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Design and Modelling of Nanorods for Display Applications

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Abstract—**There has been growing demand for fabrication of smart and functional metal oxide thin film coatings on ZnO nanowires, nanorods and arrays. In this scenario, the present work is focused to model the interaction of Gaussian electromagnetic wave (750 nm) with dense array of nanorods. Interestingly, the distance between the rods and its diameter is much smaller than the wavelength which enables to model nanorods. Under typical conditions, the rod array does not function as a diffraction grating. Instead, the rod array behaves as if it was a continuous metal sheet for light polarized along the rods, most importantly, when light polarized perpendicular to the rods, the array is almost transparent to the electromagnetic wave. Thus the perpendicular case lead to the dipole coupling between the rods, thereby coupling electromagnetic excitation between the rods also outside of the illuminated region. The software tool COMSOL Multiphysics version 5.0 is used to model the proposed novel design of nanorods.**

Keywords— Nanorods; Gaussian electromagnetic wave; Dipole coupling; Electric field.

I. Introduction

In nanotechnology, nanorods are morphology of nanoscale objects. Each of their dimensions ranges from 1nm to 100 nm. They may be synthesized from metals or semiconducting materials [1]. Standard aspect ratios are 3 to 5. Out of various synthesis procedures, direct chemical synthesis is widely being used for the production of nanorods. The role of ligands is very important in controlling the shape and size of nanorods. A combination of ligands acts as shape control agents and bond to different faces of the nanorod with different strengths. This allows different faces of the nanorod to grow at different rates, producing an elongated object. Quantum dots are also sometimes referred to as artificial atoms, a term that emphasizes that a quantum dot is a single object with bound, discrete electronic states, as is the case with naturally occurring atoms or molecules [2,3].Quantum dots exhibit properties that are intermediate between those of bulk semiconductors and those of discrete molecules. Their optoelectronic properties change as a function of both size and shape [4, 5]. Larger Quantum dots emit longer wavelengths resulting in emission colors such as orange or red. Smaller Quantum dots emit shorter wavelengths resulting in colors like blue and green, although the specific colors and sizes vary depending on the exact composition of the Quantum dots [6].

An emerging application is usage of quantum dots in micro-electro-mechanical systems. Theranosticnanomedicine is emerging as a promising therapeutic paradigm. It takes advantage of the high capacity of nanoplatforms to ferry cargo and loads onto them for both imaging and therapeutic functions. Lot of attention has been paid to the investigations on quantum dots due to their superior advantages viz., minimized energy and materials, improved reproducibility, accuracy, reliability, selectivity, sensitivity, low power consumption, ranger, color accuracy. The main important potential applications are includes transistors, solar cells, Light Emitting Diode, lasers second harmonic generation, quantum computing, and medical imaging [7]. Additionally, the small size allows quantum dots to be suspended in solution which leads to possible uses in inkjet printing and spin-coating [8]. These processing techniques result in less-expensive and less time consuming methods of semiconductor fabrication. Since photons have large bearing on nanoparticles, it is interesting to send electromagnetic waves on to the nanorods or wires of different sizes may be leading to production of variety of colors. Quantum dots are new and innovative perspective on the traditional semiconductor.

Considering the need and technical importance of quantum dots, present work is focused to manifestation of quantum dots producing different colours due to incidence of electromagnetic wave [9]. The distance between the rods and its diameter is much smaller than that wavelength of Gaussian electromagnetic wave.

II. SOFTWARE TOOL

The software tool COMSOL Multiphysics version 5.0 is used to model the proposed nanorods. Another important thing, the selection of suitable module that provides necessary mathematical equations for the modeling of proposed design. In optics, a ray is an idealized model of light, obtained by choosing a line that is perpendicular to the wave fronts of the actual light, and those points in the direction of energy flow [10]. New Ray Optics Module treats electromagnetic waves as rays in systems where the wavelength is much smaller than its encompassing geometry. Frequency and material-controlled one-click meshing to set-up infinite elements, perfectly-matched layers (PMLs), and periodic conditions.

A) Design Procedure

For any model to be designed using COMSOL will undergo following steps.

