COMSOL Multiphysics in Plasmonics and Metamateirls

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Excerpt from the Proceedings of the 2011 COMSOL Conference in Taipei

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

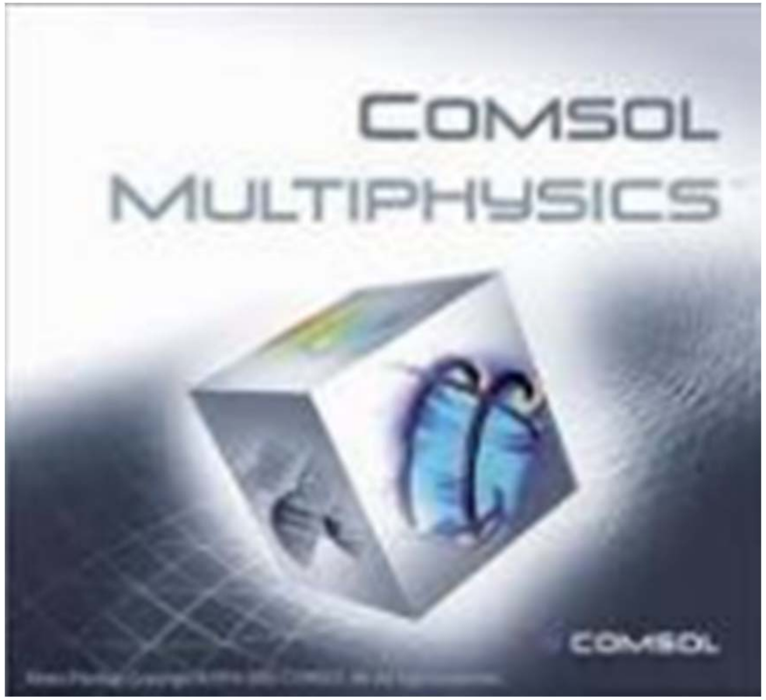
2008 Shanghai

2009 Shanghai

2010 Taipei

VIP Customer

- ☐ **COMSOL Multiphysics 3.5a, Fudan**
- ☐ **COMSOL Multiphysics 4.2a, NTU**

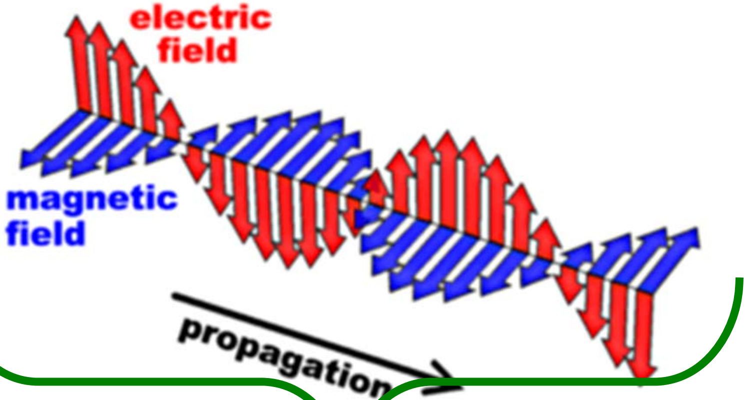


COMSOL DOCUMENTATION

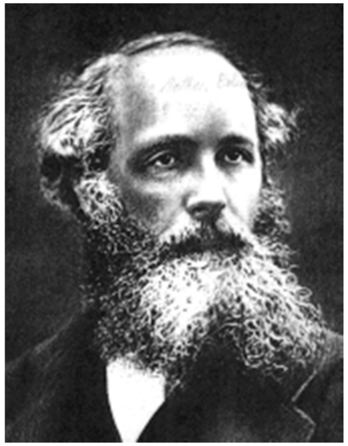
COMSOL

- AC/DC Module
- Acoustics Module
- Chemical Engineering Module
- Earth Science Module
- Heat Transfer Module
- MEMS Module
- RF Module
- Structural Mechanics Module

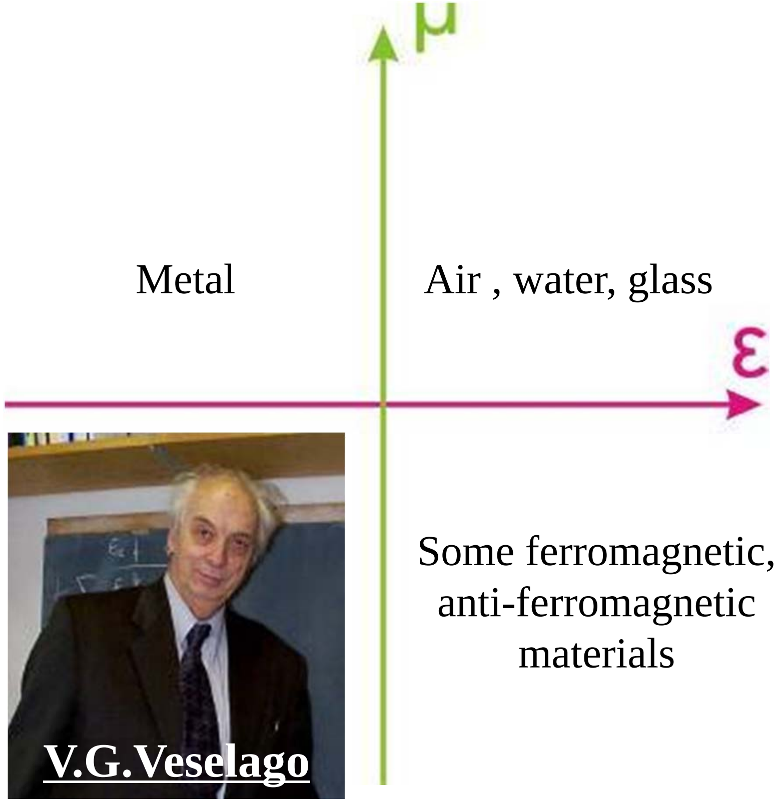
The rules obeyed by electromagnetic waves



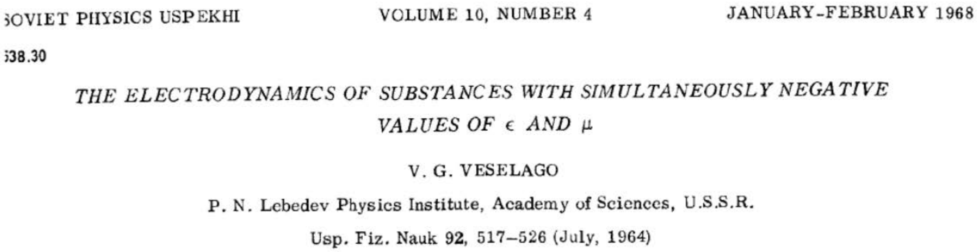
$$\begin{cases} \nabla\cdot\vec{E} = \rho\boxed{/\varepsilon} \\ \nabla\times\vec{E} = -\boxed{\mu}\dfrac{\partial}{\partial t}\vec{H} \\ \nabla\cdot\vec{H} = 0 \\ \nabla\times\vec{H} = \vec{j} + \varepsilon\dfrac{\partial}{\partial t}\vec{E} \end{cases}$$



Maxwell equations



V.G.Veselago



SOVIET PHYSICS USPEKHI VOLUME 10, NUMBER 4 JANUARY-FEBRUARY 1968

538.30

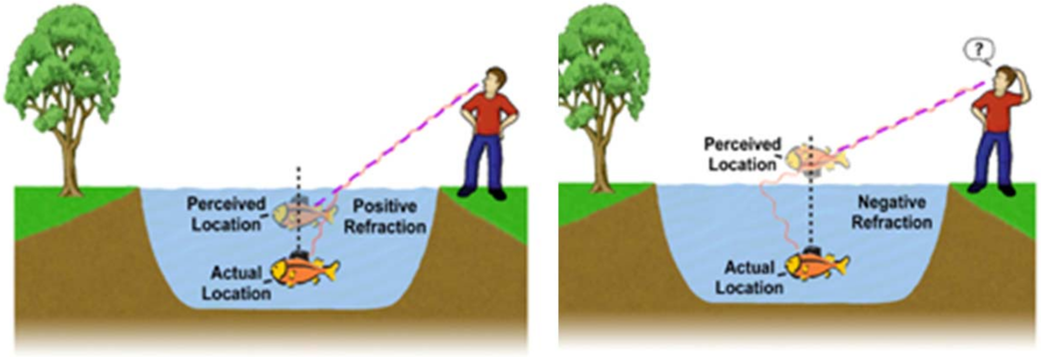
THE ELECTRODYNAMICS OF SUBSTANCES WITH SIMULTANEOUSLY NEGATIVE VALUES OF ϵ AND μ

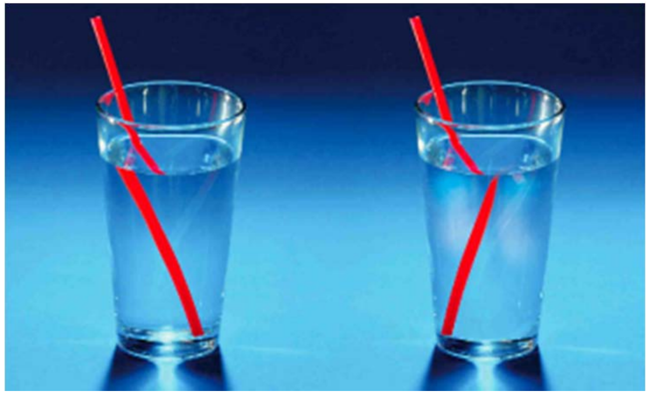
V. G. VESELAGO

P. N. Lebedev Physics Institute, Academy of Sciences, U.S.S.R.

Usp. Fiz. Nauk **92**, 517–526 (July, 1964)

