Numerical Simulations of Optical Multilayer Structure with an Embedded Octahedron Nanocrystals Using a FEM Based Approach

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***Abstract*—This theoretical study describes the optical multilayer structure models leading to investigate Surface Plasmon Polariton (SPP) to an extern applied magnetic field at visible wavelenght using a 3D-FEM based on Comsol Multiphysics software. The layered structures include the amorphous silicon c-Si octahedral nanocrystals on the interface SiO2/dielectric were investigated to enhance the SPP intensity.**

***Keywords*-Nanoplasmonics, FEM, Surface Plasmon Polariton**

I. INTRODUCTION

The rapid evolution of electronics and telecommunications has been possible by the presence of innumerable high performance devices based on silicon technology. The new applications of microelectronics, photovoltaics and photonics refer to effort to optimize the optical components. On the other hand the complexity of the junction solar cell stems from the delicate balance that exists between the different properties of the materials used and the geometric structure of the cell itself. Therefore several parameters affect the solar cell conversion efficiency. Consequently, understanding of interaction between the incident EM waves and materials is fundamental to define an accurate analysis on effects due to the presence of the nanostructures and electronic equipment.

The development of nanoplasmonic has been a topic of increasing interest in recent years. This recent progress has been possible as a result of advances in nanofabrication technology [1],[2]. Plasmonic nanoparticles are of great interest for light trapping in thin-film silicon solar cells, Ag nanoparticles can provide light-trapping performance, through excitation of charge carriers, comparable to state-of-the-art random textures in $n-i-p$ amorphous silicon solar cells. The excellent light trapping is a result of strong light scattering and low parasitic absorption of self-assembled Ag nanoparticles embedded in the back reflector. Infact, the characteristic length scale of the structures necessary to manipulate and generate surface plasmon polaritons (SPPs) in the visible and near-infrared region of the optical spectrum is in the nanometre regime. The plasmonic structures are used to increase optical absorption and the power conversion effeciency in thin-film solar cells. The principal aspects of the fabrication of Si nanocrystals in thin SiO_2 layers with the Si substrate have been considered in [3]. The Si nanocrystals are widely used for a number of solid state electronic devices, such as solar cells, solid state photosensors and thin film transistor for liquid crystal displays. Third-generation photovoltaic devices are realized in silicon nanocrystals (Si-NCs) embedded in a dielectric matrix [4], [5].

In amorphous materials, the bond lenghts and number vary slightly for different atoms in the lattice. The coordination of bonds of an atom with its closest neighbours is almost the same as in the corresponding crystalline material, but is gradually lost with more distant neighbours. Thus amorphous Si is a direct band semiconductor unlike crystalline Si, and has a high absorption coefficient with a deposition process applicable at low temperature.

The most numerous defect type, crucial for use fo a-Si in solar cells, is a dangling bond decreasing the charge carriers lifetime and mobility. To improve this situation, hydrogen (H) is incorporated into a-Si during fabrication. Hydrogenated amorphous silicon $a-Si:H$ solar cells are a low-cost alternative to bulk crystalline Si cells, offering a larger absorption coefficient across the solar radiation spectrum. Thus, an $a-Si:H$ film of thickness of 500 nm absorbs sufficient sunlight to enable efficient solar cell operation, compared to thicknesses of several tens to hundreds of microns that are required for bulk crystalline Si devices.

However, the high defect densities typically present in $a-Si:H$ thin films limit the typical minority carrier diffusion lengths to 100 nm^3, consequently, $a-Si:H$ solar cells are generally fabricated using even thinner $a-Si:H$ layers, resulting in reduced absorption of incident solar radiation. However, the significantly reduced thickness of their silicon layer makes it more difficult for them to absorb sunlight.

Therefore the capability of measuring the change of phase by the reflection of polarized light on a surface or layer structure allows a typical sensitivity of less than one nanometer for the layer thickness and for the refractive index. The thickness, homogeneity and interface qualities of the layers can be measured directly, whereas the properties related to the nanocrystal structure (like the crystallinity, the nanocrystal size or the density of the layer) can be obtained indirectly using proper optical models. From numerical simulation it is possible create a relation between the optical properties as λ_{spp} with thickness of metal in a multilayer structure. The external electric field effects on spectra and decay of photoluminescence as well as on absorption spectra were measured for CdSe nanoparticles in a polymethyl methacrylate film by Takakazu Nakabayashi and al. [6].

