

Modelling approaches for photonic metamaterials

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Main resources

EU-Brochure on *Nanostructured Metamaterials* http://ec.europa.eu/research/industrial_technolo gies/pdf/metamaterials-brochure_en.pdf



EUROPEAN / European / Industrie



Metamaterials handbook (2 volumes), edited by Filippo Capolino, CRC Press, Taylor & Frances

http://www.metamorphose-vi.org



EU project on Electromagnetic Characterization of Nanostructured Metamaterials

http://econam.metamorphose-vi.org

Metamaterials

Artificial, structured (in subwavelength scale) materials

with electromagnetic (EM) properties not-encountered in natural materials

EM properties derive from shape and distribution of constituent units (usually metallic & dielectric, of subwavelength scale)





Possibility to engineer electromagnetic properties

Interesting metamaterial regimes



Modelling approaches

- •Rigorous approaches (detailed numerical techniques, e.g. FDTD, BEM, TMM,..)
 - Input: Maxwell equations + detailed geometrical structure + material parameters of components Output: transmission/reflection, dispersion relation, electromagnetic fields, ... •RLC circuit modeling
- Homogenization (homogeneous effe approaches: Search for the equivalent homogeneous medium (ε, μ, κ, ...) with the same response as our metamaterial
 - Direct approaches (first principle approaches): From microscopic quantities to macroscopic through averaging
 Inverse (heuristic) approaches: From reflection/transmission to material parameters through inversion

Modelling approaches

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Homogenization (homogeneous effective medium)
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Modelling essentials

Maxwell's equations - determine the propagation of EM waves
Constitutive relations in the constituent media (metals + dielectrics) – represent the electromagnetic response of each material

$$\mathbf{D}(\mathbf{r}) = \varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r}) \qquad \mathbf{B}(\mathbf{r}) = \mu_0 \mathbf{H}(\mathbf{r})$$

- →Structure geometry
- Boundary conditions
- •Excitations (if any)



Maxwell's equations in matter



$$\mathbf{D} = \varepsilon \mathbf{E} = \varepsilon_0 \mathbf{E} + \mathbf{P}$$

$$\mathbf{J} = \boldsymbol{\sigma} \mathbf{E} = \frac{\partial \mathbf{P}}{\partial t}$$

$$\varepsilon = \varepsilon_0 + i \frac{\sigma}{\omega}$$







Ampere's law

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

Rigorous modelling techniques



Many free and commercial software packages – see Wikipedia

Finite Difference Time Domain (FDTD) Method

Treats: mainly finite systems along propagation direction Calculates: transmission, reflection, fields in time and frequency domain

Approach: Discretization of time-dependent Maxwell's equations in both space and time (1D-3D)

$$\mathbf{H}_{i,j}^{n} = \mathbf{H}(i\Delta x, j\Delta y, n\Delta t)$$

$$\mathbf{E}_{i,j}^{n} = \mathbf{E}[(i+1/2)\Delta x, (j+1/2)\Delta y, (n+1/2)\Delta t]$$

Maxwell's equations → algebraic difference equations

 $\mathbf{H}(t + \Delta t / 2) = \operatorname{Function}(\mathbf{E}(t), \mathbf{H}(t - \Delta t / 2))$

 $\mathbf{E}(t + \Delta t) = \operatorname{Function}(\mathbf{E}(t), \mathbf{H}(t + \Delta t / 2))$



 $\mathbf{H}(\boldsymbol{\omega}) = \mathrm{FFT}(\mathbf{H}(t))$

Yee's scheme

E(t), H(t) $E(\omega) = FFT(E(t))$

Finite Difference Time Domain (FDTD) Method (2)

Problem for dispersive materials

 $\mathbf{D}(t) \neq \mathcal{E}(t) \mathbf{E}(t)$

Constitutive relations should be discretized taking into account explicit dispersion model

Additional equations are required

Advantages of FDTD

- •With one computation →multifrequency study
- •Treats both random and periodic media
- •Treats almost arbitrary geometries
- •Not heavy computational memory requirements





Finite element method (1D-3D)

From Yinun Liu, Univ. of Cincinnati

Treats mainly finite systems but also infinite **Calculates** transmission, reflection, fields in time and frequency domain, dispersion relation

Approach: Reformulates harmonic Maxwell's equations + boundary conditions → weak form

Procedure:

- Divides structure into pieces (elements with nodes)
- Connect (assemble) the elements at the nodes to form an approximate system of equations for the whole structure
- Solve the system of equations involving unknown quantities (fields) at the nodes→ matrix inversion

Advantages

•Treats arbitrary geometries and materials

W. B. J. Zimmerman, Process Modelling and Simulation with Finite Element Methods (World Scientific, Singapore, 2004). J. Jin, The Finite Element Method in Electromagnetics (John Wiley & Sons, Inc., New York, 2002).





