# On the Role of Bounds in Topology Optimization

Christian Kern, University of Utah
Owen Miller, Yale University
Graeme Milton, University of Utah

# The Lycurgus Cup (4th Century Roman, British Museum)

Lit from in front

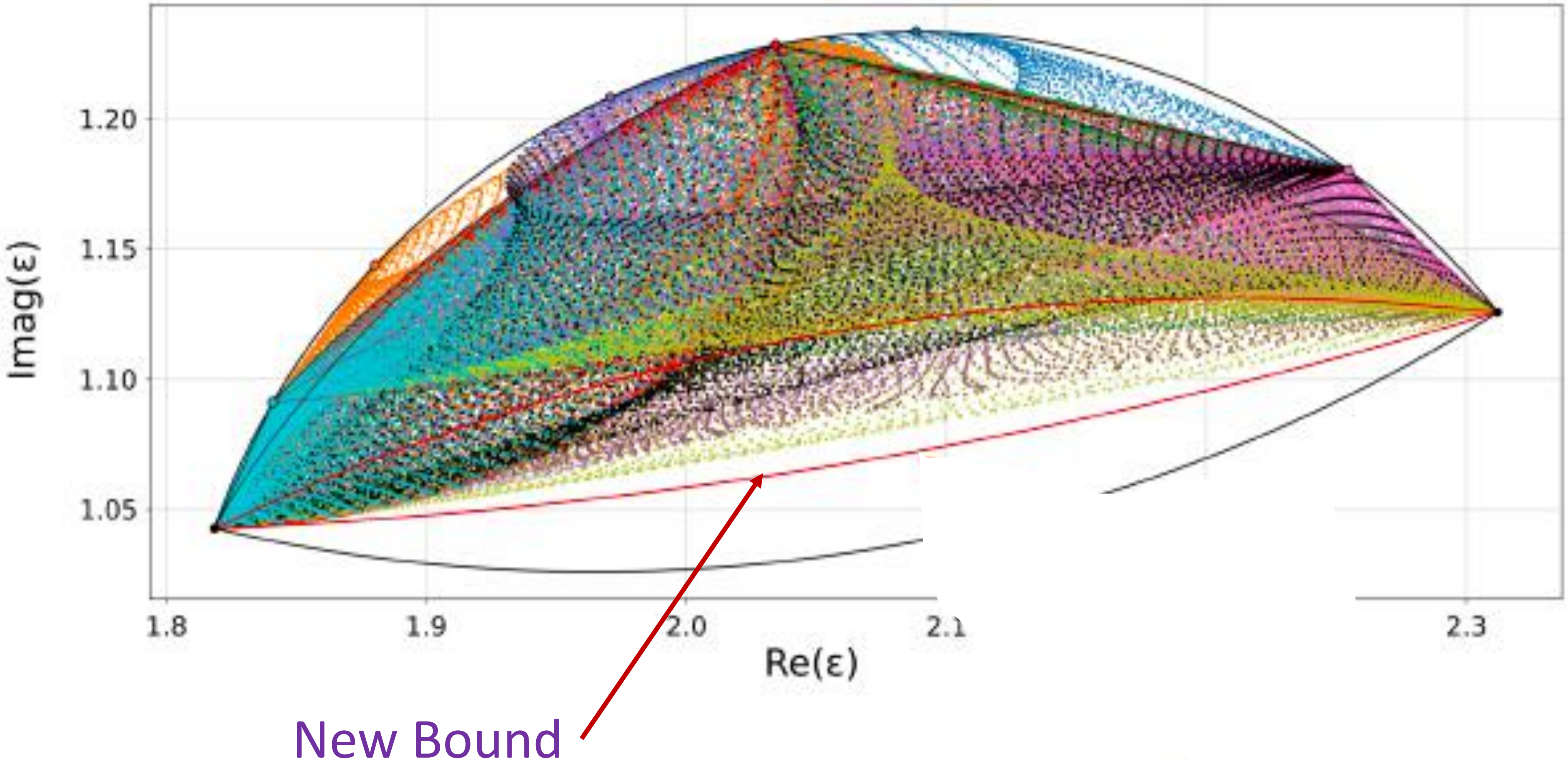
Lit from behind

# Naomi Halas's Group (2002)

Rice University

# Gold Nanoshells

# Bergman-Milton Bounds (1980) and microstructures that fill them




With Christian Kern and Owen Miller (2019)

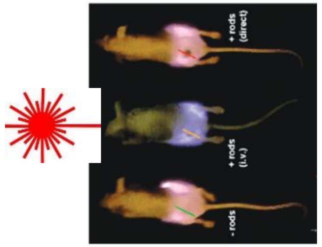
Simulations of Christian Kern

# Related example (Miller and collaborators): maximum extinction/mass of dilute nanoparticles (i.e., what is the best smoke grenade?)

*Goal*: dilute, randomly-arranged particles to absorb or scatter light over a broad bandwidth

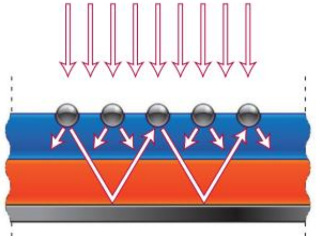
*Related applications*:

cancer therapy



*JACS* 128, 2115 (2006)

solar cells



*Nat. Mat.* 9, 205 (2010)

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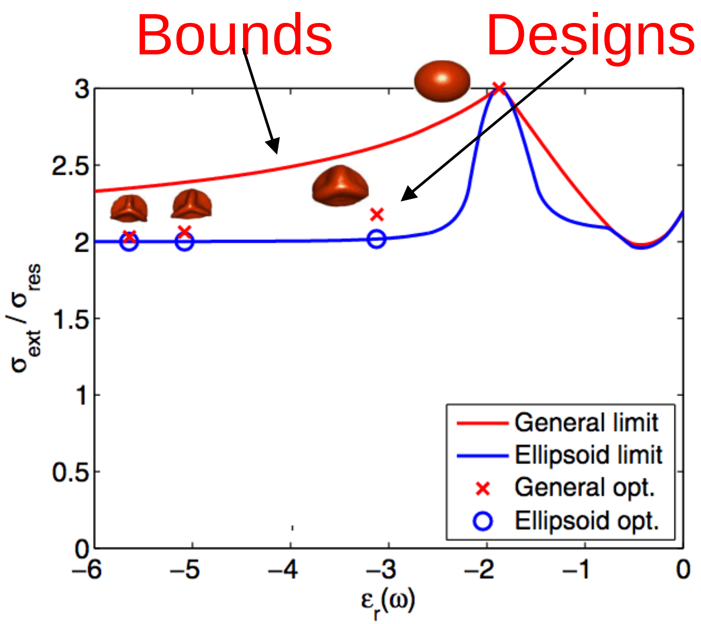



