (4\pi/3){R_{QD}}^3$)

m_0: the mass of electron

ω_0 : the resonance frequency of QD

with the parameters values for InAs [3]:

$\varepsilon_b = 12.8$

$\gamma_{QD} = 1.519 \cdot 10^{12}/s$

$\omega_0 = 2.279269 \cdot 10^{15}/s$

2.2 – Model for the Metamaterial Used in the Numerical Simulations

The designed metamaterial is a composite between the nanoparticles and the dielectric host medium. The nanoparticles are placed distributively inside the host medium such that this metamaterial composite attains its objective, i.e. specifically epsilon-near-zero (ENZ) material. The nanoparticles with permittivity $\varepsilon_{\mathbf{np}}$ are distributed inside the host medium with permittivity $\varepsilon_{\mathbf{h}}$ to reach the average permittivity of the metamaterial close to zero. Figure 2.2 shows the geometry of the model of the metamaterial designed in COMSOL Multiphysics which includes two air layers such that metamaterial is sandwiched between air layers.

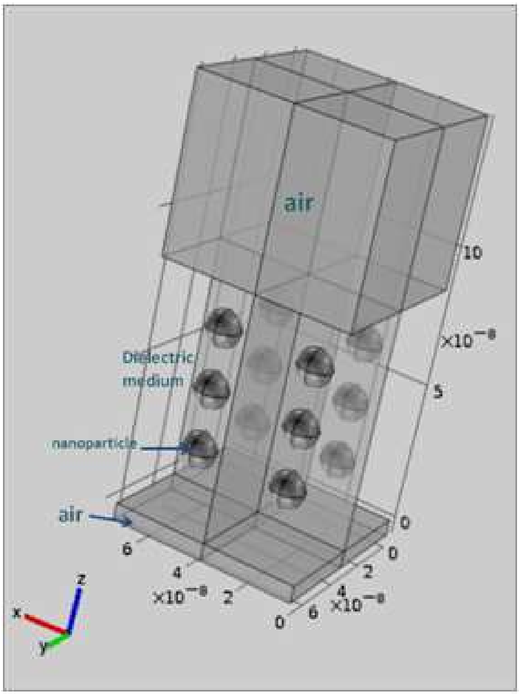


Figure 2.2 The Geometry Model of Metamaterial

2.3 – The Effective Permittivity of Material Composite

Compound of two or more constituent materials in a composite will respond to an electromagnetic field (light) as the average response from a material which is called the effective medium and is determined by its elements' properties. In metamaterials, the composite is usually made of dielectric (insulator or semiconductor) and metal. Two most famous and widely used methods to obtain the effective medium are the Maxwell Garnett Theory (MGT) and the Bruggemann effective medium theory (EMT). MGT and EMT come from the basic principles, but they use different assumptions for the composite topology.

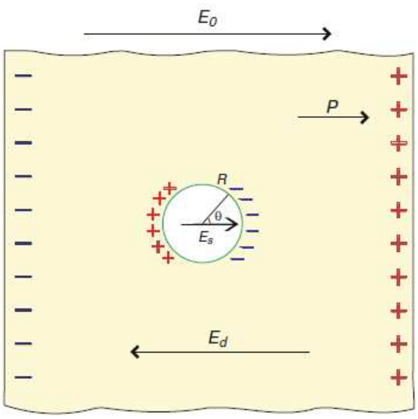


Figure 2.3. Electric Field along material's composite

The effective medium theory of a material composite is based on the Lorentz local field expression which describes the electromagnetic responses of a material in microscopic point of view. Figure 2.3 shows the Lorentz local field description in the Lorentz space and we are interested in studying only the response of the electric field in the dipole of small particle. The dipole is assumed to be a sphere with radius R. There are 3 electric field components in the Lorentz space: the external electric field $\boldsymbol{E_0}$, the depolarization field $\boldsymbol{E_d}$ (due to polarization charges P lying at the external surface on the medium) and the electric field lying on the Lorentz surface $\boldsymbol{E_s}$ (due to the polarization P). The total Lorentz field $\boldsymbol{E_L}$ are the summation of those 3 components and the summation of $\boldsymbol{E_0}$ and $\boldsymbol{E_d}$ is nothing else but the macroscopic electric field *E*. The Lorentz Field relation is written in the following equations 2.3.

$$\boldsymbol{E_L} = \boldsymbol{E_0} + \boldsymbol{E_d} + \boldsymbol{E_s} \tag{2.3a}$$

$$\boldsymbol{E_0} + \boldsymbol{E_d} = \boldsymbol{E} \tag{2.3b}$$

$$\boldsymbol{E_d} = -\frac{\boldsymbol{P}}{\varepsilon_0} \tag{2.3c}$$

$$\boldsymbol{E_s} = \frac{\boldsymbol{P}}{3\varepsilon_0} \tag{2.3d}$$

The equation 2.3 can be simplified to become the equation 2.4 which represent the Lorentz field in macroscopic point of view. In equation 2.5 and 2.6, it is shown that polarization P depends on polarizability of one dipole in molecule α , the density of the dipoles N, Lorentz electric field $\boldsymbol{E_L}$ and and dielectric constant or (relative) permeability ε . The polarizability α depends on the type of molecule. Then, after combining equation 2.5 and 2.6, Clausius-Mossotti Relation is obtained to see the relation between the material property in microscopic scale, i.e. the polarizability α and the dipoles density N; and the material properties in macroscopic scale, i.e. dielectric constant ε .

$$\boldsymbol{E_L} = \boldsymbol{E} + \frac{\boldsymbol{P}}{3\varepsilon_0} \tag{2.4}$$

$$\boldsymbol{P} = N\alpha\boldsymbol{E}_L = N\alpha\left(\boldsymbol{E} + \frac{\boldsymbol{P}}{3\varepsilon_0}\right) \tag{2.5}$$

$$\mathbf{P} = \varepsilon_0\chi_e\mathbf{E} = \varepsilon_0(1-\varepsilon)\mathbf{E} \tag{2.6}$$

$$\frac{N\alpha}{3\varepsilon_0} = \frac{\varepsilon-1}{\varepsilon+2} \tag{2.7a}$$

$$\alpha = \frac{3\varepsilon_0}{N}\frac{\varepsilon-1}{\varepsilon+2} \tag{2.7b}$$

The next step is using the Clausius-Mosotti relation for the composite material. First of all, it should be assumed that there are two constituent materials forming the composite in such a way that the volume ratio between first material with permittivity ε_1 and second material with permittivity ε_h are small enough (see Figure 2.3a). This assumption is called the Maxwell-Garnett Theory (MGT). The molecules of the first material are distributed randomly in the composite. So that the material with big volume (the second material) behaves as a medium. Then, the Clausius-Mosotti relation in equation 2.7a and the polarizability function in equation 2.7b should be modified into Clausius-Mosotti relation and polarizability in equations 2.8 and 2.9, respectively.

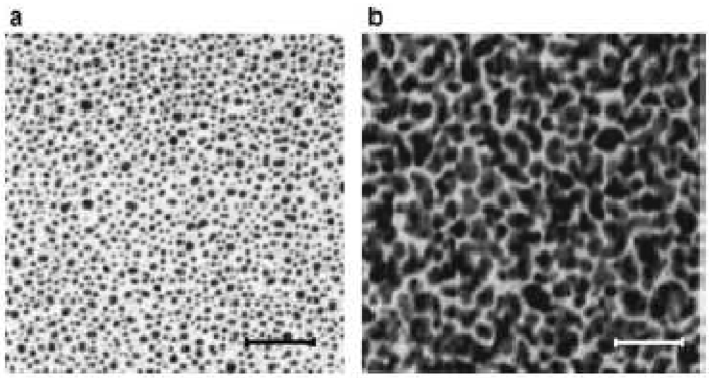


Figure 2.3 TEM images of typical metal-dielectric composites in a) MGT geometry and b) EMT geometry. The bright and the dark areas represent the host medium and the nanoparticles, respectively.

Equation 2.8 shows the modified Clausius-Mosotti relation for whole composite material such that host permittivity ε_h substitute constant 1 in equation 2.7a, because the medium is not the free space anymore, but it is the host material. Then, the polarizability function in equation 2.7b is also modified into equation 2.9. The modified polarizability equation includes the filling factor f because the microscopic polarization due to dipole moment only happens in the first material. Substituting equation 2.9 into equation 2.8 gives the effective permittivity function of material composite which is also called the formula of the Maxwell Garnett theory (MGT) in equation 2.12.

$$\frac{N\alpha}{3\varepsilon_0\varepsilon_h} = \frac{\varepsilon-\varepsilon_h}{\varepsilon+2\varepsilon_h} \tag{2.8}$$

$$\alpha = \frac{3\varepsilon_0\varepsilon_h f}{N}\frac{\varepsilon_1-\varepsilon_h}{\varepsilon_1+2\varepsilon_h} \tag{2.9a}$$

$$\text{f}= \frac{V_1}{V_1+V_h} \tag{2.9b}$$

$$\frac{N}{3\varepsilon_0\varepsilon_h}\cdot\left(\frac{3\varepsilon_0\varepsilon_h f}{N}\frac{\varepsilon_1-\varepsilon_h}{\varepsilon_1+2\varepsilon_h}\right) = \frac{\varepsilon-\varepsilon_h}{\varepsilon+2\varepsilon_h} \tag{2.10}$$

$$\frac{\varepsilon-\varepsilon_h}{\varepsilon+2\varepsilon_h} = f\left(\frac{\varepsilon_1-\varepsilon_h}{\varepsilon_1+2\varepsilon_h}\right) \tag{2.11}$$

$$\varepsilon = \varepsilon_h\frac{\varepsilon_1(1+2f)+2\varepsilon_h(1-f)}{\varepsilon_1(1-f)+\varepsilon_h(2+f)} \tag{2.12}$$

As it is described, MGT is based on assumption that no dipole moment happens in the second material, so the second material behaves as a medium. But, this assumption is only satisfied when the total volume of the first material is small enough respect to the second material and there is no dipole moment due to the interaction between two or more nanoparticles, or in the special condition such that there is no dipole moment in the second material. If the assumption of MGT cannot be required, the equation 2.11 must be modified into equation 2.13. Equation 2.13 uses the assumption that both the first and the second material behave similarly which have dipole moments each other and the host medium is the composite. So that the effective permittivity of the composite ε is nothing else but the host permittivity ε_h. This modified assumption model is called the Bruggemann effective medium theory (EMT) (see Figure 2.3b for a sketch of the resulting composite). By deriving equation 2.13, the effective permittivity of the medium based on EMT is obtained as written in equation 2.17 and 2.18. It should be noticed that the total filling fraction must be equal to 1. The effective medium equation based on EMT can also be applied to composites with more than two constituent materials and their expressions are shown in equations 2.19a and 2.19b.

$$\frac{\varepsilon-\varepsilon_h}{\varepsilon+2\varepsilon_h} = \frac{N_1\alpha_1}{3\varepsilon_0\varepsilon_h} + \frac{N_2\alpha_2}{3\varepsilon_0\varepsilon_h} \tag{2.13}$$

$$\alpha_1 = \frac{3\varepsilon_0\varepsilon_h f_1}{N_1}\frac{\varepsilon_1-\varepsilon_h}{\varepsilon_1+2\varepsilon_h} \tag{2.13b}$$

$$\alpha_2 = \frac{3\varepsilon_0\varepsilon_h f_2}{N_2}\frac{\varepsilon_2-\varepsilon_h}{\varepsilon_2+2\varepsilon_h} \tag{2.13c}$$

$$\frac{\varepsilon-\varepsilon_h}{\varepsilon+2\varepsilon_h} = f_1\frac{\varepsilon_1-\varepsilon_h}{\varepsilon_1+2\varepsilon_h} + f_2\frac{\varepsilon_2-\varepsilon_h}{\varepsilon_2+2\varepsilon_h} \tag{2.14}$$

$$f_1 + f_2 = 1 \tag{2.15}$$

$$\varepsilon = \varepsilon_h \tag{2.16}$$

$$f_1 \frac{\varepsilon_1 - \varepsilon}{\varepsilon_1 + 2\varepsilon} + f_2 \frac{\varepsilon_2 - \varepsilon}{\varepsilon_2 + 2\varepsilon} = 0 \tag{2.17}$$

$$\varepsilon = \frac{1}{4}\left[(3f_1 - 1)\varepsilon_1 + (3f_1 - 1)\varepsilon_2 \pm \sqrt{[(3f_1 - 1)\varepsilon_1 + (3f_2 - 1)\varepsilon_2]^2 + 8\varepsilon_1\varepsilon_2}\right] \tag{2.18}$$

$$\sum_i f_i \frac{\varepsilon_i - \varepsilon}{\varepsilon_i + 2\varepsilon} = 0 \tag{2.19a}$$

$$\sum_i f_i = 1 \tag{2.19b}$$

2.4 – The Effective Permittivity of the Metal-Semiconductor Nanocomposite (the Nanoparticle)

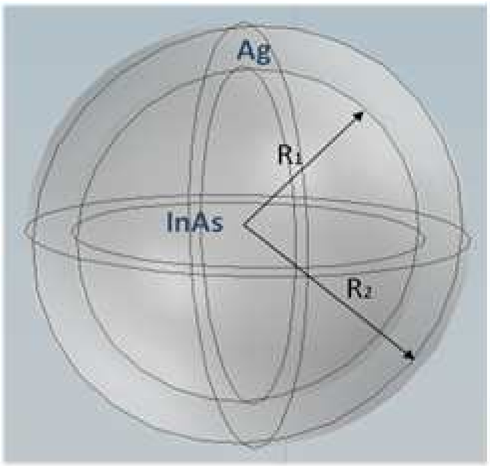


Figure 2.4 Model of the Nanoparticle

The metal-semiconductor nanoparticle as shown in figure 2.4 is a composite between the semiconductor InAs in the core and the metal Ag in the shell. The effective permittivity from the Maxwell Garnet Theory (MGT) can be used to obtain its effective permittivity of this nanoparticle such that the metal Ag behaves as a host medium. Although the volume of InAs can be larger than the volume of the host medium Ag, but the MGT assumption is still valid in this case because the metal Ag will not give dipoles moment, since Ag is not a separate molecule and always behaves as a medium. Moreover, InAs is not distributed inside the medium Ag so there is only one dipole moment. The effective permittivity of each metal-semiconductor nanoparticle is written below in the equation 2.20a and 2.20b.

$$\varepsilon_{np}(A, \rho, \omega_0) = \varepsilon_{Ag} . \frac{\varepsilon_{InAs}(1+2\rho) + \varepsilon_{Ag}(1-\rho)}{\varepsilon_{InAs}(1-\rho) + \varepsilon_{Ag}(2+\rho)} \tag{2.20a}$$

$$\rho = \frac{R_1^{\,3}}{R_2^{\,3}} \tag{2.20b}$$

where:

ρ : the fraction of the total nanoparticle volume occupied by the core material (InAs QD)

R_1: the radius of the core (InAs QD)

R_2: the radius of the shell (Ag)

2.5 – The Effective Permittivity of the Metamaterial (the Composite of the Nanoparticles and the Dielectric Host Medium)

As it is described, metal-semiconductor nanoparticles, or shortly called the nanoparticles, with permittivity ε_{np} are distributed randomly inside the dielectric host medium with permittivity ε_h . This composite is later called the metamaterial. When, the filling fraction of the nanoparticles f is small enough, the expression of the effective permittivity of the metamaterial ε_{eff} is obtained based on the Maxwell-Garnett Theory (MGT) as written in equation 2.21.

$$\varepsilon_{eff} = \varepsilon_h \frac{\varepsilon_{np}(1+2f)+2\varepsilon_h(1-f)}{\varepsilon_{np}(1-f)+\varepsilon_h(2+f)} \tag{2.21a}$$

$$f = \frac{V_{np}}{V_{np}+V_h} \tag{2.21b}$$

where:

V_{np} : the total volume of the nanoparticles

V_h : the volume of the host dielectric medium

2.6 – The Statistical Approach

The dimensions and parameters of the nanoparticlesdistributed in the host dielectric, i.e. the radius of the core R1, the radius of the shell R2, the core volume fraction ρ , the resonance frequency of quantum dot semiconductor ω_0 , the gain factor of quantum dot semiconductor A But in reality it is very difficult to fabricate nanoparticles which are distributed inside the host dielectric host medium having the same values of R_1, R_2, ρ and ω_0 , A. So that it is important to use the statistical method to study the effects of the parameter distributions in the metamaterial property, i.e. the effective permittivity of the metamaterial.

There are two parameters which are taken into account their parameter distributions, i.e. the core volume fraction ρ and the resonance frequency of quantum dot semiconductor ω_0. We do not consider the parameter distributions of R_1 and R_2 because those parameters have been covered with ρ. The gain factor A is expected to be thesame for all nanoparticles, since it is not so difficult to make uniform doping rate for pumping.

Gaussian model is used to describe the parameter distributions in the nanoparticles as written in the equation 2.22 where ρ and ρ' are the mean value and the deviate value of the core volume fraction, respectively; ω_0 and ω_0' are the mean value and the deviate value of the QD resonance freqeucy, respectively. Then, after inducing the Gaussian distribution of parameters in the Maxwell Garnett Theory (MGT), the effective permittivity of the metamaterial can be obtained as written in equation 2.23a, 2.23b and 2.23c.

$$G(\rho' - \rho, \omega_0' - \omega_0) = \frac{1}{\pi \Delta\rho \Delta\omega_0} e^{-\left(\frac{\rho' - \rho}{\Delta\rho}\right)^2} e^{-\left(\frac{\omega_0' - \omega_0}{\Delta\omega}\right)^2} \tag{2.22}$$

$$\int d\rho' \int d\omega_0' \left(\frac{\varepsilon_{np}(\omega, A, \rho', \omega'_0) - \varepsilon_h}{\varepsilon_{np}(\omega, A, \rho', \omega'_0) + 2\varepsilon_h} G(\rho' - \rho, \omega_0' - \omega_0) \right) = \frac{1}{f} \left(\frac{\varepsilon_{eff} - \varepsilon_h}{\varepsilon_{eff} + 2\varepsilon_h} \right) \tag{2.23a}$$

$$W_\omega(A, \rho | \varepsilon_h, \omega_0, \Delta\rho, \Delta\omega_0) = \int d\rho' \int d\omega_0' \left(\frac{\varepsilon_{np}(\omega, A, \rho', \omega'_0) - \varepsilon_h}{\varepsilon_{np}(\omega, A, \rho', \omega'_0) + 2\varepsilon_h} G(\rho' - \rho, \omega_0' - \omega_0) \right) \tag{2.23b}$$

$$\varepsilon_{eff} = \frac{1 + 2f W_\omega(A, \rho | \varepsilon_h, \omega_0, \Delta\rho, \Delta\omega_0)}{1 - f W_\omega(A, \rho | \varepsilon_h, \omega_0, \Delta\rho, \Delta\omega_0)} \tag{2.23c}$$

2.7 – References

[1] Y. Zeng, Q. Wu, D.H. Werner, "Electrostatic Theory for Designing Losseless Negative Permittivity Materials", Optic Letters, Vol.35, No.9 (2010).

[2] P. Holmstrom, L. Thylen, A. Bratkovsky, "Composite Metal/Quantum-Dot Nanoparticle-Array Waveguides with Compensated Loss", Applied Physics Letters 97, 073110 (2010).

[3] P. Holmstrom, L. Thylen, Bratkovsky, "Dielectric Function of Quantum Dots in the Strong Confinement Regime", Journal of Applied Physics 107, 064307 (2010).

CHAPTER 3

THEORETICAL CALCULATION IN MATLAB

Theoretical calculation aims to design the nanoparticles composite metamaterial to reach Epsilon Near Zero (ENZ) based on the theory. There are two kinds of approaches, i.e. nanoparticles with same dimensions and nanoparticles with different dimensions (radius) (statistical method). Maxwell Garnett Formula is used to analyze the first approach. Maxwell Garnett Formula assumes nanoparticles in random condtions media. Matlab is used to perform this theoretical calculation.

3.1–MATLAB Overview [1]

MATLAB is a comprehensive program which works with matrix formulation. It has several tools for programming, like numerical calculation and programming. MATLAB is not only very interactive to the user, but also the user can find many features which are easy to handle and are faster than the other traditional programming like Fortran, C or C++. One example of Matlbab's eminency is the user does not have to define variable type.

MATLAB contains 5 main components, i.e. Desktop Tools and Development Enivironment, Mathematical Function Library, the Language, Graphics, and External Interfaces. Desktop Tools and Development Environment is like the desktop of operating system in personal computer to guide user to start a program or using interface. MATLAB's language is a high level matrix language which controls flow statements, functions, data structure, input/output and object oriented programming features. Mathematical Function Library consists several mathematical function from elementary function like sine and cosine until advanced function like matrix invers, eigenvalues and Fast Fourier transform (FFT). Graphics are useful to perform the vector/matrix array in the graphic display, both 2D and 3D, such that the user can set the performance of it as it is needed to display. Then, external interfaces can be used to do interaction between MATLAB and others programming tools like Fortran, C/C++.