Commercial packages: FEMLAB CST

Disadvantages

•Not easy implementation

Multiple scattering method

Treats: Both infinite and finite (not very large) systems; both periodic and random systems

Calculates: Band structure (ω vs k), equifrequency contours, transmission/reflection, fields



Main idea: Incident wave at each scatterer = external field + scatteredwave from all the other scatterersYannopapas. Stefanou.

Yannopapas, Stefanou, Moroz, Chan, Sheng, ...

Procedure: Waves are expanded in vector spherical harmonics; final equation is a non-linear algebraic system (for eigenmodes) or a linear algebraic system (for finite slabs)

Variation: Layered Multiple Scattering Method Disadvantages

- •Heavy algebra
- •Treatment of simple-shaped scatterers only

Boundary Element Method (BEM) or Method of Moments (MoM)

Treats: Clusters of arbitrarily-shaped particles (good for particles with small surface to volume ratio)

Calculates: Scattering cross-sections, fields, density of states

Procedure: Discretizes only the boundaries, expresses the fields vs potentials, potentials vs Green's functions, requires continuity of potentials and parallel fields

Disadvantage: Produces dense matrices (→ suitable for small systems)

De Abajo, Craeye, Cappolino, ...

F. J. García de Abajo and A. Howie, Phys. Rev. B, 65, p. 115418, 2002



Parallel k



Courtesy of V. Myrosnichenko

Transfer Matrix Method (1D-3D)

Treats: Finite slabs along propagation direction; both periodic and random systems

Calculates: transmission/reflection, fields (in frequency domain)



Procedure: Divides the space in layers. Calculates transfer matrix for each layer $\vec{\mathbf{T}}_{slab} = \prod \vec{\mathbf{T}}_k$ $\begin{pmatrix} E^{k+1} \\ H^{k+1} \end{pmatrix} = \mathbf{\ddot{T}}_k \begin{pmatrix} E^k \\ H^k \end{pmatrix}$

Pendry, Bell, Transfer matrix techniques for EM waves, Photonic Band Gap Materials, 1996



Peter Markoš • Costas M. Soukouli

Fourier Modal Method or Rigorous Coupled Wave Analysis (2D-3D)

Treats: Both infinite and finite (in 1D) slabs

Calculates: Band structure (ω vs k), equifrequency contours, transmission/reflection, fields in frequency domain (sum of Bloch modes)

Main idea: All EM quantities are expanded in Fourier series \rightarrow Eigenmode problem calculating ω for each k

Procedure applied to planar metamaterials: Brakes system into layers, calculates the eigenmodes of a ^z ← single layer (2D problem) for a given ω, k_{//}



P. Lalanne, F. Lederer, G. Shvets, ...

L. Li, "New formulation of the Fourier modal method for crossed surface-relief gratings," J. Opt. Soc. Am. A 14, 2758 (1997).

From Thomas Paul thesis, Univ. of Jena

Modelling approaches

 Rigorous approaches (detailed numerical techniques, e.g. FDTD, BEM, TMM,..) Input: Maxwell equations + detailed geometrical structure + material parameters of components
 Output: transmission/reflection, dispersion relation electromagnetic fields, ...
 RLC circuit modeling Mixing rules

Homogenization (homogeneous effective medium)
approaches: Search for the equivalent homogeneous medium
(ε, μ, κ, ...) with the same response as our metamaterial

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Why homogenization?

- Offers simple and physical picture of the metamaterial response (connects the response to few, well known material parameters)
- Predicts the metamaterial response under different conditions (excitation, environment, total size)
- Offers path to metamaterial optimization and design rules
- Predicts phenomena connected with the metamaterial
- Reveals potential applications/uses of the metamaterial

Typical forms of metamaterial parameters



Artificial electric metamaterials

Artificial magnetic metamaterials

Donzelli et al, Metamaterials 3 (2009)

Questions on homogenization



- How many effective parameters are needed to characterize the metamaterial? → metamaterials classification
- Under what conditions a metamaterial can be homogenizable?
- Under what conditions effective medium parameters can be considered characteristic metamaterial parameters?