Previous state-of-the-art: coated, metal+dielectric nano-spheres

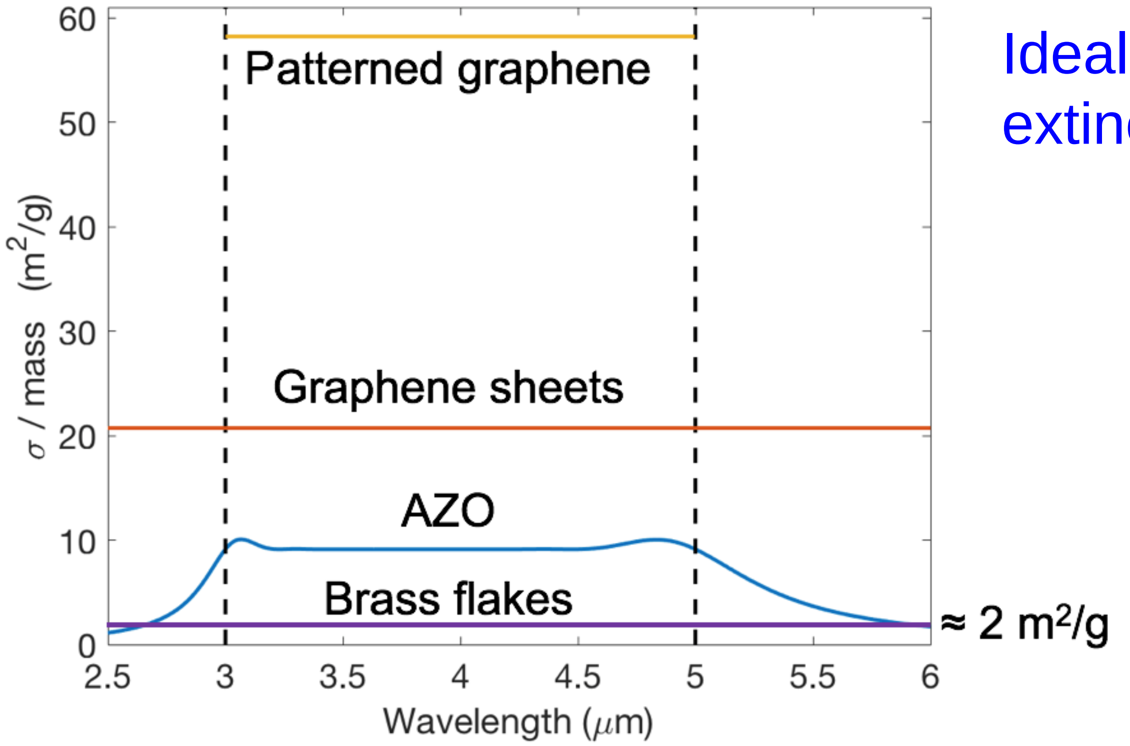
Optimal ellipsoids and more exotic designs obtained via topology optimization achieve 5-20X better performance

Via theory (e.g. Bergman-Milton approach), one can show that these structures are approaching global upper bounds

*Miller et al. Phys. Rev. Lett. 112, 123903 (2014)*

Inverse design approaches necessarily find local optima / saddle point. Analytical upper bounds provide global targets, dictating when to modify algorithms and when to stop searching.

Moreover, we could predict which *materials* to start with!




Ideal materials for extinction / mass

# Early work: Bounds coupling thermal expansion and bulk modulus and their realizabilty using topology optimization

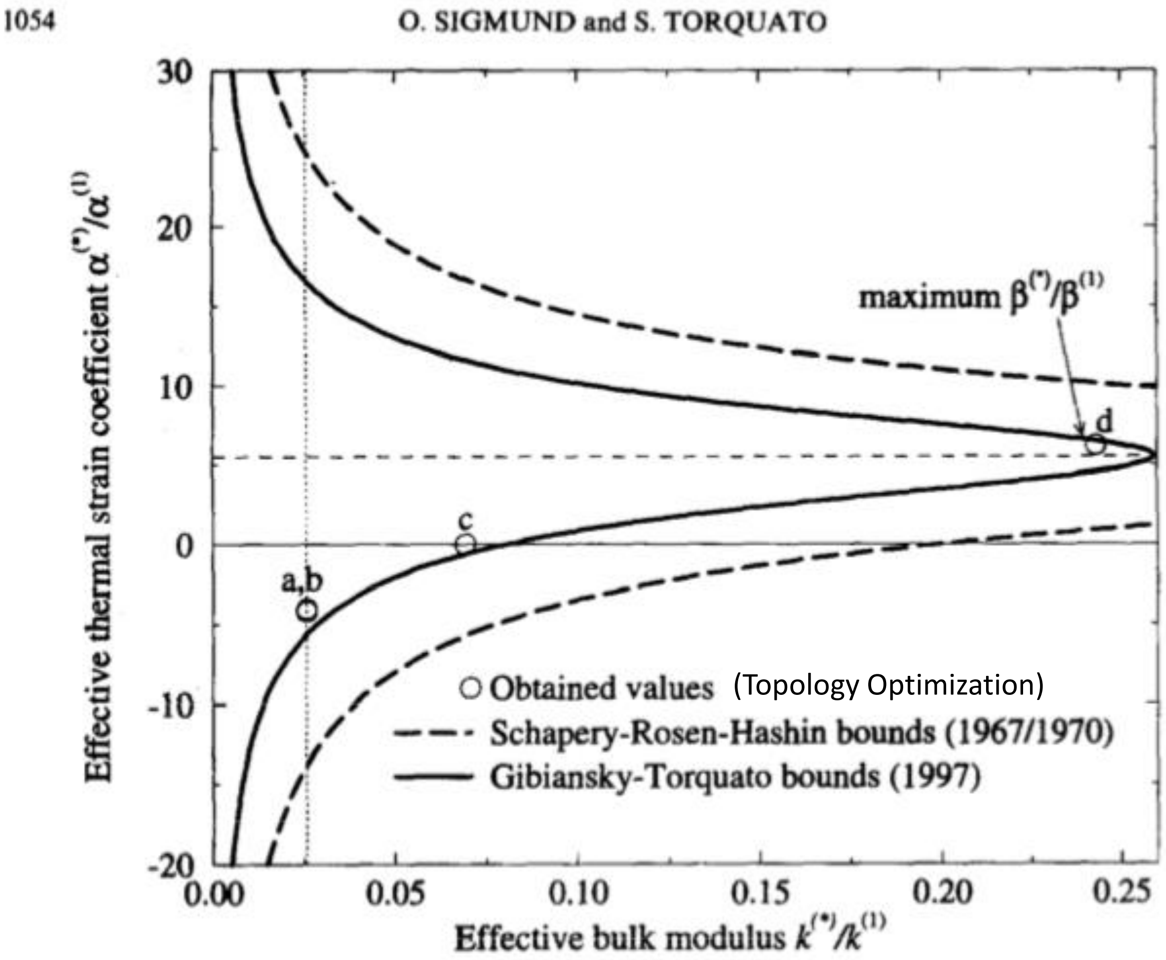



Fig. 4. Bounds for three-phase design example. The circles with letters a–d denote the obtained values for the microstructures shown in Figs 5 and 6.

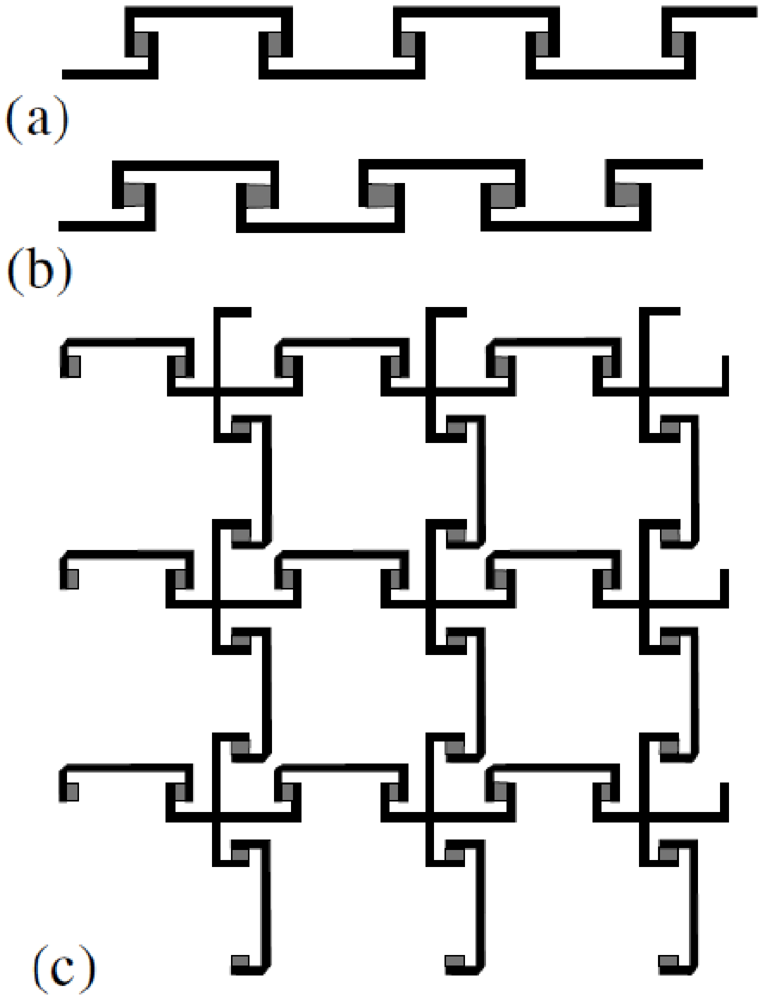
Sigmund and Torquato (1997)

