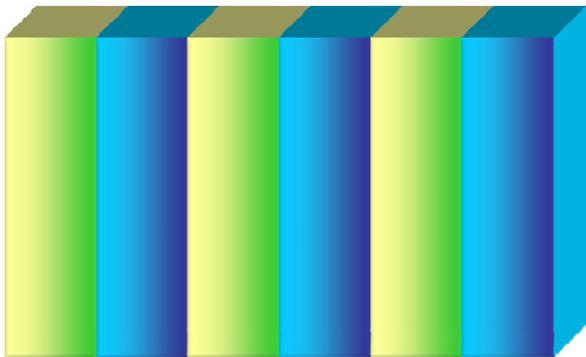# Novel phononic metamaterials for acoustic and thermal applications
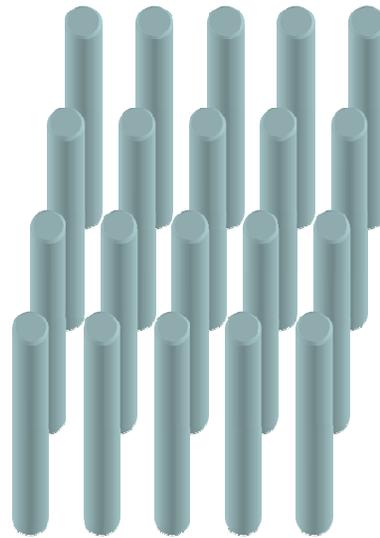
Krishna Muralidharan
Materials Science and Engineering
University of Arizona
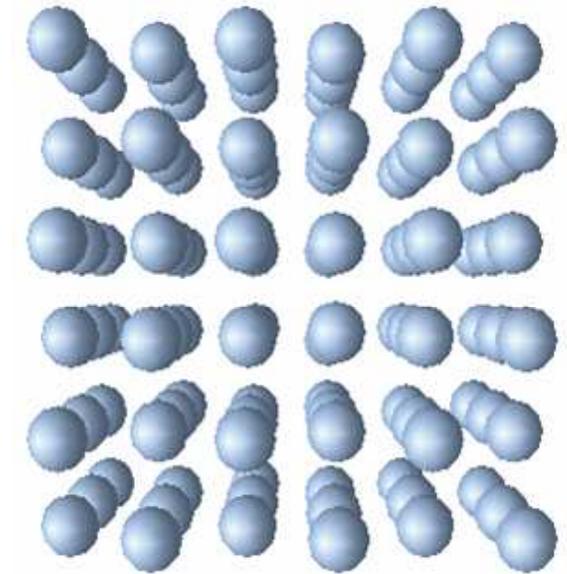
PHONONIC METAMATERIALS

• Artificially structured composite materials whose elastic constants and density are periodic functions of the position (1D, 2D, 3D)

1D: Multilayers materials

2D: Array of cylinders of circular, square, cross section embedded in a matrix

3D: Array of spherical, cubic,…inclusions embedded in a matrix

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PHYSICAL PARAMETERS

✍ **Constituents** : Solid/solid, fluid/fluid, mixed solid/fluid composites (Parameters: longitudinal and/or transverse speeds of sound, density)

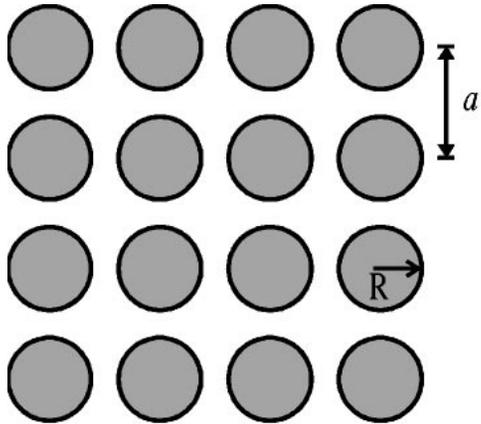✍ **Composition** : $f \equiv$ filling fraction of inclusions

✍ **Structure** : Geometry (Lattices: square array, triangular lattice, boron-nitride structure,…, lattice parameter, inclusion size and geometry).