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Metamaterial classification

For linear, *homogenizable*, metamaterials (in frequency domain)

Isotropic	Anisotropic
$\mathbf{D} = \boldsymbol{\varepsilon} \mathbf{E}$	$\mathbf{D} = \vec{\varepsilon} \mathbf{E}$
$\mathbf{B} = \boldsymbol{\mu} \mathbf{H}$	$\mathbf{B} = \ddot{\mu}\mathbf{H}$
2-parameters	18-parameters
Bi-isotropic	Bi-anisotropic
$\Box = \varepsilon \mathbf{E} + \xi \mathbf{H}$	$\mathbf{D} = \vec{\varepsilon}\mathbf{E} + \vec{\xi}\mathbf{H}$
$\mathbf{B} = \boldsymbol{\zeta} \mathbf{E} + \boldsymbol{\mu} \mathbf{H}$	$\mathbf{B} = \vec{\zeta} \mathbf{E} + \vec{\mu} \mathbf{H}$
4-parameters For reci exchange	procal media (system properties do not change by ging source and receiver position) $\vec{\varepsilon} = \vec{\varepsilon}^T, \vec{\mu} = \vec{\mu}^T, \vec{\xi} = -\vec{\zeta}^T$
Greek: isos=equal, tropos=way, i.e. isotropic=behave in equal way for all directions	

Subclasses of bi-isotropic media: Chiral

<u>Chiral media</u> (no identical with their mirror images)

- $\mathbf{D} = \boldsymbol{\varepsilon} \mathbf{E} + i\boldsymbol{\kappa} \mathbf{H}$
- $\mathbf{B} = -i\kappa\mathbf{E} + \mu\mathbf{H}$

$$n_{\pm} = \sqrt{\varepsilon\mu} \pm \kappa$$



e.g. DNA

κ=Chirality parameter

Greek: chira=hand

•Different index for left- and right-handed circularly polarized waves (circular birefringence)

handed

- •Negative index possibility
- •Optical activity (polarization rotation of a linearly polarized wave)
- •Circular dichroism (different absorption for left and right circularly polarized light)

Zheludev, Pendry, Tretyakov, Soukoulis, Wegener, Giessen, Shalaev, ...

Subclasses of anisotropic media: Uniaxial

Uniaxial media

$$\vec{\varepsilon} = \begin{pmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$

Birefringence: Different index for polarization along *z* and perpendicularly to *z*

Light polarized along the optic axis is called the extraordinary ray, and light polarized perpendicular to it is called the ordinary ray

Important example: hyperbolic dispersion relation metamaterials → **Hyperlensing, large DOS**

Narimanov, Engheta, Shalaev, Smolyaninov, Zhang, ...

Effective parameters dispersion

Temporal dispersion

1

$$\mathbf{D}(\mathbf{r},t) = \int_{0}^{t} \varepsilon_{eff}(\mathbf{r},t-t') \mathbf{E}(\mathbf{r},t') dt'$$

$$\blacktriangleright \mathcal{E}_{eff} = \mathcal{E}_{eff}(\omega)$$

Spatial dispersion?

Due to the not very small size/wavelength ratio

$$\mathbf{D}(\mathbf{r},t) = \int_{0}^{r} \varepsilon_{eff}(\mathbf{r},\mathbf{r}',t) \mathbf{E}(\mathbf{r}',t) d\mathbf{r}'$$

Response is not local in space

$$\boldsymbol{\varepsilon}_{eff} = \boldsymbol{\varepsilon}_{eff}(\mathbf{k})$$

Boundary conditions are not fulfilled Strong spatial dispersion is detrimental for homogenization

Artificial magnetism, chirality and weak spatial dispersion Silveirinha, Phys. Rev. B 75, 115104 (2007)