J. Mech. Phys. Sol. 45, 1037-1067 (1997)

Mantra: what is not obviously forbidden may actually be possible

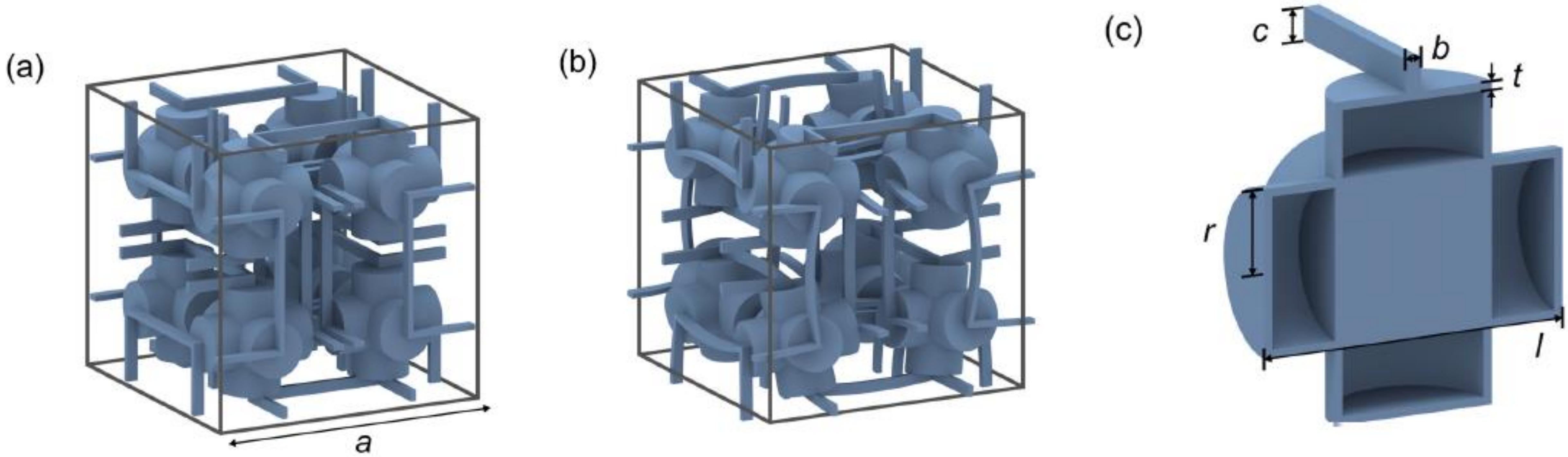
# Negative Expansion from positive expansion

Topology Optimization can help guide intuition




Original designs: Lakes (1996); Sigmund & Torquato (1996, 1997)

# One can get a similar effect for poroelasticity

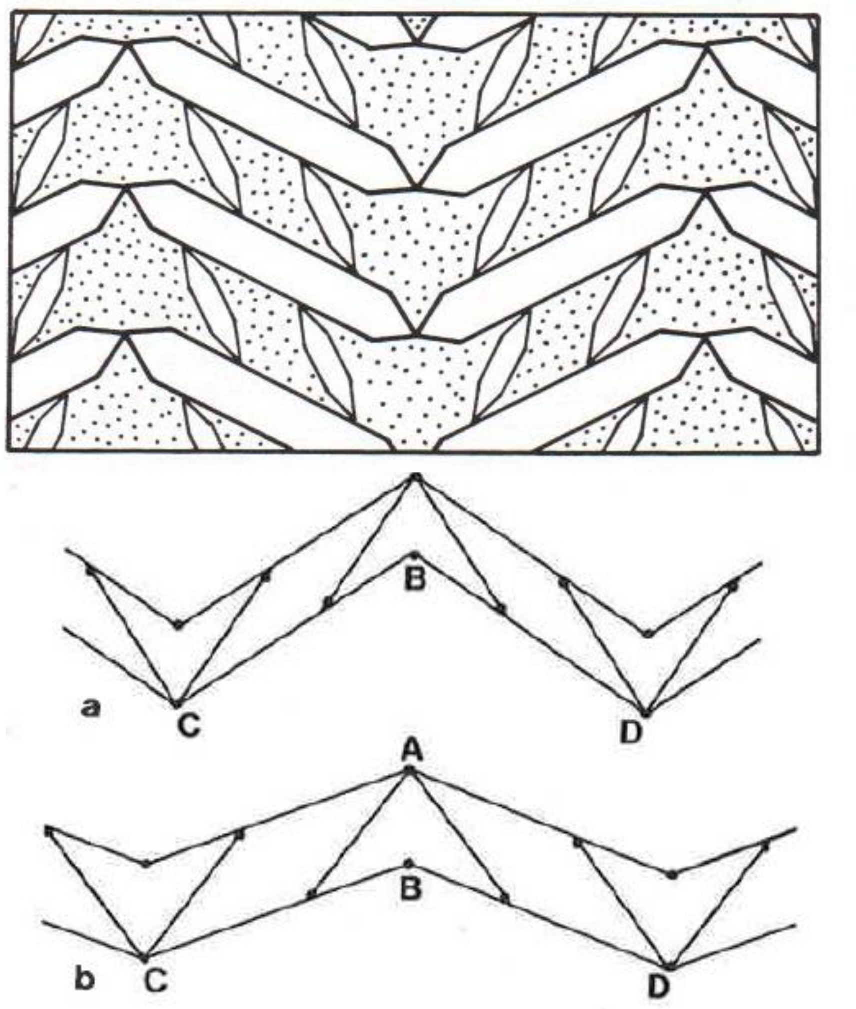



Qu, et.al 2017

Same equation,
but different physics

# Sometimes Intuition and topology optimization almost coincide:

## Auxetic materials that expand when stretched




J. Mech. Phys. Sol. 40, 1105-1137 (1992)

Larsen, Sigmund and Boustra (1997)
(Topology Optimization)

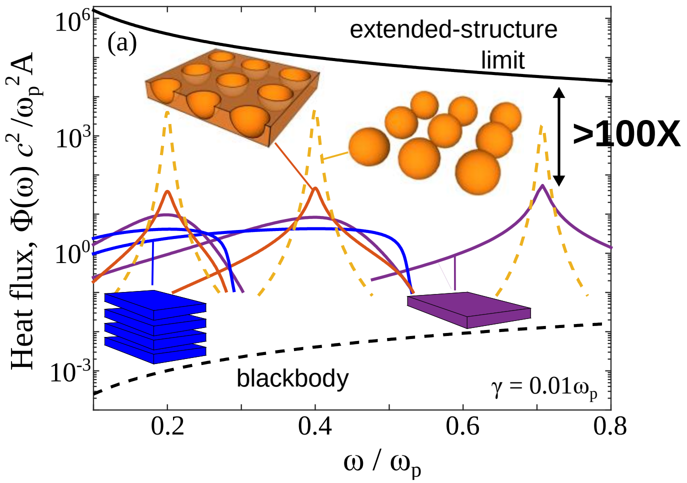
J. Microelectromech. Sys 6, 91-106 (1997)

# Near-field optics (Miller and collaborators)

For spontaneous emission, radiative heat transfer, Raman scattering, quantum entanglement between qubits, etc., *near-field* coupling can lead to dramatic rate enhancements.

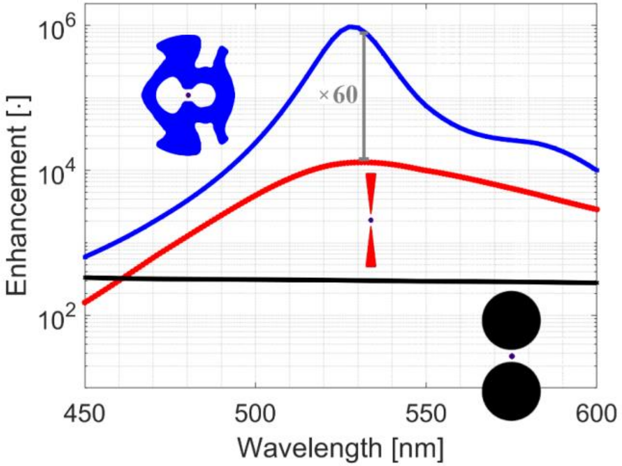
We derived bounds to these quantities, and showed that in certain frequency ranges, prototypical structures—bowtie antennas, hyperbolic metamaterials—fall far short. Opportunity for topology optimization!

