Topology Optimization and its applications to mechanics and wave propagation problems

Ole Sigmund

Department of Mechanical Engineering
Technical University of Denmark

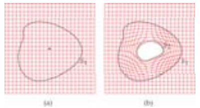
Towards Systematic Design of Metamaterials

Ole Sigmund

Department of Mechanical Engineering
Technical University of Denmark

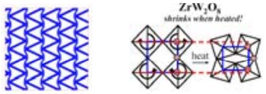
Metamaterials

Wikipedia:
*"Among electromagnetics researchers, the term is often used, quite narrowly, for **materials which exhibit negative refraction**"*



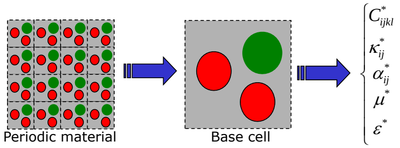
Transformation optics, Leonhardt, Pendry a.o.

DARPA (2001):
*"Metamaterials are (a new class of) ordered composites that exhibit **exceptional properties not readily observed in nature**"*



Design problem

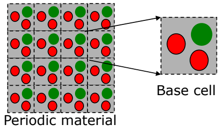
Find the periodic microstructure that has extreme or some prescribed properties



- Metamaterial design/synthesis
- Inverse problem
- **Inverse homogenization**

Sigmund (1994), IJSS, *31*, pp. 2313-2329

The Homogenization Problem



Homogenized elastic properties

$$C^*_{ijkl} = \frac{1}{Y}\int_Y \left(C_{ijkl} - C_{ijpq}\frac{\partial w_p^{kl}}{\partial y_q} \right) dY$$

Where w_p^{kl} is the solution to the equilibrium equation

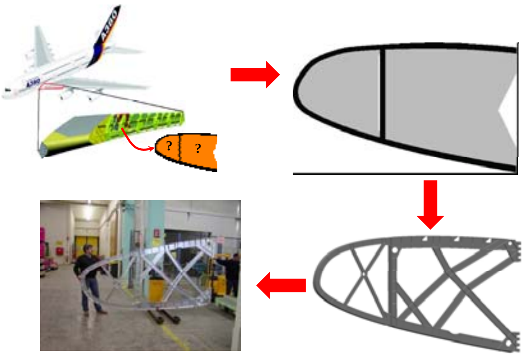
$$\int_Y C_{ijpq}\frac{\partial w_p^{kl}}{\partial y_q}\frac{\partial v_i}{\partial y_j}dY = \int_Y C_{ijpq}\varepsilon_{pq}^{0(kl)}\frac{\partial v_i}{\partial y_j}dY, \ \forall v \in V$$

$$V = \{ v : v \text{ is } Y - \text{periodic} \}$$

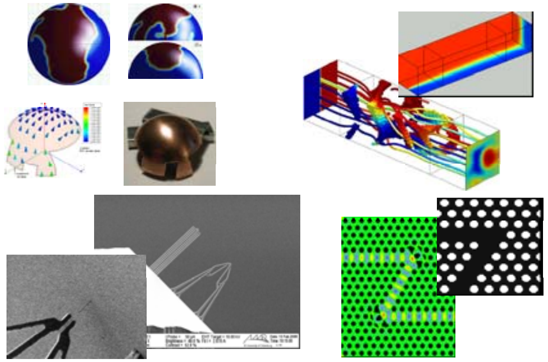
Solved by Finite Element Analysis

The Topology Optimization method

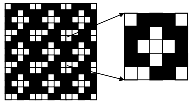
Bendsøe and Kikuchi (1988)



Other applications



The "Inverse Homogenization Problem"



$$\boxed{\begin{aligned} \min_{\boldsymbol{\rho}} :\ & \Phi(C^*_{ijkl}(\boldsymbol{\rho})) \\ s.t. :\ & \sum_{e=1}^{N} v_e\rho_e/V_0 = \mathbf{v}^T\boldsymbol{\rho}/V_0 \le f \\ :\ & g_i(C^*_{ijkl}(\boldsymbol{\rho})) \le g_i^*, \quad i = 1,\dots,M \\ :\ & \rho_e = \begin{cases} 0 \text{ (material 1)} \\ 1 \text{ (material 2)} \end{cases}, \ e = 1,\dots,N \\ :\ & \mathbf{K}(\boldsymbol{\rho})\mathbf{U}_i = \mathbf{F}_i, \quad i = 1,\dots,m \end{aligned}}$$