Tretyakov, EU-brochure

Equivalent descriptions for weak spatial dispersion

$$\mathbf{D} = \varepsilon(\mathbf{k})\mathbf{E}$$

$$\mathbf{B} = \mu_0 \mathbf{H}$$

$$\mathbf{B} = \zeta \mathbf{E} + \xi \mathbf{H}$$

$$\mathbf{B} = \zeta \mathbf{E} + \mu \mathbf{H}$$
Taylor expansion
$$\mathbf{D} = \varepsilon \mathbf{E} + a\mathbf{k} \times \mathbf{E} + \beta \mathbf{k} (\mathbf{k} \cdot \mathbf{E}) + \gamma \mathbf{k} \times (\mathbf{k} \times \mathbf{E})$$

$$\mathbf{D} = \varepsilon \mathbf{E} + a \nabla \times \mathbf{E} + \beta \nabla \nabla \cdot \mathbf{E} + \gamma \nabla \times \nabla \times \mathbf{E}$$

$$\mathbf{D} = \varepsilon \mathbf{E} + a \nabla \times \mathbf{E} + \beta \nabla \nabla \cdot \mathbf{E} + \gamma \nabla \times \nabla \times \mathbf{E}$$

$$\mathbf{Chirality term}$$

$$\mathbf{B} \sim \nabla \times \mathbf{E} / \omega$$
Artificial magnetism

Artfical magnetism and metamaterial chirality are results of weak spatial dispersion

Maxwell eqs invariant for

 $\mathbf{D}' = \mathbf{D} + \nabla \times \mathbf{Q}$ $\mathbf{H}' = \mathbf{H} - i\omega \mathbf{Q}$

Questions on homogenization



• How many effective parameters are needed to characterize the metamaterial? → metamaterials classification

• Under what conditions a metamaterial can be homogenizable?

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Conditions for homogenization

The metamaterial equifrequency surfaces should be either ellipsoids or hyperboloids



-2

-2 -1

kra

The condition is fulfilled in the limit

$$q_{eff} = \frac{\omega}{c} n_{eff} < \frac{\pi}{a} \rightarrow \lambda_{eff} = \frac{\lambda_0}{n_{eff}} > 2a$$

For resonant structures this may require $q_0 a \ll 1 \Rightarrow \lambda_0 \gg a$

For most of today's metamaterials $\lambda_0 < 10a$ Validity of effective parameters is questionable or limited

Questions on homogenization



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Effective parameters restrictions

Parameters should obey

$$\mathbf{D} = \varepsilon \mathbf{E} = \varepsilon_0 \mathbf{E} + \mathbf{P}$$
$$\mathbf{B} = \mu \mathbf{H}$$

Causality: (cause precedes the effect) Polarization P(t) depends on electric field E(t'<t)

$$\frac{\partial(\omega\varepsilon)}{\partial\omega} \ge 1 \qquad \frac{\partial(\omega\mu)}{\partial\omega} \ge 1$$

For low-loss ε , μ , n should be increasing functions of frequency

Passivity: Energy does not grow

 $\operatorname{Im}(\varepsilon) > 0, \operatorname{Im}(\mu) > 0$

$$\operatorname{Re}(z) = \operatorname{Re}(\sqrt{\mu / \varepsilon}) > 0$$

 $\operatorname{Im}(n) = \operatorname{Im}(\sqrt{\mu\varepsilon}) > 0$

Effective parameters requirements

To be considered as characteristic bulk continuous medium parameters effective parameters should be $\mathbf{D} = \vec{\varepsilon}\mathbf{E} + \vec{\xi}\mathbf{H}$ $\mathbf{B} = \vec{\zeta}\mathbf{E} + \vec{\mu}\mathbf{H}$

- Independent of system thickness
- Independent of direction of propagation
- +
- Fulfilling the causality and passivity requirements

If no, applicability of parameters is restricted (e.g. to the specific excitation conditions)

Homogenization approaches

Direct approaches: From microscopic quantities (or fields) to macroscopic through "averaging" → material parameters



Heuristic (inverse) approaches: From reflection/transmission (propagated wave features) to material parameters through inversion → wave parameters

From microscopic to macroscopic quantities



Approach: Consideration of the metamaterial as collection of electric and/or magnetic dipoles

 $p.vs.E_{loc} \rightarrow P.vs. < E >$ $m.vs.B_{loc} \rightarrow M.vs. < B >$

Problem: Calculate P vs <E> and M vs

p.vs.E_{loc} or m.vs.B_{loc} by simple EM formulas C. Simovski, J. Optics 13, 013001 (2011) RLC circuit formulas

Averaging Maxwell equations

Smith & Pendry, J. Opt. Soc. Am. B 23, 391 (2006)



Other approaches: Silveirinha, Alu, Shvets, ...