**Orders-of-Magnitude Enhancements**




*Miller et al. PRL 2015, Opt. Exp. 2016, PRX 2019*

**Very recent top-opt designs from collaborators, outperforming state-of-art**

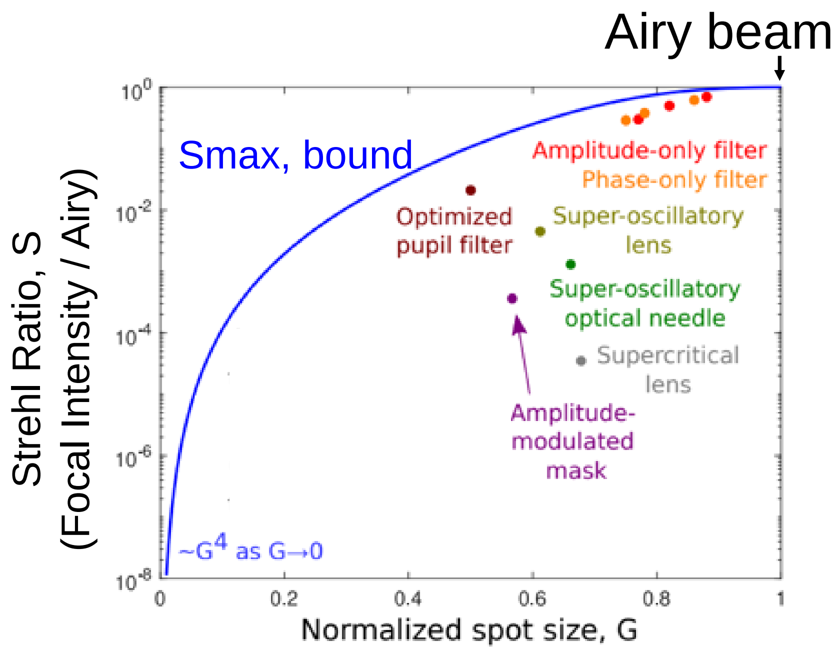



*Christiansen et al. arXiv:1911.05002 (2019)*

# Beating the diffraction limit (Miller and collaborators)

It has long been known that sub-diffraction-limited optical beams are possible, with potential ramifications for imaging. Problem: large sidelobes obscure the signal. Question: how much can the sidelobes be reduced?

We derived general upper bounds, and compare them to the best designs from the literature

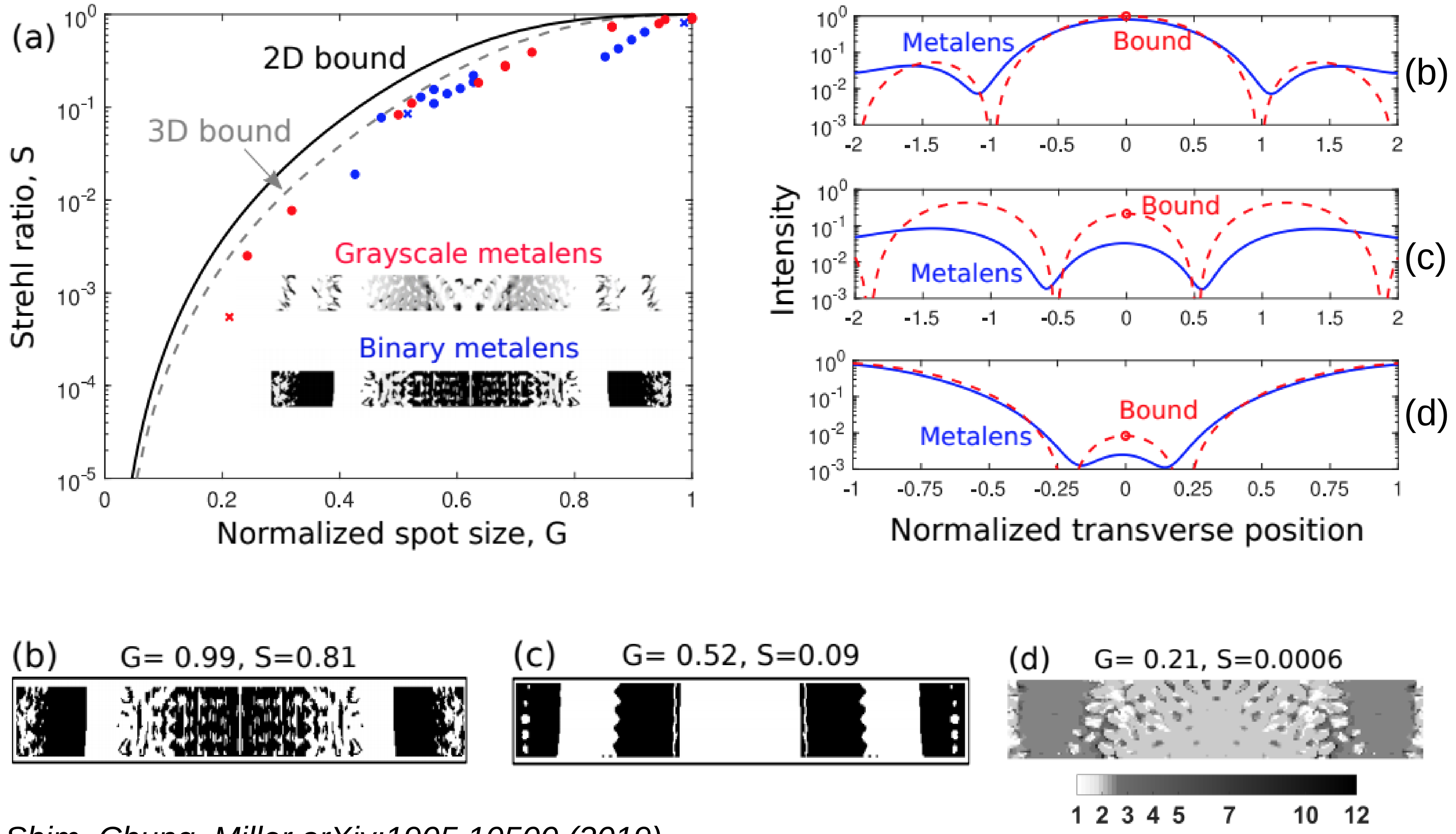



There is significant room for improvement!