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i. Geometry
ii. Addition of Materials
iii. Addition of Physical Interface
iv. Simulation
v. Analysis (Change of Materials, Inputs and Dimensions)
vi. Exploring Optimum output conditions

B) Geometry

The main idea is to model a nanorods first that followed by array of nanorods. Further, manifestation of incident of electromagnetic wave on to an array of rods along with analysis. The beam propagates in negative y-direction. It is very important to note that the wavelength of incident electromagnetic wave matches with the spot radius of the beam (750 nm). The rod of radius 20 nm is designed and the array of such many rods was modeled with internal separation of 150 nm. Figure 1 shows that half of the beam illuminates the first part of the array of rods. Thus, most of the 40 rods in the model have a very low illumination. The designed array of nanorods was shown in Figure 1. By providing specific minimum and maximum values for X and Y axes ($-0.5x10^{-6}$ to $0.5x10^{-6}$), the perfect match layer was done and shown in Figure 2. To this layer, selective domains were added that enable to verify interaction of Gauss electromagnetic wave with array of nanorods.

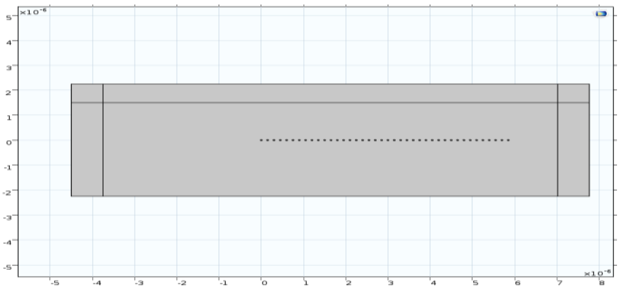

Fig 1: Geometrical array of nanorods

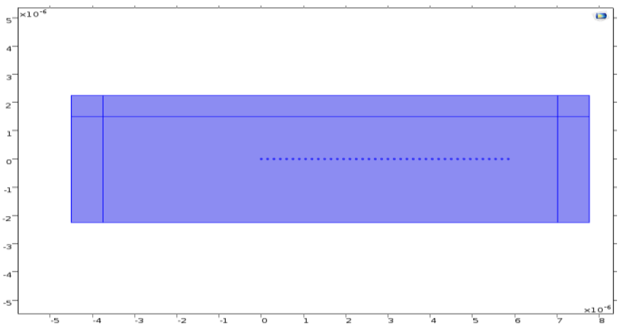

Fig 2: Perfectly matched layer

C) Parameters and physical interface

Add parameters for the Gaussian light beam, the geometric domains, and the critical material parameter for the nanorod. Now add functions used for describing the input Gaussian beam. Define the radius of curvature function, R, as a piecewise function, since it is infinite when its argument is zero.

Table 1

Parameters

S.No	Name of the parameters	Value
1	Wave length (wl)	$7.5000e^{-7}$m
2	Frequency (f)	3.9972e141s
3	Spot radius (w0)	$7.5000e^{-7}$m
4	Rayleigh range (z0)	$2.3562e^{-6}$m
5	Propagation constant (k)	8.3776e61/m
6	Electric Field Amplitude (E0)	1[V/m]
7	Radiusof Nanorods (r_NP)	2.0000e-8m
8	Number of Nanorods (N_NP)	40
9	Separation between Nanorods (dx_NP)	1.5000e-7m
10	Plasma Frequency for Nanorods (omega_p)	1.1509e16 1/s
11	Width of air domain for axis x(w_air_left)	3.7500e-6m
12	Width of air domain for x (w_air_right)	7.0200e-6m
13	Width of air domain (w_air)	1.0770e-5m
14	Height of air domain (h_air)	3.0000e-6m
15	Thickness of PML domain (d_PML)	7.5000e-7m

The rods are metallic, with a dispersion formula for the relative permittivity given by

$$\varepsilon(\omega)=1-\omega p^2/\omega^2 \quad \text{....................(1)}$$

Where the angular frequency is defined by

$$\omega=2\pi c/\lambda \quad \text{..............................(2)}$$

ωp is the plasma frequency. The plasma frequency is set to zero, resulting in a negative relative permittivity similar to that of gold.

D) Addition of materials

The default material be air. The material properties of the nanorods will later be defined in a wave equation feature.

Electromagnetic Waves, Frequency Domain (EWFD)

Calculate the first solution for light polarized along the out-of-plane z-direction. Solve for the scattered field and set the field to a propagating 2D Gaussian beam. In Electromagnetic Waves, Frequency Domain (ewfd) having Scattered field consists the Eb vector it has some values that are x=0,y=0,z=E(x,y). Because there are no in-plane field components in this case, it suffices to compute the solution for the out-of-plane component.

Meshing

After giving terminal and ground, applied meshing to the structure of selective regions. Meshing is done in-order to distribute the applied pressure equally on the device. Create a swept mesh for the PML regions.