Homogenization through S-parameter inversion (1)

T and R of a homogeneous slab

Nicholson-Ross-Weir (NRW) method

$$E_{0}e^{ikx}$$

$$E_{0}e^{ikx}$$

$$E_{t}e^{ikx}$$

$$E_{t}e^{ikx}$$

$$E_{t}e^{ikx}$$

$$r = E_{t} / E_{0}$$

$$r: Reflection amplitude t: Transmission amplitude t$$

$$r = -t \exp(+ikd)i(z-1/z)\sin(nkd)/2$$

 $z = \sqrt{\frac{\mu}{\varepsilon}}$

Homogenization through S-parameter inversion (2)

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

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

 $\mathcal{E} = n / z$

$$\mu = nz$$

Lifting ambiguities using causality arguments

• $\operatorname{Re}(z) > 0$

•Im(*n*)>0

•*n* continuous function of ω

•Apply for small *d*



PRB, 65, 195103 (2002)

Representative results and ambiguities



k

Alternative retrieval approaches

Periodic effective medium approach

- Treatment of metamaterial as a periodic medium made of alternating resonant and air slabs
- Th. Koschny, et al, *Phys. Rev. B* 71, 245105 (2005)

Wave propagation approach

- Impedance from single interface Refractive index from modulation of propagating field
- Andryieuski et al, *Phys. Rev. B* 80, 193101 (2009)
- Many more!!! Also for anisotropic and bianisotropic materials







Discrepancies between retrieved and averaged effective params

Wave (retrieved) parameters often do not obey

$$<$$
 D >= \mathcal{E}_{eff} $<$ E >

$$<$$
 H >= (1 / μ_{eff}) $<$ **B** >

Averaged parameters often do not give correct scattering properties



Reason?

Impedance obtained through R/T-parameter retrieval implies surface averaged fields

Impedance obtained through averaging procedure implies volume averaged fields



RLC circuit description (1)







RLC circuit description (2)



 $F \sim$ volume fraction of the resonator within unit cell



Mixing rules



A. Sihvola, Electromagnetic mixing formulas and applications, 1999

Quasi-static effective medium approaches: Mixing rules

Give effective permittivity (or permeability) of a system of scatterers in the long wavelength limit

Valid for wavelengths $\lambda_{host} >> r$, $\lambda_{scat} >> r$

Offer

- Quick approach to assess metamaterial properties
- Path to tailor the metamaterial response

Most simple and widely used •Maxwell-Garnett (or Claussious Mossoti) •Bruggeman



A. Sihvola, *Electromagnetic mixing formulas and applications*, 1999

Maxwell-Garnett approach

$$\frac{\varepsilon_{eff} - \varepsilon_o}{\varepsilon_{eff} + 2\varepsilon_o} = f \frac{\varepsilon_i - \varepsilon_o}{\varepsilon_i + 2\varepsilon_o}$$

Also Reyleigh formulation

f: filling ratio, ε : dielectric function



$$\frac{\varepsilon_{eff} - \varepsilon_o}{\varepsilon_{eff} + 2\varepsilon_o} = \frac{na}{3\varepsilon_i}$$

(1) C-M formulation

Suitable for nonsymmetric composites

 $\mathbf{p} = a\mathbf{E}_{loc} \rightarrow \mathbf{P} = \varepsilon_0(\varepsilon_{eff} - 1)\mathbf{E}$

Uses polarizability (*a*) in the static limit & interaction among scatterers

Extended Maxwell-Garnett: Eq. (1) with *a* **non-static polarizability Predicts magnetic response from non-magnetic composites** Rupin, Tretyakov, Yannopapas, ...

Other approaches

Bruggeman

Requires vanishing of averaged polarization of the actual medium relative to the effective medium

$$f \frac{\varepsilon_{i} - \varepsilon_{eff}}{\varepsilon_{i} + \varepsilon_{eff}} + (1 - f) \frac{\varepsilon_{o} - \varepsilon_{eff}}{\varepsilon_{o} + \varepsilon_{eff}} = 0$$



Suitable for symmetric composites – (interconnected phases)

Averaging

$$\varepsilon_{eff} = f \varepsilon_i + (1 - f) \varepsilon_o$$

If the applied field is parallel to the interfaces