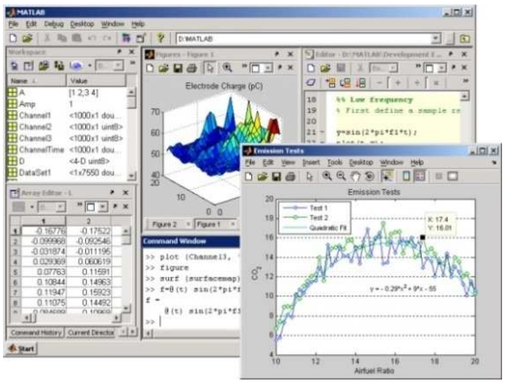


Figure 3.1 MATLAB Desktop

3.2–MATLAB Implementation in Calculation of the Metamaterial Variables

There are some fundamental theoretical equations which are used to compute the metamaterial properties, as it has been described in Chapter 2, i.e.:

- The effective permittivity of silver (Ag) by Drude Model

$$\varepsilon_{Ag}(\omega) = \varepsilon_{\infty} + \frac{{\omega_p}^2}{\omega^2 - i\omega\Gamma_{Ag}} \tag{3.1}$$

$$\varepsilon_{\infty} = 1$$

$$\Gamma_{Ag} = 3.00 \cdot 10^{14}/s$$

$$\omega_p = 1.38 \cdot 10^{16}/s$$

- The effective permittivity of the InAs Quantum Dot:

$$\varepsilon_{InAs}(\omega) = \varepsilon_b + A\frac{{\omega_0}^2}{(\omega^2 - {\omega_0}^2) - 2i\gamma_{QD}} \tag{3.2}$$

$$\varepsilon_b = 12.8$$

$$\gamma_{QD} = 1.519 \cdot 10^{12}/s$$

$$\omega_0 = 2.279269 \cdot 10^{15}/s$$

- The effective permittivity of the metal-semiconductor nanoparticle

$$\varepsilon_{np}(A, \rho, \omega_0) = \varepsilon_{Ag} \cdot \frac{\varepsilon_{InAs}(1+2\rho) + \varepsilon_{Ag}(1-\rho)}{\varepsilon_{InAs}(1-\rho) + \varepsilon_{Ag}(2+\rho)} \tag{3.3a}$$

$$\rho = \frac{{R_1}^3}{{R_2}^3} \tag{3.3b}$$

- The effective permittivity of the metamaterial

$$\varepsilon_{eff} = \varepsilon_h \frac{\varepsilon_{np}(1+2f) + 2\varepsilon_h(1-f)}{\varepsilon_{np}(1-f) + \varepsilon_h(2+f)} \tag{3.4a}$$

$$f = \frac{V_{np}}{V_{np} + V_h} \tag{3.4b}$$

3.2.1–MATLAB Computation Results

- **Permittivity of Ag (by Drude Model)**
  The computational result of permittivity

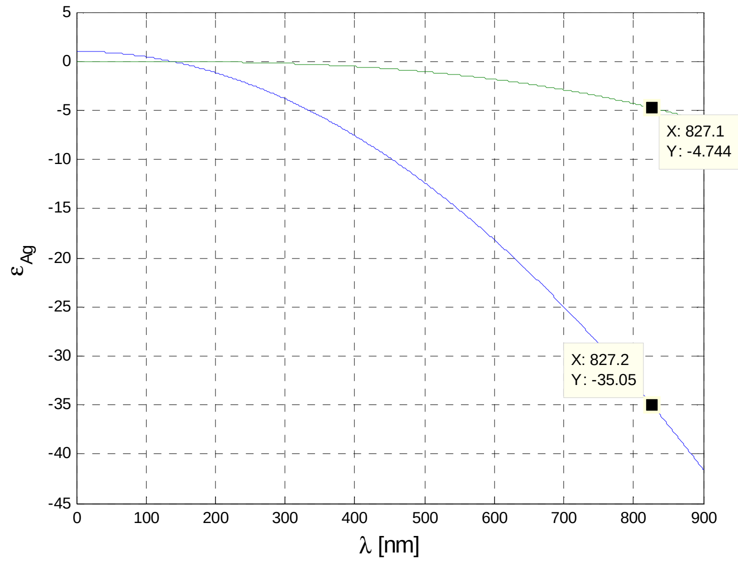


Figure 3.2 Computation Result for the Permittivity of Silver in Several Range of Wavelength

- **Permittivity of InAs (by Quantum Dot Model)**
  The result:

  A = `3.203320623998E-03 (gain factor)`

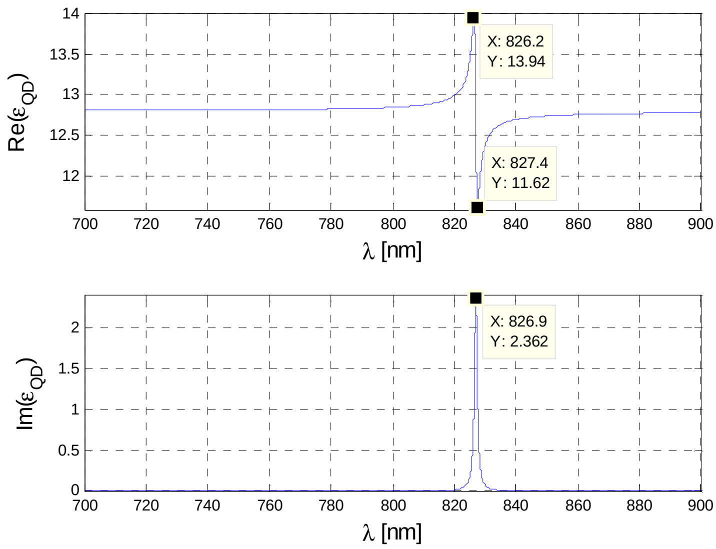


Figure 3.3 Computation Result for the Permittivity of InAs in Several Range of Wavelength

- **Permittivity of the Metal-Semiconductor Nanoparticle (Ag-InAs)**

  ρ = 0.498272867240438 (filling fraction)

  The result:

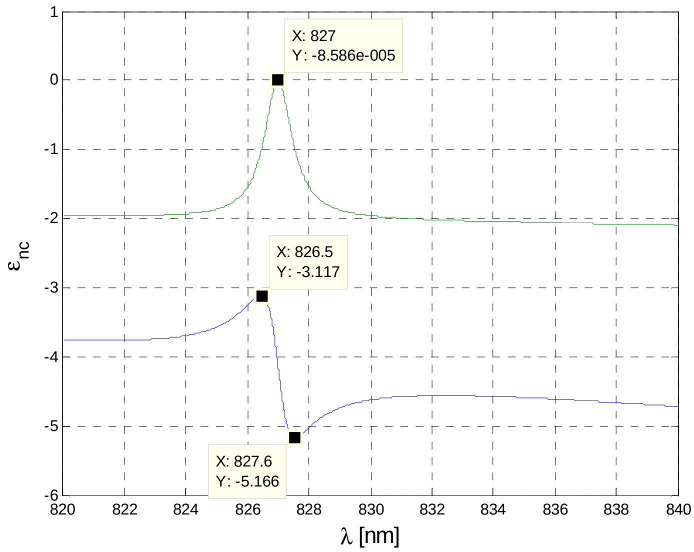


Figure 3.4 Computation Result for the Permittivity of the Metal-semiconductor nanoparticles in Several Range of Wavelength

- **Permittivity of the Metamaterial (the Composite of Nanoparticles and Host Dielectrics) by Fixed Methods**

  $\varepsilon_h = 2.2022$ (the host dielectric constant)

  f = 0.02 (the filling fraction)

  The result:

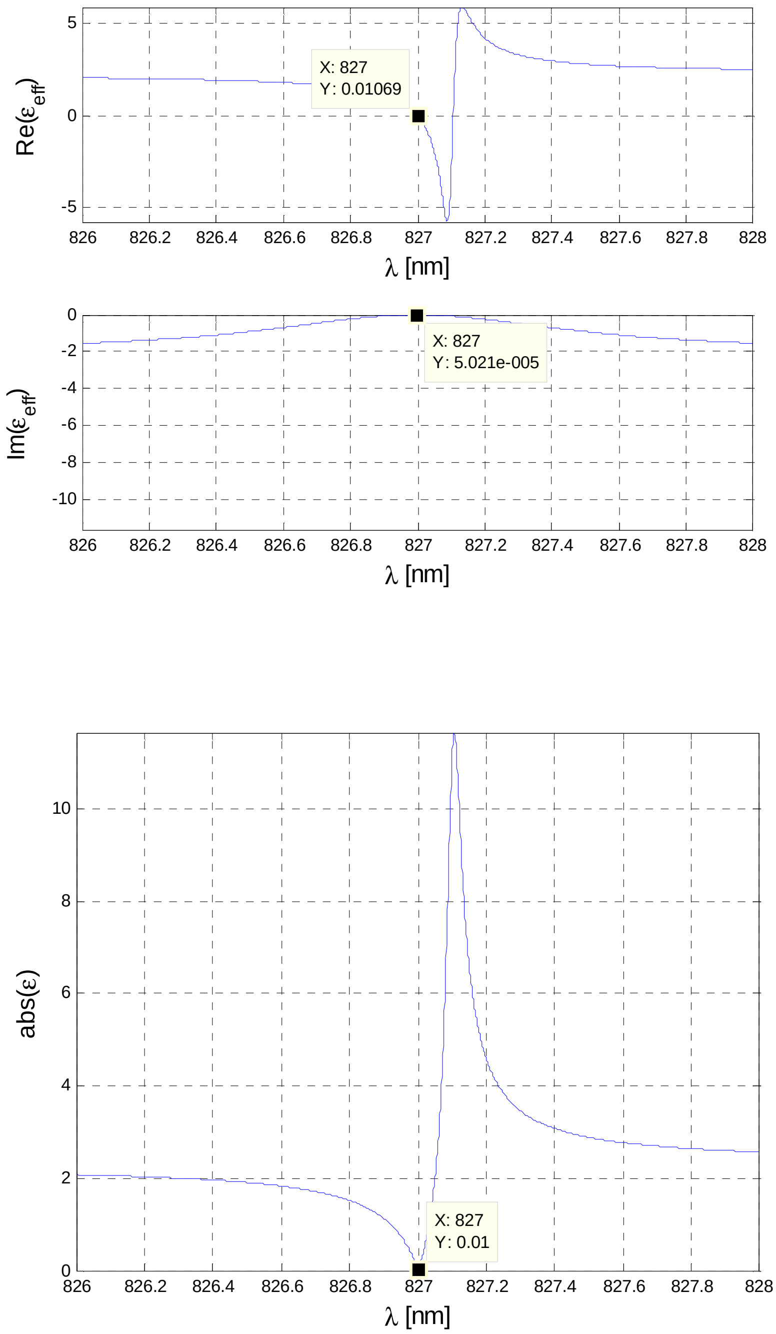


Figure 3.5 Computation Result for the Permittivity of the Metamaterial Permittivity and Its Modulus in Several Range of Wavelength by Fixed Methods

- **Permittivity of the Metamaterial (the Composite of Nanoparticles and Host Dielectrics) by Fixed Methods**

  $\varepsilon_h = 2.2022$ (the host dielectric constant)

  f = 0.02 (the filling fraction)

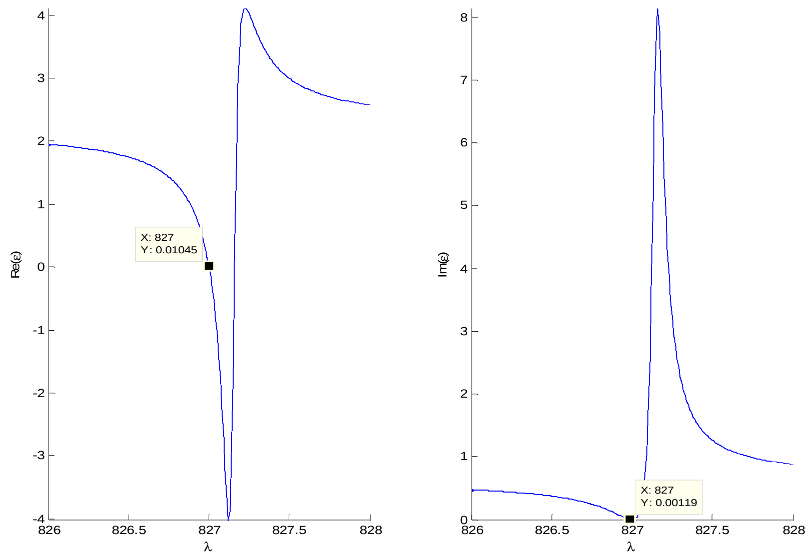


Figure 3.6a Computation Result for the Permittivity of the Metamaterial Permittivity and Its Modulus in Several Range of Wavelength by Statistical Methods when $\Delta\rho = 0, \Delta\omega = 0$

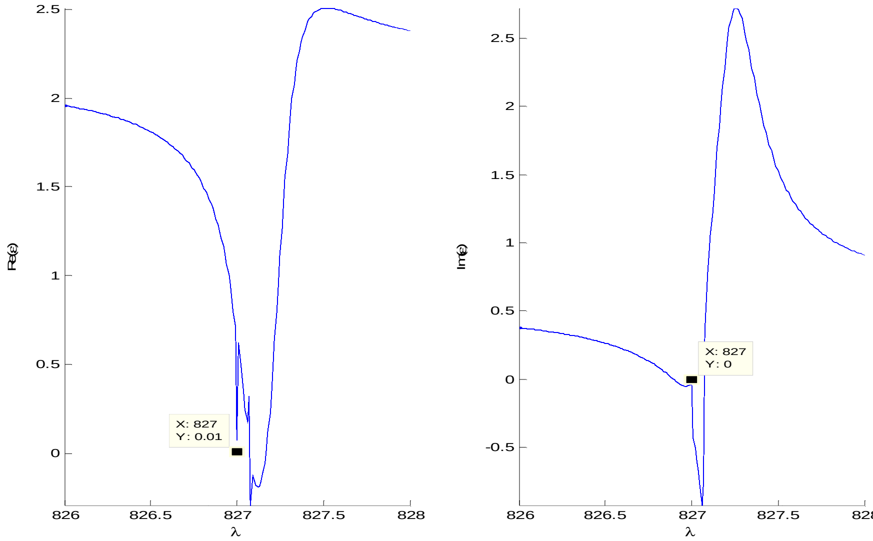


Figure 3.6b Computation Result for the Permittivity of the Metamaterial Permittivity and Its Modulus in Several Range of Wavelength by Statistical Methods when $\Delta\rho = 0.01, \Delta\omega = 0$

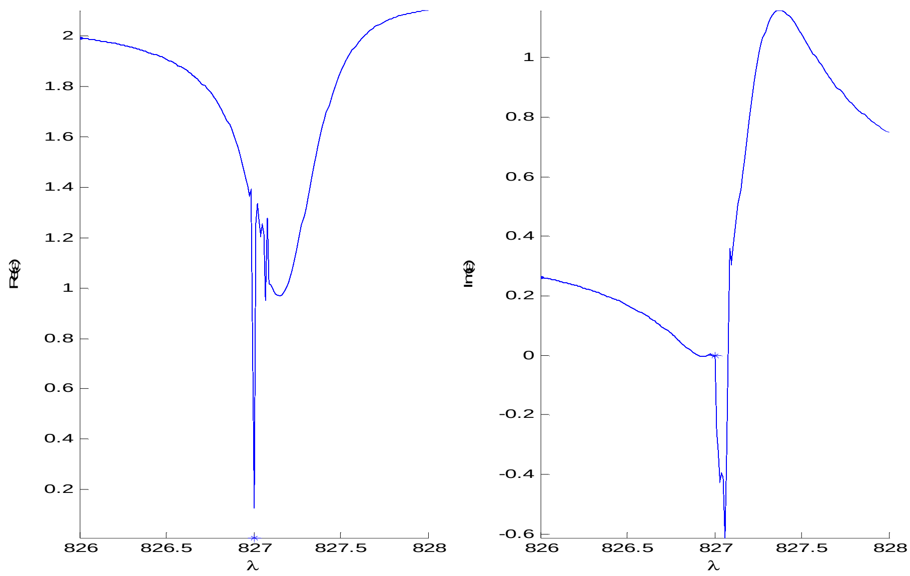


Figure 3.6b Computation Result for the Permittivity of the Metamaterial Permittivity and Its Modulus in Several Range of Wavelength by Statistical Methods when $\Delta\rho = 0.02, \Delta\omega = 0$

3.2.2 - Numerical Computation of in MATLAB to Obtain ENZ Metamaterial by Fixed Method and by Statistical Method

To reach the metamaterial with epsilon-near-zero (ENZ), the independent variables of the metamaterial have to be set such that the effective permittivity of the metamaterial becomes zero or relatively close to zero. The independent variables of the metamaterial which determines the effective permittivity are InAs' gain factor (A), the filling factor of the nanoparticle (ρ), the filling factor of the metamaterial (f) and the wavelength λ . As it is seen in Figure 3.5 and 3.6 , there exists dispersion of the effective permittivity respect to the wavelength and it is impossible to get epsilon-near-zero for all wavelength. So that we have to determine in which specific wavelength we want to get epsilon-near-zero.

MATLAB is able to make numerical computation to determine those independent variables based to get the goal, i.e. epsilon -near-zero, as seen in the appendix. The results of MATLAB numerical computation to obtain the optimal value of ρ, A,R1 and R2 by fixed method and by statistical method are shown in table 5.1 and table 5.2.

Table 5.1 The optimal Parameters to Reach ENZ in 827 nm by fixed method

Filling Fraction (F)	ρ	A	R1 [nm]	R2 [nm]
0.02	0.4983	3.203E-03	5	6.306876
0.03	0.5010	3.175E-03	5	6.295296
0.04	0.5037	3.149E-03	5	6.284194
0.05	0.5063	3.123E-03	5	6.273537
0.06	0.5087	3.098E-03	5	6.263302
0.07	0.5112	3.075E-03	5	6.253461
0.08	0.5135	3.052E-03	5	6.243992
0.09	0.5157	3.030E-03	5	6.234878
0.1	0.5179	3.009E-03	5	6.226095

Table 5.1 The optimal Parameters to Reach ENZ in 827 nm by statistical method ($\Delta\omega = 0$)

$\Delta\rho$	ρ	A	R1 [nm]	R2 [nm]
0.000	0.5010	3.175E-03	5	6.295296
0.01	0.5092	3.262E-03	5	6.261435
0.02	0.523	2.262E-03	5	6.205871

3.3–Refference

[1] http://www.mathworks.com

CHAPTER 4

COMSOL SIMULATION

4.1 – Introduction of COMSOL Multiphysics

COMSOL Multiphysics is a solver to simulate physical models based on partial differential equation (PDE) by Finite Element Method (FEM). One of its excellences is it can solve any physical problems in the same time for 1 dimension until 3 dimensions geometry with Cartesian or spherical coordinate. The physical systems handled by COMSOL Multiphysics is ranging from electrics, acoustics, structural mechanics, heat transfer, MEMS, RF until chemical engineering and earth science. Because of its user friendly with CAD application, COMSOL Multiphysics becomes popular to be used by engineering, scientist and students for academic or industrial purposes[1].

In this chapter, the physical model of COMSOL Multiphysics which is used is only the electromagnetic waves interface (EWI), since the optical system of the metamaterial has been covered by this model. By the electromagnetic model which is encountered in COMSOL, simulation process can be done. Simulation is the important and the effective way to study the microscopic electromagnetic response. It is very difficult, not to say impossible, doing microscopic electromagnetic study by analytical calculation because it has complicated boundary value problems. It is expected that simulation in specific model (geometry and physical system) which represents the real condition is able to analyze the inhomogeinity of the metamaterial in this research, i.e. the composite of the dielectric and the metal-semiconductor nanocomposite.

4.2 – Electromagnetic Waves Interface (EWI) Model in COMSOL Multiphysics

Electromagnetic waves interface model aims to solve the electric field problem for time harmonic domain in the linear medium. The studies (simulations) which are able to be done by this model are frequency domain, eigenfrequency, mode analysis and boundary-mode analysis. The frequency domain study is used to find the solution in single input frequency or multiple input frequencies. The eigenfrequency study is able to get the resonance frequency and its eigenmodes in cavity problems. The mode analysis is capable to find allowed propagating modes and its transmission line for 2D cross-sections in waveguides. Then, boundary mode analysis is applied to study the boundaries representing waveguide ports and only the electric field variant of the time harmonic equation can to be solved. To make simulation for our metamaterial model, the frequency domain study is selected because we want to analyze the electromagnetic response of the metamaterial in different frequencies of electromagnetic waves (light).