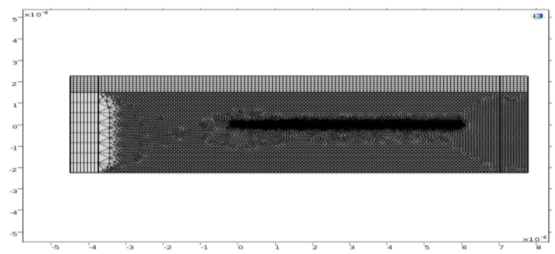

Fig 3: Meshing of PML.

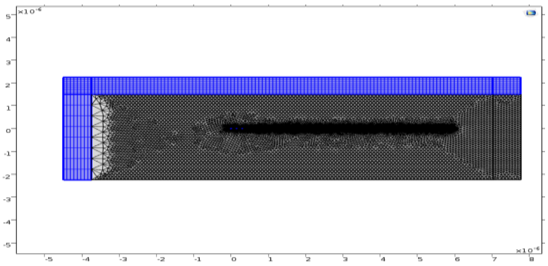

Fig 4: Mapping of PML

III. SIMULATION

Simulation is a process of using a computer to create conditions that are like those in real life. By changing variables in the simulation, prediction may be made about the behaviour of the system. It is a tool to virtually investigate the behaviour of the system under study. After defining the geometry of the proposed model, materials are added, which gives a solid design.

IV. RESULTS AND DISCUSSIONS

Simulation has been carried out for proposed design with the necessary inputs such as focusing polarized light beam along grating vector direction (*x*-direction) or in z-direction that lead to significant optical changes from nanorod array. Figure 5 shows the norm of the electric field for the Gaussian beam. In this configuration, the light beam is polarized in the *x*-direction, that is, in the direction of the grating vector. As seen from the surface plot, the nanorod array illuminates half of the Gaussian light beam. However, for this polarization there is no noticeable reflection or diffraction from the nanorod array.

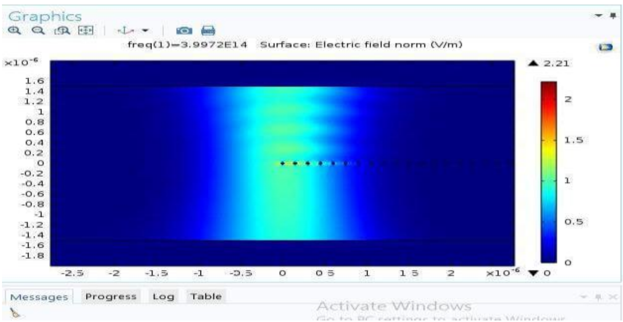

Fig 5: Surface plot of the electric field norm.

The electric field of the Gaussian light beam is polarized in the x direction where figure 6 shows a zoom-in of the left most part of the nanorod array and the center of the light beam. The plot shows that there is a dipolar coupling between the rods. As per figure 6, the polarization of the beam is in the x direction that reveals no diffraction or reflection from nanorod array. Figure 7 shows that the coupling between the nanorods extends much longer than the intensity distribution of the exciting Gaussian light beam. When the light beam is polarized along the rods, that is, in the *z* direction (the out-of-plane direction), the interaction between the beam and the nanorod array is much stronger.

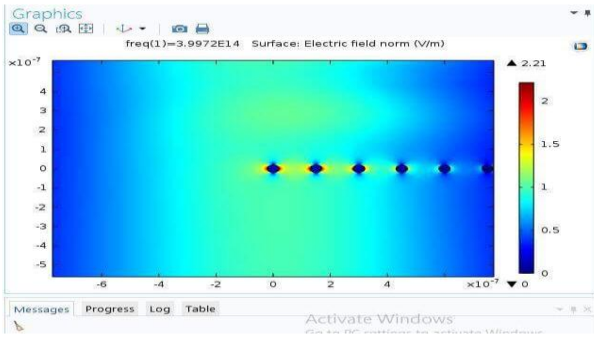

Fig 6: Zoom-in on the centre of the Gaussian beam and the left-most nanorods.

Fig 7: Line plot of the x component of the electric field (blue line) and the Gaussian beam background field (green line). The beam is polarized in the x direction.