The major aim of the deposition of amorphous Si nanoparticels on the SiO_2 film is to improve solar light harvesting and lead to increased efficiencies due to excitation of surface plasmons polaritons. In this paper, the excitation of the SPP is due to the combination of the amorphous silicon nanocrystal related to the presence of SiO_2/air and the exiting external electric field source with wavelenght spanning from 300 to 700 nm. The numerical calculations and simulations for the resolution of electromagnetic field have been developed to solve Maxwell's equation with the Finite Element Method (FEM) using the commercial software packages Comsol Multiphysics. This theoretical work used a 3D-FEM modeling based on Comsol Multiphysics software to investigate the SPP in a multilayer structure of SiO_2 interfaces with dielectric substrate containing the embedded small octahedral amorphous silicon nanocrystals.

The multilayer structures have a very important role in Renewable energies integration in electric generation systems to promote their use and then the economic development and growth of rural areas and less developed countries have to be considered so as their management problems [7], [8].

II. Theory: Model Drude for Surface Plasmon Polariton

Metals have different optical properties as dielectric function compared to semiconductors and dielectric due to their electronic band structure. In the Drude model Maxwells equations describe an electromagnetic wave in a medium of conductivity σ, and net zero charge.

$$\begin{aligned} \nabla \cdot E &= \frac{\rho_{free}}{\epsilon} \\ \nabla \times E &= -\frac{\partial B}{\partial t} \\ \nabla \cdot B &= 0 \\ \nabla \times B &= \mu \frac{\partial J}{\partial t} + \mu \epsilon E \end{aligned} \tag{1}$$

In the absence of external charge and current densities, the curl equations can be combined to yield the wave equation:

$$\nabla^2 E + k_0^2 \epsilon E = 0 \tag{2}$$

This equation has plane wave solutions with complex wavevectors

$$\vec{E} = \vec{E_0} e^{i(\vec{k}\cdot\vec{x}-\omega t)} \tag{3}$$

$$k^2 = \mu\varepsilon\omega^2 + i\mu\sigma\omega = \mu\varepsilon\left(\omega^2 + \frac{i\sigma\omega}{\varepsilon}\right) \tag{4}$$

The distance over which the wave drops to $1/e$ its original value is known as the penetration or skin depth. Therefore it is the expression for the penetration depth by taking the square root of the expression for k^2 and reinserting it into the plane wave solution $\vec{E} = \vec{E_0} e^{i(Re[\vec{k}]\cdot\vec{x}-\omega t)} e^{-Im[\vec{k}]\cdot\vec{x}}$. It follows that the $1/e$ distance is $\delta_p = \frac{1}{Im[k]}$. For the metals as silver, gold and copper the electric field of optical waves falls to $1/e$ of its initial value in a few nm.

Surface plasmons represent coupling of an electromagnetic field to the kinetic motion of free charge carriers. Surface plasmons exist at the boundary between dielectric and conductor. Oscillation of surface charge density σ is the source of the electric fields. A discontinuity of the normal component of the external electric field at the boundary of dielectric and conductor with dielectric functions ε_d and ε_c, respectively:

$$E_{z1} - E_{z0} = 4\pi\sigma \tag{5}$$

where E_{z1} and E_{z0} are the normal components of electric field in the conductor and dielectric respectively. The wave function for a traveling charge density wave is:

$$\sigma(x,t) = \sigma_0 e^{i(K_x x - \omega t)} \tag{6}$$

K_x is the wave vector along the boundary. The charge oscillations are coupled with external electric field (E_x, E_z), which has components normal to the surface and in the propagation direction, and the transverse magnetic field (H). The SPP is a p-polarized electromagnetic wave because its electric field vector E lies in the plane (x, z) defined by the surface normal and the propagation vector while the magnetic field vector H is perpendicular to this plane. The wave function for the normal component of the electric field is

$$E_z = A\, e^{i(K_x x + K_z z - \omega t)} \tag{7}$$

where K_z is mostly imaginary. This causes exponential decay from interface, making SPPs evanescent waves. The energy density can exceed that of the incident radiation that excites the SPP. The wave vectors K_x and K_z are related according to the following:

$$K_x^2 + K_{zd,zc}^2 = \varepsilon_{d,c}\,(\omega/c)^2 \tag{8}$$

where $\varepsilon_{d,c}$ is the complex dielectric function of the dielectric or conductor, respectively. The dispersion relation for the nonradiative SPP mode can be derived by applying Maxwells equations together with the continuity conditions for E and H. For p-polarized oscillations ($E_y, H_x = H_z = 0$), boundary conditions yield, obtaining the surface plasmon wave vector