The Maxwell Equationsare the core of the EWI model to solve the electric field $\boldsymbol{E}$. The governing Maxwell equation which is used for the time-harmonic and eigenfrequency is written in equation 4.1.

$$\nabla \times (\mu^{-1}\nabla \times \boldsymbol{E}) - {k_0}^2 \left(\varepsilon - \frac{i\sigma}{\omega\varepsilon}\right)\boldsymbol{E} = \boldsymbol{0} \quad (4.1a)$$

$$k_0 = \omega\sqrt{\varepsilon_0\mu_0} = \frac{\omega}{c_0} \quad (4.1b)$$

$$c = 3 \cdot 10^8\ m/s \quad (4.1c)$$

$$\omega = 2\pi\nu \quad (4.1d)$$

where:

μ : the relative permeability

ε : the relative permittivity

σ: the conductivity

ν: the frequency of electromagnetic wave [Hz]

c: the speed of light in air/vacuum

For nonmagnetic and linear materials with $\mu = 1$ and $\varepsilon = n^2$ where n is the refractive index of material, equation 4.1a can be written in equation 4.2.

$$\nabla \times (\nabla \times \boldsymbol{E}) - {k_0}^2 n^2 \boldsymbol{E} = 0 \quad (4.2)$$

4.3 – Modelling and Simulation of the Metamaterial in COMSOL Multiphysics

4.3.1–Geometry of the Metamaterial

The geometry model in COMSOL simulation aims to model the real condition of the metamaterial properties (alloy of the dielectric and the metal-semiconductor nanocomposites) and its interaction with electromagnetic waves. It divides into three layers, i.e. two air layers for the incident wave and for the transmitted wave; and the metamaterial layer. The metamaterial layer is sandwiched between two air layers such that there are numbers of metal-semiconductor nanocomposites (the nanoparticles) distributed in order inside host dielectric material. The dimension of nanoparticles are fixed and uniform for all. Figure 4.1 shows the description of model geometry for 4 nanoparticles.

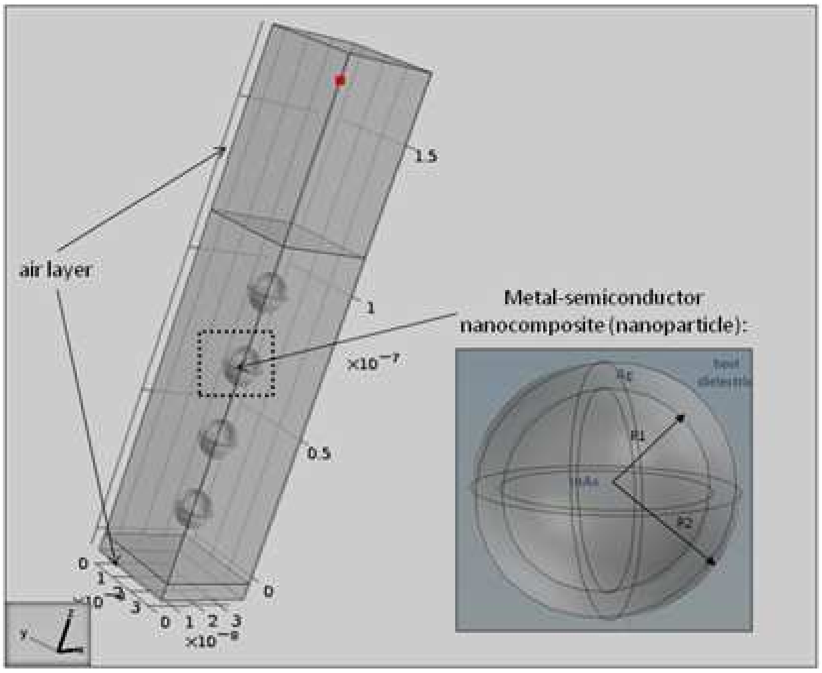


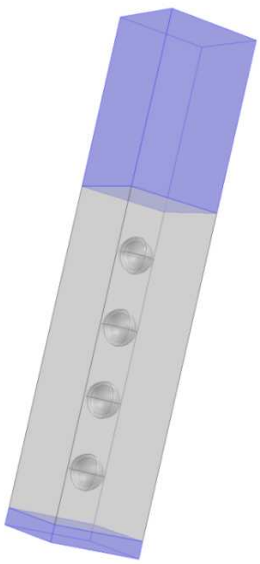
Figure 4.1 Geometry Model of the Metamaterial

4.3.2–The Model of Materials

The model of Materials which are used in COMSOL simulation are exactly similar with materials model in analytical calculation, i.e. Drude Model for silver, Quantum Dot (QD) model for semiconductor InAs. These models determined directly their permittivity. The permittivity of host dielectric (PMMA) is constant. Figure 4.2, 4.3, 4.4 and 4.5 shows the material's of air, the host dielectric, the metal (silver) and the semiconductor, respectively in geometry model.

In Electromagnetic Waves Interface (EWI) Model, 3 material contents (properties), i.e. electric conductivity, relative permittivity and relative permeability, should be filled completely to solve the Maxwell Equation written in equation 4.1a. COMSOL Multiphysics has included these contents immediately when the built-in materials (the materials which has been defined in COMSOL material's library) are selected. The users can also define their material and properties by themselves.

The material's model of air which is shown in Figure 4.2 is applied for air layer. Its material contents are taken from built-in materials in COMSOL material's library with electric conductivity, relative permeability and relative permittivity are equal to 0, 1 and 1. It means that the air layers are completely transparent media to transfer light/electromagnetic wave.

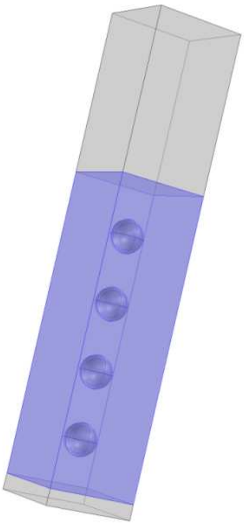


Material Contents

	Property	Name	Value
✓	Electric conductivity	sigma	0
✓	Relative permeability	mur	1
✓	Relative permittivity	epsilonr	1

Figure 4.2 Material's Model of Air

The material's model of the host dielectric which is shown in Figure 4.3 is applied its geometry in the metamaterial layer. As explained before, the metamaterial layer has two component, i.e. the host dielectric and the nanoparticles; and every nanoparticle contains two element, i.e. the semiconductor (InAs) in the core and the metal (Ag) in the shell. Material contents of the host dielectric medium (PMMA) are defined with electric conductivity, relative permeability and relative permittivity are equal to 0, *ep_h* and 1. *ep_h* is set to be constant with value 2.2022.



Material Contents

	Property	Name	Value
✓	Electric conductivity	sigma	0
✓	Relative permittivity	epsilonr	ep_h
✓	Relative permeability	mur	1

Figure 4.3 Material's Model of the Host Dielectric

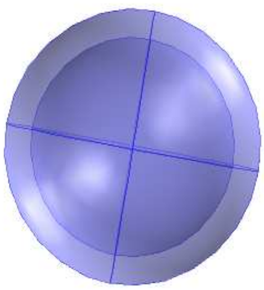
The material contents of silver (Ag) for every nanoparticle in metamaterial layer are defined with electric conductivity, relative permeability and relative permittivity are equal to 0, *ep_Ag* (or, ε_{Ag}) and 1. Permittivity of silver, ε_{Ag} , has dispersion relation respect to the frequency of electromagnetic wave and is expressed by Drude Model as written in equation 4.3.

$$\varepsilon_{Ag}(\omega) = \varepsilon_{\infty} + \frac{\omega_p{}^2}{\omega^2 - i\omega\Gamma_{Ag}} \tag{4.3}$$

$$\varepsilon_{\infty} = 1$$

$$\Gamma_{Ag} = 3.00 \cdot 10^{14}/s$$

$$\omega_p = 1.38 \cdot 10^{16}/s$$



Material Contents

	Property	Name	Value
✓	Electric conductivity	sigma	0
✓	Relative permittivity	epsilonr	ep_Ag
✓	Relative permeability	mur	1

Figure 4.4 Material's Model of the Silver by Drude Model

The model of the semiconductor (InAs) in this metal-semiconductor nanocomposite (the nanopartcle) is expressed by Quantum Dot model. Its material contents are defined with electric conductivity, relative permeability and relative permittivity are equal to 0, *ep_QD* (or, ε_{QD}) and 1. Permittivity of InAs which is modeled by Quantum Dot, ε_{QD}, has dispersion relation respect to the frequency of electromagnetic wave as written in equation 4.4.

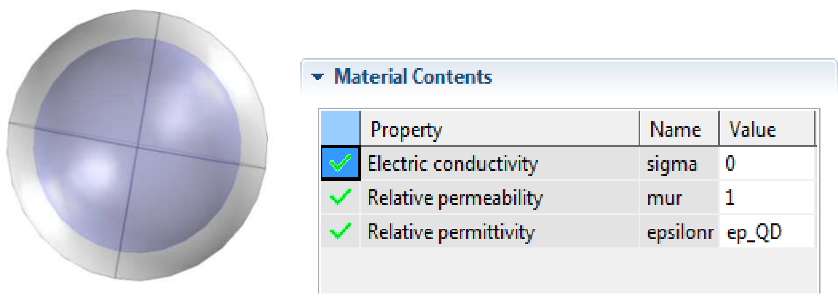
$$\varepsilon_{InAs}(\omega) = \varepsilon_b + A\frac{{\omega_0}^2}{(\omega^2 - {\omega_0}^2) - 2i\gamma_{QD}} \tag{4.4}$$

$\varepsilon_b = 12.8$

$\gamma_{QD} = 1.519 \cdot 10^{12}/s$

$\omega_0 = 2.279269 \cdot 10^{15}/s$

A: the gain factor, which is selected by analytical calculation in Chapter 2



	Property	Name	Value
✓	Electric conductivity	sigma	0
✓	Relative permeability	mur	1
✓	Relative permittivity	epsilonr	ep_QD

Figure 4.5 Material's Model of InAs by Quantum Dot Model

4.3.3–Boundary Conditions

4.3.3.1 – Scattering Boundary Conditions

Scattering boundary conditions are used to model the condition of electric field from the incident (incoming) light and the scattered (outgoing) light. Scattering BC assumes the boundaries are transparent medium for scattered wave and incoming plane wave that are normal to the boundary. The scattered plane wave of electric field **E** in scattering BC is expressed in equation 4.3.

$$\boldsymbol{E} = \boldsymbol{E}_{sc}e^{-i\boldsymbol{k}(\boldsymbol{n}\cdot\boldsymbol{r})} + \boldsymbol{E}_0 e^{-i\boldsymbol{k}(\boldsymbol{k}\cdot\boldsymbol{r})} \tag{4.5}$$

$\boldsymbol{E}_0$: the incident plane wave which travels in the direction **k**

$\boldsymbol{E}_{sc}$: the scattered (outgoing) wave

There are 2 scattering boundary conditions applied in geometry model, i.e for incoming light and for outgoing light, as shown in figure 4.6. Both scattering boundary conditions of incoming light and outgoing light are placed in the air layer. The type of electromagnetic wave is transverse magnetic (TM) with incident angle equal to 0^o such that the electric field is parallel to the plane of incident. The plane of incident is formed by x- and z- axis, so that the electric field **E** in scattering boundary conditions (and also in whole domain) is always parallel with x-axis. The incident electric field $\boldsymbol{E_1}$ in the first scattering BC and the transmitted electric field $\boldsymbol{E_2}$ in the second scattering BC are $1\hat{k}\ V/m$ and $\mathbf{0}\ V/m$, respectively.

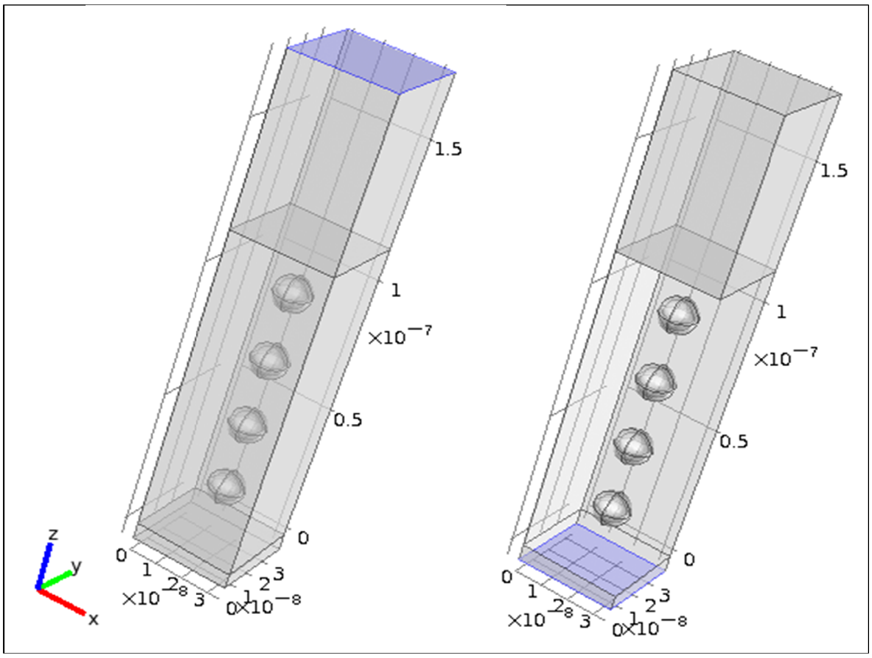


Figure 4.6 Scattering Boundary Conditions

4.3.3.2 – Periodic Boundary Conditions

Periodic boundary conditions are used in the boundary of metamaterial layer and air layers in x and y axis. It means that there are infinite air and metamaterial layers in Cartesian space, which means there are many nanoparticles inside host dielectric medium sandwiched by air layers. The thickness of metamaterial in z-axis (or, the distance between two air layer's boundary) is fixed and does not change. Figure 4.7 shows the periodic boundary conditions which are applied in x axis and y axis.

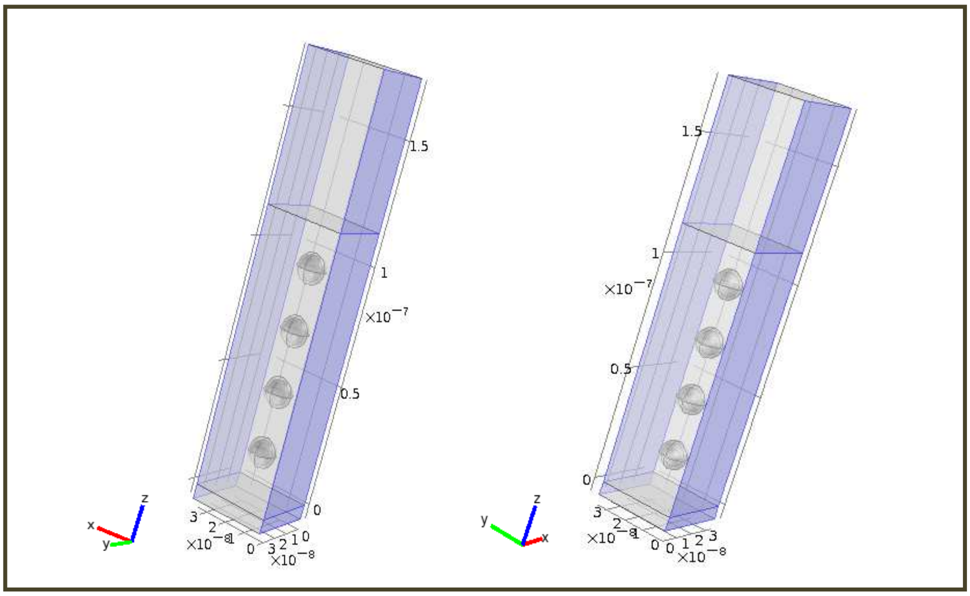


Figure 4.7 Periodic Boundary Conditions

4.3.4–Meshing the Geometry Model

The model of the metamaterial in COMSOL Multiphysics use tretrahedral meshes, as shown in Picture 4.8. The size of meshes for the nanoparticles and the dielectric host medium are smaller than the size of meshes for air layers. It is done like that because the differential of physical variables respect to the space domain in the metamaterial layer (the nanoparticles and the dielectric host medium) are larger than the differential of physical variables in the air layers. COMSOL Multiphysics can set the size of meshes automatically and adapt with contours and interfaces.

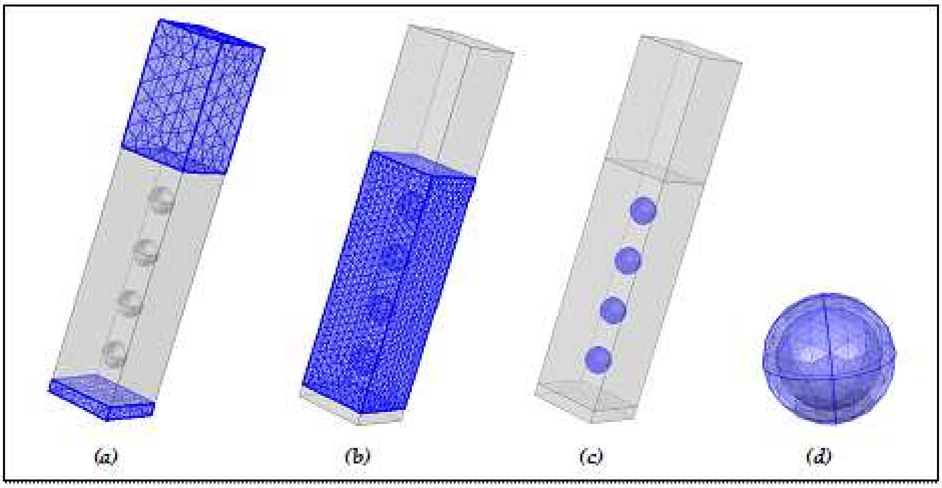


Figure 4.8 Meshing of Geometry Models

4.3.5–Simulation Study

The simulation of the metamaterial study is done for several wavelengths of electromagnetic waves in frequency domain. COMSOL Multiphysics is able to perform parametric sweep for every variable. In our study, we make sweep of wavelength (which is related to the frequency), then the simulation gives solutions of electric field $\boldsymbol{E}$ for every electromagnetic wavelength (frequency)in all space domains. But, the solution only can be found in every mesh, not in every point of domain, because the model uses Finite Element with discretization of increment. The solution of the electric field $\boldsymbol{E}$in every mesh can be represented in many forms, like modulus (norm), complex value, etc. Figure 4.9 shows the solution of electric field norm in space domain for specific electromagnetic wavelength (frequency) obtained by simulation in COMSOL Multiphysics.

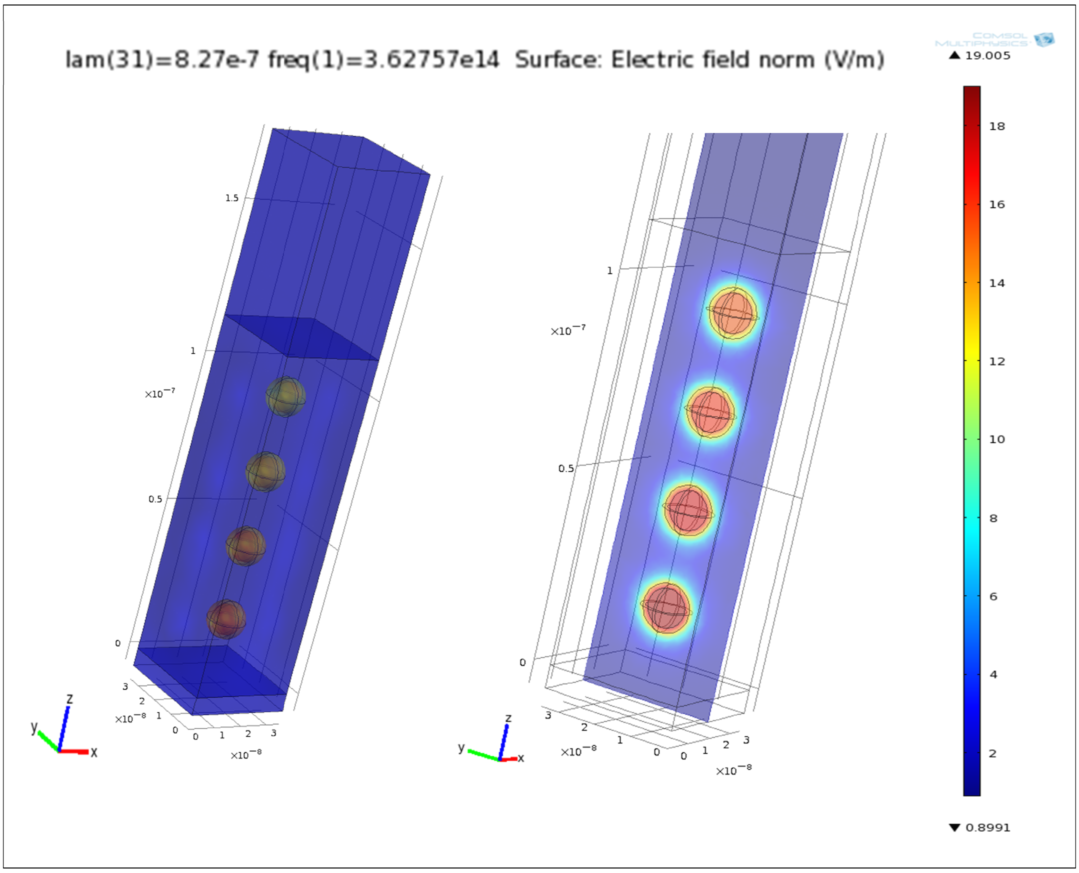


Figure 4.9 Electric Field Norm Solution in Space Domain

4.4 – Processing the Simulation Data

4.4.1–Point Probe

The point probe is taken in the second air layer where the transmitted wavelength propagates (Figure 4.10). COMSOL Multiphysics can give the electric field solution there respect to the parametric sweep of electromagnetic wavelengths. The electric field result in point probe will be processed (in MATLAB) to get the average permittivity of the metamaterial model. The point probe position and its probing result are shown in Figure 4.10 and 4.11, respectively.