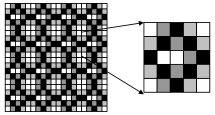
where $C_{ijkl}(\rho_e) = (1-\rho_e)C^1_{ijkl} + \rho_e C^2_{ijkl}$

0/1 Integer problem

- Combinations: N=10, M=5 => 252
  N=20, M=10 => 185.000
  N=40, M=20 => $1.4 \cdot 10^9$
  N=100, M=50 => 10^{29}

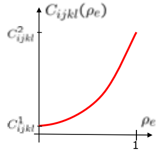
$$\boxed{\frac{N!}{(N-M)!M!}}$$

Continuous variables



Element stiffness interpolation:

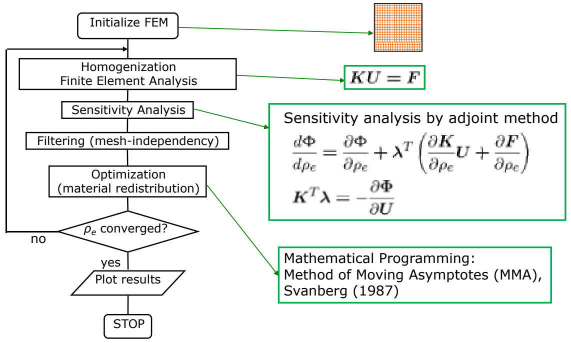
$$\boxed{\begin{aligned} \min_{\boldsymbol{\rho}} :\ & \Phi(C^*_{ijkl}(\boldsymbol{\rho})) \\ s.t. :\ & \sum_{e=1}^{N} v_e\rho_e/V_0 = \mathbf{v}^T\boldsymbol{\rho}/V_0 \le f \\ :\ & g_i(C^*_{ijkl}(\boldsymbol{\rho})) \le g_i^*, \quad i = 1,\dots,M \\ :\ & \mathbf{0} \le \boldsymbol{\rho} \le \mathbf{1} \\ :\ & \mathbf{K}(\boldsymbol{\rho})\mathbf{U}_i = \mathbf{F}_i, \quad i = 1,\dots,m \end{aligned}}$$



$p > 1$

where $C_{ijkl}(\rho_e) = (1-\rho_e)^p C^1_{ijkl} + \rho_e^p C^2_{ijkl}$

The Topology Optimization process



Initialize FEM

Homogenization
Finite Element Analysis

$KU = F$

Sensitivity Analysis

Filtering (mesh-independency)

Optimization
(material redistribution)

ρ_e converged?

no

yes

Plot results

STOP

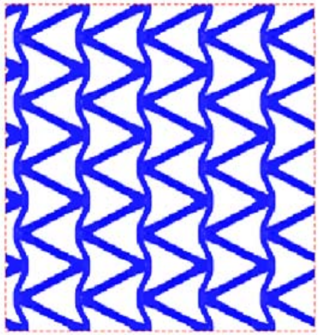
Sensitivity analysis by adjoint method

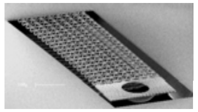
$$\frac{d\Phi}{d\rho_e} = \frac{\partial \Phi}{\partial \rho_e} + \boldsymbol{\lambda}^T \left(\frac{\partial \boldsymbol{K}}{\partial \rho_e} \boldsymbol{U} + \frac{\partial \boldsymbol{F}}{\partial \rho_e} \right)$$

$$\boldsymbol{K}^T \boldsymbol{\lambda} = -\frac{\partial \Phi}{\partial \boldsymbol{U}}$$

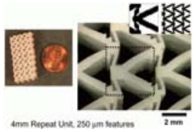
Mathematical Programming:
Method of Moving Asymptotes (MMA),
Svanberg (1987)