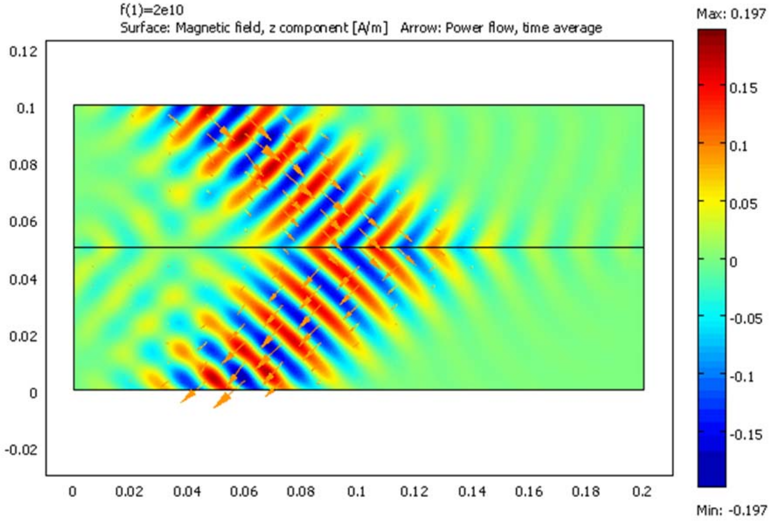
Negative refraction

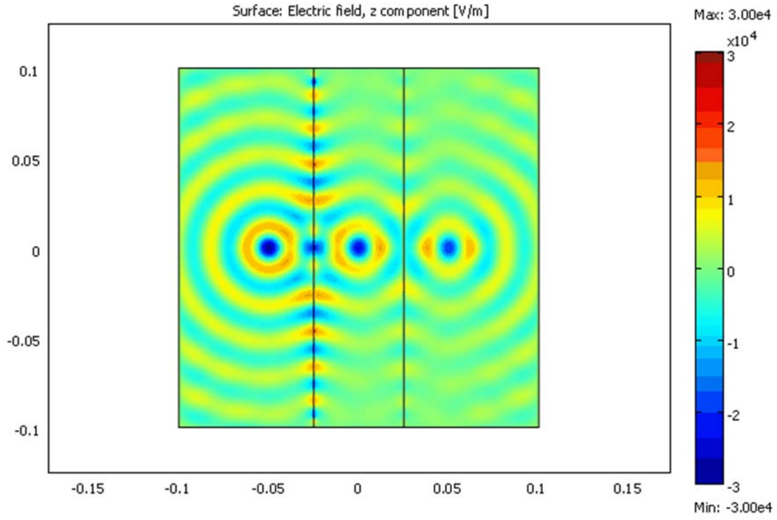




Negative Refraction

Super Lens





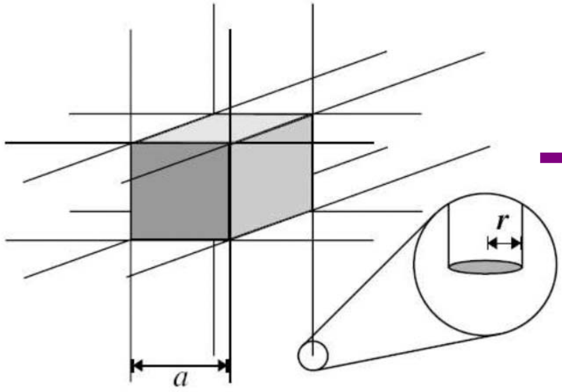
Experimental demonstration

J. B.Pendry

D. R. Smith

-ε

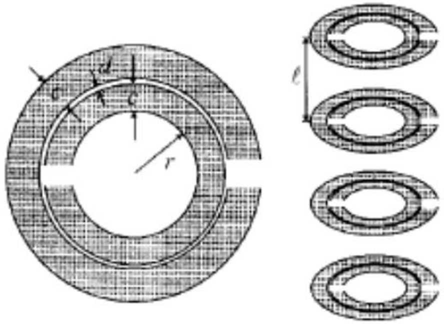
Electric atom



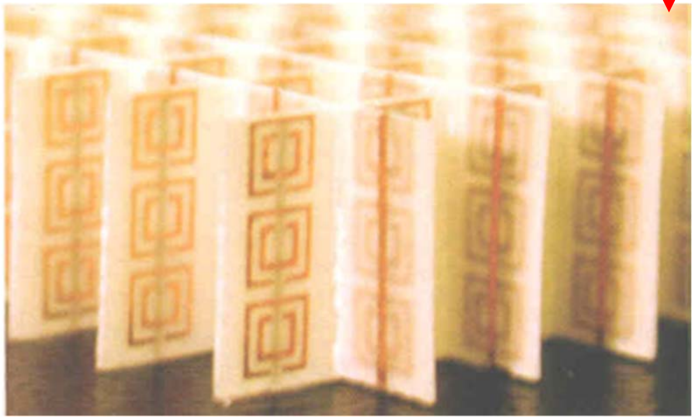
PRL 76, 4773 (1996)

+

Magnetic atom **-μ**

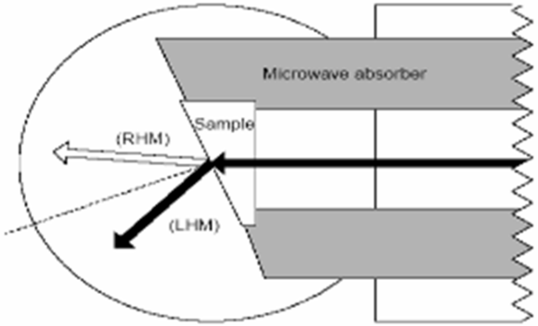


IEEE Trans. Microwave Theory Tech. 47, 2075 (1999)



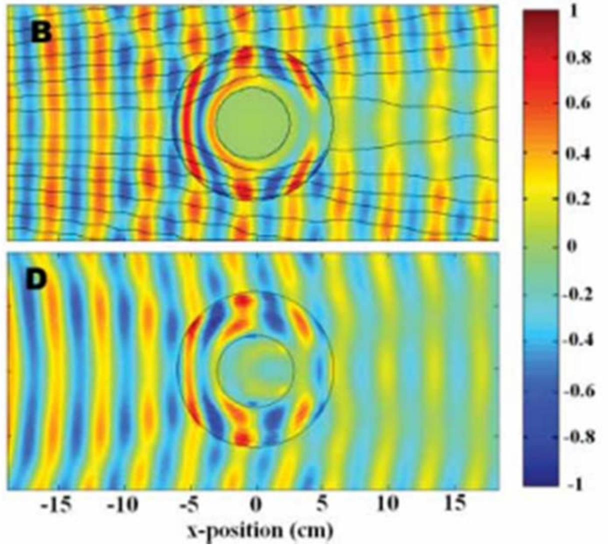
Science 292, 77(2001)

First experimental verification of negative refraction **-n**



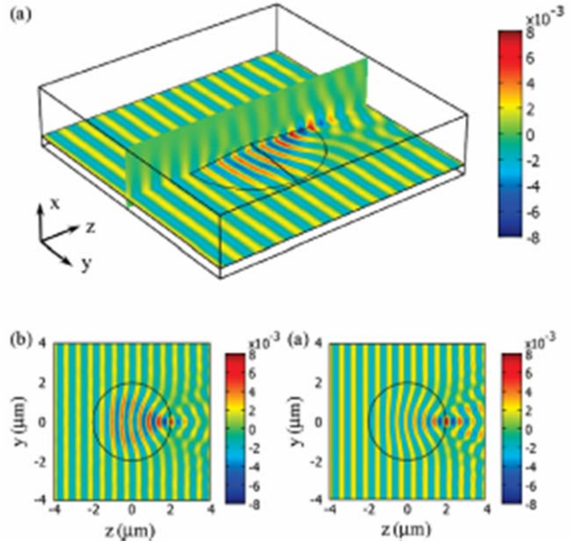
Simulation and Experiments

EM Cloaking



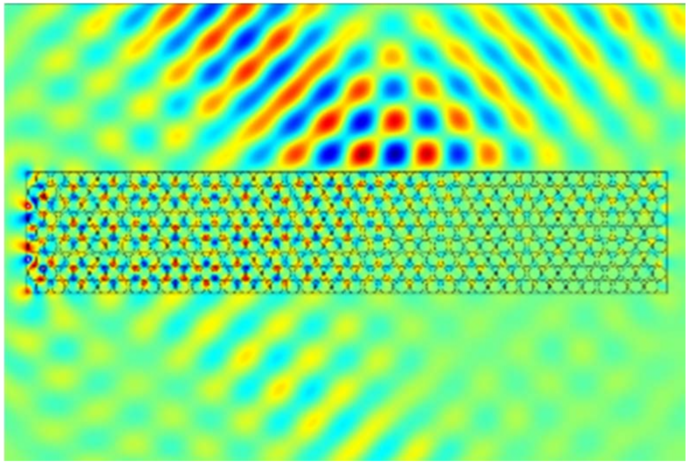
Science 314,997 (2006)

Plasmonic Luneburg Lens



Nano Lett. 10, 1991 (2010)

Negative refraction in PC



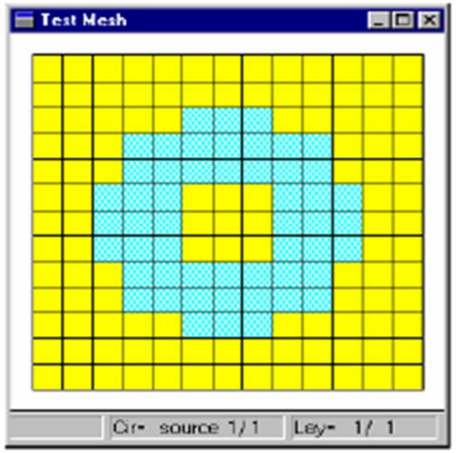
PRL 97,073905(2006)

☐ **FEM Simulation is a powerful tool to design the metamaterial and investigate its properties.**