V. CONCLUSION

An array of nanorods and interaction light beam is modelled using COMSOL Multiphysics version 5.0. Quantum dot can be synthesized to be essentially any size, and therefore produce essentially any wavelength of light. When the polarization of the beam is in the x direction then the nanorod array illuminates half of the Gaussian light beam that reveals no diffraction or reflection from nanorod array. The coupling between the nanorods extends much longer than the intensity distribution of the exciting Gaussian light beam. When the light beam is polarized along the rods, that is, in the *z* direction (the out-of-plane direction), the interaction between the beam and the nanorod array is much stronger. Due to their physiochemical properties, quantum dots may used in different field by altering their surface property, internal structures, preparation techniques, coating material etc. The future looks bright and exciting on all the possible applications of quantum dots.

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REFERENCES

[1] *Gyu-Chul Yi, Chunrui Wang & Won Il Park. "Nanorods synthesis, characterization and applications". Semiconductor Science and Technology. 20 (4): S22–S34. doi:10.1088/0268-1242/20/4/003.*

[2] *M. Lax, W.H. Louisell, and W.B. McKnight, "From Maxwell to paraxial wave optics," Physical Review A, vol. 11, no. 1, pp. 1365–1370, 1975.*

[3] *Ashoori, R. C. (1996). "Electrons in artificial atoms". Nature. 379 (6564):2. Bibcode:1996 Nature.379..413A. doi:10.1038/379413a0.*

[4] *Kastner, M. A. (1993)."Artificial Atoms". Physics today. 46 (1):20. doi:10.1063/1.881393.*

[5] *Murray, C. B.; Kagan, C. R.; Bawendi, M. G. (2000). "Synthesis and Characterization of Mono-disperse Nano-crystals and Close-Packed Nanocrystal Assemblies". Annual Review of Materials Research 30 (1). doi:10.1146/annurev.matsci.30.1.545.*

[6] *Brus, L.E. (2007). "Chemistry and Physics of Semiconductor Nano-crystals" (PDF). pg no. 2 Retrieved 7 July 2009. "Quantum Dots". Nanosys – Quantum Dot Pioneers.pg no. 2Retrieved 2015-12-04.*

[7] *Ramírez, H. Y., Flórez J., and Camacho A. S., (2015). "Efficient control of coulomb enhanced second harmonic generation from excitonic transitions in quantum dot ensembles". Phys. Chem. Chem. Phys. 1(8): pg no2 23938. doi:10.1039/C5CP03349G.*

[8] *Coe-Sullivan, S.; Steckel, J. S.; Woo, W.-K.; Bawendi, M. G.; Bulović, V. "Large-Area Ordered Quantum-Dot Monolayer's via Phase Separation during Spin-Casting". Advanced Functional Materials. 1 (9):2. doi:10.1002/adfm.200400468.*

[9] *M. Lax, W.H. Louisell, and W.B. McKnight, "From Maxwell to paraxial wave optics," Physical Review A, vol. 11, no. 1, pp. 1365–1370, 1975.*

[10] *Moore, Ken (25 July 2005). "What is a ray?". ZEMAX Users' Knowledge Base. Retrieved 30 May 2008.*

[11] *Appell D 2002 Nanotechnology: wired for success Nature 419 553.*

[12] *Samuelson L 2003 Self-forming nanoscale devices Mater. Today 6 22.*

[13] *Duan X F, Huang Y, Cui Y, Wang J F and Lieber C M 2001 Indium phosphide nanowires as building blocks for nanoscale electronic and optoelectronic devices Nature 409 66*

[14] *Cui Y, Wei Q, Park H and Lieber C M 2001 Nanowire nanosensors for highly sensitive and selective detection of biological and chemical species Science 293 1289.*

[15] *Xia Y N, Yang P D, Sun Y G, Wu Y Y, Mayers B, Gates B, Yin Y D, Kim F and Yan H Q 2003 One-dimensional nanostructures: synthesis, characterization, and applications Adv. Mater. 15 353.*

[16] *Wang Z L 2000 Characterizing the structure and properties of individual wire-like nanoentities Adv. Mater. 12 1295.*

[17] *Hu J, Odom T W and Lieber C M 1999 Chemistry and physics in one dimension: synthesis and properties of nanowires and nanotubes Acc. Chem. Res. 32 435.*

[18] *Yang P D and Lieber C M 1996 Nanorod-superconductor composites: a pathway to materials with high critical current densities Science 273 1836.*

[19] *Morales A M and Lieber C M 1998 A laser ablation method for the synthesis of crystalline semiconductor nanowires Science 279 208.*

[20] *Peng X G, Wickham J and Alivisatos A P 1998 Kinetics of II-VI and III-V colloidal semiconductor nanocrystal growth: 'focusing' of size distributions J. Am. Chem. Soc. 120 5343*