Material with negative Poisson's ratio



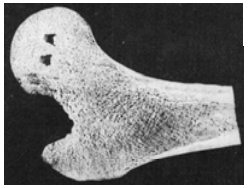


DTU Nanotech

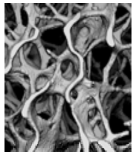


Halloran, UofM

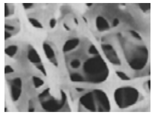
Bone microstructures



Head of Femur
(Gibson and Ashby (1988))



Bone microstructure
(Scanned by Odgaard)



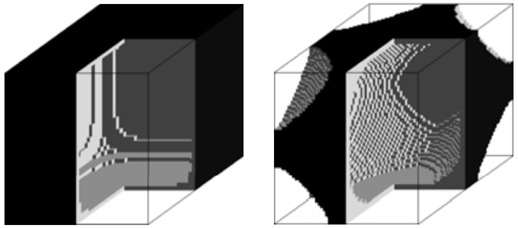
Bone microstructure
(Fazzalari et al. (1989))

It has been claimed that bone structure is optimized with respect to stiffness

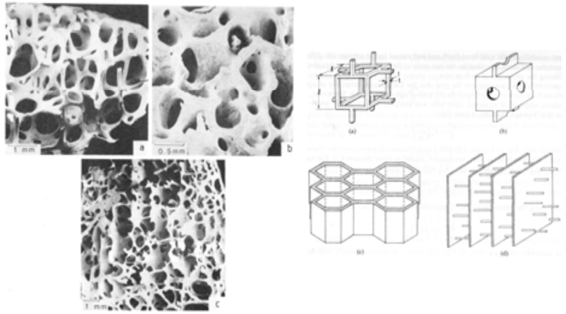
Is this true?

Optimized "Bone" microstructures

Maximize bulk modulus for hydrostatic load and volume constraint 30%



Practical observations in bone microstructures



All pictures taken from Gibson and Ashby (1988)

A two-physics competition problem

Elasticity problem: $\nabla \cdot \boldsymbol{\sigma} = 0$ $\quad E(\rho_e) = \rho_e^p E^0$

Porous flow: $\nabla \cdot (\kappa \nabla p) = 0$ $\quad \kappa(\rho_e) = (1-\rho_e)^p \kappa^0$

$$\begin{aligned} \max_{\boldsymbol{\rho}} :& \quad k^H(\boldsymbol{\rho}) \\ s.t. :& \quad \mathbf{v}^T \boldsymbol{\rho} / V_0 \leq f \\ :& \quad \kappa^H(\boldsymbol{\rho})) \geq \kappa^*, \\ :& \quad 0 < \rho_{min} \leq \boldsymbol{\rho} \leq 1 \end{aligned}$$

Comparison with theoretical bounds

Hashin Strikhman: k*=0.1294 (density = 0.3)

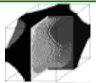
Cubic symmetry:

Closed cell: k^H=0.127

Open cell (κ^H>40%): k^H=0.081

Isotropy:

Closed cell: k^H=0.123



Open cell (κ^H>40%): k^H=0.085

Material with negative thermal expansion

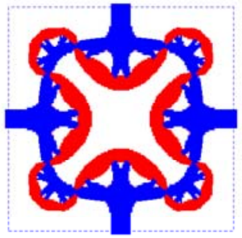
🟦 $\alpha^1 = 1$

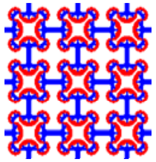
🟥 $\alpha^2 = 10$

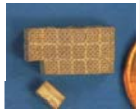
$E^1 = E^2 = 1$

$$C_{ijkl}(\rho_e^1, \rho_e^2) = (\rho_e^2)\left[(1-\rho_e^1)C_{ijkl}^1 + \rho_e^1 C_{ijkl}^2\right]$$