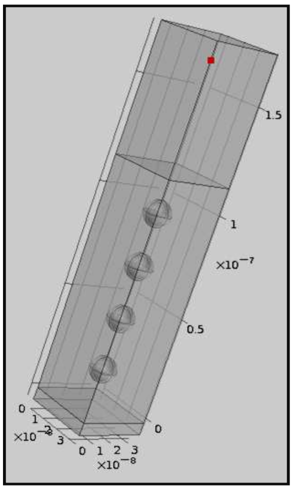


Figure 4.10 The point probe in the second air layer

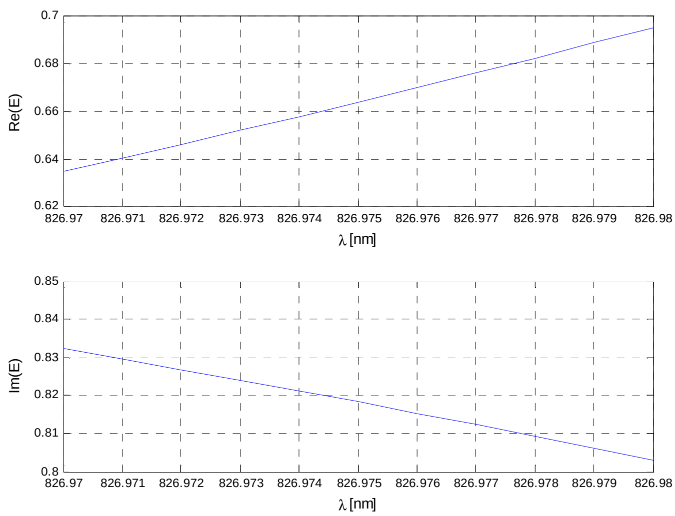


Figure 4.11 The electric field magnitude in the point probe

4.4.2–Retrivial Lambda

The retrivial lambda in this research is a process to obtain permittivity of the metamaterial from the available information (the variable) in the simulation result, i.e. the electric field **E**. This process should be done because the Electromagnetic Waves Interface (EWI) model in COMSOL Multiphysics cannot give the permittivity value directly. Figure 4.12 shows the scheme of the vector field (electric field **E**and wave vector **k**) in 2 air layers. As written before, the simulation uses TM mode with incident angle equal to 0^o so that the electric field always parallel to that plane of incident in all layers.

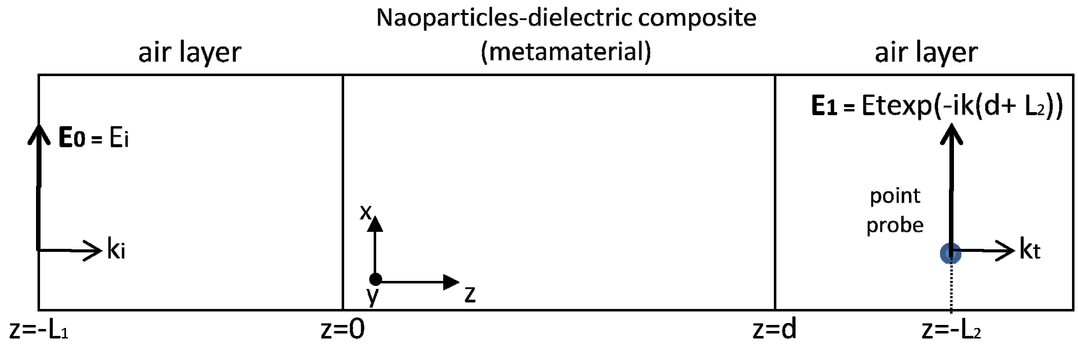


Figure 4.12 The scheme of vector of fields in all domains

Based on Smith, et.al [1], the transmission coefficient for waves incident normally to the face of one-dimensional (1-D) slab of continuous material (in vacuum/air) with length *d* and permeability $\mu = 1$ is expressed in equation 4.4.

$$t = \frac{1}{\cos(nkd)+\frac{i}{2}\left(n+\frac{1}{n}\right)\sin(nkd)} e^{ikd} \tag{4.4}$$

In our geometry, the transmission coefficient is the ratio between 'the magnitude' of transmitted electric field E_t at z>d (and also in point probe) and 'the magnitude' of incident electric field E_0 at z<0. After some algebraic manipulations, the relation between electric fields in 2 points (E_t and E_0) and permittivity of metamaterial n can be obtained as shown in equation 4.7 and 4.8. Although the simulation does not make homogenization in metamaterial layer such that there are many complicated interactions between electromagnetic wave, the nanoparticles and the host dielectric , but the transmitted electric field in the second air layer (z>d) is expected to become the average response of metamaterial.

$$t = \frac{E_t}{E_i} \tag{4.5}$$

$$\frac{E_1}{E_0} = \frac{1}{cos(nkd) + \frac{i}{2}\left(n + \frac{1}{n}\right) sin\,(nkd)} e^{-ikL_2} \tag{4.6}$$

$$\frac{E_0}{E_1} = cos(nkd) + \frac{i}{2}\left(n + \frac{1}{n}\right) sin(nkd)\, e^{ikL_2} \tag{4.7}$$

$$\varepsilon = \sqrt{n} \tag{4.8}$$

The retrivial process can be obtained by numerical calculation in MATLAB to get the average permittivity of the metamaterial for each frequency/wavelength. The code can be seen in the attachment.

4.5–Simulation of Geometry Model Variations and Their Permittivity Results

Simulation is done by changing the configuration of geometry model of the metamaterial. The metal-semiconductor nanocomposites (the nanoparticles) are designed with fixed dimension and are distributed in order inside the host dielectric medium with several distribution patterns of the nanoparticles inside the host medium. The simulation aims to see the permittivity of the metamaterial for each geometry structure when it interacts with polarized EM waves (TM waves) then to compare its permittivity with analytical result.

4.5.1– Simulation of 1 Cell with 4 Nanoparticles

4.5.1.1-Regular Distribution

In this model, 4 nanoparticles are placed regularly along z-axis in one cell which is duplicated periodically along x-axis and y-axis, and the distance is kept in such a way so that they will not cross each other. The filling fraction of the total volume of the nanoparticles respect to the total volume of the metamaterial is fixed to be 0.03 . Based on the theoretical calculation in Chapter 3, the to reach epsilon-near-zero (ENZ) at the wavelength 827.00 nm, the core radius R_1 and the shell radius R_2 should be 5 nm and 6.29 nm; with the gain of Quantum Dot A is $3.175 \cdot 10^{-3}$.

To make the filling fraction become 0.03 in the COMSOL geometry model, the dimension of metamaterial layer's domain Lx, Ly, Lz(=*d*) are fixed in 35 nm, 35 nm and 113.8 nm, respectively. The distance between the outer boundaries of the nanoparticles are uniform, i.e. 12.7 nm (or, 18.99 nm from their centre points). Measured from the outer boundaries the outermost nanoparticles, their distances with air layers are 12 nm and 13 nm in lower part and in upper part, respectively. This geometry model can be seen in Figure 4.13.

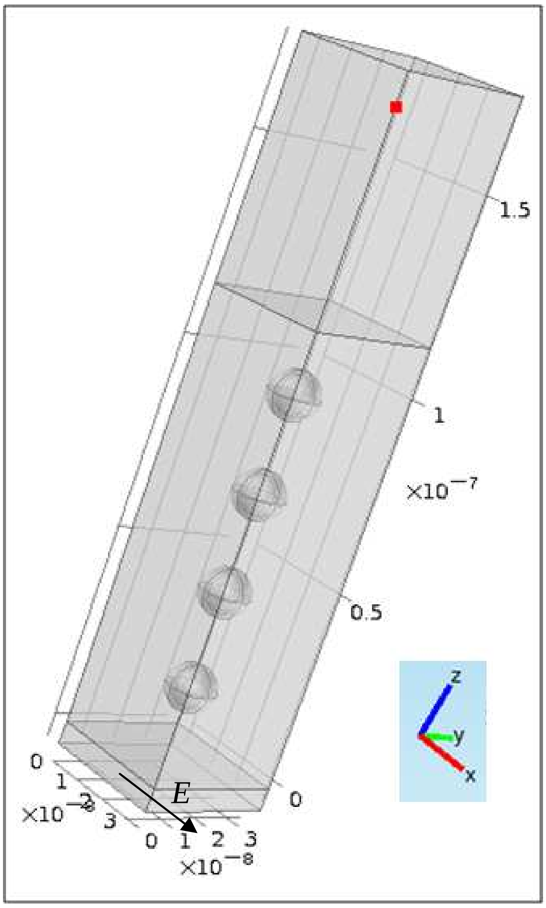


Figure 4.13 The geometry of 4 nanoparticles model in regular distribution

The simulation is done in frequency domain of TM mode (p-polarization) electromagnetic incident waves in which the polarization electric field **E** is always parallel to x-axis in all domains. The result that we want to obtain is the effective permittivity of the metamaterial as the function of the electromagnetic wavelength. As known, electromagnetic wavelength λ is same as the light speed in vacuum *c* divided with frequency ν. The wavelength of incident light ranging from 826.970 nm to 827.010 nm.

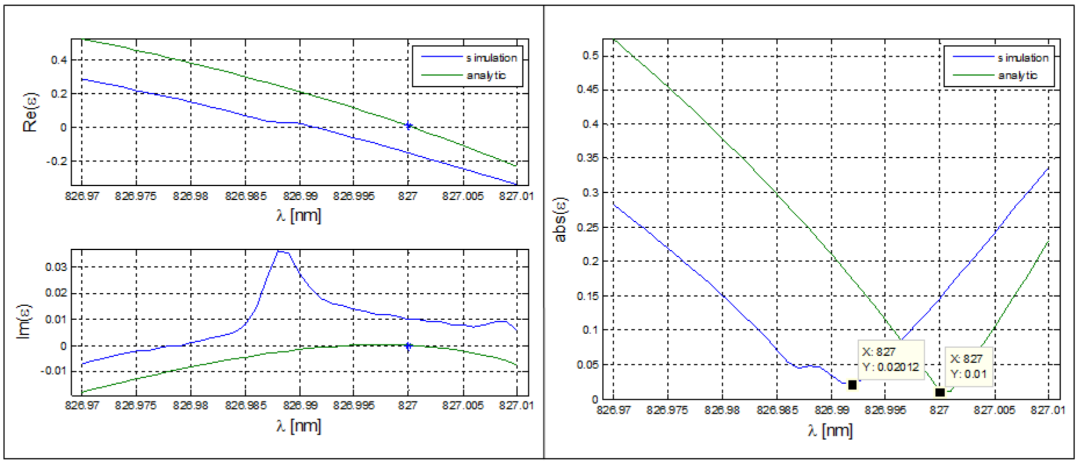


Figure 4.14 The simulation result of 4 nanoparticles model in regular distribution

Figure 4.14 shows the comparisons between the permittivity of the metamaterial obtained by COMSOL simulation in the regular distribution and obtained by theoretical calculation in MATLAB, for several range of wavelengths. The COMSOL simulation reaches the epsilon-near-zero (ENZ) close to the expected frequency which has been calculated by the theoretical calculation in MATLAB. But, the simulation has resonance from 826.985 nm until 826.995 such that the permittivity due to the surface Plasmon polariton excitation, or we can call that resonance as *the plasmonic resonance* (it will be discussed in the next Chapter). . The results obtained by the theoretical calculation in MATLAB do not have plasmonic resonances because the nanoparticles are distributed randomly in the host dielectric medium.

In the next simulations, we will make variations of the nanoparticles positions in the cell to see if the plasmonic resonance position and its pick point will move or not The variation of the nanoparticles configuration in the geometry model is important, because we want to make simulations whose results are close to the theoretical expectations. But, COMSOL Multiphysics cannot make the random distribution like in the theoretical model or assumption. Then, if we find a geometrical model configuration whose simulation result show plasmonic resonance is small enough, we can use that geometrical model configuration as an ideal geometry model that represents a random distribution of the nanoparticles in the host dielectric medium. Moreover, the variation of the geometry model configuration is useful to see how the plasmonic resonance behaves respect to nanoparticles positions and light polarizations.

4.5.1.2-Variation 4.1.I

In this variation, 4 nanoparticles which were placed regularly along z-axis in one periodic cell, are modified. 2 nanoparticles in the middle are moved away from each other along z-axis, as shown in Figure 4.15. The movement is done for every 1 nm, so that for every one movement, the distance between 2 nanoparticles in the middle turn into 2 nm. The filling fraction of the total volume of the nanoparticles respect to the total volume of the metamaterial is still 0.03, and the dimension of the nanoparticles are $\mathbf{R_1 = 5\ nm}$ and $\mathbf{R_2 = 6.29\ nm}$. These dimensions are uniform for all nanoparticles.

The dimension of metamaterial layer's domain Lx, Ly, Lz(=*d*) are 35 nm, 35 nm and 113.8 nm, respectively. Measured from the outer boundaries the outermost nanoparticles, their distances with air layers are still similar with the regular form, i.e. 12 nm and 13 nm in lower part and in upper part, respectively.

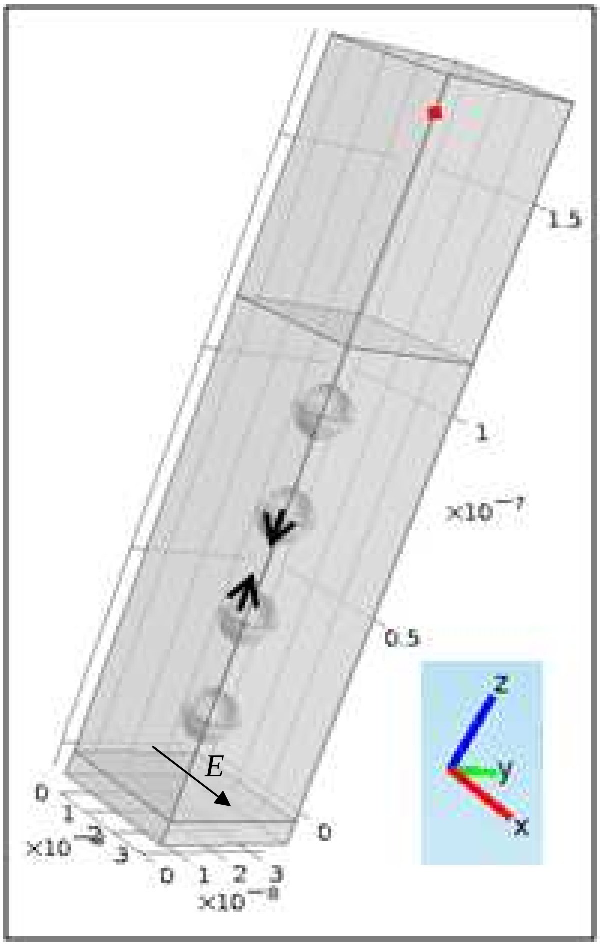


Figure 4.15 The geometry of variation 4.1.I

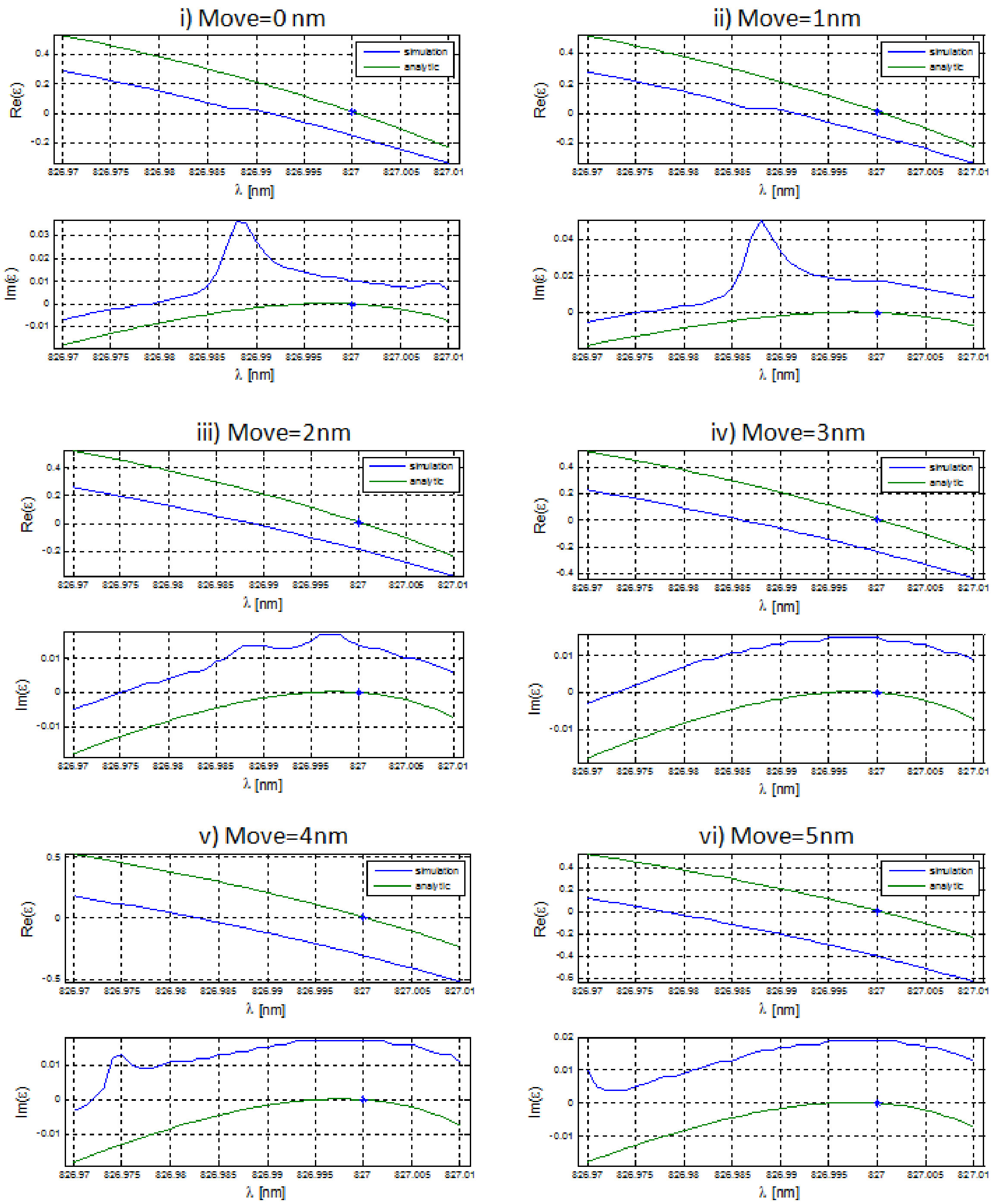


Figure 4.16 The Permittivity Graphics of Variation 4-1-A for saveral movements

Figure 4.16 is the simulation results of variation 4.1.I for movement of nanoparticles in the middle every 1 nm. They show that the plasmonic resonance become smaller at the first time when we move away the nanoparticlese in the middle, but the plasmonic resonance become larger anymore when we move more. In this variation the wavelebgth of the plasmonic peak resonance shift to the left side (blue shift) when the nanoparticles movement is larger,

4.5.1.3 Variation 4.1.II

In this variation, 4 nanoparticles which were placed regularly along z-axis in one periodic cell, are modified. 2 nanoparticles in the middle approach each other along z-axis, as shown in Figure 4.17 The movement is done for every 1 nm, so that for every one movement, the distance between 2 nanoparticles in the middle turn into 1 nm. The filling fraction of the total volume of the nanoparticles respect to the total volume of the metamaterial is still 0.03, and the dimension of the nanoparticles are $\mathbf{R_1 = 5\ nm}$ and $\mathbf{R_2 = 6.29\ nm}$. These dimensions are uniform for all nanoparticles.

The dimension of metamaterial layer's domain Lx, Ly, Lz(=*d*) are 35 nm, 35 nm and 113.8 nm, respectively. Measured from the outer boundaries the outermost nanoparticles, their distances with air layers are still similar with the regular form, i.e. 12 nm and 13 nm in lower part and in upper part, respectively.