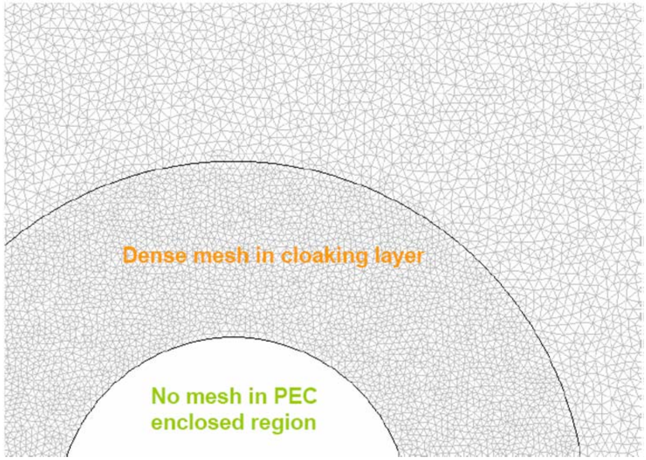
Comparison of FEM and FDTD

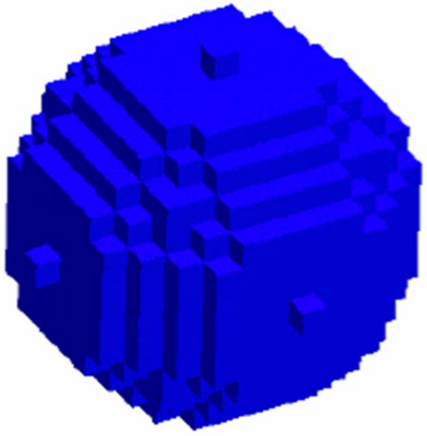
FDTD

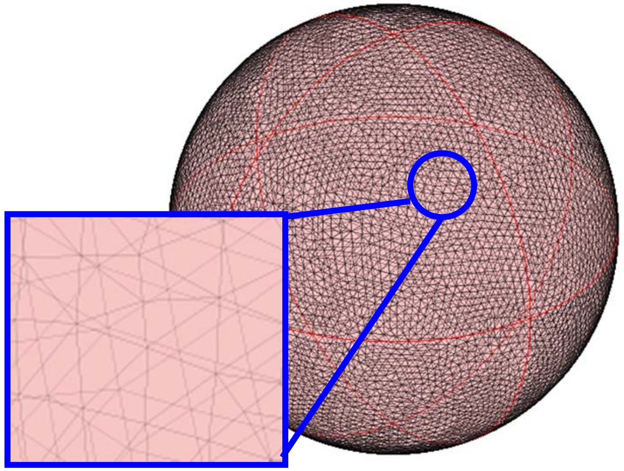
FEM



effect can also be seen in three dime







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

Outlook

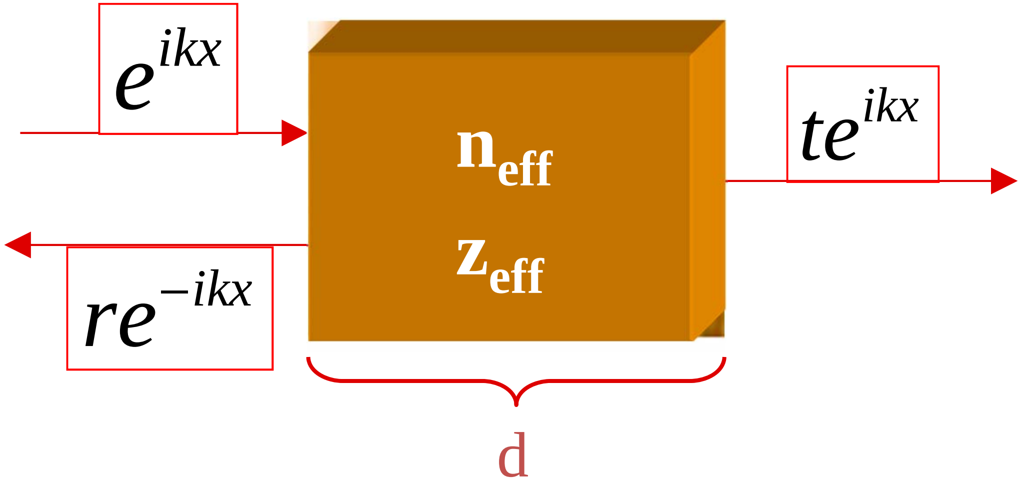
- ☐ Introduction;
- ☐ Our works:
  - Effective-medium properties of metamaterials: A quasi-mode theory;
  - 2D complete band gaps from 1D photonic crystal;
  - Optical microcavities;
- ☐ Conclusions.

Section I

Effective-medium properties of meta-materials: A quasi-mode theory

Ref: Shulin Sun, S. T. Chui, Lei Zhou, Phys. Rev. E 79, 066604 (2009)

[1] How to determine effective-medium properties;



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

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

$$n=\sqrt{\varepsilon}\sqrt{\mu};\, z=\frac{\sqrt{\mu}}{\sqrt{\varepsilon}}$$

$$\varepsilon_{eff} = \frac{n_{eff}}{z_{eff}},\ \mu_{eff} = n_{eff}\, z_{eff}$$

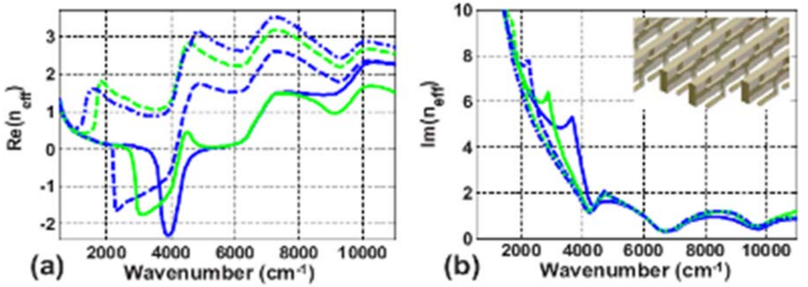
S-Parameter Retrieval Method

[PRB, 65, 195103 (2002)]

[2] Problems in traditional effective-medium method

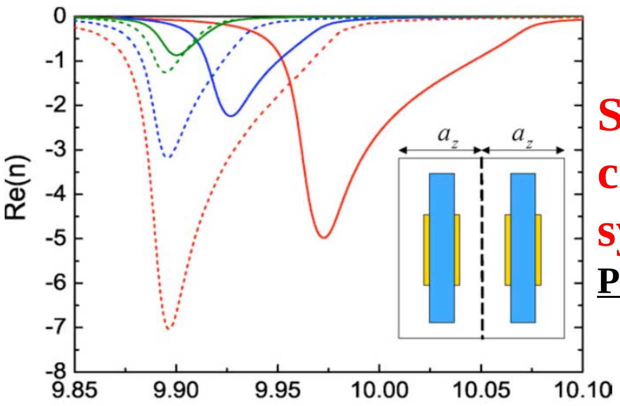
$$n_{eff} = \frac{1}{kd}\cos^{-1}\left(\frac{1}{2t}\left[1-\left(r^2-t^2\right)\right]\right)+\frac{2\pi m}{kd}$$

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



Effective medium changes while unit cell increases

PRB 77, 035126 (2008)

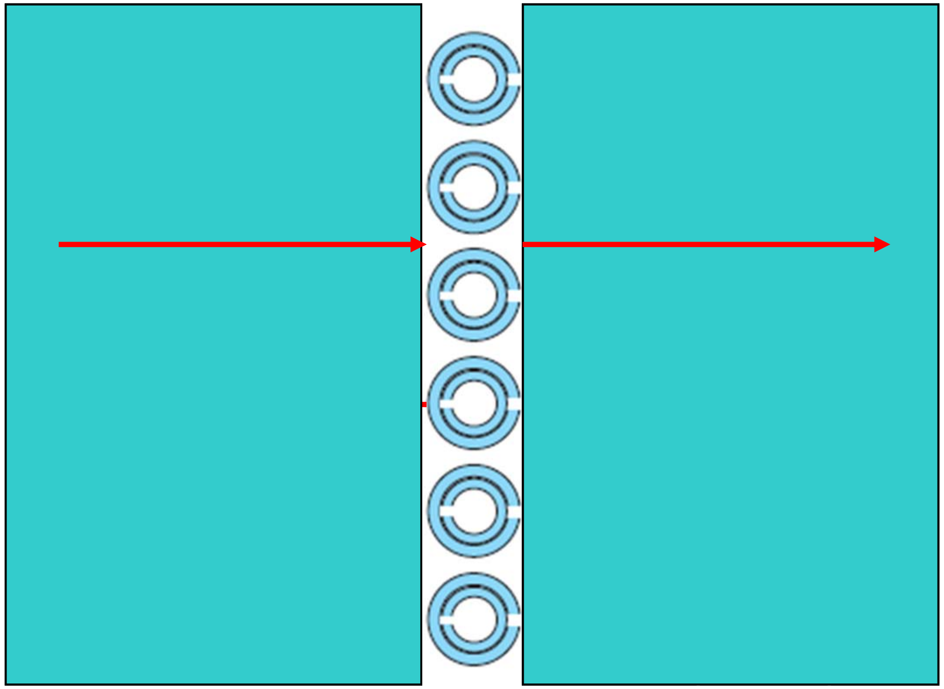


Strong coupling system

PNFA 6,96 (2008)

Quasi-mode Method to determine effective EM properties

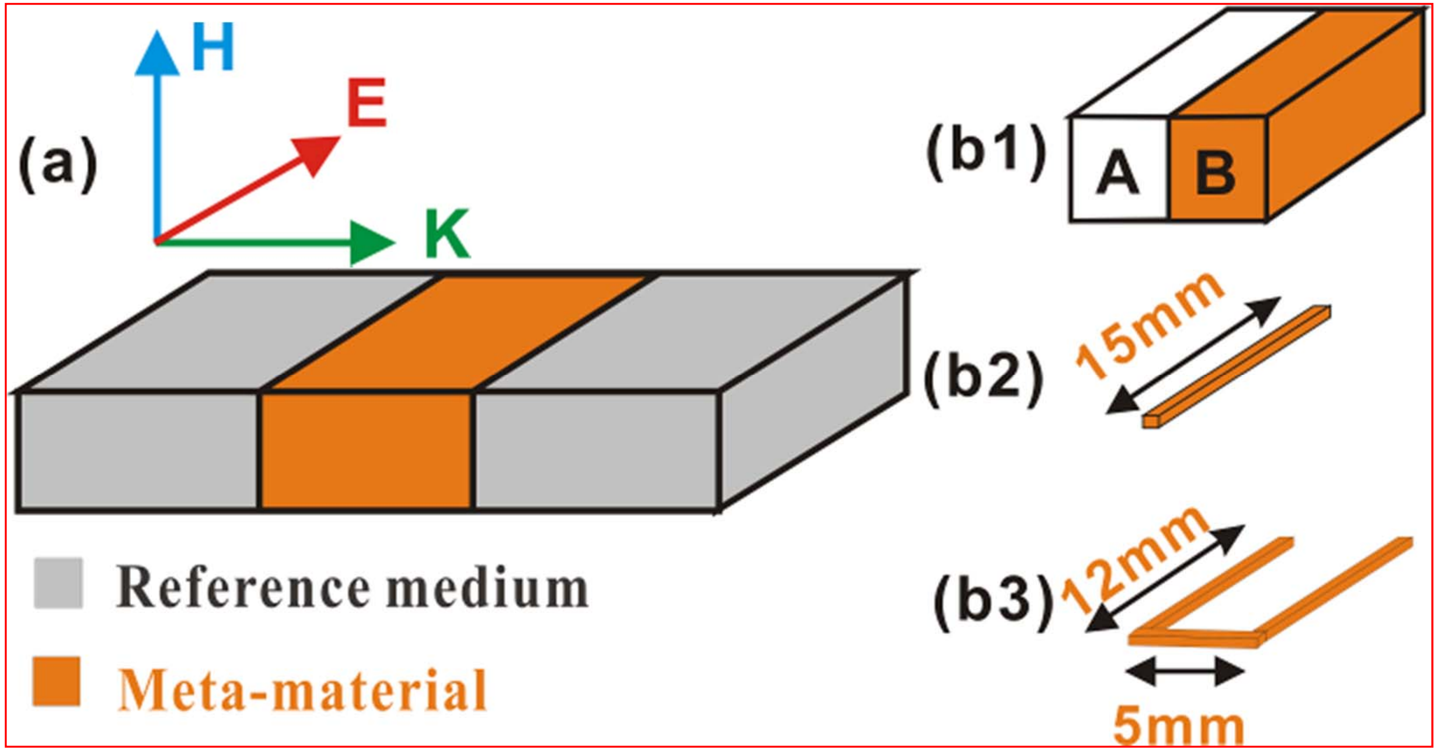
Meta-materials



Vary $\varepsilon_{ref},\mu_{ref}$ → **Scattering loss self-energy** → 0 → $\varepsilon_{eff}=\varepsilon_{ref}$ $\mu_{eff}=\mu_{ref}$

