COMSOL Multiphysics in Plasmonics and Metamaterials

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Outlook

- Introduction;
- Our works:
  - Effective-medium properties of metamaterials: A quasi-mode theory;
  - 2D complete band gaps from 1D photonic crystal;
  - Optical microcavities;
- Conclusions.
User history of COMSOL Multiphysics

2008    Shanghai

2009    Shanghai

2010    Taipei
VIP Customer

- COMSOL Multiphysics 3.5a, Fudan
- COMSOL Multiphysics 4.2a, NTU
• AC/DC Module
• Acoustics Module
• Chemical Engineering Module
• Earth Science Module
• Heat Transfer Module
• MEMS Module
• **RF Module**
• Structural Mechanics Module
The rules obeyed by electromagnetic waves

\[ \nabla \cdot \vec{E} = \rho / \varepsilon \]
\[ \nabla \times \vec{E} = -\mu \frac{\partial}{\partial t} \vec{H} \]
\[ \nabla \cdot \vec{H} = 0 \]
\[ \nabla \times \vec{H} = j + \varepsilon \frac{\partial}{\partial t} \vec{E} \]

Maxwell equations

Metal

Air, water, glass

Some ferromagnetic, anti-ferromagnetic materials

\[ \mu \]

\[ \varepsilon \]

V.G. Veselago
Negative refraction

Negative Refraction

Super Lens
Experimental demonstration

Electric atom

-\varepsilon

PRL 76, 4773 (1996)

Magnetic atom

-\mu


First experimental verification of negative refraction

Science 292, 77(2001)

J. B. Pendry

D. R. Smith
**Simulation and Experiments**

**EM Cloaking**

*Science 314,997 (2006)*

**Plasmonic Luneburg Lens**

*Nano Lett. 10, 1991 (2010)*

**Negative refraction in PC**

*PRL 97,073905(2006)*

- **FEM Simulation** is a powerful tool to design the metamaterial and investigate its properties.
Comparison of FEM and FDTD

Conclusion: FEM has more freedom of mesh setup to define the complex structure more accurately.
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Section I

Effective-medium properties of metamaterials:
A quasi-mode theory

[1] How to determine effective-medium properties;

\[ n_{\text{eff}} = \frac{1}{kd} \cos^{-1} \left( \frac{1}{2t} \left[ 1 - (r^2 - t^2) \right] \right) + \frac{2\pi m}{kd} \]

\[ z_{\text{eff}} = \pm \sqrt{\frac{(1 + r)^2 - t^2}{(1 - r)^2 - t^2}} \]

\[ n = \sqrt{\varepsilon} \sqrt{\mu}; z = \frac{\sqrt{\mu}}{\sqrt{\varepsilon}} \]

\[ \varepsilon_{\text{eff}} = \frac{n_{\text{eff}}}{z_{\text{eff}}}, \mu_{\text{eff}} = n_{\text{eff}} z_{\text{eff}} \]

S-Parameter Retrieval Method

[PRB, 65, 195103 (2002)]
[2] Problems in traditional effective-medium method

\[ n_{\text{eff}} = \frac{1}{kd} \cos^{-1}\left( \frac{1}{2t} \left[ 1 - \left( r^2 - t^2 \right) \right] \right) + \frac{2\pi m}{kd} \]

\[ z_{\text{eff}} = \pm \sqrt{\frac{(1+r)^2 - t^2}{(1-r)^2 - t^2}} \]

Effective medium changes while unit cell increases
PRB 77, 035126 (2008)

Strong coupling system
PNFA 6,96 (2008)
Quasi-mode Method to determine effective EM properties

Meta-materials

Vary $\varepsilon_{\text{ref}}, \mu_{\text{ref}}$  \quad \Rightarrow \quad \text{Scattering loss self-energy}  \quad \Rightarrow \quad 0

$\varepsilon_{\text{eff}} = \varepsilon_{\text{ref}}$

$\mu_{\text{eff}} = \mu_{\text{ref}}$

Simulation setup

Cross section of wire: 0.2mm × 0.5mm (y × z)
Lattice constant: 16mm × 6mm × 7.5mm (x × y × z)
Effective medium properties of metallic wire

At a single frequency we tune $\varepsilon_{\text{ref}}$ and $\mu_{\text{ref}}$ to search the highest DOS and determine the effective EM properties.