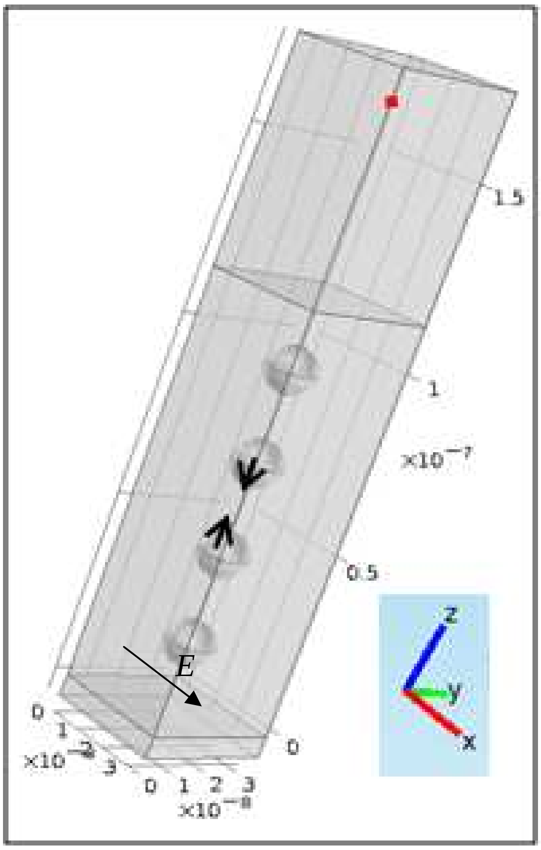


Figure 4.17 The geometry of variation 4.1.II

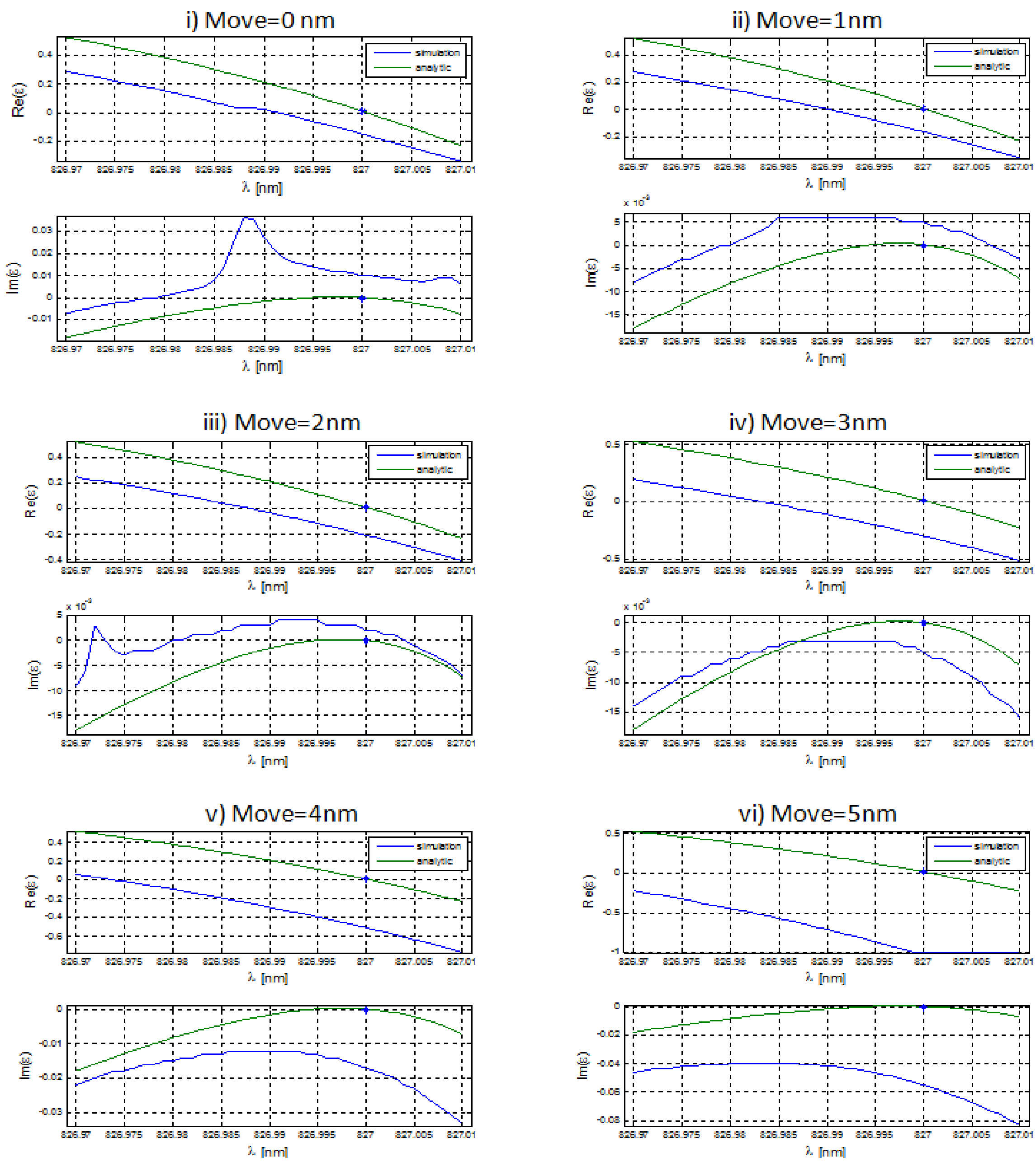


Figure 4.18 The Permittivity Graphics of Variation 4.1.II for saveral movements

Figure 4.18 is the simulation results of variation 4.1.II for movement of nanoparticles in the middle every 1 nm. They show that the plasmonic resonance becomes smaller very fast, faster than something happens in the variation 4.1.I. Although the plasmonic resonance decreases quite fast when the movements are done more, but thedifferences between the permittivity obtained by simulation and the permittivity obtained by the theoretical calculation becomes larger. In this variation the wavelength of the plasmonic peak resonance shift to the left side (blue shift) when the nanoparticles movement is larger.

4.5.1.4 Variation 4.1.III-x

In this variation, 4 nanoparticles which were placed regularly along z-axis in one periodic cell, are modified. 2 nanoparticles in the middle move in x-axis with the same direction, as shown in Figure 4.19 The movement is done for every 1 nm. The filling fraction of the total volume of the nanoparticles respect to the total volume of the metamaterial is still 0.03, and the dimension of the nanoparticles are $\mathbf{R_1 = 5\ nm}$ and $\mathbf{R_2 = 6.29\ nm}$. These dimensions are uniform for all nanoparticles.

The dimension of metamaterial layer's domain Lx, Ly, Lz(=*d*) are 35 nm, 35 nm and 113.8 nm, respectively. Measured from the outer boundaries the outermost nanoparticles, their distances with air layers are still similar with the regular form, i.e. 12 nm and 13 nm in lower part and in upper part, respectively.

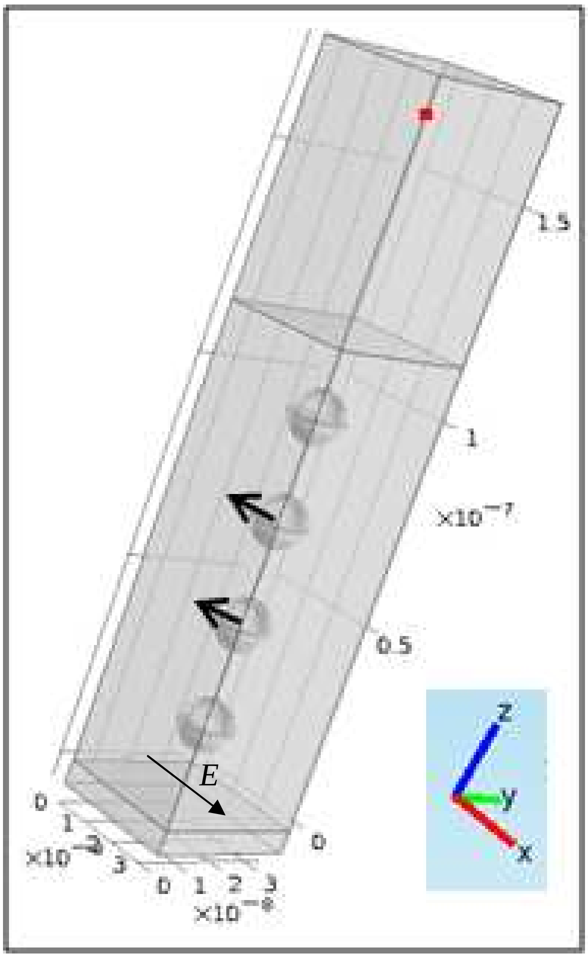


Figure 4.19 The geometry of variation 4.1.III-x

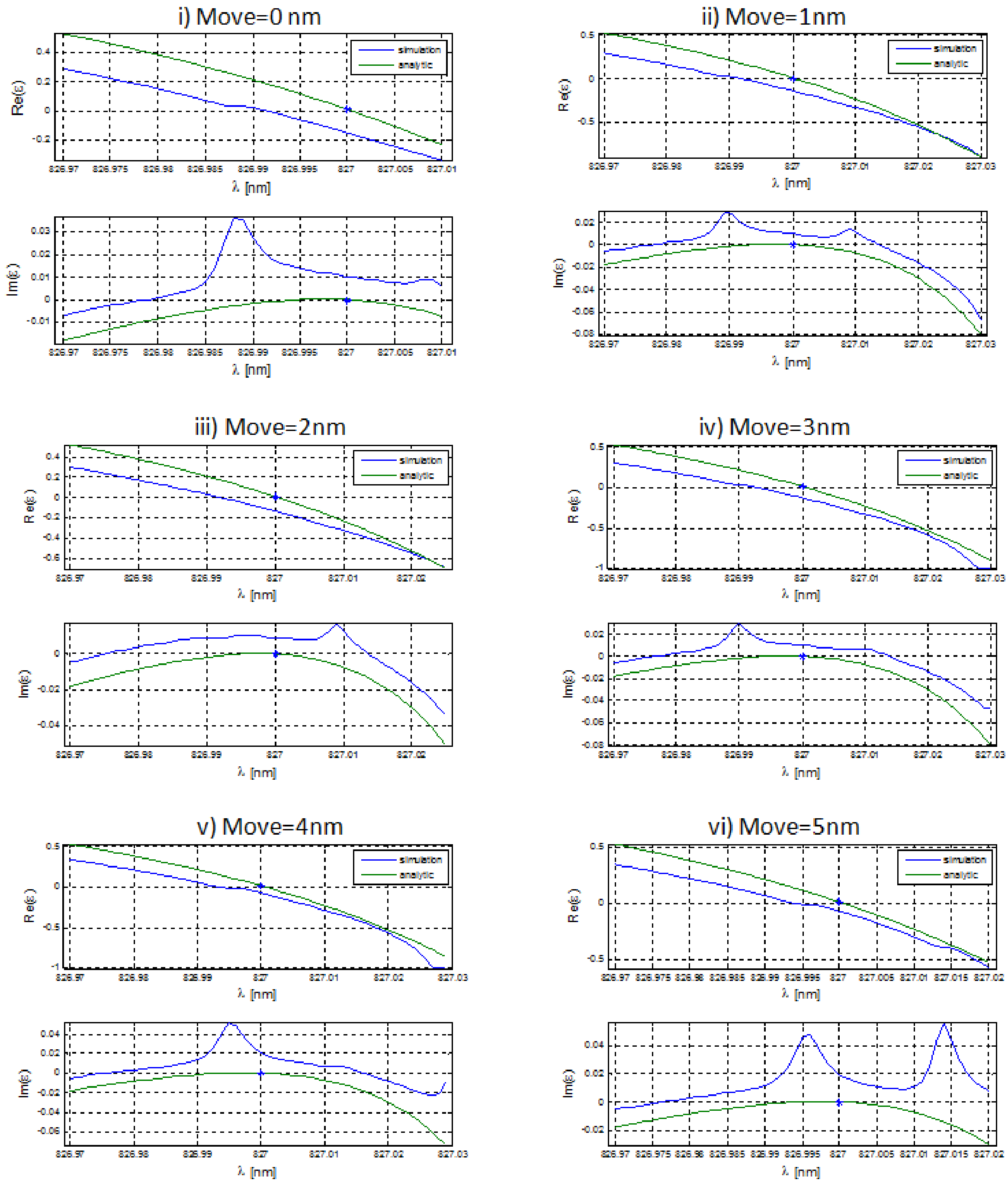


Figure 4.20 The Permittivity Graphics of Variation 4.1.III-x for saveral movements

Figure 4.20 is the simulation results of variation 4.1.III-x for movement of nanoparticles in the middle every 1 nm. They show that the plasmonic resonance pattern is not predictable we move the nanoparticlese in the middle, and some movements in this variation there are more than one plasmonic resonance. In this variation, we cannot determine precisely the shifting pattern of the plasmonic peak resonance respect to the movement of 2 nanoparticles in the middle.

4.5.1.5 Variation 4.1.III-y

In this variation, 4 nanoparticles which were placed regularly along z-axis in one periodic cell, are modified. 2 nanoparticles in the middle move in y-axis with the same direction, as shown in Figure 4.21. The movement is done for every 1 nm. The filling fraction of the total volume of the nanoparticles respect to the total volume of the metamaterial is still 0.03, and the dimension of the nanoparticles are $\mathbf{R_1 = 5\ nm}$ and $\mathbf{R_2 = 6.29\ nm}$. These dimensions are uniform for all nanoparticles.

The dimension of metamaterial layer's domain Lx, Ly, Lz(=*d*) are 35 nm, 35 nm and 113.8 nm, respectively. Measured from the outer boundaries the outermost nanoparticles, their distances with air layers are still similar with the regular form, i.e. 12 nm and 13 nm in lower part and in upper part, respectively.

Figure 4.22 is the simulation results of variation 4.1.III-y for movement of nanoparticles in the middle every 1 nm. They show that the plasmonic resonance decreases quite fast when the nanoparticles in the middleare moved in y-direction..

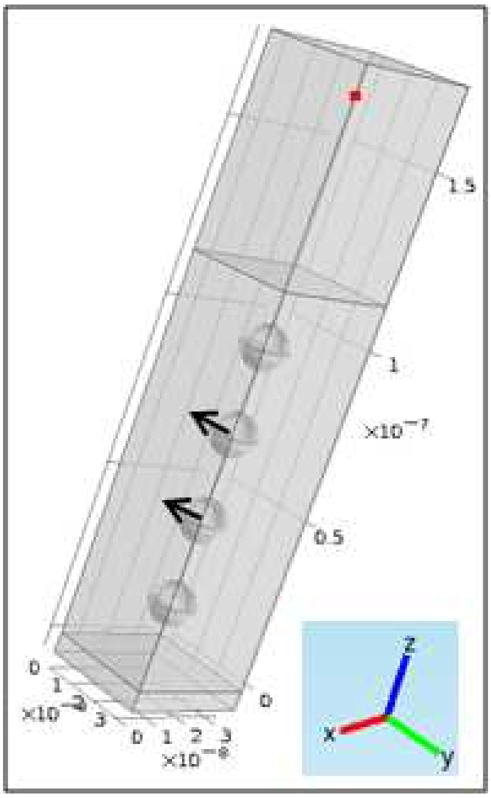


Figure 4.21 The geometry of variation 4.1.III-y

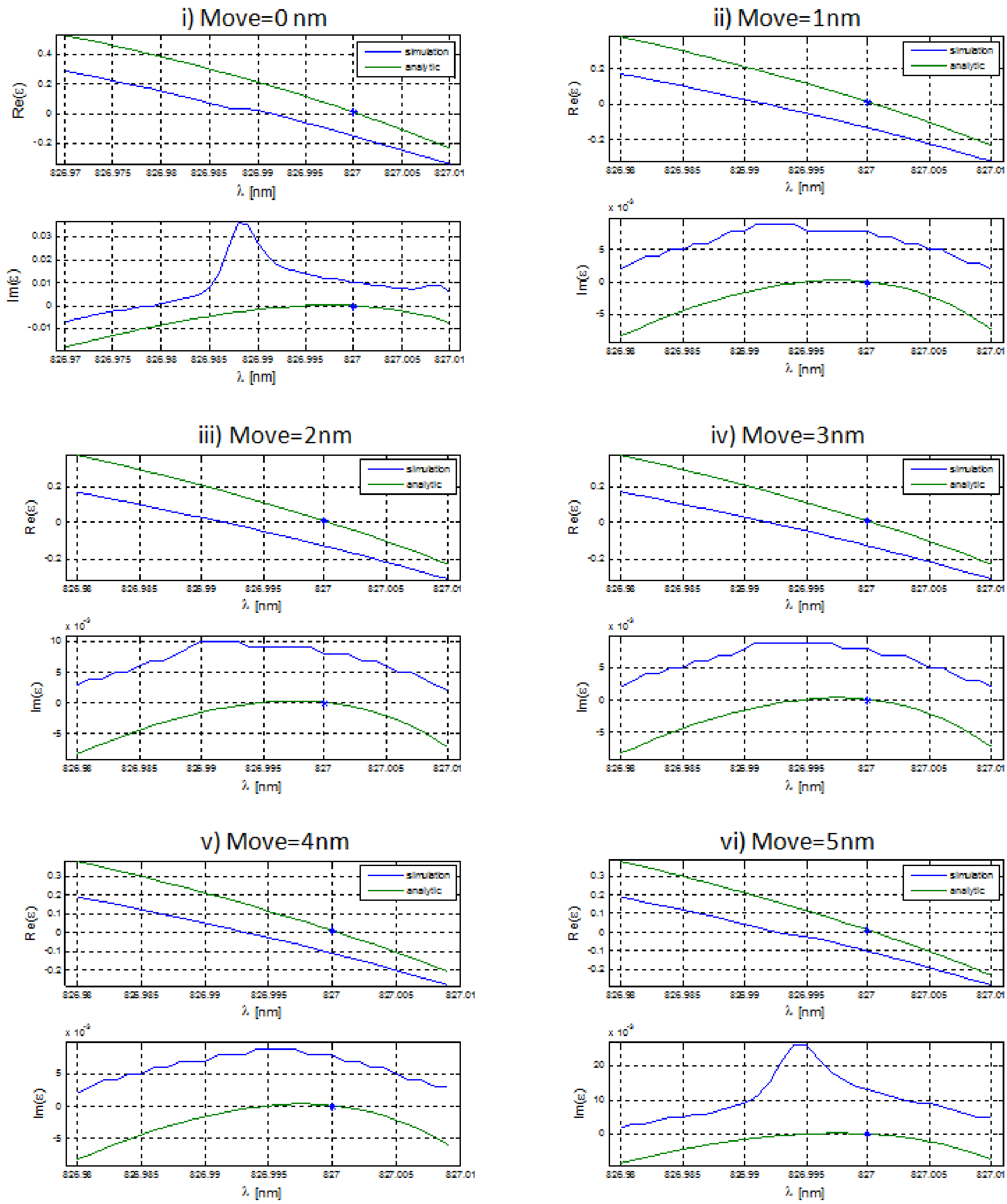


Figure 4.22 The Permittivity Graphics of Variation 4.1.III-y for saveral movements

4.5.1.6 Variation 4.1.IV-x

In this variation, 4 nanoparticles which were placed regularly along z-axis in one periodic cell, are modified. 2 nanoparticles in the middle move in x-axis with opposite direction, as shown in Figure 4.23. The movement is done for every 1 nm. The filling fraction of the total volume of the nanoparticles respect to the total volume of the metamaterial is still 0.03, and the dimension of the nanoparticles are $\mathbf{R_1 = 5\ nm}$ and $\mathbf{R_2 = 6.29\ nm}$. These dimensions are uniform for all nanoparticles.

The dimension of metamaterial layer's domain Lx, Ly, Lz(=*d*) are 35 nm, 35 nm and 113.8 nm, respectively. Measured from the outer boundaries the outermost nanoparticles, their distances with air layers are still similar with the regular form, i.e. 12 nm and 13 nm in lower part and in upper part, respectively.