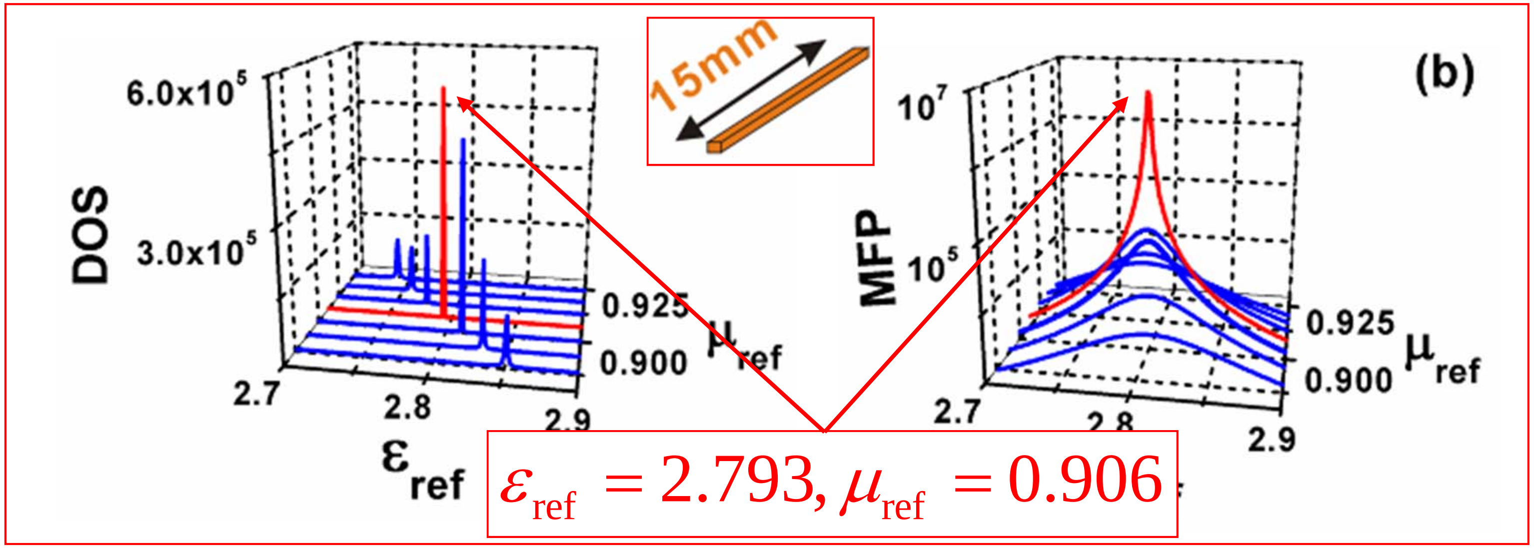
Shulin Sun, S. T. Chui, Lei Zhou, Phys. Rev. E 79, 066604 (2009)

Simulation setup



Cross section of wire: **0.2mm×0.5mm (y×z)**
Lattice constant: **16mm×6mm×7.5mm (x×y×z)**

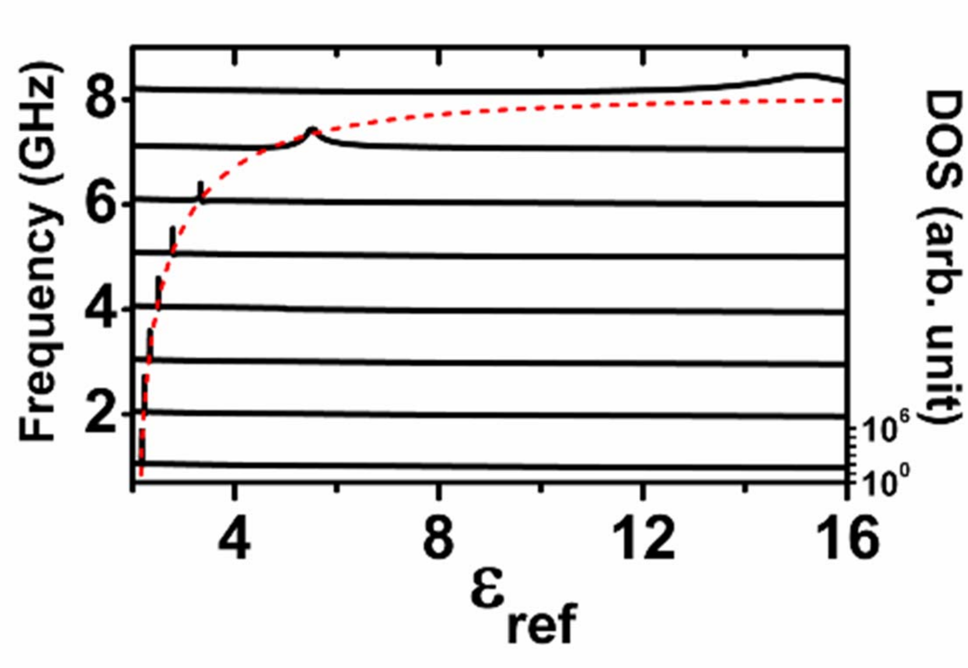
Effective medium properties of metallic wire



$$\varepsilon_{ref} = 2.793, \mu_{ref} = 0.906$$

At a single frequency we tune ε_{ref} and μ_{ref} to search the highest DOS and determine the effective EM properties.

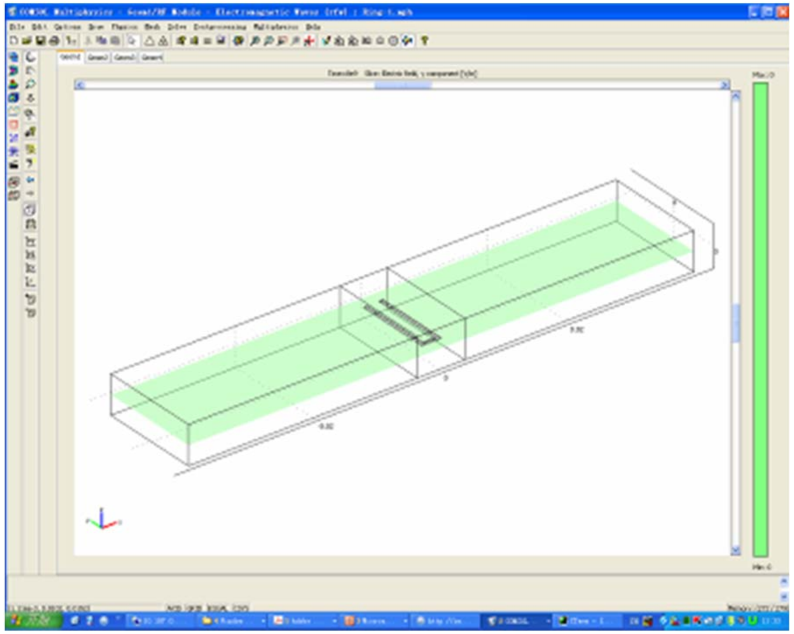
Dispersion of effective permittivityε_{eff}

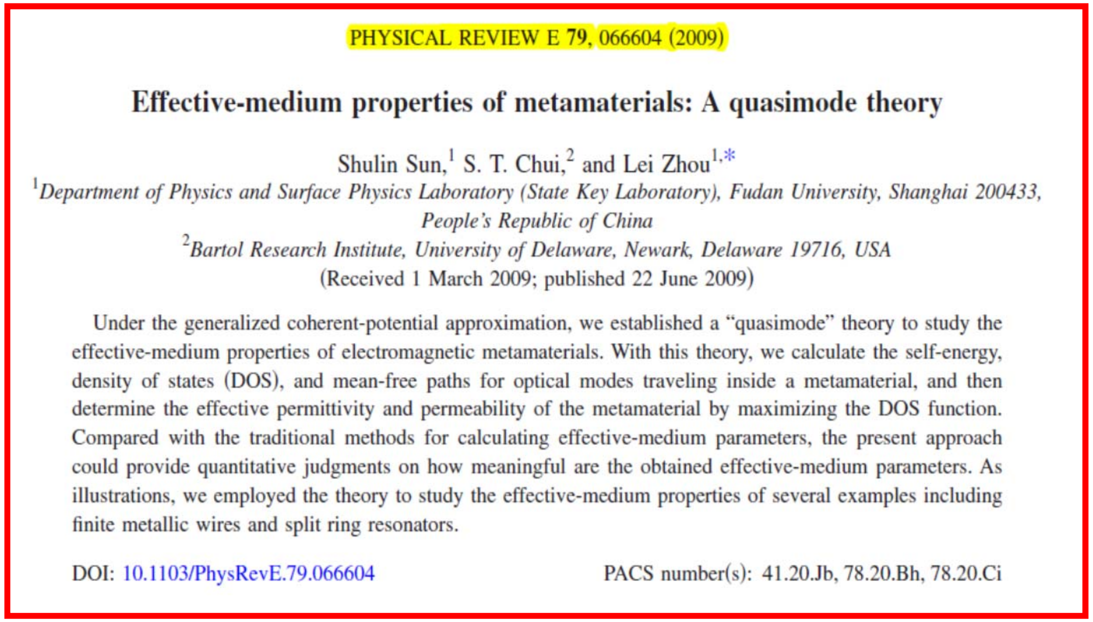


- ➢Peaks of DOS broaden and decrease while frequency increases.

- ➢It means uncertainty range of effective parameters is more and more large that effective medium description gradually breaks down.

Simulation Setup





PHYSICAL REVIEW E **79**, 066604 (2009)

Effective-medium properties of metamaterials: A quasimode theory

Shulin Sun,[1] S. T. Chui,[2] and Lei Zhou[1,*]
[1]*Department of Physics and Surface Physics Laboratory (State Key Laboratory), Fudan University, Shanghai 200433, People's Republic of China*
[2]*Bartol Research Institute, University of Delaware, Newark, Delaware 19716, USA*
(Received 1 March 2009; published 22 June 2009)

Under the generalized coherent-potential approximation, we established a "quasimode" theory to study the effective-medium properties of electromagnetic metamaterials. With this theory, we calculate the self-energy, density of states (DOS), and mean-free paths for optical modes traveling inside a metamaterial, and then determine the effective permittivity and permeability of the metamaterial by maximizing the DOS function. Compared with the traditional methods for calculating effective-medium parameters, the present approach could provide quantitative judgments on how meaningful are the obtained effective-medium parameters. As illustrations, we employed the theory to study the effective-medium properties of several examples including finite metallic wires and split ring resonators.