$\varepsilon_{\text{ref}} = 2.793, \mu_{\text{ref}} = 0.906$
Dispersion of effective permittivity $\varepsilon_{\text{eff}}$

- Peaks of DOS broaden and decrease while frequency increases.
- It means uncertainty range of effective parameters is more and more large that effective medium description gradually breaks down.
I try to seek the simulation method for about half a year.
As far as I know, comsol is the only commercial software which can solve my problem.

Section II

2D complete gaps from 1D photonic crystal

3D Complete Photonic Band Gap (PBG)

\[ \varepsilon_1 = 1, \mu_1 = 1, \varepsilon_2 = -6, \mu_2 = -1.38, d_1 = 1.5\lambda / 2\pi, d_2 = 1.4\lambda / 2\pi \]

Complete band gaps can never be realized in 1D right-handed periodic structures.

\[ \varepsilon_2 = \mu_3 = -6, \mu_2 = \varepsilon_3 = -1.38, d_2 = d_3 = 0.7\lambda / 2\pi \]

Ilya V. Shadrivov et. al., PRL 95, 195903 (2005)
Whether we can confine the light in two or three dimensional space using a one dimensional system?

Green Function

Comsol Simulation

S.L. Sun et. al., PRE 53,066602 (2007)
Kivshar et al, PRL 95,195903(2005)
Section III

Optical Microcavities

Ref: Hongxing Dong, et al., Appl. Phys. Lett. 97, 223114 (2010);
Optical Microcavity

Fabry-Pérot microcavity

Whispering gallery microcavity


Other kinds of Microcavities

Peidong Yang, et al., Science 292, 1897 (2001)

Plasmonic Laser

- The first experimental demonstration of plasmon laser.
- Small size, hybrid plasmonic waveguide, low loss;


Introduction of ZnO Nanowire

WGM of photon

\[ 6R_i = \frac{hc}{nE} \left[ N + \frac{6}{\pi} \arctan(\beta \sqrt{3n^2 - 4}) \right] \]

WGM of exciton polariton

Indium oxide octahedra optical microcavities


vapor-phase transport method

Indium and oxygen vapor as source materials

Reaction temperature 950 °C

\[ \text{N}_2 \rightarrow \text{O}_2 \rightarrow \text{N}_2 \rightarrow \text{In}_2\text{O}_3 \]

\[ 950^\circ \text{C} \]

\[ \text{In}_2\text{O}_3 \text{ octahedra are very regular and nearly perfect in shape with sizes ranging from 0.5 to 2.5 } \mu\text{m} \]

Single-crystalline with BCC lattice

The SEM, TEM and SAED of In\textsubscript{2}O\textsubscript{3} octahedrons

\[ \langle 110 \rangle, \langle 100 \rangle, \langle 111 \rangle \]
Because of this confocal configuration, the spatial resolution can be up to sub-micrometer
The photoluminescence (PL) spectrum

Bow-tie like model

an angle of incidence of 35°

Plane wave model

Cauchy dispersion formula

The factor $\beta$ depends on polarization, for TM mode (the electrical component of light $E \perp$ rhombic cross section), $\beta=n^{-1}$ and for TE mode ($E \parallel$ rhombic cross section), $\beta=n$. 

$n_\parallel = 1.81 + \frac{7.16 \times 10^4}{\lambda^2}$
Numerical Simulation

- All the modes observed experimentally are identified by FEM simulated spectrum.
Conclusions

- COMSOL Multiphysics is a powerful and necessary simulation tools for me.
- COMSOL Multiphysics offers many freedoms for the postprocessing.
- COMSOL Multiphysics has powerful connection with other softwares-Matlab, Autocad, etc.
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