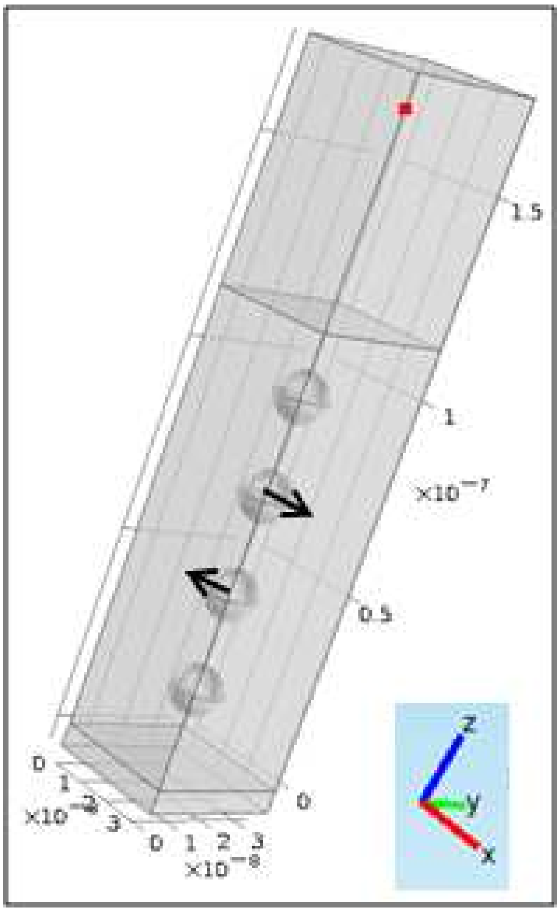


Figure 4.23 The geometry of variation 4.1.IV-x

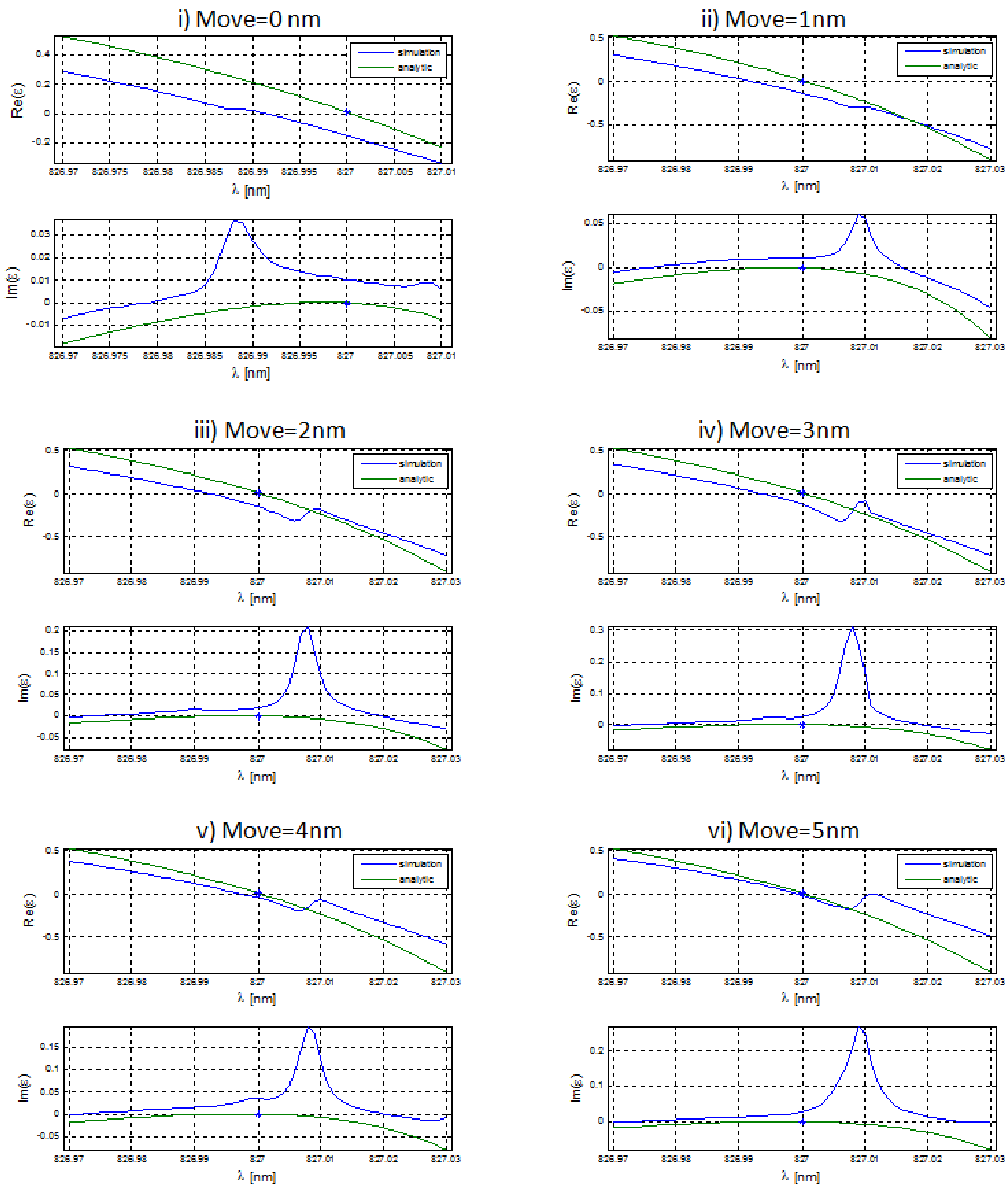


Figure 4.24 The Permittivity Graphics of Variation 4.1.IV-x for saveral movements

Figure 4.24 is the simulation results of variation 4.1.IV-x for movement of nanoparticles in the middle every 1 nm. They show that the plasmonic resonance pattern is not predictable we move the nanoparticlese in the middle, and some movements in this variation there are more than one plasmonic resonance. In this variation, we cannot determine precisely the shifting pattern of the plasmonic peak resonance respect to the movement of 2 nanoparticles in the middle.

4.5.1.7 Variation 4.1.IV-y

In this variation, 4 nanoparticles which were placed regularly along z-axis in one periodic cell, are modified. 2 nanoparticles in the middle move in y-axis with opposite direction, as shown in Figure 4.25. The movement is done for every 1 nm. The filling fraction of the total volume of the nanoparticles respect to the total volume of the metamaterial is still 0.03, and the dimension of the nanoparticles are $\mathbf{R_1 = 5\ nm}$ and $\mathbf{R_2 = 6.29\ nm}$. These dimensions are uniform for all nanoparticles.

The dimension of metamaterial layer's domain Lx, Ly, Lz(=*d*) are 35 nm, 35 nm and 113.8 nm, respectively. Measured from the outer boundaries the outermost nanoparticles, their distances with air layers are still similar with the regular form, i.e. 12 nm and 13 nm in lower part and in upper part, respectively.

Figure 4.26 is the simulation results of variation 4.1.IV-y for movement of nanoparticles in the middle every 1 nm. They show that the plasmonic resonance decreases quite fast when the nanoparticles in the middleare moved in y-direction..

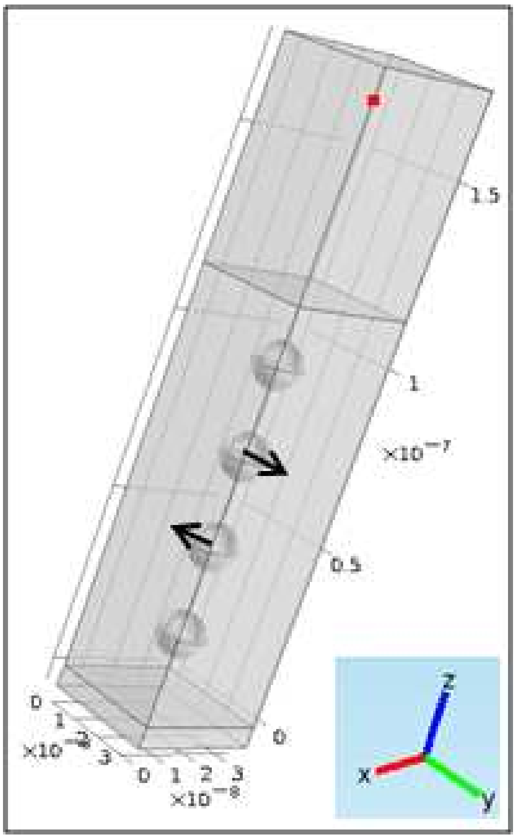


Figure 4.25 The geometry of variation 4.1.IV-y

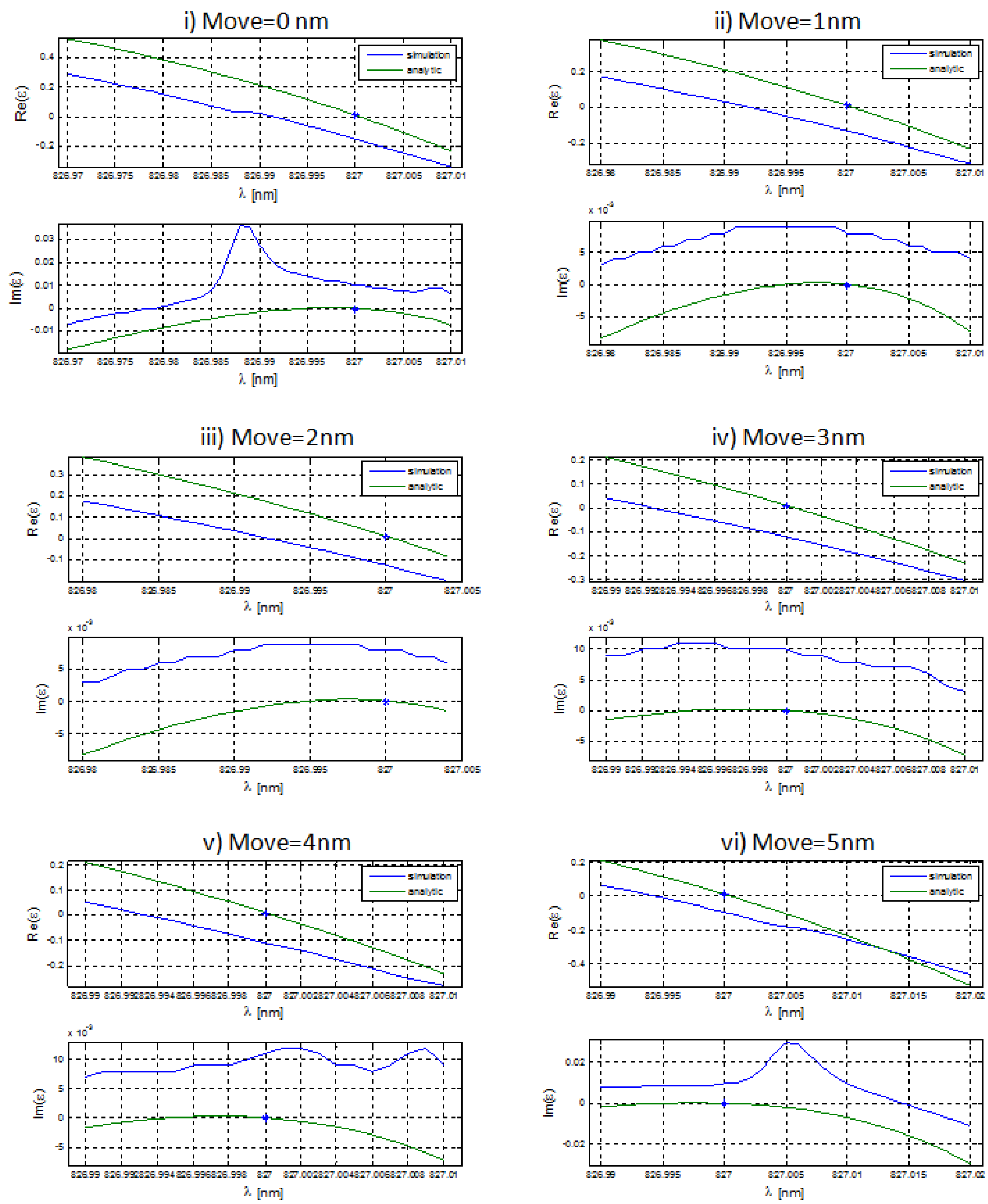


Figure 4.26 The Permittivity Graphics of Variation 4-1-D2 for saveral movements

4.5.2 – Simulation of 4 Cells with 16 Nanoparticles

4.5.2.1 Variation 4.4.I

This variation is an integration between the variation 4.1.I and 4.1.II in 4 cells. In Figure 4.27 we can see that the variation 4.1.I is applied in the first and the third cell, and the variation 4.1.II is applied in the second and the fourth cell. The light polarization is parallel to x-axis. The idea is to see if this configuration model can approach the homogeneity assumed in the theoretical MGT model, so that the plasmonic resonance can be reduced.

Figure 4.28 shows how the variation 4.4.I can reduce the plasmonic resonance in a good way, although when we move the nanoparticles too far, the plasmonic resonance is generated again and cannot be predicted.

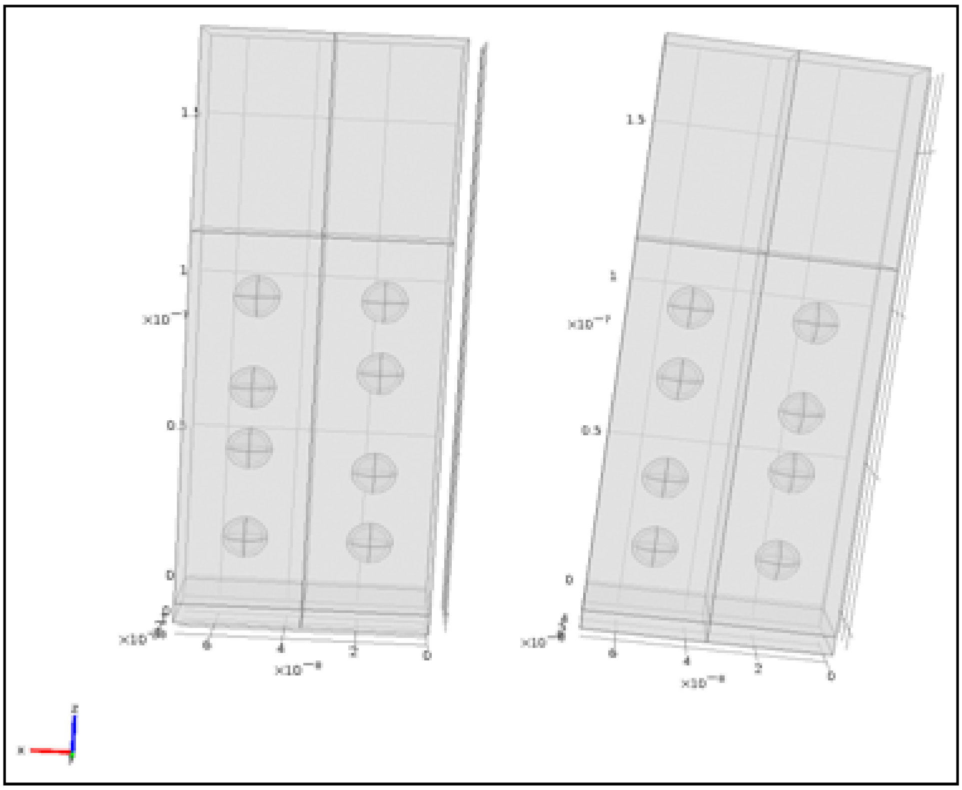


Figure 4.27 The geometry of variation 4-4-I

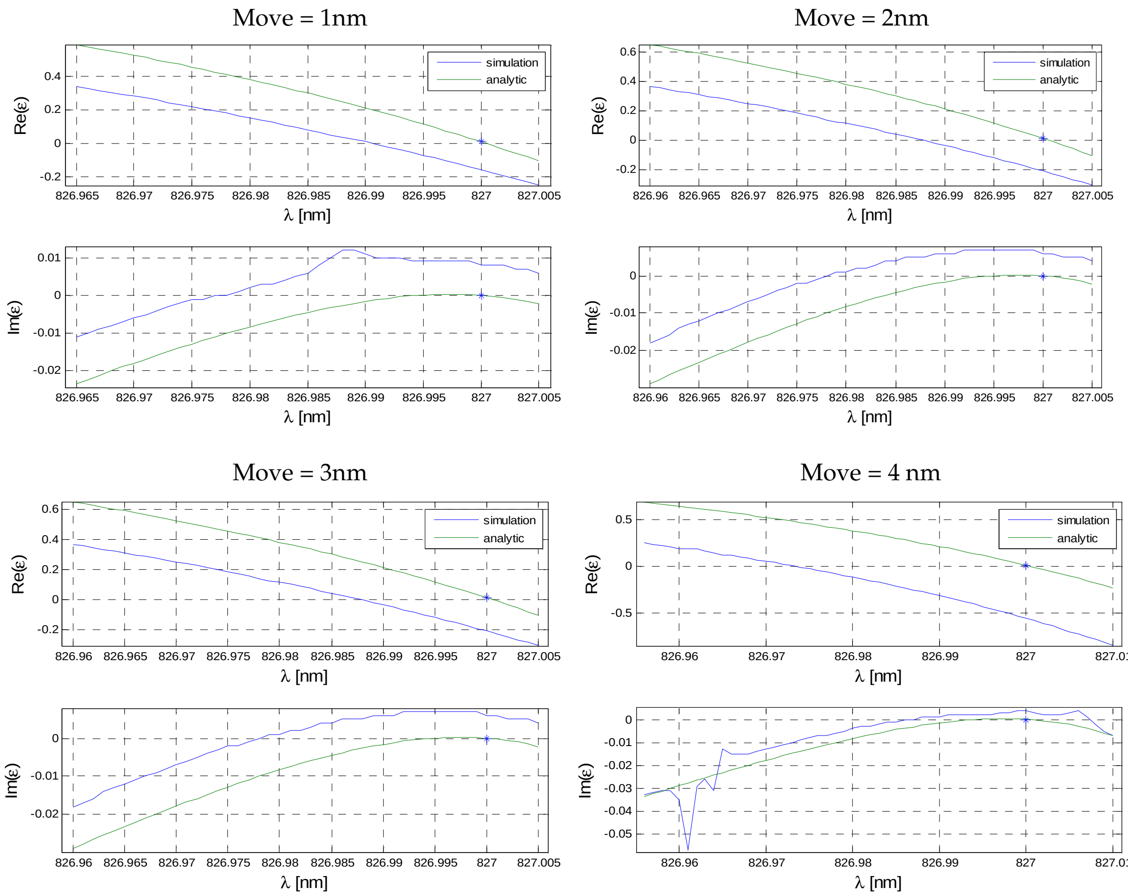


Figure 4.28 The Permittivity Graphics of Variation 4.4.I for saveral movements

4.5.2.2 Variation 4.4.II

This variation is a modification between the variation 4.1.III-x and 4.1.IV-x. The light polarization comes is parallel to x-axis. In Figure 4.29 we can see that the variation 4.1.III-x is applied in the first and the third cell, and the variation 4.1.IV-x is applied in the second and the fourth cell. The light polarization is parallel to x-axis. The idea is to see if this configuration model can approach the homogeneity assumed in the theoretical MGT model, so that the plasmonic resonance can be reduced.

Figure 4.30 shows how the variation 4.4.II generates more plasmonic resonances, instead reduces it. It can be concluded that this variation is not suitable to approach the randomness of the Maxwell Garnett Theory (MGT) assumption

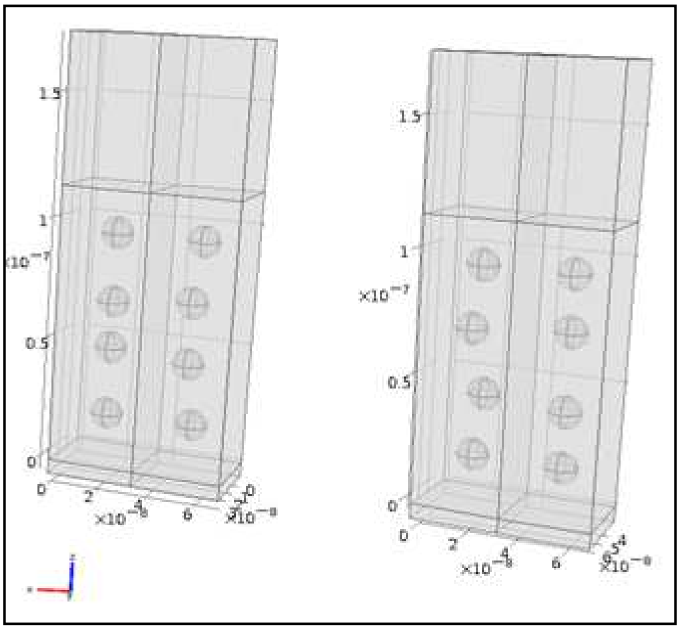


Figure 4.29 The geometry of variation 4.4.II

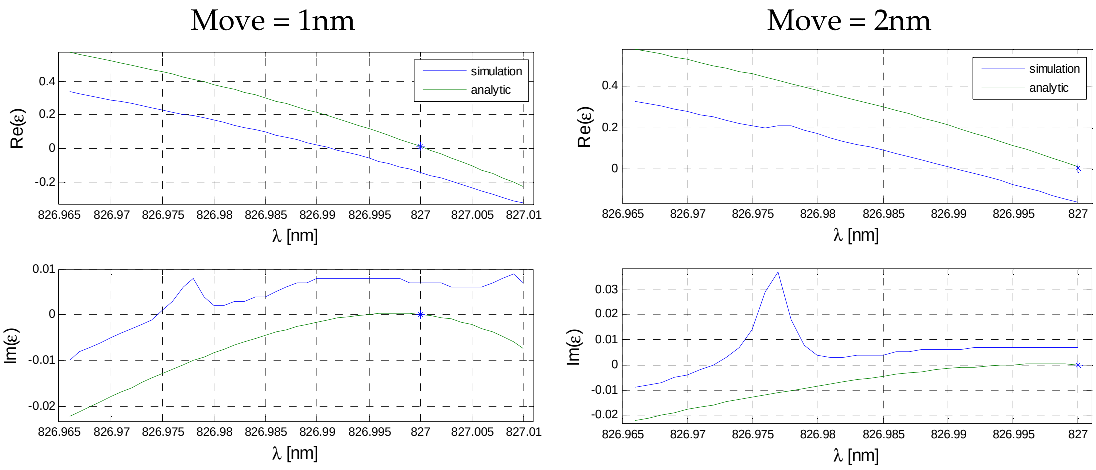


Figure 4.30 The geometry of variation 4.4.II

4.6 – References

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CHAPTER 5

DISCUSSION OF RESULT

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5.1 – The Aims of Simulations

The simulation in COMSOL Multiphysics aims to study the electromagnetic responses of the metamaterial when it interacts with electromagnetic waves and to induce its material properties (i.e. the permittivity). It is almost impossible to simulate the model of the metamaterial in COMSOL as done in the analytical/theoretical model (the real geometry and particles distribution), because there are many limitations of COMSOL, like available features and capacity of memory. As written in the previous chapter, COMSOL can only model the simplified geometry of the metamaterial with certain boundary conditions. Still, those COMSOL models are expected to be represented the analytical model.