$\alpha^* = -4.02$





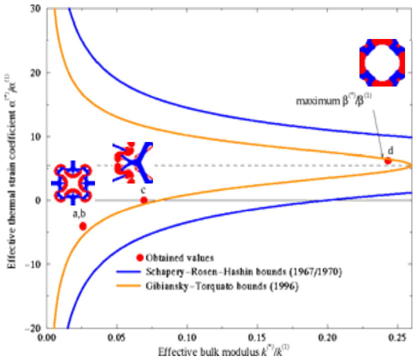


Sigmund and Torquato, APL, *69*, 3203-3205 (1996)

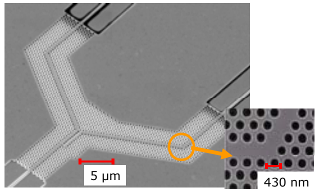
Halloran, UofM

Comparisons with bounds for thermal expansion

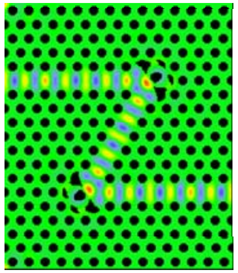
Sigmund and Torquato, APL, *69*, 3203-3205 (1996)



Photonic crystal based waveguides

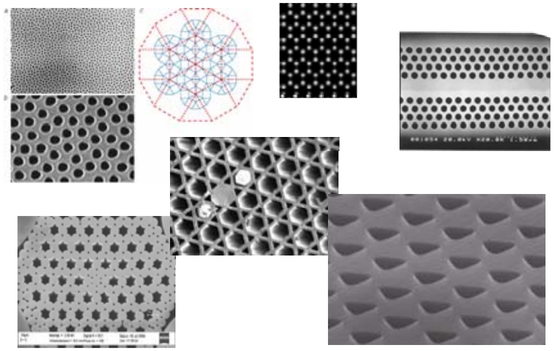


Yablonovitch, John a.o.

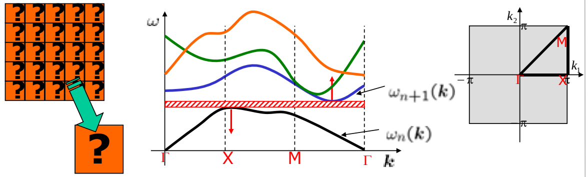


Borel et al, (2004-2007)
Jensen and Sigmund (2004,2005)

What microstructure maximizes the band gap?



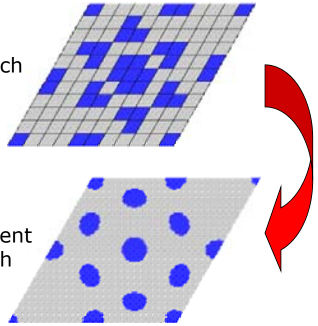
Band gap optimization



Maximize relative band gap between bands *n* and *n+1*:

$$\frac{\Delta\omega_n}{\omega_n^0} = 2\frac{\min\limits_{\boldsymbol{k}} : \omega_{n+1}(\boldsymbol{k},\boldsymbol{\rho}) - \max\limits_{\boldsymbol{k}} : \omega_n(\boldsymbol{k},\boldsymbol{\rho})}{\min\limits_{\boldsymbol{k}} : \omega_{n+1}(\boldsymbol{k},\boldsymbol{\rho}) + \max\limits_{\boldsymbol{k}} : \omega_n(\boldsymbol{k},\boldsymbol{\rho})}$$

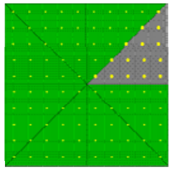
Two-step approach



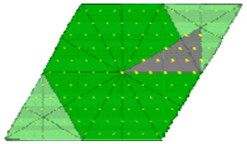
Make exhaustive search on **coarse mesh**

Fine design by gradient approach on fine mesh

Coarse discretization



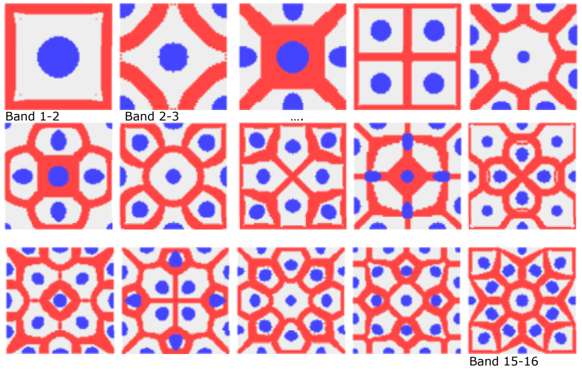
Square cell:
10 by 10 elements
15 variables
2^{15} =33768 combinations
6298 combinations after reduction