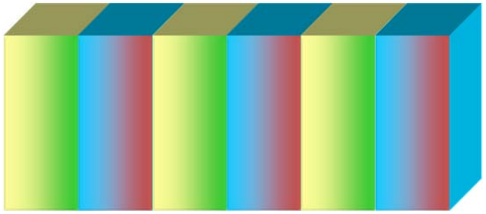
DOI: 10.1103/PhysRevE.79.066604 PACS number(s): 41.20.Jb, 78.20.Bh, 78.20.Ci

- ❖ **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.**

[32] Comsol Multiphysics by COMSOL ©, ver. 3.5, network license (2008).

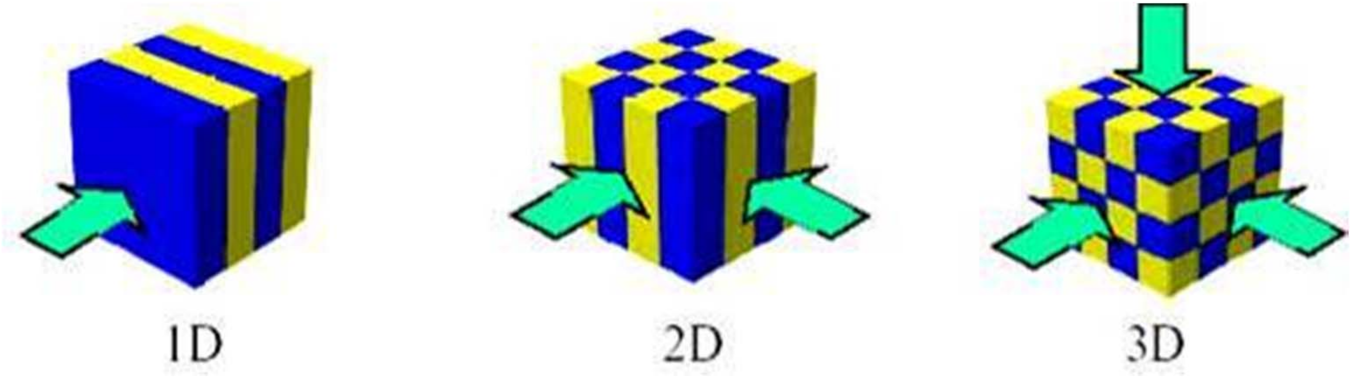
Section Ⅱ

2D complete gaps from 1D photonic crystal



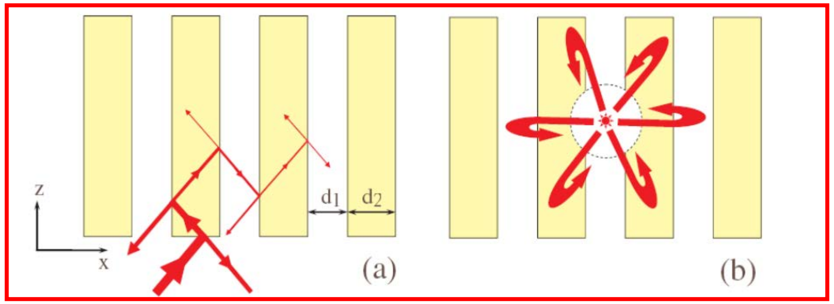
Ref: Shulin Sun, Xueqin Huang, Lei Zhou, Phys. Rev. E 75, 066602 (2007)

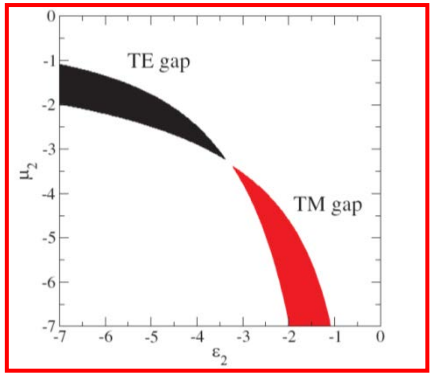
Photonic crystal



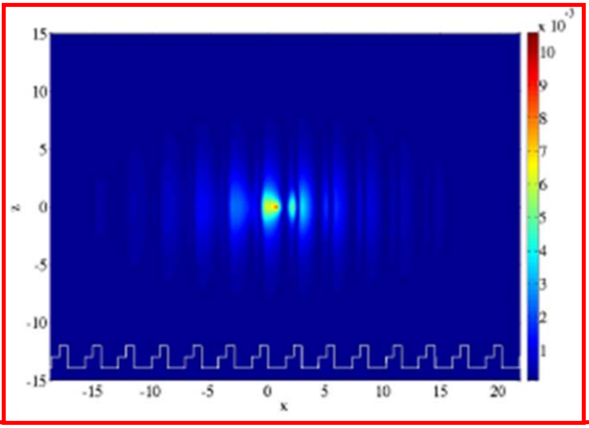
3D Complete Photonic Band Gap (PBG) ⟷ **3D Photonic Crystal**

[3] Complete Gaps in 1D Left-Handed Photonic Crystal





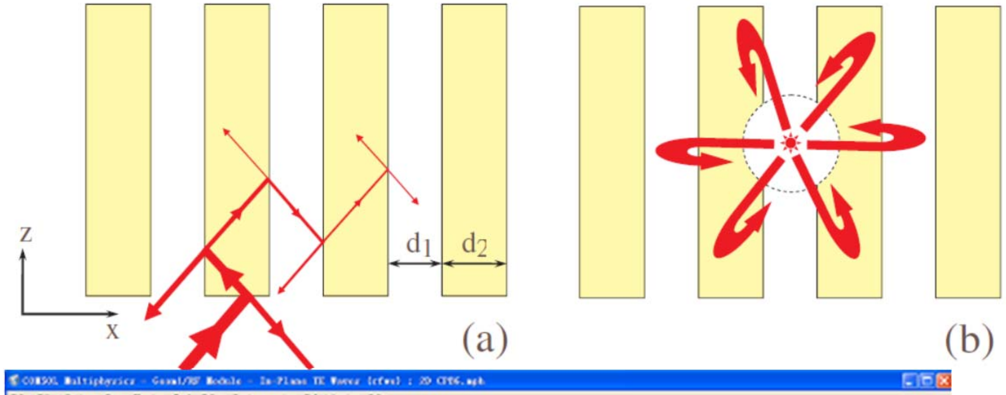
$$\varepsilon_1=1,\mu_1=1,\varepsilon_2=-6,\mu_2=-1.38,d_1=1.5\lambda/2\pi,d_2=1.4\lambda/2\pi$$



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

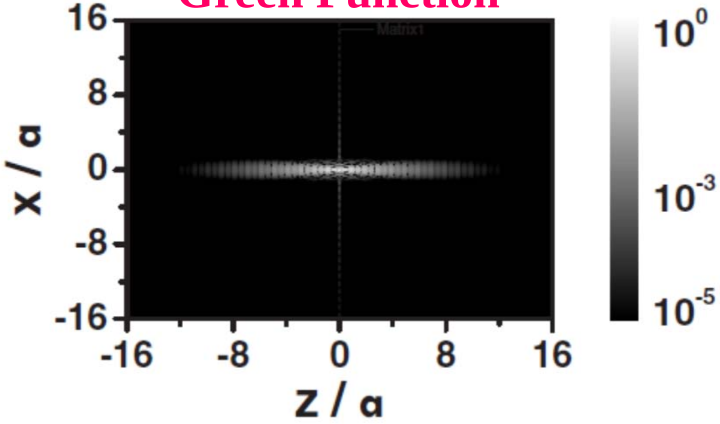
$$\varepsilon_2=\mu_3=-6,\mu_2=\varepsilon_3=-1.38,d_2=d_3=0.7\lambda/2\pi$$

Ilya V. Shadrivov et. al., PRL 95,195903(2005)

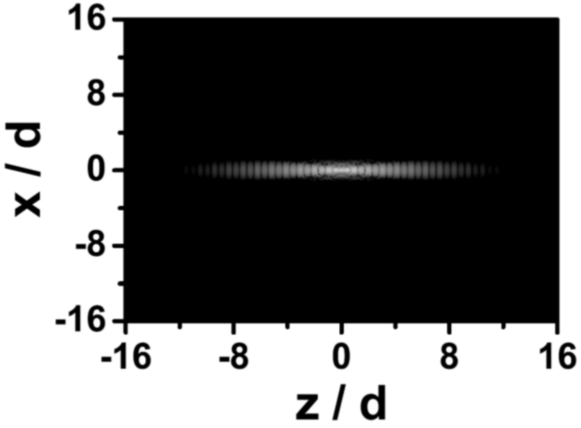


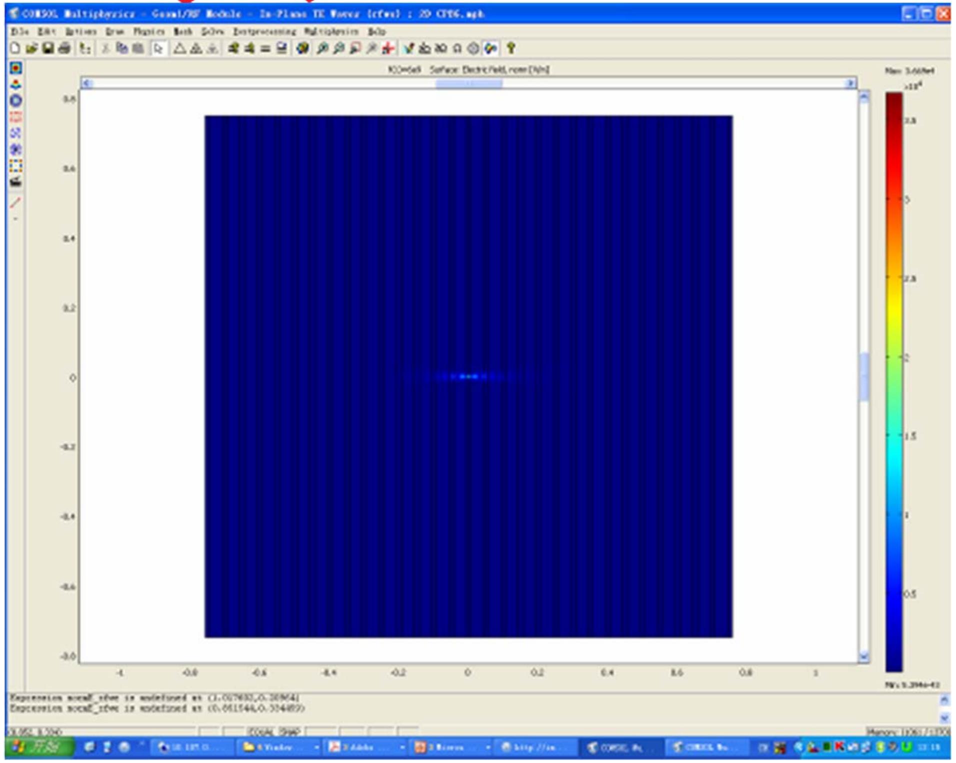
Whether we can confine the light in two or three dimensional space using a one dimensional system?