$$K_{SPP}(\omega) = (\omega/c)\sqrt{\frac{\varepsilon_d \varepsilon_c}{\varepsilon_d + \varepsilon_c}} \tag{9}$$

which describe propagation and damping, respectively. According to the Drude model for metals, the electrons in a conductor behave like an ideal gas, and the real part of the dielectric constant for a conductor varies as

$$\varepsilon_c(\omega) = 1 - \frac{\omega_p^2}{\omega^2} \tag{10}$$

where the plasma frequency is:

$$\omega_p^2 = \frac{Ne^2}{m\epsilon_o} \tag{11}$$

N is free electron density, m and e, the mass and charge of electron, and ϵ_0 the permittivity of free space. The field intensity of SPPs also decreases exponentially both in conductor and dielectric. The dispersion relationship using this approximation elucidates an important physical phenomena. Below the plasma frequency is imaginary and waves are attenuated as they enter the metal. Above the plasma frequency becomes real allowing for traveling waves. These traveling waves are waves in the electron plasma and at the plasma frequency they are completely longitudinal. The quantum of a plasma oscillation is known as a plasmon. Surface plasmon polaritons (SPP's), can occur at any interface. The basic structure of a propagating SPP is of an evanescent wave, decaying exponentially in intensity normal to the interface, and oscillating in the direction of propagation. Traditionally, to find the solutions that constitute confined surface waves one assumes that a wave exists at the boundary and solves for the appropriate boundary conditions. The wavelength of the SPP is defined by:

$$\lambda_{SPP} = \frac{2\pi}{Re[K_{SPP}]} \tag{12}$$

L_{SPP} is the SPP propagation length, physically the energy dissipated through the metal heating and it is the propagation distance. Where:

$$L_{SPP} = \frac{1}{Im[K_{SPP}]} \tag{13}$$

III. MODEL DEVELOPMENT

This theoretical work used a 3D-FEM modeling based on Comsol Multiphysics software to investigate the SPP in a multilayer structure of SiO2 interfaces with dielectric (air) substrate containing the embedded small octahedral amorphous silicon nanocrystals.

The numerical procedure for FEM allows the approximate solutions of partial differential equations (PDE) over a model with specified boundary conditions. It is thereby a procedure that may be used to solve many different kind of problems in physics. A three-dimensional model of the structure is created and constraints and parameters are applied on each subdomain and boundary, defining the necessary expressions for the incident wave, and setting the optical properties of the different domain. The finished models are then exported to the program Comsol Multiphysics chosen as environment for the application tool. Thus, parasolid geometries are modified in COMSOL Multiphysics to add the original CAD design the external physical effects to simulate such as the optical effects. The interesting model consists of octahedrons nanoparticles centered, deposited and embedded on the SiO2 surface (interface) of multilayer structure. The modes of SPP excitation depends on the size and shape of a-Si nanoparticles. The nanocrystals mostly have an lenght octahedral shape of 140 nm with optical property. Octahedron has a pyramid on the top and a pyramid on the bottom, it is a square bipyramid in any of three orthogonal orientations. The SiO2/dielectric multilayer structure is shown in the fig. 2