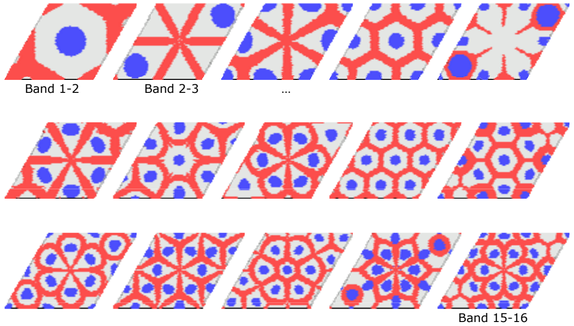
Rhombic cell:
11 by 11 elements
16 variables
2^{16} =65536 combinations
15450 combinations after reduction

Reduction: f<10%, f>90%, isolated elements, translational copies

Composite TE (red) and TM (blue) structures

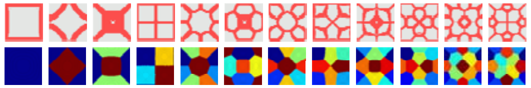


Composite TE (red) and TM (blue) structures



Geometrical quality measures

- Mesh quality factor (not too good)
- Air filling fraction (pretty good but) not good for design
- Perimeter of cell walls (for TE walls, pretty good)
- Packing factors
- Cybulski et al., “Minimization of the Renyi entropy production in the space-partitioning process”, Phys Rev. E, **71**, 046130 (2005)



Conjecture

Optimal photonic band gap structures
for gaps between band n *and* n+1
can be found by a purely geometric rule:

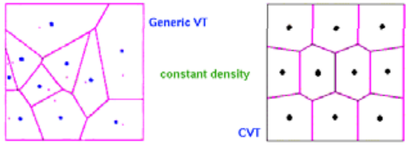
TM-polarization:
n elliptic rods with centers defined by the generators of the optimal *centroidal Voronoi tesselation*

TE-polarization:
The walls of above tesselation

Centroidal Voronoi tesselation

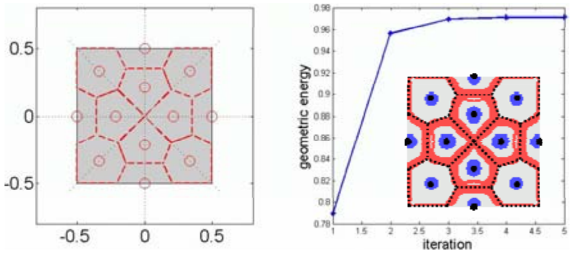
A Voronoi tessellation is called centroidal when the generating point of each Voronoi cell is also its mean (center of mass).

It can be viewed as an optimal partition corresponding to an optimal distribution of generators