Green Function



Comsol Simulation





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

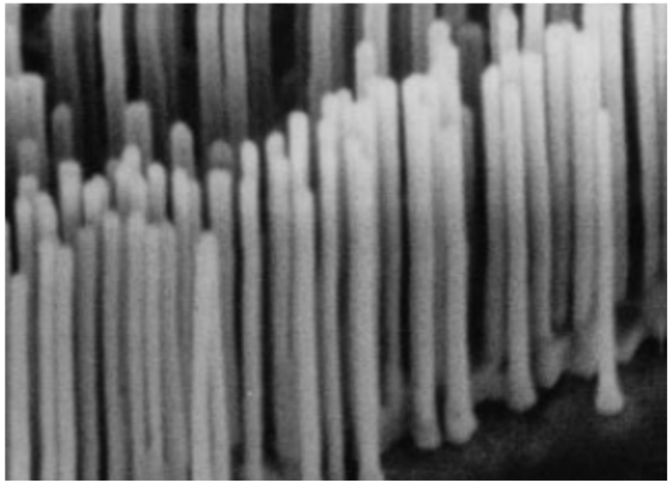
Section Ⅲ

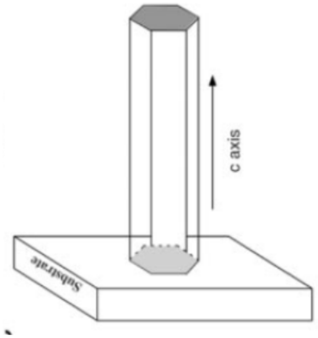
Optical Microcavities

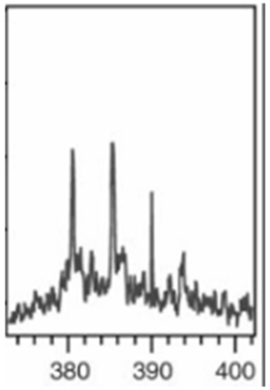
Ref: Hongxing Dong, *et al*., Appl. Phys. Lett. 97, 223114 (2010);
Hongxing Dong, *et al*., Appl. Phys. Lett. 98, 011913 (2011).

Optical Microcavity

Fabry-Pérot microcavity



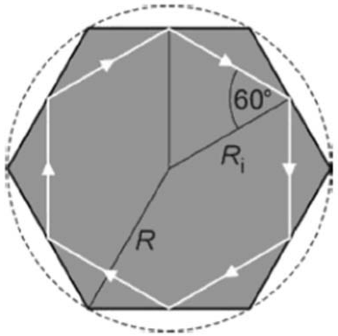


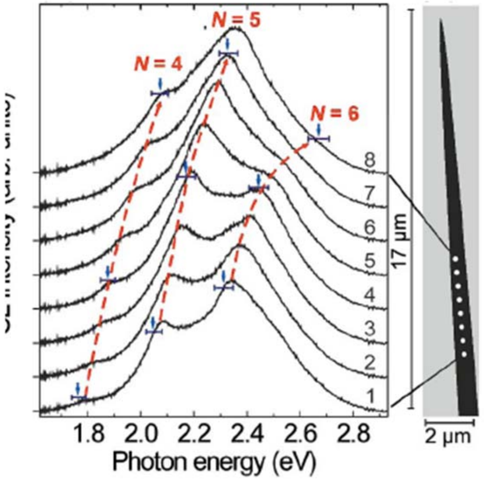


Peidong Yang, *et al.*, Science 292, 1897 (2001)

Whispering gallery microcavity

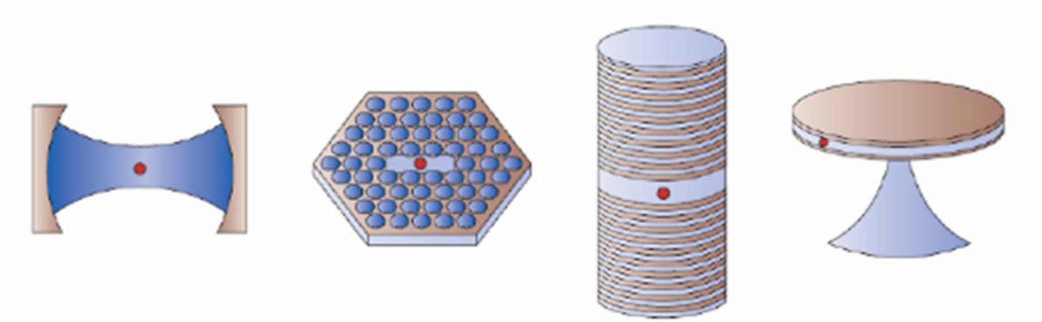
$$6R_i = \frac{hc}{nE}\left[N + \frac{6}{\pi}\arctan(\beta\sqrt{3n^2 - 4})\right].$$





Thomas Nobis, *et al.*, PRL 93,103903 (2004)

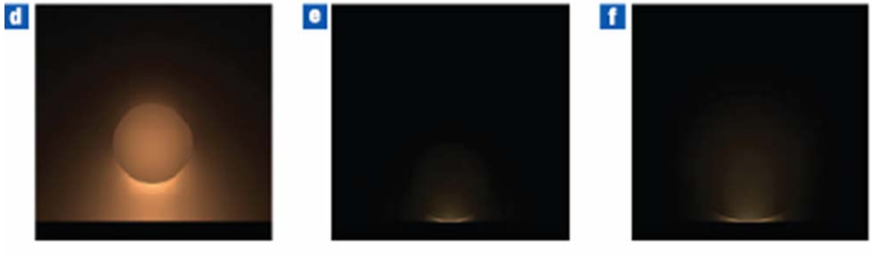
Other kinds of Microcavities

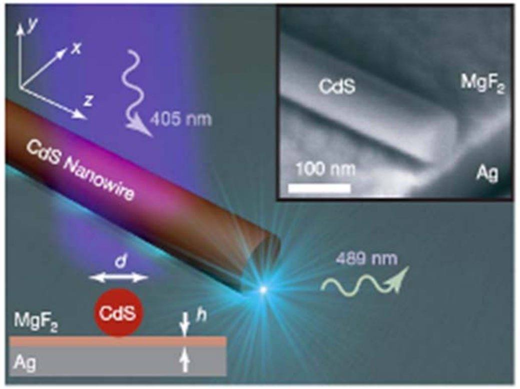


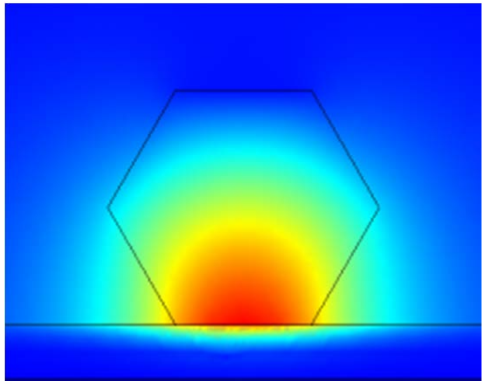
G. Khitrova, *et al.*, Nature Physics 2, 81 (2006)

Plasmonic Laser

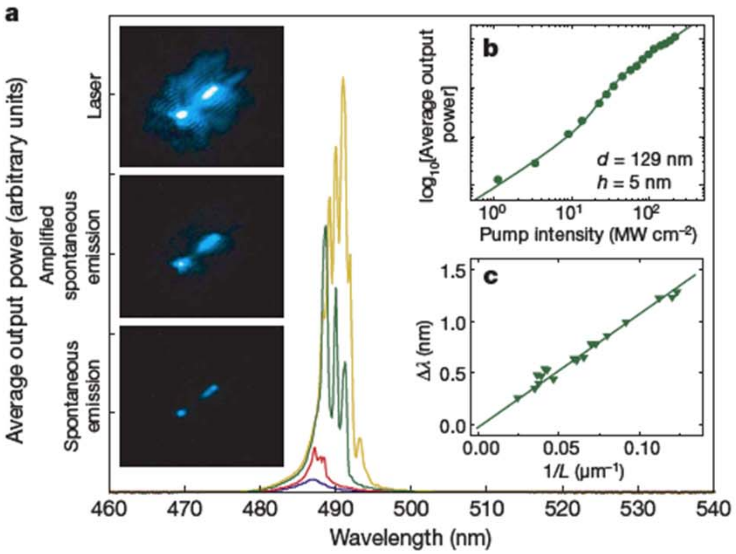
- ☐ **The first experimental demonstration of plasmon laser.**
- ☐ **Small size, hybrid plasmonic waveguide, low loss;**