Apply topology optimization…

*Shim, Chung, Miller arXiv:1905.10500 (2019)*

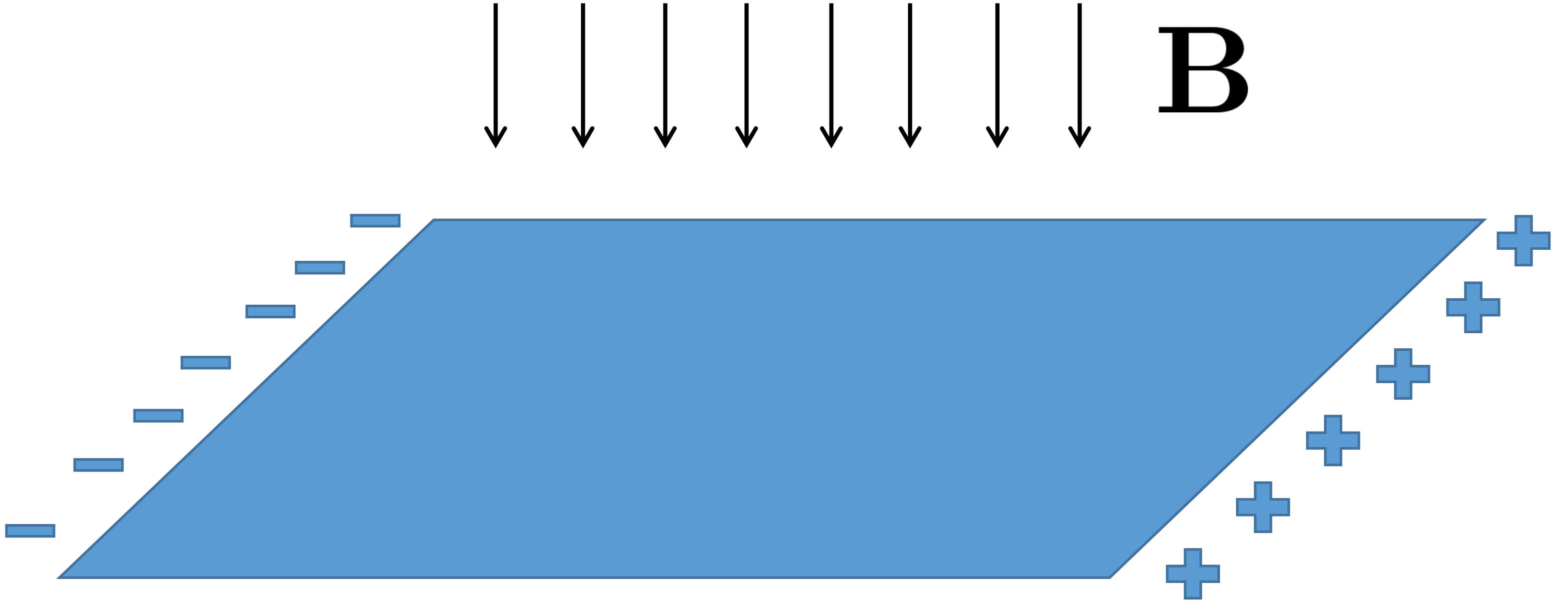
# Topology optimization of super-resolving metasurfaces approaching fundamental limits (Miller and collaborators)




*Shim, Chung, Miller arXiv:1905.10500 (2019)*

Sometimes the geometries one obtains, even by intuition (guided by mathematics), are not at all simple

One interesting example:




Hall Voltage

Can one reverse the Hall Voltage by playing with microstructure?

$$\mathbf{F} = q\mathbf{v} \times \mathbf{B}$$

# Geometry suggested by artist Dylon Whyte

Picture Courtesy Dylon Whyte

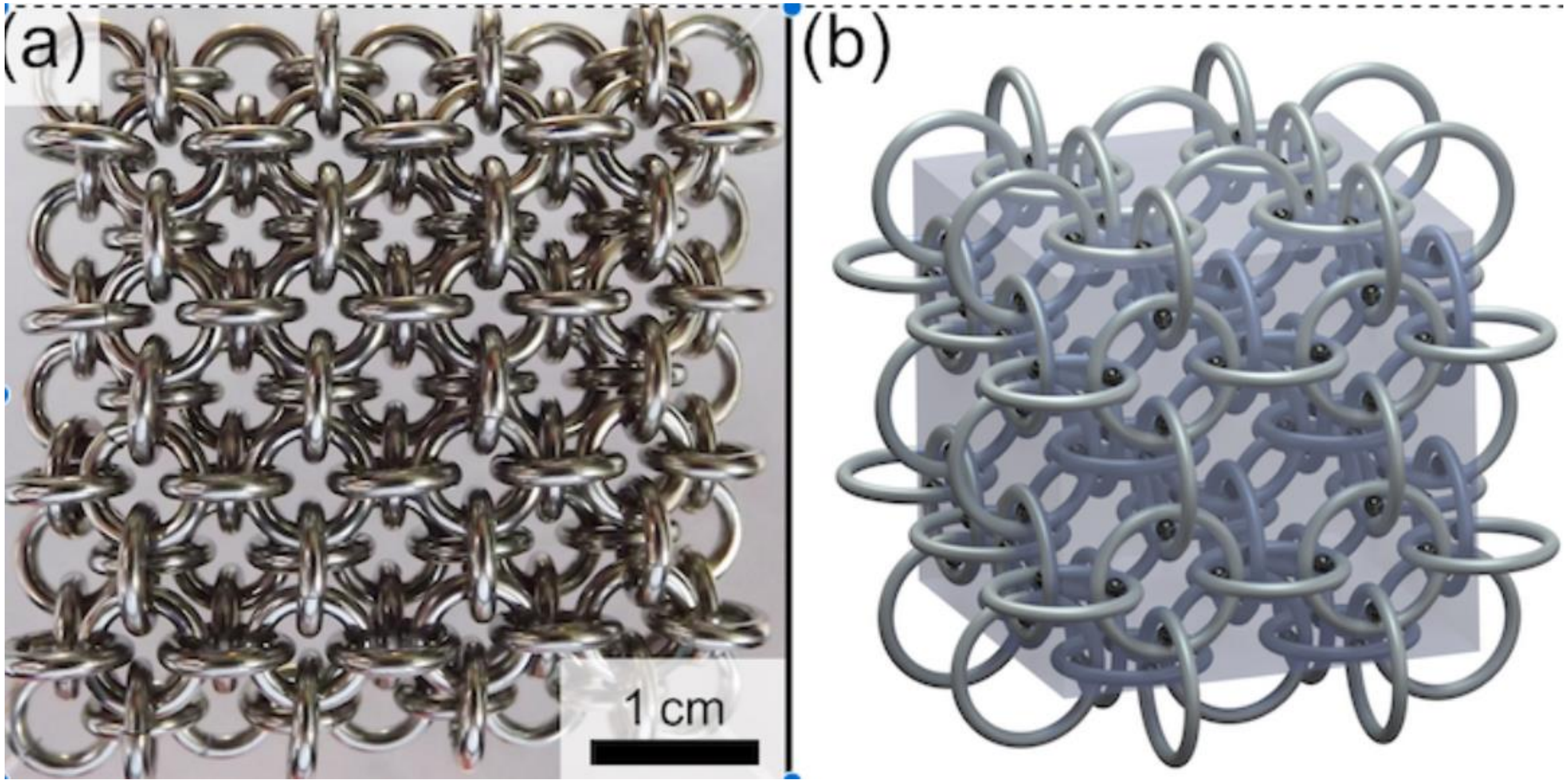
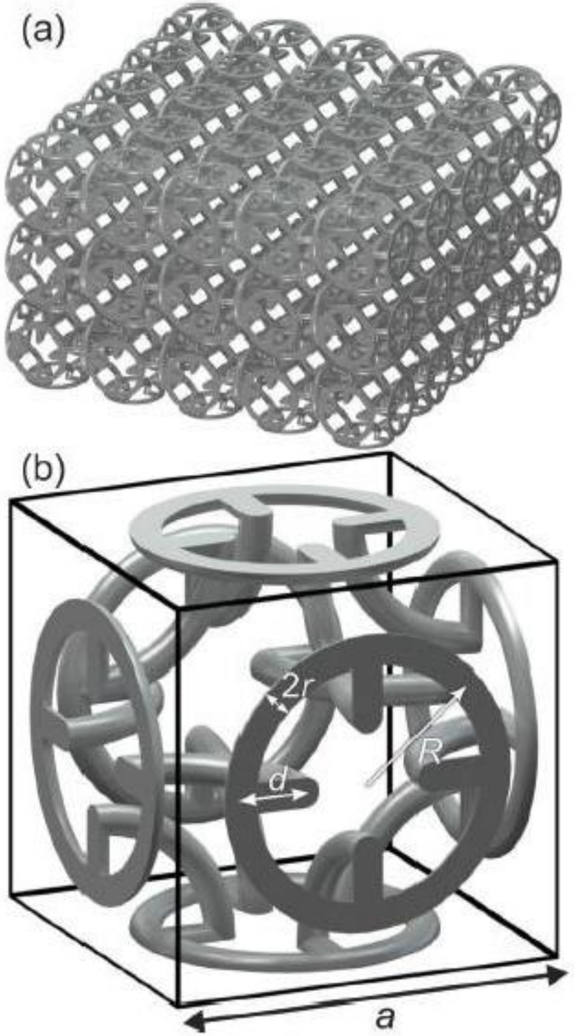