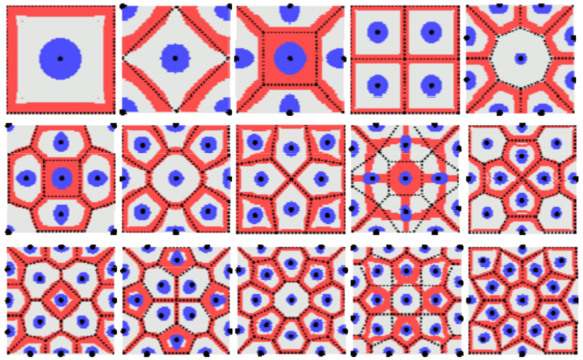


Lloyd's algorithm

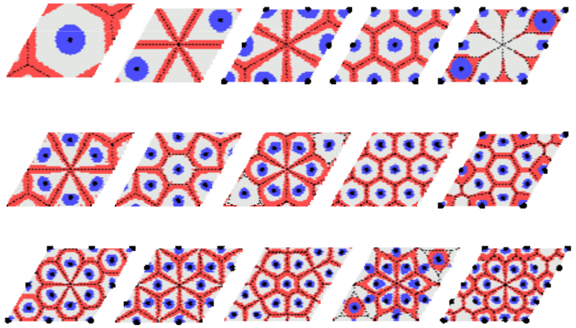
Example: *n=10*



Composite TE and TM structures



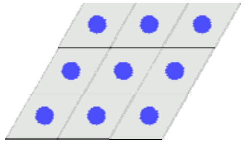
Composite TE and TM structures



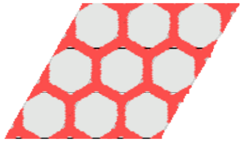
"Geometric properties of optimal photonic band gap structures"

Sigmund & Hougaard, *PRL*, **2008**, *100*, 153904

The overall optimal planar photonic band gap structures are:

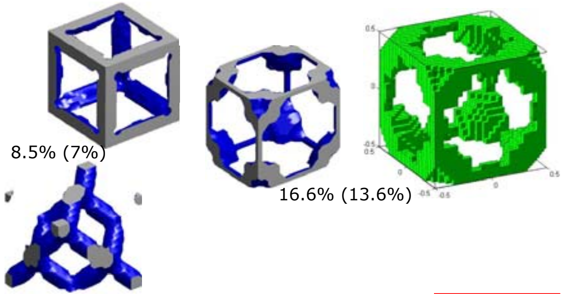


TM: 48%



TE: 52%

What about 3d?



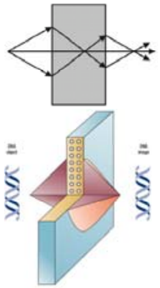
By Niels Aage

Issues: Discretization, CPU-time, parallellization, symmetries

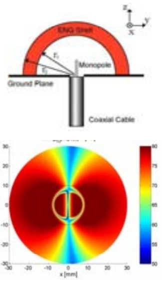
---

Electromagnetic metamaterials

Cloaking



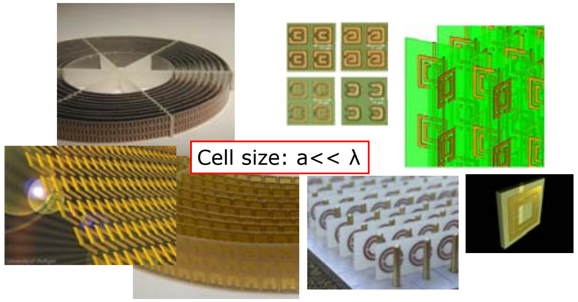
Super lensing



Antennas

Small antennas for hearing aids

Electromagnetic metamaterials



Cell size: a<< λ

Microwave regime: a ~ 1cm
Optical regime: a ~ 100nm

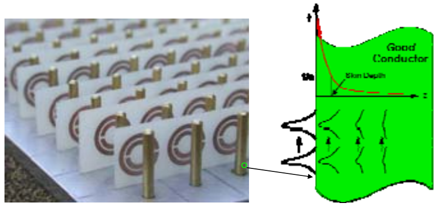
Challenges in EM metamaterial design (I)

- Skin depth issue for FE discretization

Skin depth in Copper, δ<1 μm
Cell size ~ 1 cm
FE-discretization ~ 20.000^3

Skin depth

$$\delta = \frac{1}{\sqrt{\pi f \mu \sigma}}$$



Maxwell's equations

Maxwell's equation for harmonic waves

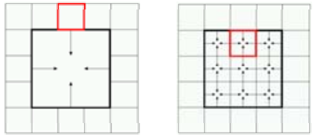
$$\nabla \times (\frac{1}{\mu_r}\nabla \times \mathbf{E}) + \frac{\omega^2}{c^2}\left(\epsilon_r(\rho) - i\frac{\sigma(\rho)}{\omega\epsilon_0}\right)\mathbf{E} = 0$$