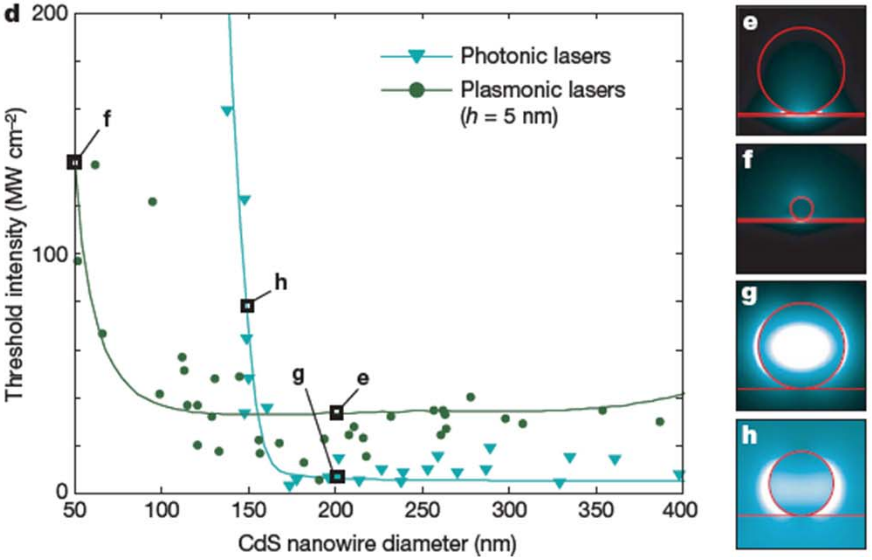






R. F. OULTON, et. al., Natrure photonics. 2,496(2008)



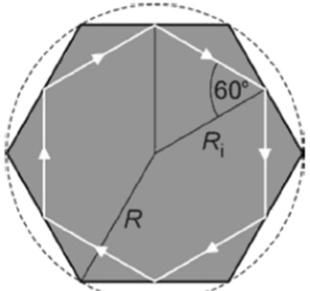


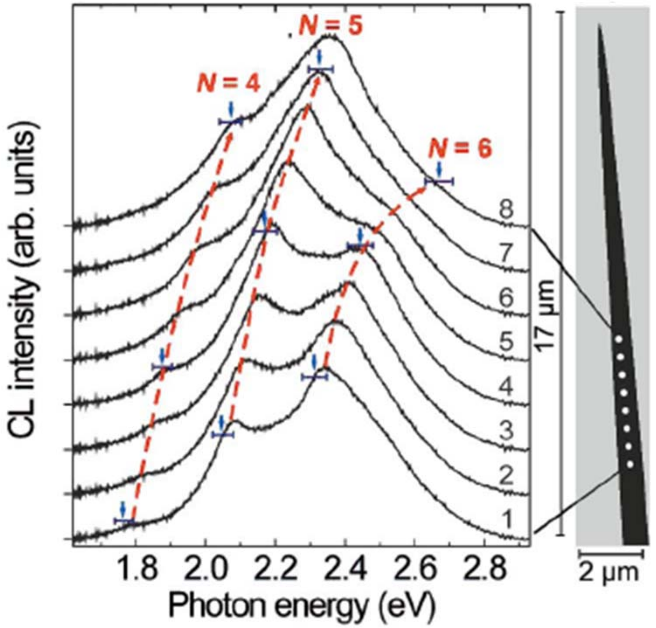
Rupert F. Oulton, et. al., Nature 461, 629 (2009)

Introduction of ZnO Nanowire

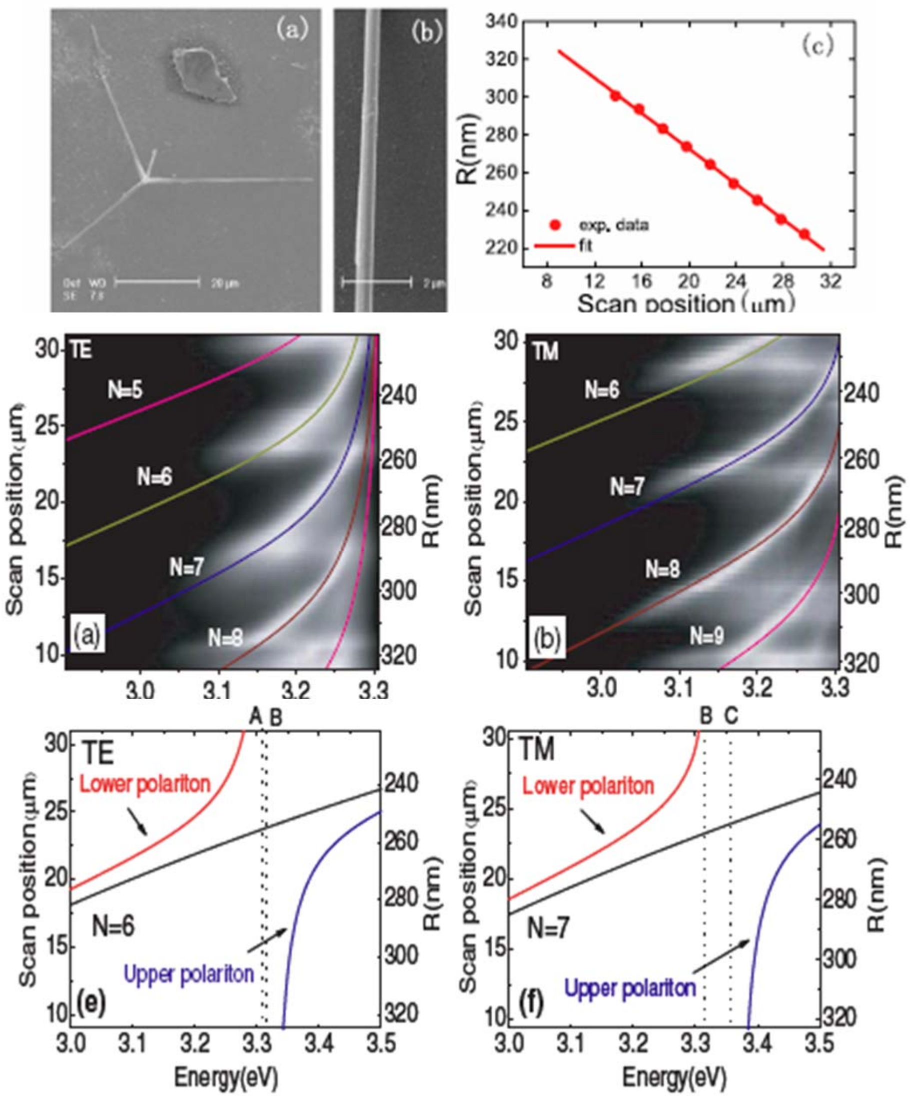
WGM of photon

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





WGM of exciton polariton



Thomas Nobis, *et al.*, PRL 93,103903 (2004) **Liaoxin Sun, et. al., PRL 100, 156403 (2010)**

Indium oxide octahedra optical microcavities

Hongxing Dong, *et al.*, Appl. Phys. Lett. 97, 223114 (2010)

vapor-phase transport method

Indium and oxygen vapor as source materials

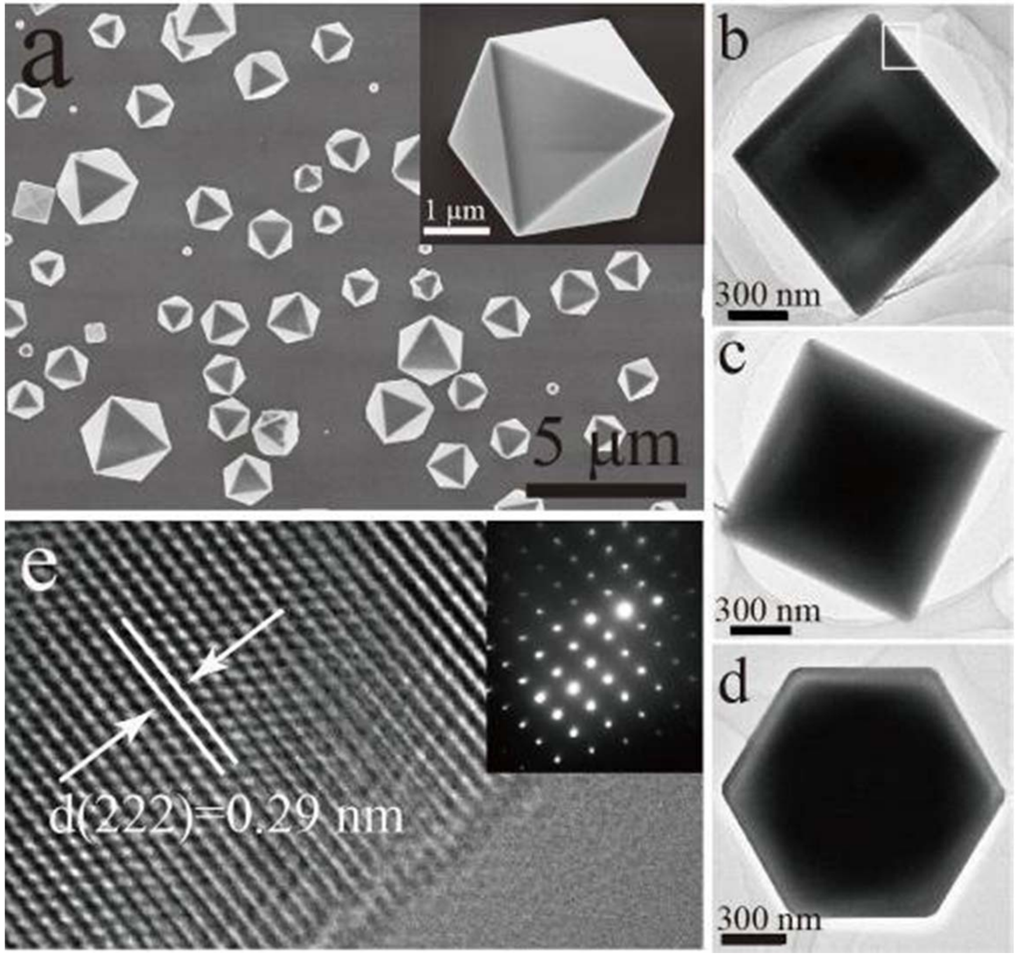
Reaction temperature 950 ℃

$$\xrightarrow{N_2}\xrightarrow[950℃]{O_2}\xrightarrow{N_2} In_2O_3$$

In_2O_3 octahedra are very regular and nearly perfect in shape with sizes ranging from 0.5 to 2.5 μm