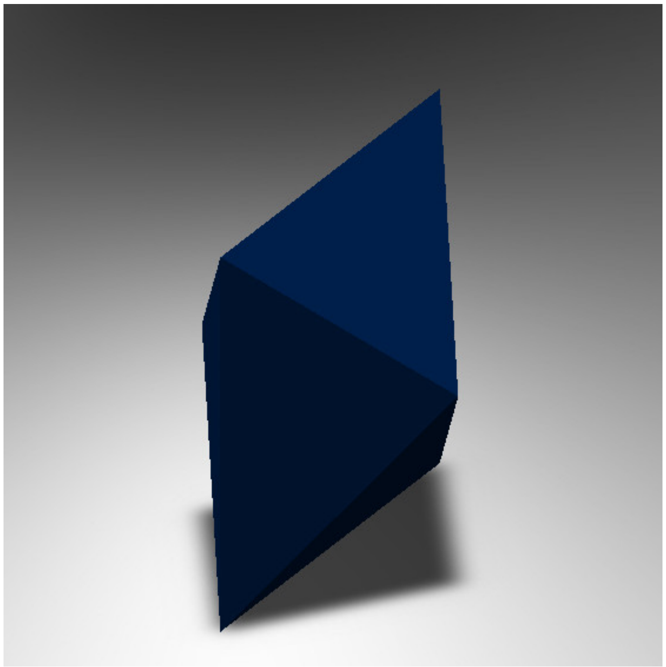

Fig. 1. 3D Octahedron of amorphous silicon (a-Si) nanocrystals modeling

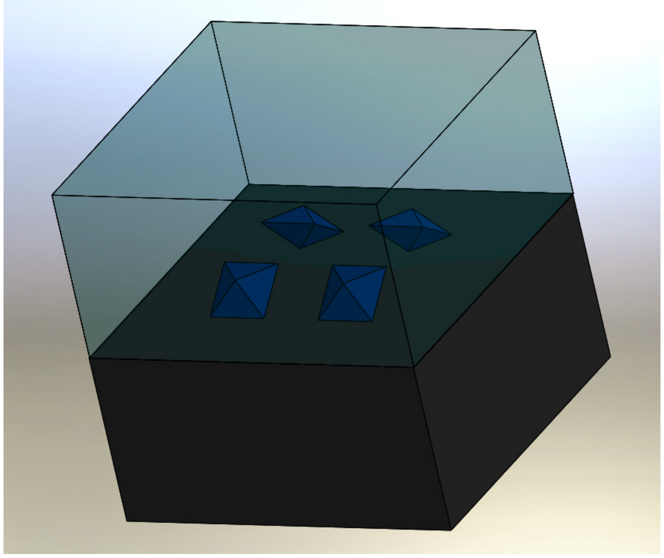

Fig. 2. 3D Multilayer structure with embedded amorphous silicon (a-Si) nanocrystals modeling

The thickness of the dielectric/SiO2 is fixed at 300nm. The dimension of the domain is 600 nm x 600 nm.

In the system the incoming electric field is a TM-polarized

Parameter	Value	Unit
ε_{air}	8.8590e-12	F/m
n_{air}	1	
n_{SiO2}	1.52	
k_{SiO2}	1e-5	
λ	Varies from 300 to 700	nm

plane wave, in order to excite the SPP associated to the nanoparticels. It was considered the contribution of surface plasmon-polariton in the model with two different layers, air and the insulator SiO2 (Silicon dioxide) substrate, where are embedded the amorphous silicon's nanocrystals (a-Si) in the centre of structure.Amorphous silicon has distinct advantages such as high refractive index, low absorption loss at telecommunication wavelengths of 1550 nm , capability of low-temperature (200-400C) plasma-enhanced chemical vapor deposition (PECVD) on almost any substrates, and even possibility for active modulation and detection. Recently, it has emerged as an important material for integrated Si photonics. A very low propagation loss of $2-3dB/cm$ at 1550 nm has been reported for$a-Si:H$ wire waveguides, which is comparable to the crystalline Si counterparts with the same dimensions.For this work the refractive index and the extinction coefficient of SiO2 are respectively 1.52 and $1e-5$ as shown in the below table the optical and electrical data used for the SPP analysis:

The $a-Si$ nanocrystals have excellent optical and electric properties, including a high index refractive and extinction coefficient at different wavelenghts in and near the visible part of the spectrum. It is very common to find the description of the optical properties of solids in terms of the index of refraction n. The general relationship of n and epsilon is $n=\sqrt{\varepsilon}$. When the radiation passes through a medium, some part of it will always be attenuated,taken into account the complex refractive index: $n = n + ik$ where the real part n is the refractive index and indicates the phase velocity, while the imaginary part k is the "extinction coefficient". The refractive index of $a-Si$ nanocrystals, as in all cases,decreased monotonically with increasing wavelength:

These surface polaritons are induced and generated by electromagnetic radiation emitting in the visible region of the spectrum, using different wavelenghts. The boundary condition chosen for the surface of dielectric and SiO2 is perfectly matched layer (PML) , meaning that is an artificial absorbing layer for wave equations. The PML is used to limit the reflections from kind of open, free-space, boundaries. For boundaries the conditions for the perfect electric conductor is given by:

$$\hat{n} \times E = 0 \tag{14}$$

In model the Cartesian axis system are chosen in such way that the z-axis is normal to the xy plane of the layers. The electromagnetic wave is assumed normal to the xy layer. The surface polariton modes are found at the interface $SiO2/air$ where one of the face of amorphous silicons nanocystals sits on interface of the substrate $SiO2/air$. Numerical simulations