Resolving the skin depth issue

Impedance BC

$$\boldsymbol{n}\times(\frac{1}{\mu_r}\nabla\times\mathbf{E}) - i\frac{\omega}{c}f(\rho)\sqrt{\left(\epsilon_r - i\frac{\sigma}{\omega\epsilon_0}\right)}\times(\mathbf{E}\times\boldsymbol{n}) = 0$$

Cut through square conductor

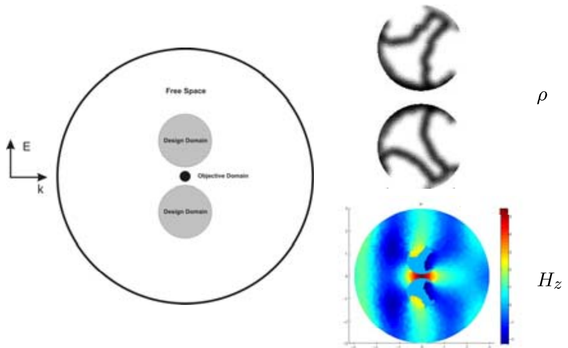


Conventional discretization

TopOpt discretization

Aage, Mortensen and Sigmund (2009), submitted

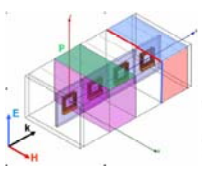
2D test case, field concentrator



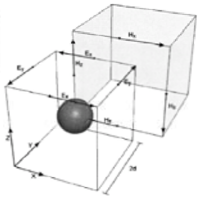
Aage, Mortensen and Sigmund (2009), submitted

Challenges in EM metamaterial design (II)

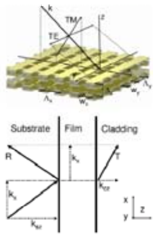
- Extracting effective properties



Field summation
Lerat *et al.* (2006)



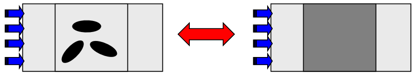
Field averaging
Smith and Pendry (2006)



S-parameter extraction
Smith *et al.* (2002) a.o.

"Classical" homogenization approaches

Parameter retrieval from S-paramters



$$n^H = \frac{1}{kd}\left(\cos^{-1}\left[\frac{1}{2S_{21}}(1 - S_{11}S_{22} + S_{21}^2)\right] + 2p\pi\right)$$

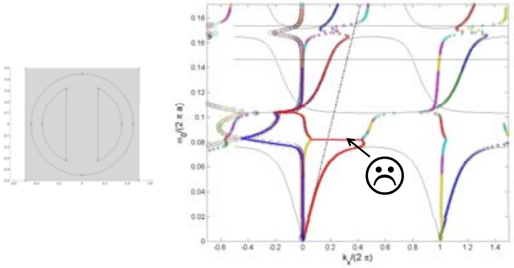
$$z^H = \sqrt{\frac{(1+S_{11})(1+S_{22}) - S_{21}^2}{(1-S_{11})(1-S_{22}) - S_{21}^2}}$$

$$\epsilon^H = n^H z^H$$

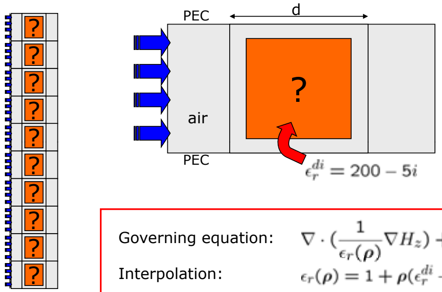
$$\mu^H = n^H / z^H$$

Smith et al. (2005)

Dis-continuous branches



2D Electromagnetic Metamaterial design



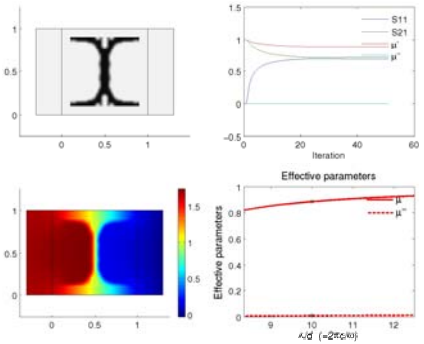
$$\epsilon_r^{di} = 200 - 5i$$

Governing equation: $\nabla \cdot (\frac{1}{\epsilon_r(\rho)}\nabla H_z) + \frac{\omega^2}{c^2}H_z = 0$