To study the reliability of the COMSOL model (geometry and boundary conditions), the analytical model and its computational result are treated as a reference for simulations. Some steps have to be done. First, geometry models in COMSOL moreless represent the geometry model of the analytical model (based on the Maxwell Garnett Theory). Second, boundary conditions of geometry models in COMSOL must be made in such a way that they approximate the conditions in analytical model. Then, the result obtained from analytical calculation and the results obtained from simulation must be compared.

Comparing the analytical results and the simulation results is very important in this research. Beside to study the reliability of COMSOL model, it can also evaluate the analytical model, i.e. how it works in specific case or conditions. The analytical model of the metamaterial in this research uses the Maxwell Garnett Theory (MGT) with some assumption, i.e. a lot of nanoparticles are distributed randomly inside the dielectric host medium, no interaction happens between one nanoparticle and the other nanoparticle(s) when the metamaterial responses electromagnetic waves (the interaction only occurs between nanoparticle and the host dielectric medium), and the filling fraction is quite small. Although COMSOL simulation can fix the filling fraction, but it is difficult to distribute nanoparticles in completely random situation and to neglect the interaction between a nanoparticle to the other nanoparticles. Indeed, those limitations in COMSOL simulation can be treated as special case and maybe there are some phenomena in COMSOL simulation which are not covered by the analytical model.

To make reach the goals, several simulations have been done, i.e.:

1. Study the plasmonic resonance behavior in regular distribution of nanoparticles in the box of dielectric host medium. It is done by changing number of nanoparticles in the box, but keeping the filling fraction.
2. Choose one study case in point 1, then make variation of nanoparticles distribution systematically by changing the distances between nanoparticles in x direction, y direction, z direction and combination of them. Beside studying their plasmonic behavior, these simulations are useful to find in which distributions the average respons of the metamaterial approximates the Maxwell Garnett Theory (MGT) assumption.

Thoses simulation studies have been done in the Chapter 4. In this Chapter we will analyze the simulation results obtained in the previous Chapter and induce some conclusions.

5.2 – The Microscopic Responses

Comparing the simulation results and theoretical calculations is the important things to study the responses of the metamaterial in microscopic scale. As explained before, analytical calculation use the Maxwell Garnett Theory (MGT) as the basis in which it assumes that the nanoparticles are distributed totally random inside the dielectric host medium, so there is no any fields generated due to the interaction between them. But, the comparison results (Chapter 4) shows that there are differences between the theoretical results and the simulation result, as can be seen again in the Figure 5.1 and 5.2

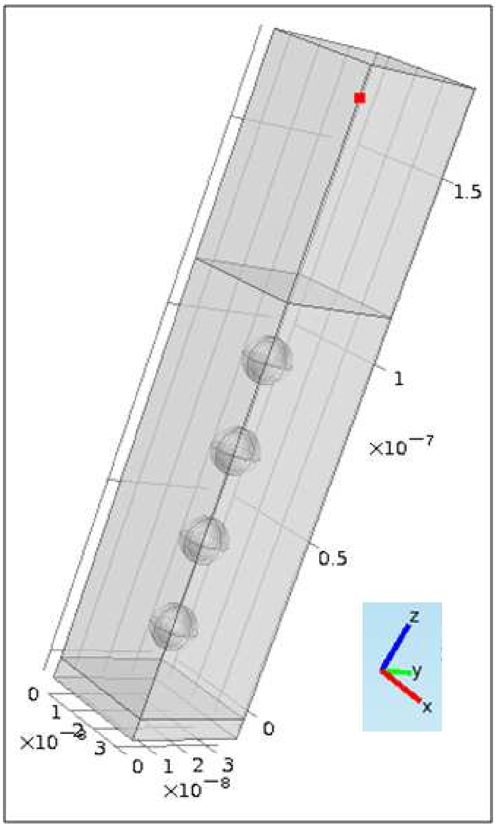

Figure 5.1 Geometry Model of COMSOL Simulation in Regular Distribution

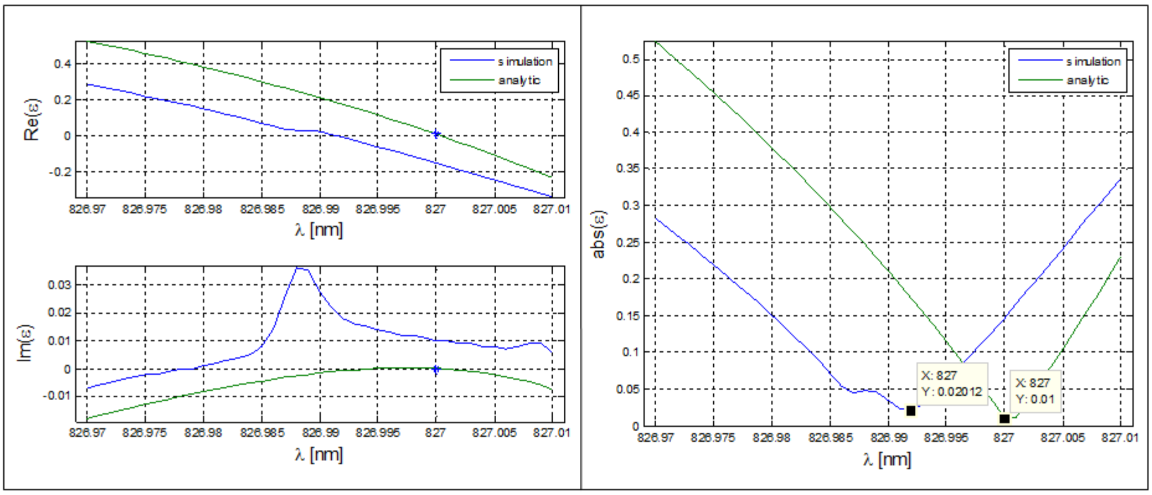

Figure 5.2 The comparison between theoretical and simulation results of the dispersion relation of the permittivity

The comparison results between theoretical calculation and simulation in regular distribution shows the similarity between them. The real part and the imaginary part of permittivity obtained by simulation behaves like the permittivity obtained by analytical calculation. But, it exists big resonance of imaginary when electromagnetic wave with lambda=826.987 is applied due to the surface Plasmon phenomena, which is called surface Plasmon polariton (SPP) excitation.

Starting from the comparison in the regular distribution, we will see how the SPP excitation behave in each simulation of geometry model/comparison, then find in which distributions the average respons of the metamaterial approximates the Maxwell Garnett Theory (MGT) assumption. But, firstly it is important to see the explanations of the microscopic effects occurring in the metamaterial.

5.2.1-The Near Field Effect

The near field effect is the outer electric fields which interact and make dipole moment with microscopic nanoparticle. This near effect field is not considered by Clausius-Mosotti relation model which is derived to be the MGT formula. MGT formula is used as the basis of analytical method to calculate the effective permittivity of the metamaterial for every light frequency/wavelength. Instead using MGT formula, COMSOL Multiphysics compute the electromagnetic response in every mesh point of geometry model, so that the near field effect will be considered and gives different result respect to the analytical calculation.

The dipole moment due to near field can be caused by the interaction between two or more nanoparticles in the medium that can be described by using the electric field in slab. When the assumption of the Maxwell Garnett Theory (MGT) is used, only one particle determines the dipole moment and polarization in microscopic scale.

$$\boldsymbol{E_L} = \boldsymbol{E_0} + \boldsymbol{E_d} + \boldsymbol{E_s} + \boldsymbol{E}_{near} \tag{5.1a}$$

$$\boldsymbol{E_0} + \boldsymbol{E_d} = \boldsymbol{E} \tag{5.1b}$$

$$\boldsymbol{E_d} = -\frac{\boldsymbol{P}}{\varepsilon_0} \tag{5.1c}$$

$$\boldsymbol{E_s} = \frac{\boldsymbol{P}}{3\varepsilon_0} \tag{5.1d}$$

But, because there are more than 1 nanoparticle (x nanoparticles) interact in the slab (when $\boldsymbol{E_{near}}$ is applied) equation 2.4 should be modified into equation….

$$\boldsymbol{E_s} + \boldsymbol{E_{near}} = x\boldsymbol{E_s} = x\frac{\boldsymbol{P}}{3\varepsilon_0} \tag{5.2}$$

$$\boldsymbol{E_L} = \boldsymbol{E} + x\frac{\boldsymbol{P}}{3\varepsilon_0} \quad (5.3)$$

$$\boldsymbol{P} = N\alpha\boldsymbol{E}_L = N\alpha\left(\boldsymbol{E} + x\cdot\frac{\boldsymbol{P}}{3\varepsilon_0}\right) \quad (5.4)$$

$$\mathbf{P} = \varepsilon_0\chi_e\mathbf{E} = \varepsilon_0(1-\varepsilon)\mathbf{E} \quad (5.5)$$

$$\frac{N\alpha}{3\varepsilon_0} = \frac{\varepsilon-1}{x\varepsilon+(3-x)} \quad (5.6)$$

$$\alpha = \frac{3\varepsilon_0}{N}\frac{\varepsilon-1}{x\varepsilon+(3-x)} \quad (5.7)$$

Then, using modified Clausius-Mosotti relation and polarizability for whole composite material with permittivity ε_h

$$\frac{N\alpha}{3\varepsilon_0\varepsilon_h} = \frac{\varepsilon-\varepsilon_h}{x\varepsilon+(3-x)\varepsilon_h} \quad (5.8)$$

$$\alpha = \frac{3\varepsilon_0\varepsilon_h f}{N}\frac{\varepsilon_1-\varepsilon_h}{x\varepsilon_1+(3-x)\varepsilon_h} \quad (5.9a)$$

$$\mathrm{f} = \frac{V_1}{V_1+V_h} \quad (5.9b)$$

$$\frac{N}{3\varepsilon_0\varepsilon_h}\cdot\left(\frac{3\varepsilon_0\varepsilon_h f}{N}\frac{\varepsilon_1-\varepsilon_h}{x\varepsilon_1+(3-x)\varepsilon_h}\right) = \frac{\varepsilon-\varepsilon_h}{x\varepsilon+(3-x)\varepsilon_h} \quad (5.10)$$

$$\frac{\varepsilon-\varepsilon_h}{x\varepsilon+(3-x)\varepsilon_h} = f\left(\frac{\varepsilon_1-\varepsilon_h}{x\varepsilon_1+(3-x)\varepsilon_h}\right) \quad (5.11)$$

$$\varepsilon = \varepsilon_h\frac{\varepsilon_1(x+(3-x)f)+(3-x)\varepsilon_h(1-f)}{x\varepsilon_1(1-f)+\varepsilon_h((3-x)+xf)} \quad (5.12)$$

The numbers of interacted nanoparticles contribute the deviation of the effective permittivity of the metamaterial. But, it is difficult to specify how many particles interacted inside the dielectric medium by analytical approach, because until now it has not been founded the method to do it. The only way is just comparing the simulation result with the analytical/theoretical calculation result such that same parameters have to be fixed, i.e. the dimension of nanoparticles R1 and R2, the filling fraction f.

5.2.2-The Surface Plasmon Polariton (SPP) Excitation, or the Plasmonic Effect

The resonance of permittivity result obtained by COMSOL simulation in several wavelength range is caused by Surface Plasmon Polariton (SPP), or *the plasmonic effect.* The plasmonic effect in the microscopic unit structure of our metamaterial model can induce the near effect field when the distances between two or more than nanoparticles are small enough so that the evanescent wave generated by SPP in one nanoparticle surface can interact with another evanescent waves in other nanoparticles. Then, as explained before, those interactions will change the macroscopic electromagnetic response of the metamaterial in some range of the wavelength.

5.2.2.1 – The Description of the Surface Plasmon Polaritons (SPP)

Plasmon is a quasi particle (plasma) generated from oscillation of collective electrons density in metal. The relationship between 'plasmon and electron oscillation' is analogue with the relationship between 'photons and electromagnetic radiation', or 'phonons with crystal vibration'. Although Plasmon is a kind of plasma, but the equations of the wave vectors and propagation constants associated with SPPs can be derived from Maxwell's equation [2].

When collective electron density oscillations are coupled with external electromagnetic waves (photons) in the surface between metal and dielectric, it gives the special type of Plasmon, which is called Surface Plasmon (SPs). Surface Plasmon Polaritons (SPPs) is also common to call it, since polariton in general means a quasi-particle consisting of two particles, like 'photon-phonon coupling' or 'photon-plasmons'. Term 'polariton' inserted in 'Surface Plasmons (SPs)' aims to state that 'plasmons in the surface between metal and dielectric' are caused by the coupling between 'photons and oscillations of the electrons'.

By definition, SPPs are *propagating solutions of Maxwell's equations at the interface between a dielectric and a metal, which are bound to that interface*. They are the resonant interaction between electromagnetic waves and the oscillations of free electrons at the metal interface and have an evanescent response into the metal and the dielectric [4]. The physics of SPP can be treated as the part of plasma behaviour based on Drude Model in metal [2]. In metal nanoparticles inside host dielectric medium, localized SPR (LSPR) can occur as a microscopic phenomena of the unit structure [3].

The wave vectors of SP is always mismatch with the wave vector of its electromagnetic couple, because SP's mode is confined is evanescent. The dispersion relation between SP's wave vector and the wave vector of its electromagnetic couple in absence of incident field is expressed in equation 5.13. k'_{SP} and k''_{SP} express the propagation and the loss of SP wave. As mentioned, SP mode is evanescent, so that it will disappear very fast due to the loses which is related with its imaginary part with the propagation length (equation 5.14).

The dispersion relation between SP propagation respect to the electromagnetic waves varying with dielectric permittivity can be seen in Figure 5.3.

$$k_{SP} = k_0 \sqrt{\frac{\varepsilon_d \varepsilon_m}{\varepsilon_d + \varepsilon_m}} = k'_{SP} + k''_{SP} \tag{5.13}$$

k_{SP} : the wave vector of SP

ε_d : the permittivity of dielectric

ε_m : the permittivity of metal, which is expressed by Drude Model

k_0 : the wave vector of electromagnetic wave in vacuum

$$L_P = \frac{1}{2k''_{SP}} \tag{5.14}$$

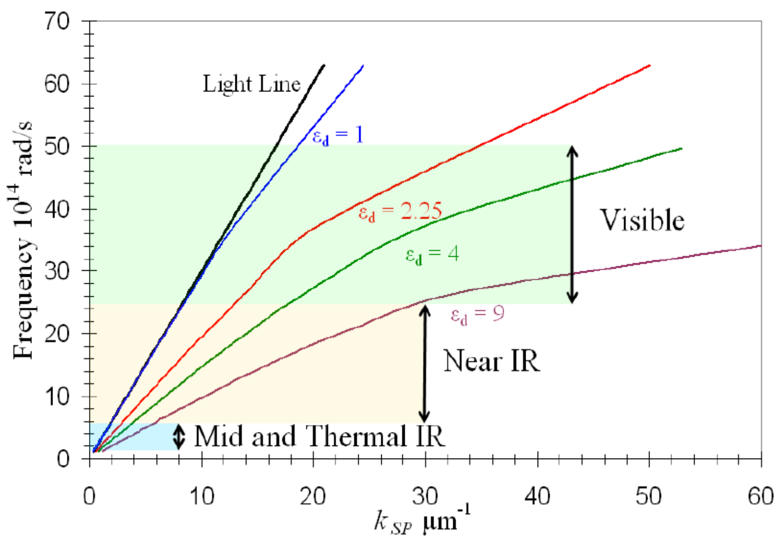

Figure 5.3 Surface Plasmon Dispersion Relationship for Different Dielectric Permittivities [2]

5.2.2.2 – The Localized Surface Plasmon Resonance (LSPR)

The Local Surface Plasmon Resnonace (LSPR) is important to be studied in our metamaterial simulation, because the plasmonic resonance which have been seen in the last chapter is changed when the mutual distances of the nanoparticles are moved. Based on researches of C. Noguez [4] and E. Hutter et al [5], LSPR exist due to the interaction between metal-nanoparticles and the external electric field $\vec{E}_{ext}$ which generates the induced electric field $\vec{E}_{ind}$ (Figure 5.4). The induced electric field $\vec{E}_{ind}$ is generated by evanescent wave (SPR) and can influence the wave propagation inside the host dielectric.

They study how the electromagnetic interaction between the nanoparticles and substrate (the host dielectric medium) which generates induced electric field depends on the separation between the nanoparticles. The results of their studies show that when the nanoparticles are larger, the plasmonic peak resonance becomes larger, and vice versa. This result is satisfied when the separation movement is parallel or perpendicular to the light polarization (see Figure 5.5)

It should be noticed that our metamaterial model is a little bit different with respect to these LSPR experiments. In these experiments, the distances of the nanoparticles are still uniform for all when the separation movement is done. On the other hand, the distances of the nanoparticles in our simulation (in all variations) are not uniform when the separation movement is done such that some nanoparticles become closer and the others become more far. But, these experiments is still useful to state that the plasmonic resonances in our metamaterial simulations are dominantly caused by the Localized Surface Plasmon Resonance (LSPR).

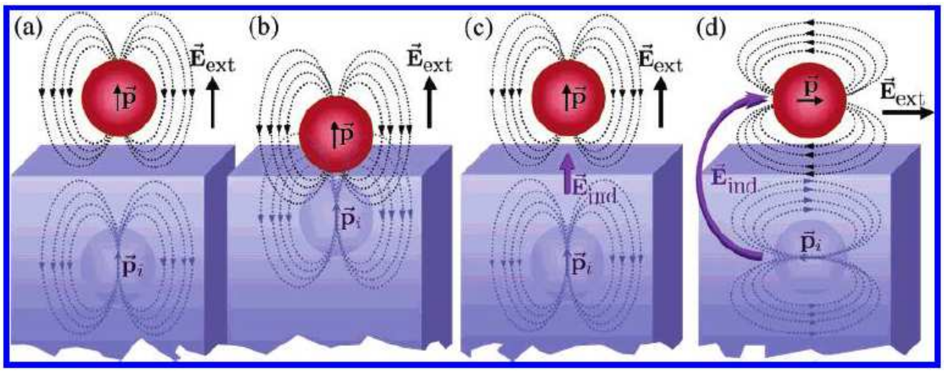

Figure 5.4 .(a and b) Electromagnetic Interaction between the nanoparticles and substrate as a function of the separation, modelled using the image method induced local field for an applied field (c) normal and (d) parallel to the interface[4]

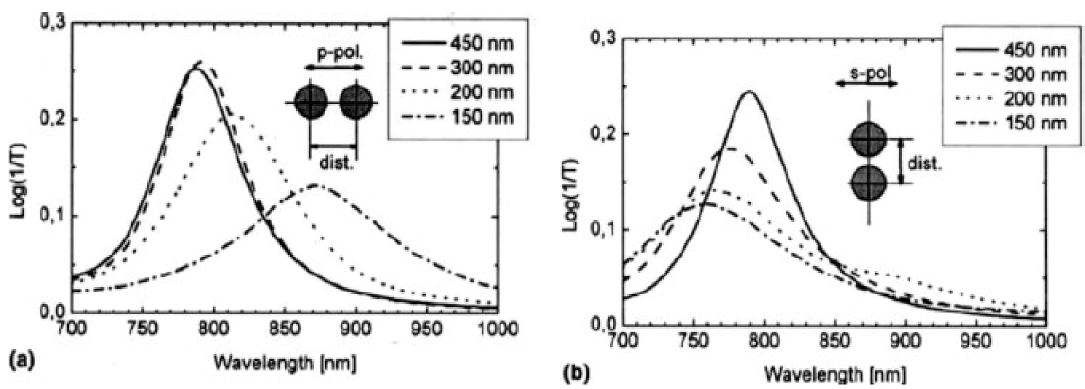

Figure 5.5 extinction spectra (1/T) of gold NPs (d=150nm) obtained by experimental result at several frequencies with (a)parallel and (b)orthogonal polarization of light excitation [5]

5.3 References

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CONCLUSION

Based on the studies and the results obtained in the previous chapters, we can conclude some important points below:

1. The simulation results of the developed metamaterial model is capable to verify the epsilon near zero condition when the metamaterial interacts with the electromagnetic wave whose wavelength is close to the wavelength obtained by the theoretical calculation.
2. Plasmonic resonances occur in the simulation because the full electromagnetic model employed in the Comsol Multiphysics program enabled us to verify the existence of Localized Surface Plasmon Resonances (LSPR) occurring between neighbouring nanoparticles. The plasmonic resonances do not occur in the theoretical calculation because the used Maxwell Garnett Theory assumes that the nanoparticles are totally random distributed inside the host dielectric medium and the surface plasmon excitation is not included.
3. Moreover the full electromagnetic analysis developed in this thesis predicts that a change in the mutual position of the nanoparticles in the model results in a change of the plasmonic resonance behaviour. For our simulation with p-polarized (TM) incident wave such that the electric field vector is always parallel to the x-axis in all domains, moving particles in the y-direction is the most effective way to neglect the interaction between nanoparticles, comparing with moving particles in the x-direction or z-direction.