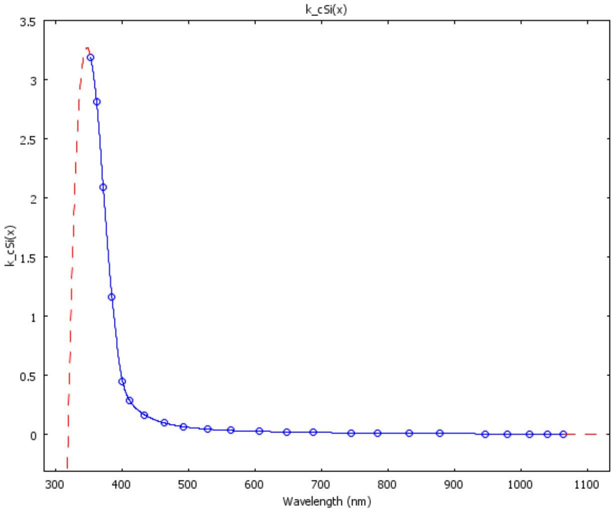

Fig. 3. Extinction coefficient of a-Si nanocrystals

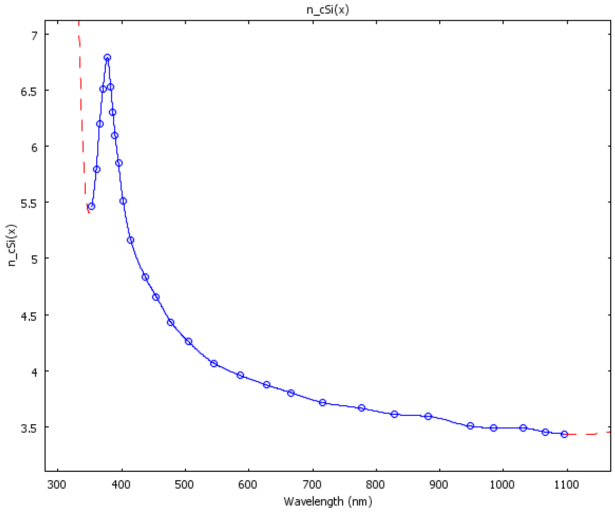

Fig. 4. Refractive index of a-Si nanocrystals

confirm the role of the octahedron photonic crystal in the coupling mechanism as shown in the Fig. 5. The information about the SPP has been established by simulations for the interaction the nanocrystals with the electromagnetic field.

IV. CALCULATION AND RESULTS

We have investigated the excitation of the SPP in an extension of the simple metal surface at visible frequencies in a-Si nanocrystals in two layer system.The method of analyses for SPP's is essentially the same of heterostructure or single flat surface , however, because of the additional interface the dispersion relation becomes more complex.It is possible to excite surface polaritons of amorphous Si (a-Si) at frequencies at which a-Si has a positive real component of the permittivity and a large imaginary component. These modes on films of a-Si have similar or even superior characteristics to those on gold films, with longer propagation lengths and similar confinement