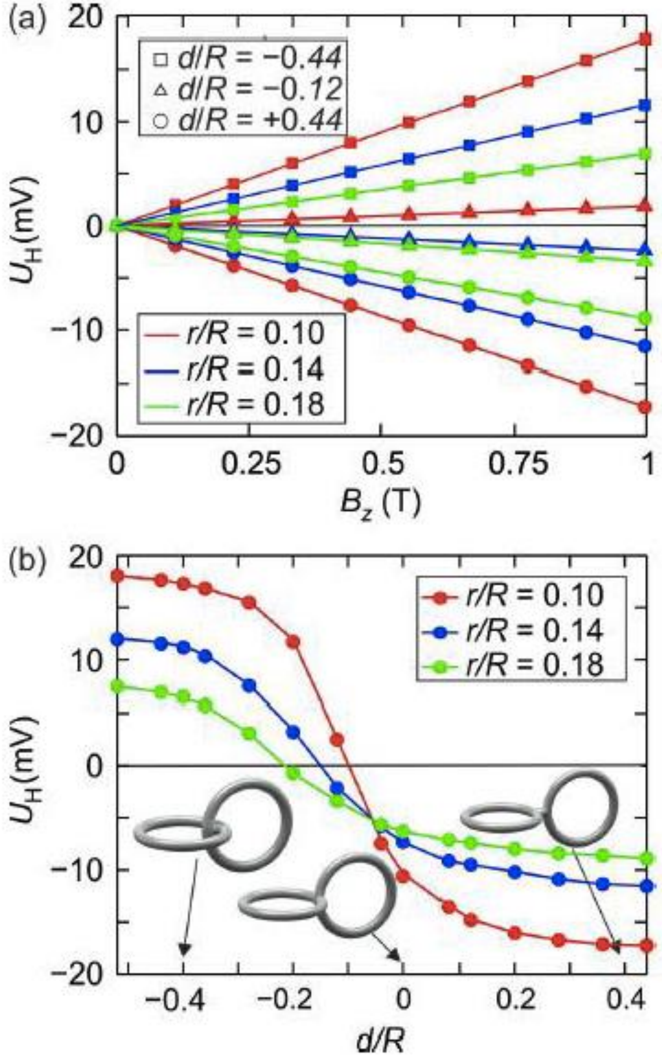

Image Courtesy Christian Kern

## A material with cubic symmetry having a Hall Coefficient opposite to that of the constituents (with Mark Briane)

Arch. Rat. Mech. Anal. 193, 715-736 (2009)

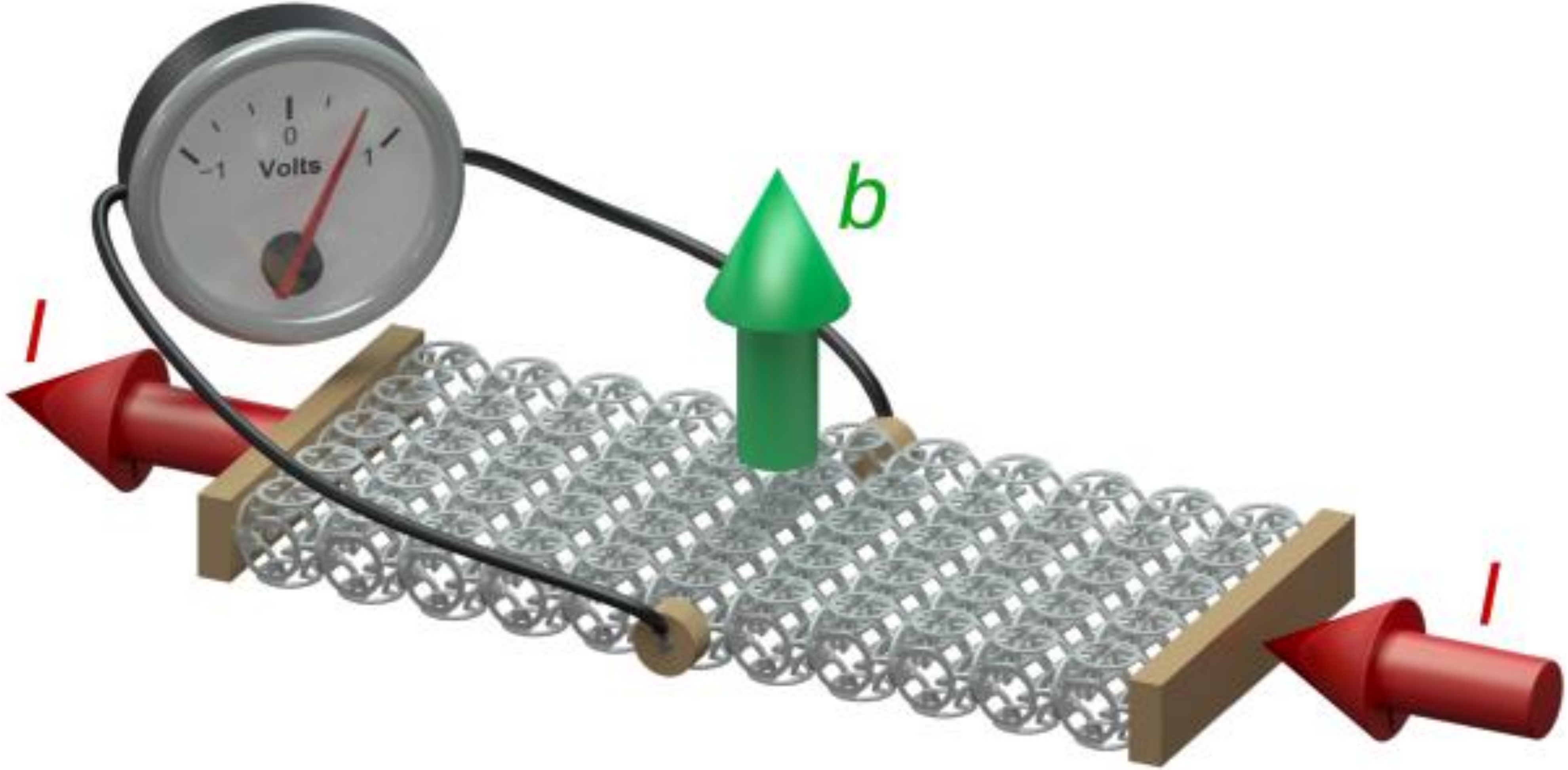
# Simplification of Kadic et.al. (2015)