Interpolation: $\epsilon_r(\rho) = 1 + \rho(\epsilon_r^{di} - 1)$

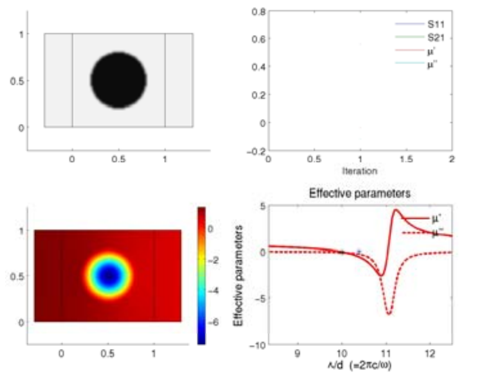
Objective function: $\min\limits_{\rho} : \mu'$

Challenges in EM metamaterial design (III)

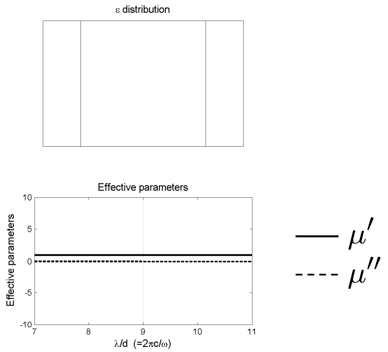


μ=0.89+0.00i, $|S_{11}|$= $|S_{22}|$= 0.69, $|S_{21}|$= 0.72

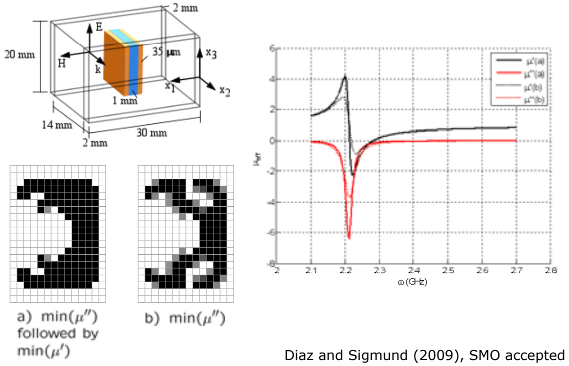
Circular inclusion



2D design example



First 3D design examples



a) min(μ'') followed by min(μ')

b) min(μ'')

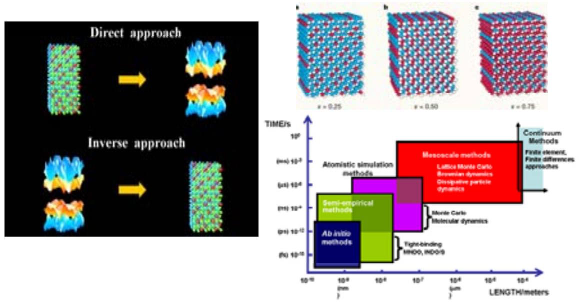
Diaz and Sigmund (2009), SMO accepted

Conclusions

- Metamaterials in a wide range of physical disciplines can be systematically synthesized using topology optimization
- Our (presently) biggest challenge is to determine effective propeties of electromagnetic metamaterials **consistently**
- More results on the way

Future work (”bridging to another scale”)

”**The inverse band-structure problem** of finding an **atomic configuration** with given electronic properties”
Franceschetti and Zunger, Nature 402, 60-63, (1999)



Thank you for your attention!

More info at
www.topopt.dtu.dk
www.topant.dtu.dk

Sponsors:
FTP – TopAnt project (Danish Technical Research Agency)
*HTF – w. DTI and Widex (*Danish Nat. Adv. Tech. Foundation)
DCSC – (Danish Center for Scientific Computing)
Elite Research Prize (Danish Minister of Science)
EURYI (EU)