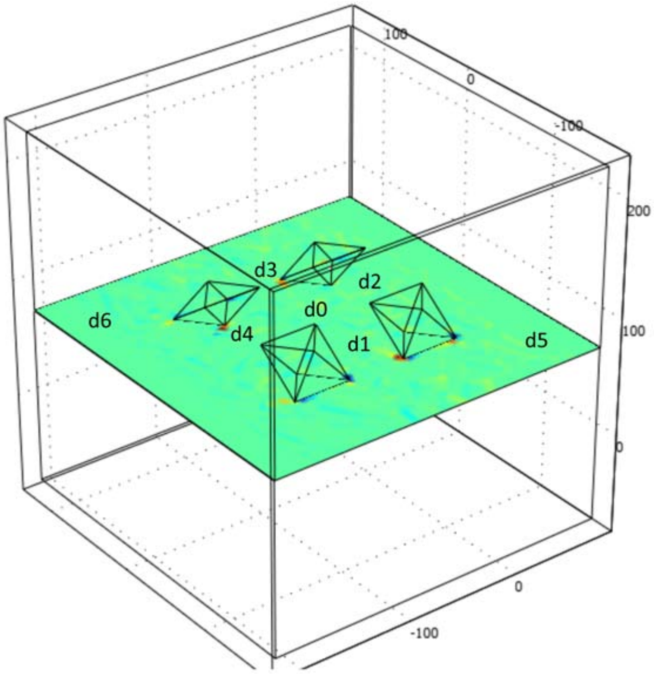

Fig. 5. Multilayer structure with amorphous silicon (a-Si) nanocrystals

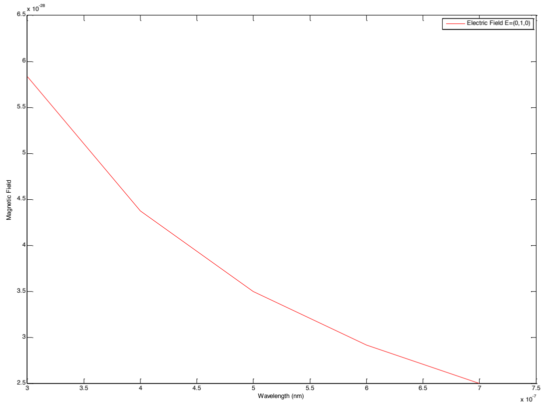

Fig. 6. Magnetic Field vs wavelenght calculated in d0 (see Fig. 5)

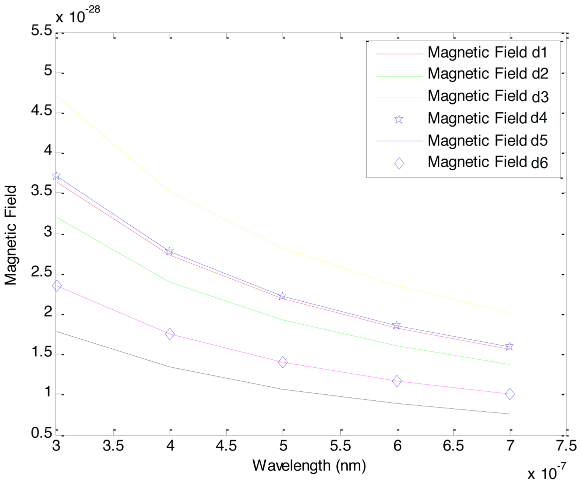

Fig. 7. Magnetic Field vs wavelenght calculated in d1, d2, d3, d4, d5, d6 (see Fig. 5)

to the thin film. The result obtained from FEM calculations are the complex description of the fields in terms of H_z.

The magnetic field decreases when the wavelenght is increased in the range from 300 to 700 nm. Carefully studying the magnetic field can reveal that the peak is shifting to lower wavelenght, maximum energy is at 300 nm at different magnetic field calculated on the interface nanocrystals/SiO2. Systematic work has illustrated considering the interaction of the SPP with the nanocrystal on interface of SiO2.

Surface Plasmons are a result of the mutual-coupling between photons and collectively oscillating electrons at the dielectric/amorphuos silicon interface. The electromagnetic energy of the surface plasmons are nicely confined in the vicinity of the interface.It is calculated the magnetic field across different directions respect to the nanocrystals to provide the interactions between the nanocrystals and SiO2 surface. This approach is consisted to calculate and relate the magnetic field at different wavelenght and directions on surface SiO2. The electromagnetic waves of SPP are detected travelling along vertical, horizontal and diagonal directions of nanocrystals positions as function of different wavelenghts throught the interface SiO2/dielectric as shown in the Fig. 6 and Fig. 7. The intensity of SPP is influenced by nanoparticels distance and disposition. Applying the magnetic field, both the real and the imaginary part of the SPP wavevector K_{SPP} are modified.

V. CONCLUSION

The plasmonic applications represent an interesting attraction due to the confinement of signals and light in structures with the possibility to work in the optical near field, localizing the surface plasmon polaritons known as electromagnetic (EM) waves that propagate along metallic nano-structure. The materials and technologies play an important role in the development of plasmonics.

For this reason, in the literature there are a large variety of optimization techniques by using soft computing techniques [9] in order to improve the conversion efficiency of solar cells [10], [11], [12], [13].

This study describes the implementation and development of the application tool Comsol Multiphysics for the simulation of the mechanisms and the interaction of the SPP with the a-Si nanocrystals on interface of SiO2/dielectric. To obtain a high efficiency the models are initially created within Comsol Multiphysics where it is easy to create a geometry, apply boundary conditions, define the necessary expressions, e.g. for the incident wave, and set the optical properties of the different domains. We show the interactions between EM and a-Si nanocrystals located on layer of nanostructure.

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