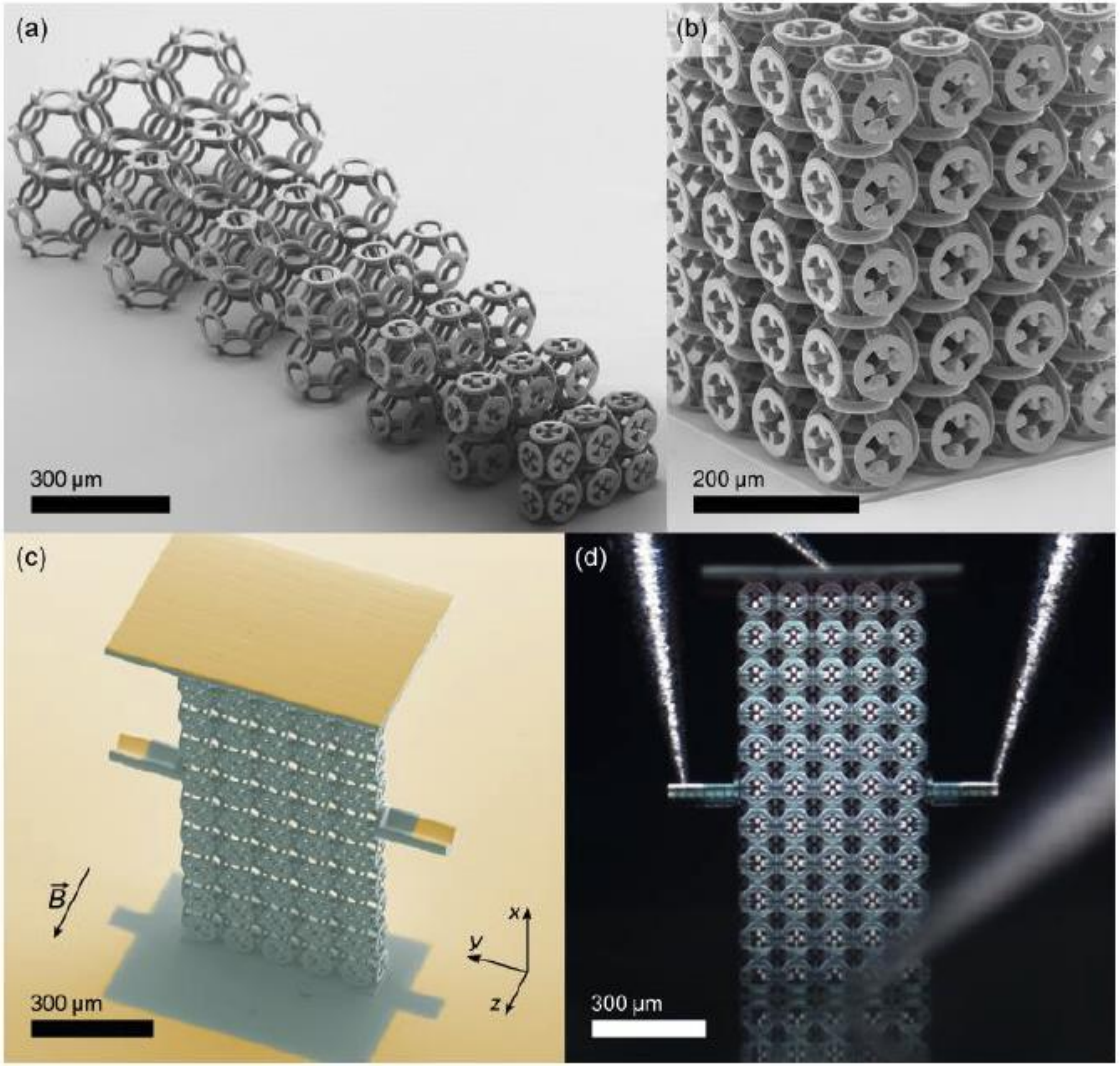




Phys. Rev. X 5, 021030 (2015)

# Experiment: Kern et.al (2017)




Phys. Rev. Lett. 118, 016601 (2017)

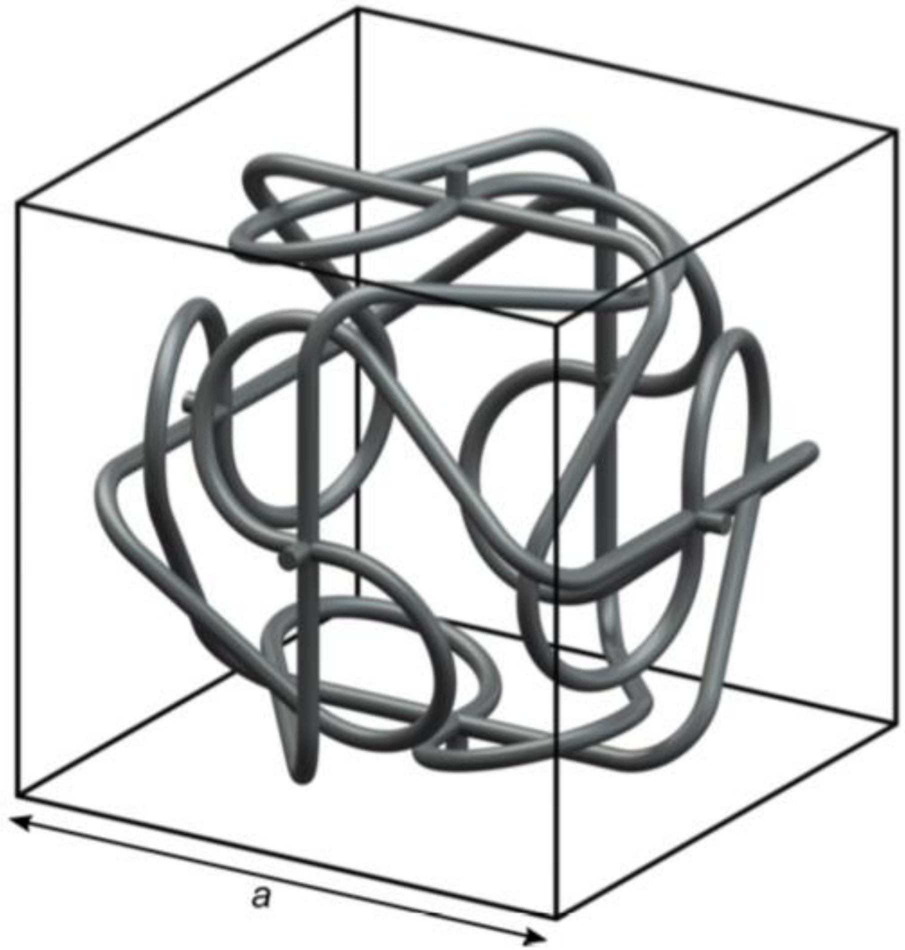






# Experimental realization of Kern, Kadic, and Wegener

# Alternate Structure of Christian Kern:




New J. Phys. ,20 193, 083034 (2018)

One can also get novel effects
Such as the parallel Hall effect

Arch. Rat. Mech. Anal. 193, 715-736 (2009)

Phys.Rev. Applied 7, 044001 (2017)

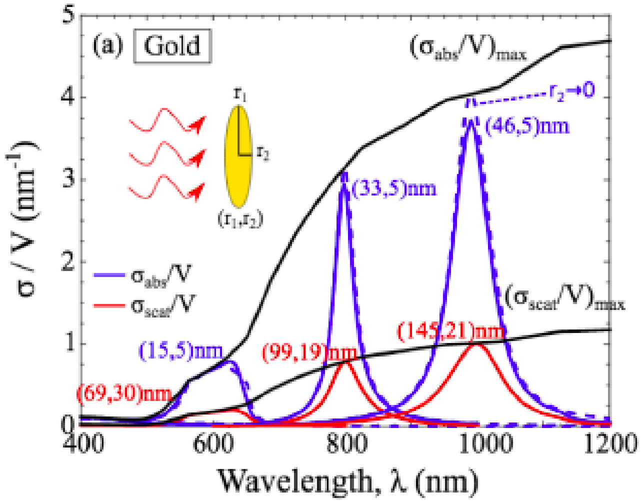
What will topology optimization give?

# On the importance of bounds for topology optimization

We've seen examples where bounds identify opportunities for improvement via topology optimization.

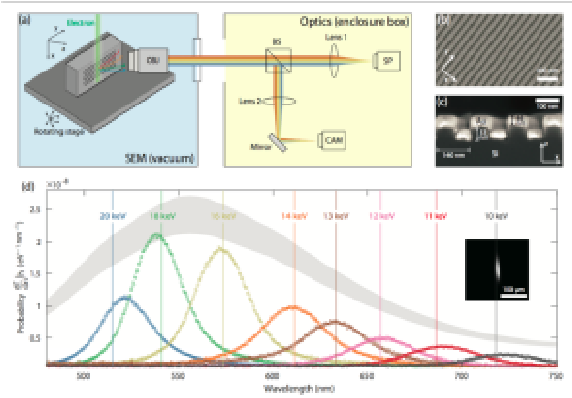
Equally important: areas where known or simple structures can already achieve global bounds, where we learn not to bother with topology optimization! We've also seen this in a few cases:

**Plane-wave scattering**



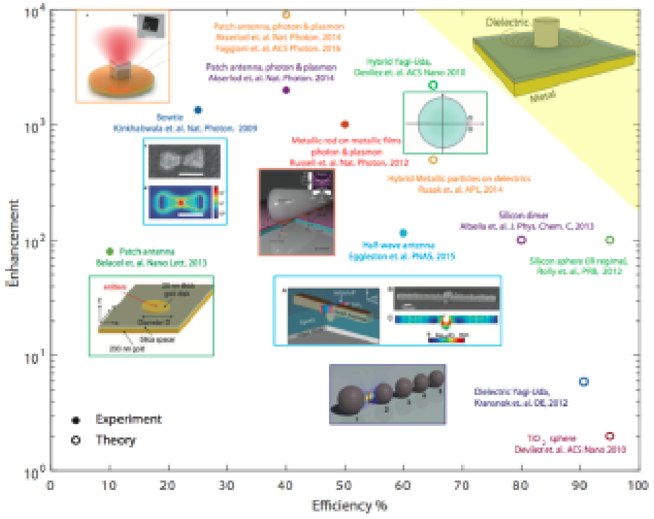

*Opt. Exp. 24, 3329 (2016)*

**Smith-Purcell radiation**



*Nat. Phys. 14, 894 (2018)*

**High-efficiency plasmonic resonators**



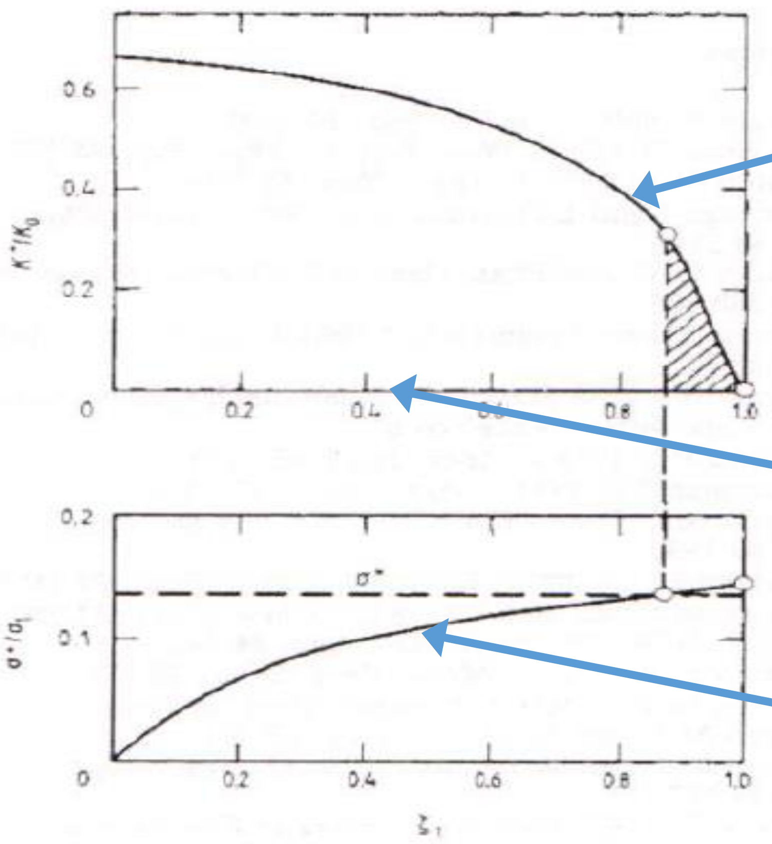

*Nano Lett. 17, 3238 (2017)*

# Finally: Bounds for Multiphysics Problems:

One approach: eliminate geometric parameters common to bounds for the different physical problems:

effective
bulk modulus

effective
conductivity




Upper bound on bulk modulus

Horizontal axis is the geometric parameter

Lower bound on conductivity

Illustrating the process through which a measurement of effective conductivity of a porous insulating material filled with a conducting fluid leads to an upper bound on the bulk modulus of the porous frame.

With J. Berryman
J.Phys.D: Appl. Phys. 21, 87-94

# Alternate Approach:

Given $m$ different (linear) physics problems where the tensors entering their constitutive laws are $\mathbf{L}_1(\mathbf{x})$,$\mathbf{L}_2(\mathbf{x})$,...,$\mathbf{L}_m(\mathbf{x})$ the idea of Gibiansky and Cherkaev is to introduce a "supertensor"

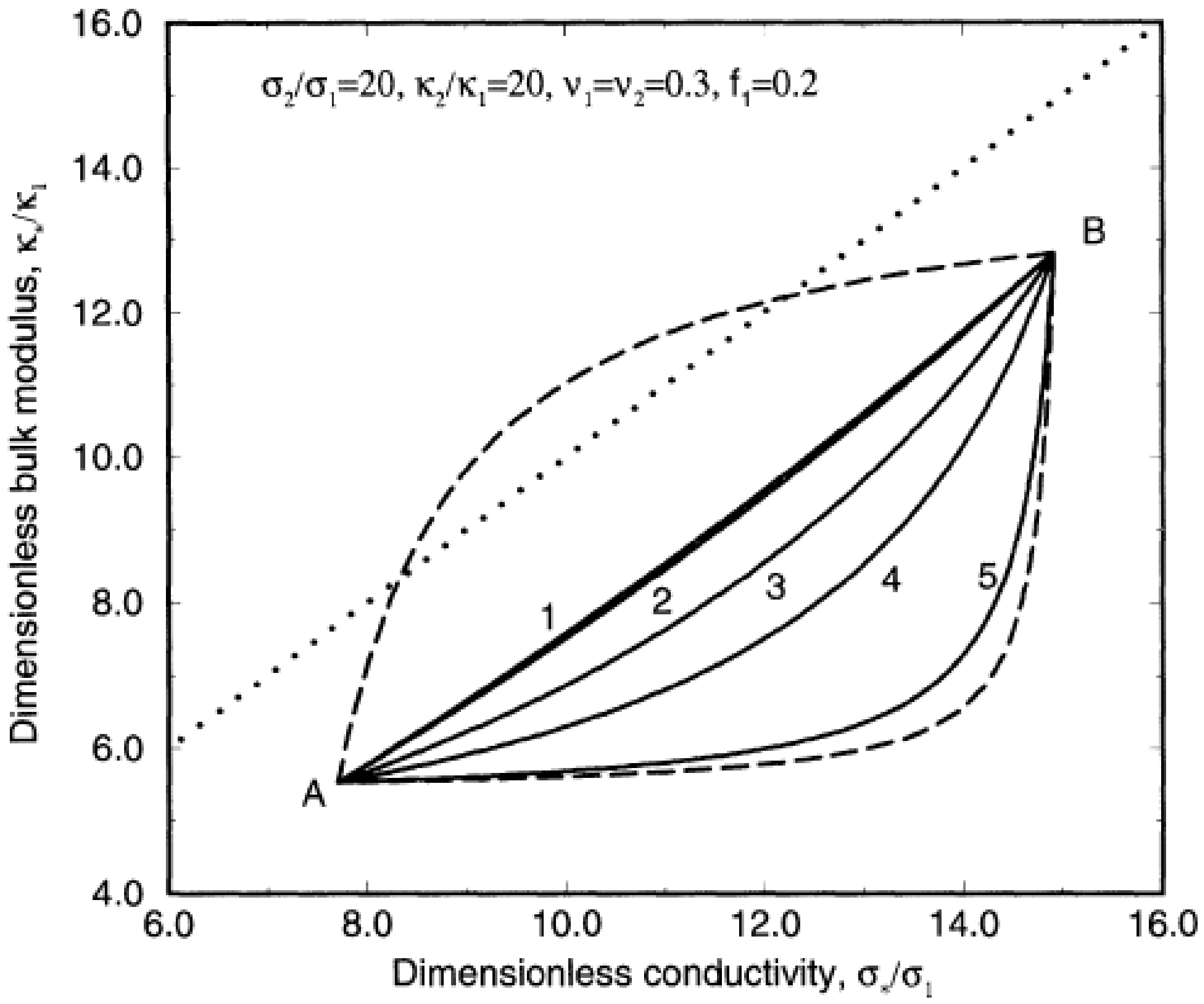
$$\underbrace{\begin{pmatrix} \mathbf{L}_1(\mathbf{x}) & 0 & 0 & \dots & 0 \\ 0 & \mathbf{L}_2(\mathbf{x}) & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \mathbf{L}_m(\mathbf{x}) \end{pmatrix}}_{\mathbf{L}(\mathbf{x})}$$

and seek bounds on the associated effective tensor

$$\underbrace{\begin{pmatrix} \mathbf{L}_1^* & 0 & 0 & \dots & 0 \\ 0 & \mathbf{L}_2^* & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \mathbf{L}_m^* \end{pmatrix}}_{\mathbf{L}^*}$$

# Example:

*L. V. Gibiansky and S. Torquato*




Proc.Roy.Soc. Lond. A, 452, 253-283 (1996)

There are many things I have not talked much about, including:

- Bounds for non-linear problems
- Bounds on the response of a body containing one or more inclusions (can be useful for the inverse problem of determining something about the inclusion)
- Bounds on the response in the time domain

***Thank-you for listening***