In conclusion both the developed theoretical and simulation calculations allow to determine the physical conditions to fabricate nanoparticles in a core/shell geometry in which a semiconductor (core) is surrounded by a thin metal shell. We demonstrated that the epsilon-near-zero condition is completely fulfilled when the induced gain in the semiconductor by external electromagnetic pumping beam (with a photon energy greater than the semiconductor gap) compensates the metal absorption effects.

Future studies:

We foresee that the developed models can be used in future studies to design more simple geometries in which, for example, single metal nanoparticles with diameters close to 1-2 nanometer, are uniformly distributed in a host that contains specific dyes. In this case the dye is externally pumped to produce the gain that allows to compensate the metal absorption. In this example the theoretical and simulation models will make use of the Bruggemann Effective Medium Theory.

Other investigations will concern the study of the plasmonic interactions deeply in the geometry of the metamaterial. Finally, it will be possible to study the nonlinear properties of metamaterials in the epsilon near zero conditions.

APPENDIX: MATLAB® CODE

Permittivity of Ag Computation (by Modified Drude Model):

```
clear function
clear all
close all

%Setting parameter
F   = 0.02
rho = 0.498272867240438
A   = 3.203320623998E-03

%%
%Permittivity of Silver (Drude Model)
eb=1;
wp=13.8*10^15;
g=3*10^14;
c=3*10^8;
con=2*pi*c;

wa=(0:0.1:900);
w=con./(wa*1E-9)

e_ag=eb-((wp.^2)./(w.^2 - w*g*i));
e1_ag=real(e_ag);
e2_ag=imag(e_ag);

figure(1)
subplot (2,1,1)
plot(wa,e1_ag)
axis([min(wa)-0.001,max(wa)+0.001,min(e1_ag)-0.001,max(e1_ag)+0.001])
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('Re(\epsilon_A_g)','fontsize',12)

subplot (2,1,2)
plot(wa,e2_ag)
axis([min(wa)-0.001,max(wa)+0.001,min(e2_ag)-0.001,max(e2_ag)+0.001])
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('Im(\epsilon_A_g)','fontsize',12)

figure(2)
plot(wa,e1_ag,wa,e2_ag)
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('\epsilon_A_g','fontsize',12)
```

Permittivity of InAs Computation (by Quantum Dot Model)

```
%Quantum Dot
eb=12.8;
w0=2.279269*10^15;
g=1.519*10^12;
A=3.203320623998E-03;

e_QD = eb + ((A*w0^2)./((w.^2-w0^2)-2*w*g*i));
e1_QD = real(e_QD)
e2_QD = imag(e_QD)
n_QD = sqrt(e_QD);


figure(1)
subplot (2,1,1)
plot(wa,e1_QD)
axis([min(wa)-0.001,max(wa)+0.001,min(e1_QD)-0.001,max(e1_QD)+0.001])
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('Re(\epsilon_Q_D)','fontsize',12)

subplot (2,1,2)
plot(wa,e2_QD)
axis([min(wa)-0.001,max(wa)+0.001,min(e2_QD)-0.001,max(e2_QD)+0.001])
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('Im(\epsilon_Q_D)','fontsize',12)

figure(2)
plot(wa,e1_QD,wa,e2_QD)
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('\epsilon_Q_D','fontsize',12)
```

Permittivity of the Metal-Semiconductor Nanoparticle Computation (Ag-InAs)

```
%Metal-Semiconductor Nanoparticle (AgInAs)
r=rho;

e_1=e_QD;
e_2=e_ag;
e_c = (e_2.*(e_1*(1+2*r)+2*e_2*(1-r)))./(e_1*(1-r)+e_2*(2+r));
e1_c=real(e_c);
e2_c=imag(e_c);

n_c = sqrt(e_c);

figure(1)
subplot (2,1,1)
plot(wa,e1_c)
axis([min(wa)-0.001,max(wa)+0.001,min(e1_c)-0.001,max(e1_c)+0.001])
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
```

```
ylabel('Re(\epsilon_n_p)','fontsize',12)

subplot (2,1,2)
plot(wa,e2_c)
axis([min(wa)-0.001,max(wa)+0.001,min(e2_c)-0.001,max(e2_c)+0.001])
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('Im(\epsilon_n_p)','fontsize',12)

figure(2)
plot(wa,e1_c,wa,e2_c)
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('\epsilon_n_c','fontsize',12)
```

Permittivity of the Metamaterial Computation (the Composite of Nanoparticles and Host Dielectrics)

```
f=F;
e_mg = (e_h.*(e_c*(1+2*f)+2*e_h*(1-f)))./(e_c*(1-f)+e_h*(2+f));
e1_mg = real(e_mg)
e2_mg = imag(e_mg)
n_mg = sqrt(e_mg);

ep_mod = sqrt(e1_mg.^2+e2_mg.^2);

figure(1)
subplot (2,1,1)
plot(wa,e1_mg)
axis([min(wa)-0.001,max(wa)+0.001,min(e1_mg)-0.001,max(e1_mg)+0.001])
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('Re(\epsilon_e_f_f)','fontsize',12)

subplot (2,1,2)
plot(wa,e2_c)
axis([min(wa)-0.001,max(wa)+0.001,min(e2_mg)-0.001,max(e2_mg)+0.001])
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('Im(\epsilon_e_f_f)','fontsize',12)

figure(2)
plot(wa,e1_mg,wa,e2_mg)
set(gca,'fontsize',8)
% set(gca,'YTick',-0.30:0.05:0.60)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('\epsilon_e_f_f','fontsize',12)

figure (3)
plot(wa,ep_mod)
hold, plot(827.000,0.01,'*')
axis([min(wa)-0.001,max(wa)+0.001, 0, max(ep_mod)+0.001])
set(gca,'fontsize',8)
```

```
% set(gca,'YTick',0:0.05:max(ep_mod))
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('abs(\epsilon)','fontsize',12)
```

Numerical Computation of in MATLAB to Get Corresponding Variables (A and ρ) for ENZ Metamaterial by Fixed Method

```
function res=tailoring;

close all
clear all
clc
format long

wav=827;
om=(2*pi*3e+8)/(wav*1e-9);

epAg=EpAg(om);
epb=12.8;


eph=2.2022;

ep=0.01;

rho=(4:0.001:6)*1E-01;
A=(3:0.0001:3.3)*1E-03;

F=0.03;     %fill the filling fraction


Q0=eph*(1+(2/F)*((ep-eph)/(ep+2*eph)))/(1-(1/F)*((ep-
eph)/(ep+2*eph)));



for jr=1:length(rho)
    jr
for jA=1:length(A)
        epQD=epb+A(jA)*Lor(om);
        Q(jr,jA)=epAg*(epQD*(1+2*rho(jr))+2*epAg*(1-
rho(jr)))/(epQD*(1-rho(jr))+epAg*(2+rho(jr))  );
end
end



MQ=abs(Q-Q0).^2;
[jr jA]=find(eq(MQ,min(min(MQ))));



figure('Position',[100            100            1000            700])
%http://www.mathworks.com/help/techdoc/ref/figure_props.html
```

```
subplot(1,3,1),  mesh(rho,A,real(Q)'),  xlabel('\rho'),  ylabel('A'),
zlabel('Re(Q)')
%http://www.mathworks.com/help/techdoc/ref/subplot.html?BB=1&BB=1
subplot(1,3,2),  mesh(rho,A,imag(Q)'),  xlabel('\rho'),  ylabel('A'),
zlabel('Im(Q)')  %http://www.mathworks.com/help/techdoc/visualize/f0-
45715.html
subplot(1,3,3),     hold,     contour(rho,A,imag(Q)',[0     0.001]),
xlabel('\rho'),                                          ylabel('A'),
plot(rho(jr),A(jA),'*')%http://www.mathworks.com/help/techdoc/creatin
g_plots/f10-2524.html




%plotting epsilon efficace

lam=826:1e-5:828;
omm=(2*pi*3e+8)./(lam*1e-9);


epS=EpAg(omm).*(   (epb+A(jA)*Lor(omm))          *(1+2*rho(jr))   +
2*EpAg(omm)*(1-rho(jr)) )...
    ./(  (epb+A(jA)*Lor(omm))*(1-rho(jr)) + EpAg(omm)*(2+rho(jr)));
G=(epS-eph)./(epS+2*eph);
epeff=eph*(1+2*F*G)./(1-F*G);

figure
subplot(1,2,1),   hold,   plot(lam,real(epeff)),   xlabel('\lambda'),
ylabel('Re(\epsilon)'), plot(wav,ep,'*'), axis tight
subplot(1,2,2),   hold,   plot(lam,imag(epeff)),   xlabel('\lambda'),
ylabel('Im(\epsilon)'), plot(wav,0,'*'), axis tight

%More about advanced plot function:
%http://www.mathworks.com/help/techdoc/creating_plots/f6-20079.html

clc
disp('RESULT')
disp(' ')
disp(strcat('rho.....=',num2str(rho(jr))))
disp(strcat('A.......=',num2str(A(jA))))
disp(strcat('R1......=',num2str(5)))
disp(strcat('R2......=',num2str(5/(rho(jr)^(1/3)))))


save merda


function res=EpAg(oom)
res=(1-(13.8e+15)^2./(oom.^2+1i*0.3e+15*oom));

function res=Lor(oom)
res=(2.279269e15)^2./(oom.^2-(2.279269e15)^2+1i*2*oom*(1.519e+12));
```

Numerical Computation in MATLAB to Get Corresponding Variables (A and ρ) for ENZ Metamaterial by Statistical Method

```
function res=res;
close all
clear all
clc

format long

global eph om0 Drho Dom0

eph=2.2022;
wav=827;
wav0=827;

om=(2*pi*3e+8)/(wav*1e-9);
om0=(2*pi*3e+8)/(wav0*1e-9);
Drho=1e-10;      %rho variation
Dom0=om0*(1e-10/wav0);    %omega variation

f=0.02;      %filling fraction


epeff=0.01;     %effective epsilon target



WT=(1/f)*((epeff-eph)/(epeff+2*eph));


rho=0:2e-1:1;
A=0:1e-3:0.008;
for jr=1:length(rho)
    disp(strcat(num2str(jr),'_',num2str(length(rho))))
for jA=1:length(A)
       WWW(jr,jA)=W(A(jA),rho(jr),om);
end
end
MQ=abs(WWW-WT).^2;
[jr jA]=find(eq(MQ,min(min(MQ))));




figure('Position',[100 100 1000 700])
subplot(1,3,1),  mesh(rho,A,real(WWW)'),  xlabel('\rho'),  ylabel('A'),
zlabel('Re(W)')
subplot(1,3,2),  mesh(rho,A,imag(WWW)'),  xlabel('\rho'),  ylabel('A'),
zlabel('Im(W)')
subplot(1,3,3),   contour(rho,A,imag(WWW)',[0   0]),   xlabel('\rho'),
ylabel('A'), plot(rho(jr),A(jA),'*')




x0=[A(jA) rho(jr)].';
dA=1e-10;
dr=1e-10;
FLA=1;

h=20;       %step
```

```
while FLA
    plot(x0(2),x0(1),'o')
    xlim([rho(1) rho(length(rho))]);
    ylim([A(1) A(length(A))]);

    x0(1);
    WW=W(x0(1),x0(2),om);
    F0=[real(WW-WT) imag(WW-WT)].';

dWA=(W(x0(1)+dA,x0(2),om)-WW)/dA;
dWr=(W(x0(1),x0(2)+dr,om)-WW)/dr;

    J(1,1)=real(dWA);
    J(2,1)=imag(dWA);
    J(1,2)=real(dWr);
    J(2,2)=imag(dWr);

    x=x0-inv(J)*F0/h;

    clc
    dist=norm(x-x0)/norm(x0)

    h=30+4*(log(dist)/log(10));

    x0=x;
    drawnow
    FLA=gt(dist,1e-6);
end

AL=x0(1)
rhoL=x0(2)


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%

lam=wav-1:1e-2:wav+1;
omm=(2*pi*3e+8)./(lam*1e-9);

figure('Position',[100 100 1000 700])
subplot(1,2,1),   hold,   xlabel('\lambda'),   ylabel('Re(\epsilon)'),
plot(wav,epeff,'*')
subplot(1,2,2),   hold,   xlabel('\lambda'),   ylabel('Im(\epsilon)'),
plot(wav,0,'*')

for j=1:length(omm);
    WW=W(AL,rhoL,omm(j));
    ep(j)=((1+2*f*WW)/(1-f*WW))*eph;
    subplot(1,2,1), plot(lam(1:j),real(ep)), axis tight, drawnow
    subplot(1,2,2), plot(lam(1:j),imag(ep)), axis tight, drawnow
end



plo(AL,rhoL,om)
```

```
save merda

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function res=W(A,rho,om)
global eph om0 Drho Dom0

difDrho=Drho/40;
difDom0=Dom0/40;

rhop=rho-3*Drho:difDrho:rho+3*Drho;
om0p=om0-3*Dom0:difDom0:om0+3*Dom0;

epAg=EpAg(om);
epb=12.8;

for jr=1:length(rhop)
for jo=1:length(om0p)
       epQD=epb+A*Lor(om,om0p(jo));
       ES=epAg*(epQD*(1+2*rhop(jr))+2*epAg*(1-rhop(jr)))/(epQD*(1-
rhop(jr))+epAg*(2+rhop(jr)));
       IN(jr,jo)=((ES-eph)/(ES+2*eph))*(1/(pi*Drho*Dom0))*exp(-
((rhop(jr)-rho)/Drho)^2 -((om0p(jo)-om0)/Dom0)^2);
end
end

res=difDrho*difDom0*sum(sum(IN));



%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function res=EpAg(oom)
res=(1-(13.8e+15)^2./(oom.^2+1i*0.3e+15*oom));



%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function res=Lor(oom,om0);
Gamma=1.519*1e+12;
res=om0^2./(oom.^2-om0^2+1i*2*oom*Gamma);



%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function res=plo(A,rho,om)
global eph om0 Drho Dom0

difDrho=Drho/35;
difDom0=Dom0/35;

rhop=rho-3*Drho:difDrho:rho+3*Drho;
om0p=om0-3*Dom0:difDom0:om0+3*Dom0;

epAg=EpAg(om);
```

```
epb=12.8;

for jr=1:length(rhop)
for jo=1:length(om0p)
       epQD=epb+A*Lor(om,om0p(jo));
       ES=epAg*(epQD*(1+2*rhop(jr))+2*epAg*(1-rhop(jr)))/(epQD*(1-
rhop(jr))+epAg*(2+rhop(jr)));
       DE(jr,jo)=(1/(ES+2*eph))*exp(-((rhop(jr)-rho)/Drho)^2       -
((om0p(jo)-om0)/Dom0)^2);
end
end

figure ('Position',[200 200 600 500])
mesh(rhop,2*pi*3e+17./om0p,log(abs(DE))'),      xlabel('\Delta\rho'),
ylabel('\Delta\lambda')
title('Resonance modes')
```

Retrivial Lambda

```
clear all
close all
clc

epR=-1.2:.001:1.2;
epI=-1.2:.001:1.2;
%L1=20;
d=113.7469603;
L1=10;
L2=50;
fid=fopen('4.1.txt')
C=textscan(fid, '%n %n', 'delimiter', ',', ...
'treatAsEmpty', {'NA', 'na'}, ...
'commentStyle', '%')
A=C{1}
B=C{2}

QQ=B.';
fclose (fid);
clear AAA

n=length(A)


wa=A';
% wa=826.99:0.01:827.01;

%%
F   = 0.03;
rho = 0.501027392331435;
A   = 0.003175418931221;

eb=1;
wp=13.8*10^15;
g=3*10^14;
c=3*10^8;
con=2*pi*c;
```

```
w=con./(wa*1E-9);

e_ag=eb-((wp.^2)./(w.^2 - w*g*i));
e1_ag=real(e_ag);
e2_ag=imag(e_ag);

e1=e1_ag; %make a simple definition of real part of permit
e2=e2_ag; %make a simple definition of imaginary of permit
n1_ag= sqrt((e1+(sqrt(e1.^2+e2.^2)))/2); %real refractive index
n2_ag= sqrt((-e1+(sqrt(e1.^2+e2.^2)))/2); %real refractive index
n_ag = n1_ag + n2_ag*i;

eb=12.8;
w0=2.279269*10^15;
g=1.519*10^12;
A=A;

e_QD = eb + ((A*w0^2)./((w.^2-w0^2)-2*w*g*i));
e1_QD = real(e_QD);
e2_QD = imag(e_QD);
n_QD = sqrt(e_QD);

r=rho;

e_1=e_QD;
e_2=e_ag;
e_c = (e_2.*(e_1*(1+2*r)+2*e_2*(1-r)))./(e_1*(1-r)+e_2*(2+r));
e1_c=real(e_c);
e2_c=imag(e_c);

n_c = sqrt(e_c);

e_h = 2.2022;
n_h = e_h^2;

f=F;
e_mg = (e_h.*(e_c*(1+2*f)+2*e_h*(1-f)))./(e_c*(1-f)+e_h*(2+f));
e1_mg = real(e_mg);
e2_mg = imag(e_mg);
n_mg = sqrt(e_mg);

ep_mod_an = sqrt(e1_mg.^2+e2_mg.^2);


%%
for jj=1:length(wa)
    jj
    wav=wa(jj);
    Q=QQ(jj);

    k=2*pi/wav;
    EE=exp(-1i*k*(L2));

for jR=1:length(epR)
for jI=1:length(epI)
            ep=epR(jR)+1i*epI(jI);
            n=sqrt(ep);
            F(jR,jI)=abs(cos(n*k*d)+0.5*1i*(n+1/n)*sin(n*k*d)-
Q*EE)^2;
```

```
end
end
    F0=min(min(F));
    A(2,jj)=F0;
    [nR nI]=find(eq(F,F0));
A(1,jj)=epR(nR)+1i*epI(nI);
end
%%
res=A;
ep_r=A(1,:);

ep_r.';

ep_mod = sqrt(real(ep_r).^2+imag(ep_r).^2);
ep_mod.'

Z1= wa,real(ep_r);
Z2 = wa,imag(ep_r);
Z3 = wa,ep_mod;
%%
%http://www.mathworks.com/help/techdoc/creating_plots/f6-20079.html

ep_r1=real(ep_r);
ep_r2=imag(ep_r);

figure(1)
subplot(2,1,1)
plot(wa,real(ep_r),wa,e1_mg)
hleg1 = legend('simulation','analytic')
hold, plot(827.000,0.01,'*')
axis([min(wa)-0.001, max(wa)+0.001, min(min(min(e1_mg),real(ep_r)))-
0.001, max(max(e1_mg),max(real(ep_r)))+0.001])
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('Re(\epsilon)','fontsize',12)


subplot(2,1,2)
plot(wa,imag(ep_r),wa,e2_mg)
hold, plot(827.000,0.00,'*')
axis([min(wa)-0.001, max(wa)+0.001, min(min(min(e2_mg),imag(ep_r)))-
0.001, max(max(e2_mg),max(imag(ep_r)))+0.001])
set(gca,'fontsize',8)
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('Im(\epsilon)','fontsize',12)


(real(ep_r))';
(imag(ep_r))';


figure (2)
plot(wa,ep_mod,wa,ep_mod_an)
hleg1 = legend('simulation','analytic')
hold, plot(827.000,0.01,'*')
axis([min(wa)-0.001, max(wa)+0.001, 0, max(ep_mod)+0.01])
```

```
axis([min(wa)-0.001, max(wa)+0.001, 0,
max(max(ep_mod),max(ep_mod_an))+0.001])
set(gca,'fontsize',8)
set(gca,'YTick',0:0.1:max(max(ep_mod),max(ep_mod_an)))
grid on
xlabel('\lambda [nm]','fontsize',12)
ylabel('abs(\epsilon)','fontsize',12)

ep_mod';
```

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