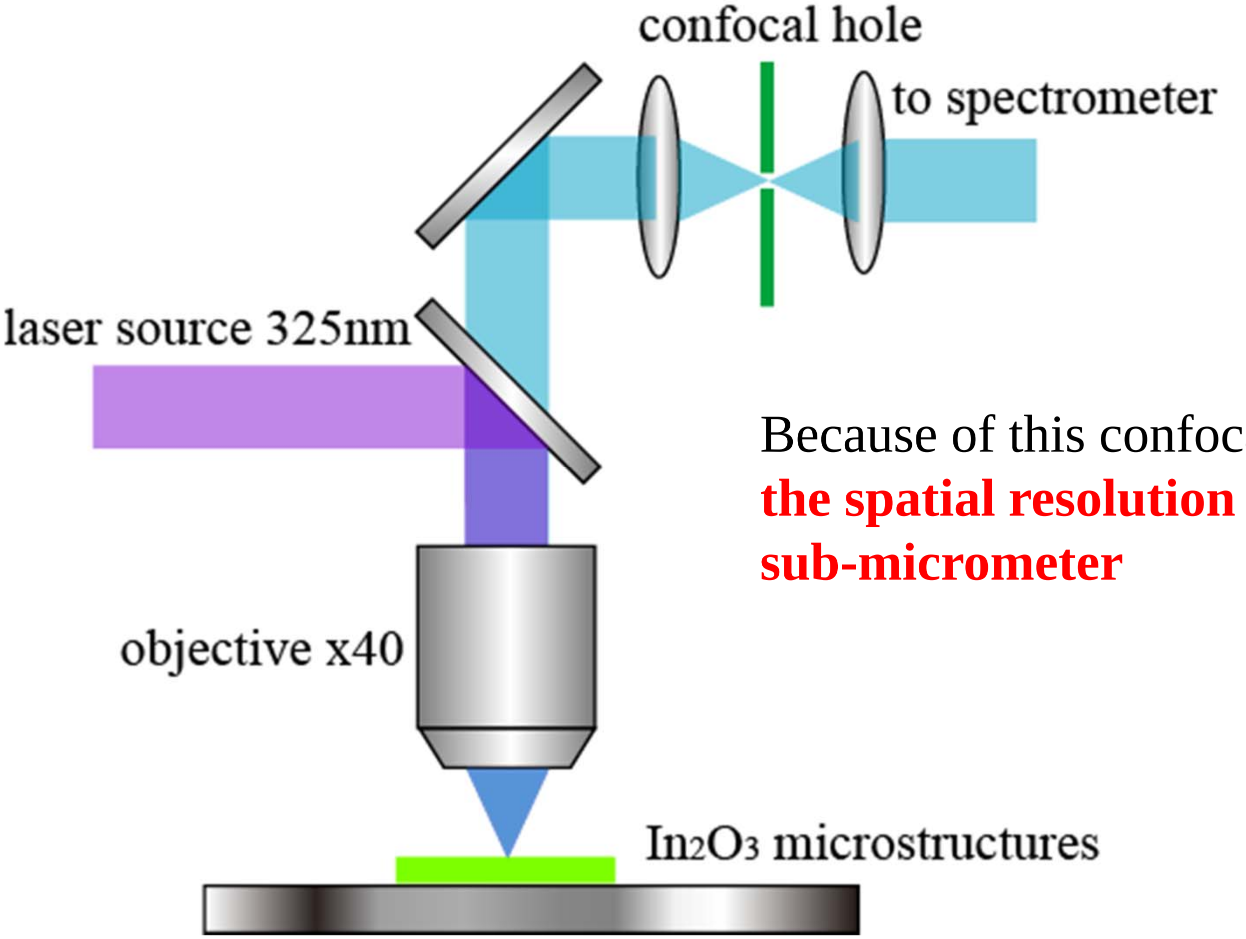
Single-crystalline with BCC lattice

The SEM, TEM and SAED of In_2O_3 octahedrons



<110>, <100>, <111>

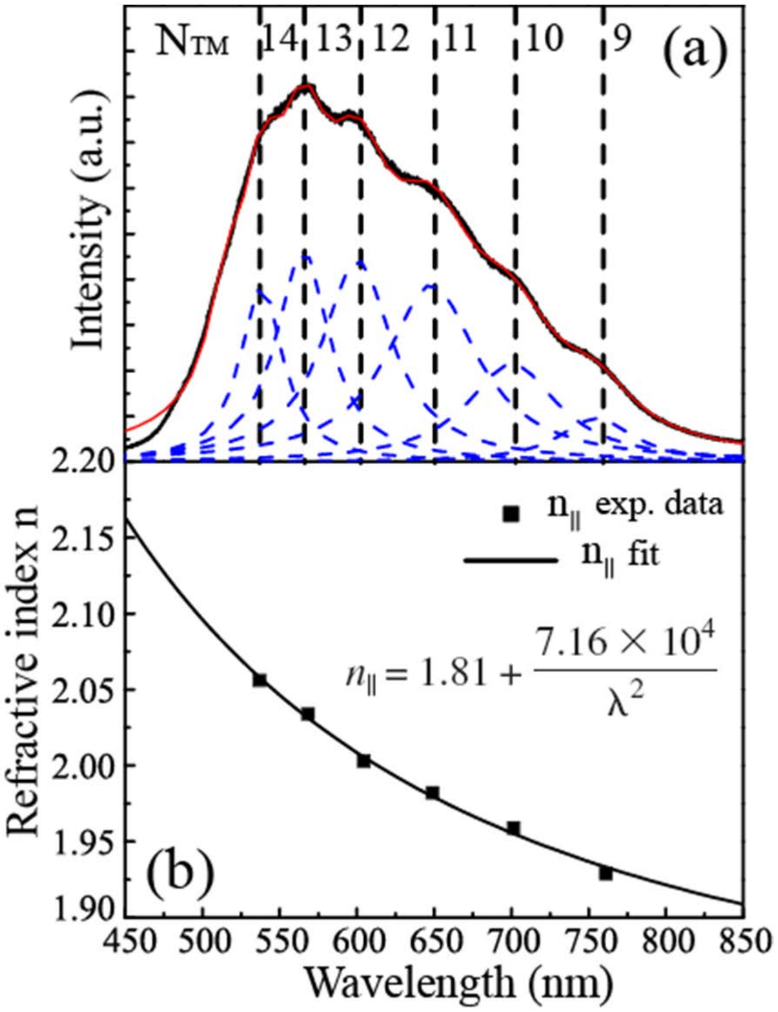
Optical experimental setup



Because of this confocal configuration, **the spatial resolution** can be up to **sub-micrometer**

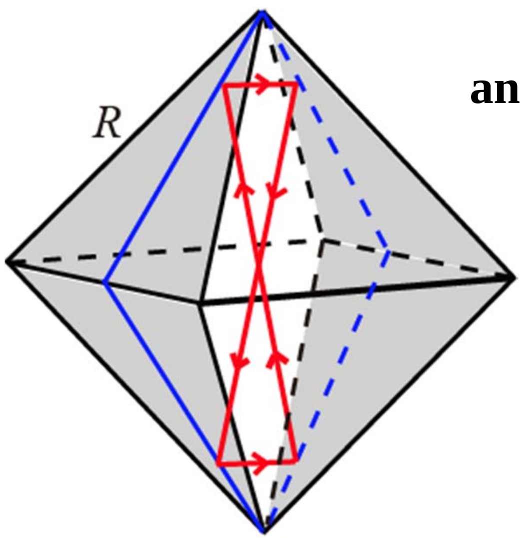
The micro-confocal spectroscopic system diagram.

The photoluminescence (PL) spectrum



Cauchy dispersion formula

Bow-tie like model



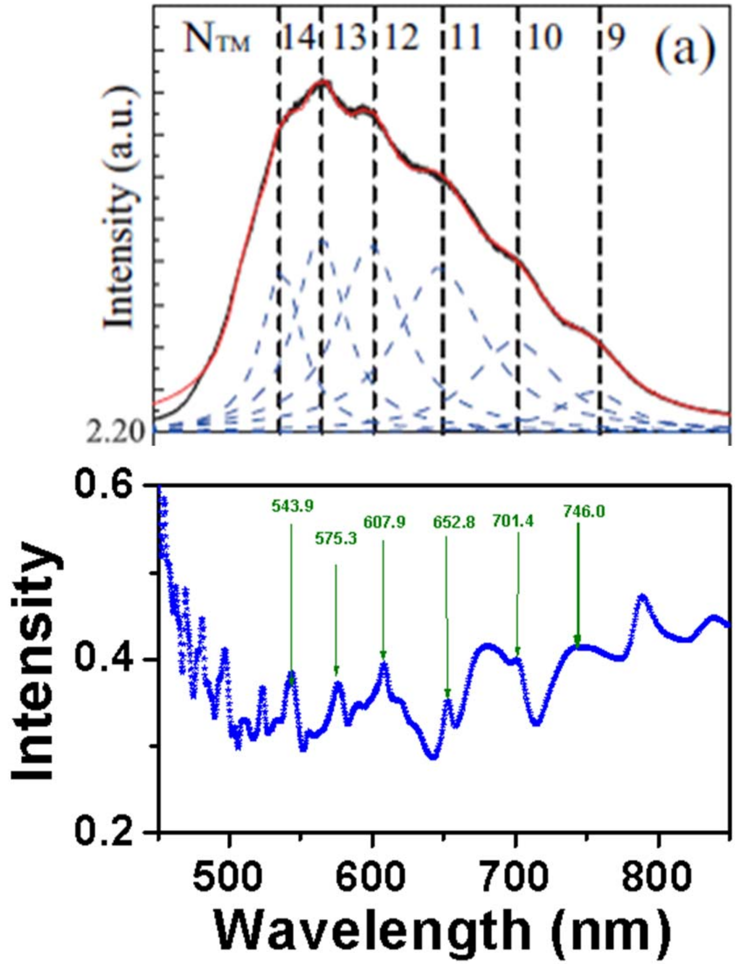
an angle of incidence of 35°

Plane wave model

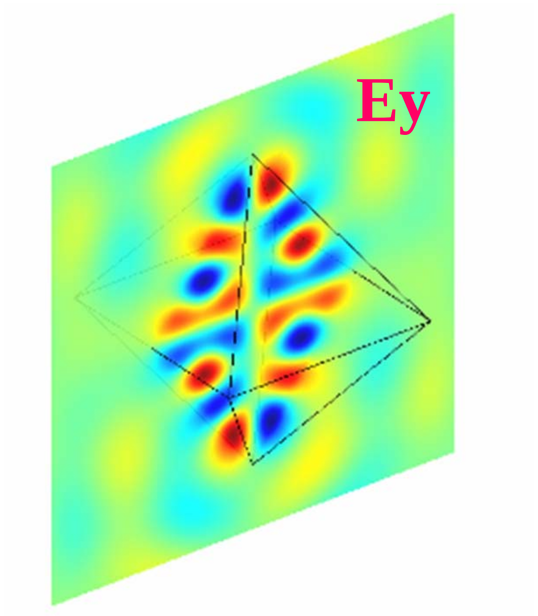
$$R = \frac{3hc}{8nE}\left[N + \frac{4}{\pi}\arctan\left(\beta\sqrt{\frac{n^2-3}{2}}\right)\right]$$

The factor β 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), $\beta = n$.

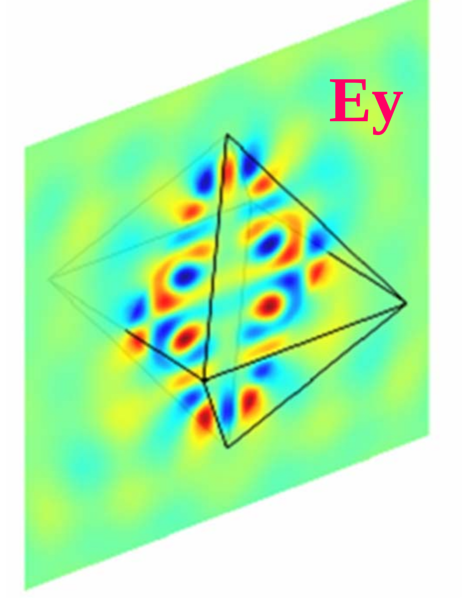
Numerical Simulation



N=9



N=14



☐ **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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  許坤霖, 崔春山, ********