Phononic Crystals

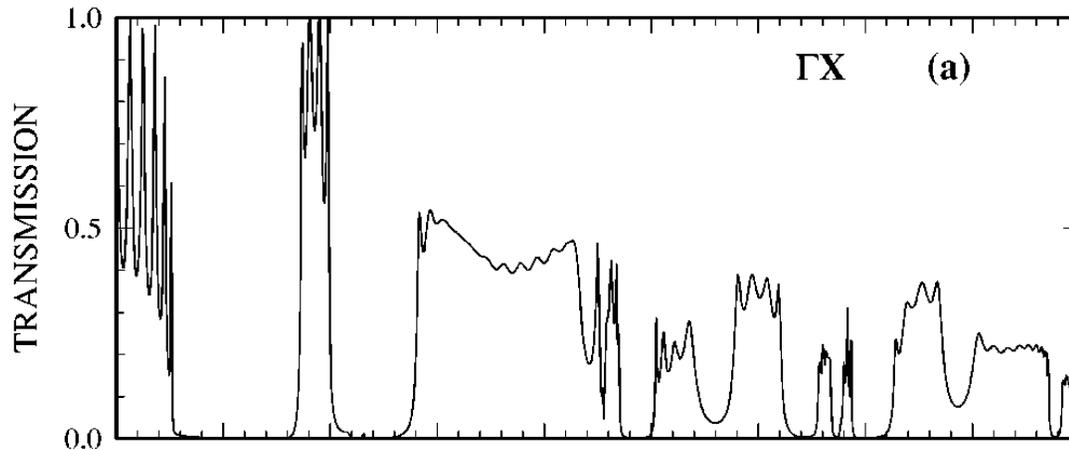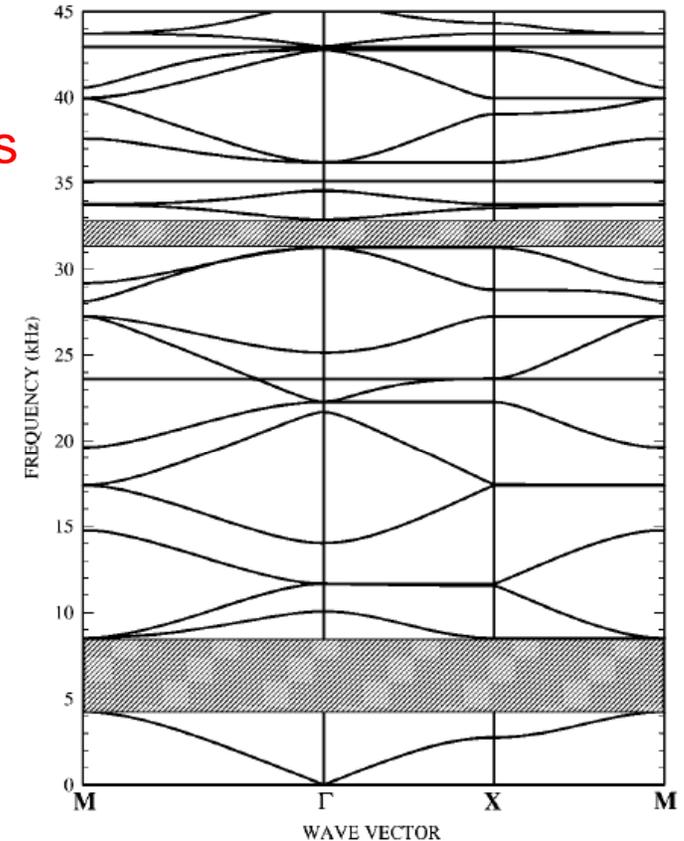d = Na = (a) 2.7155 nm   Ma = 1.6293 nm
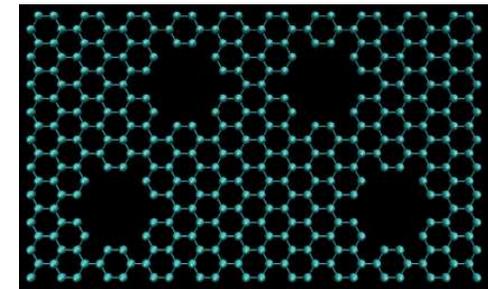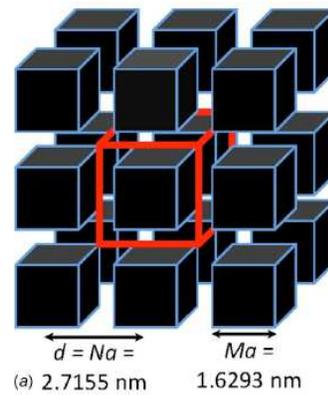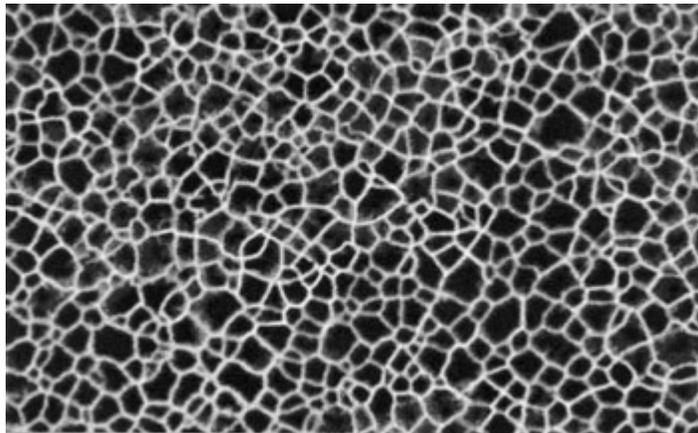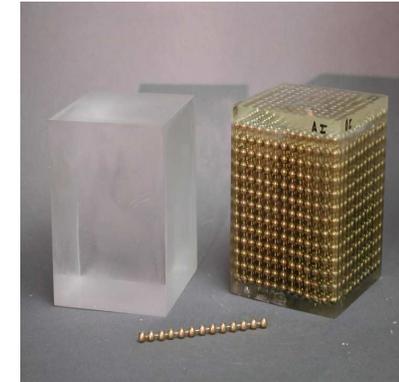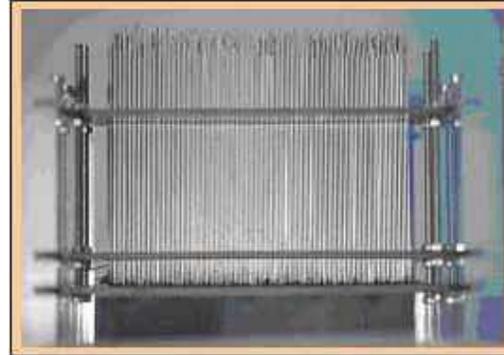
Early Work in Phononics

Bandgap Structures:

2-D structure with copper rods
- Bragg scattering

- **Ranges of certain frequencies cannot be transmitted.**
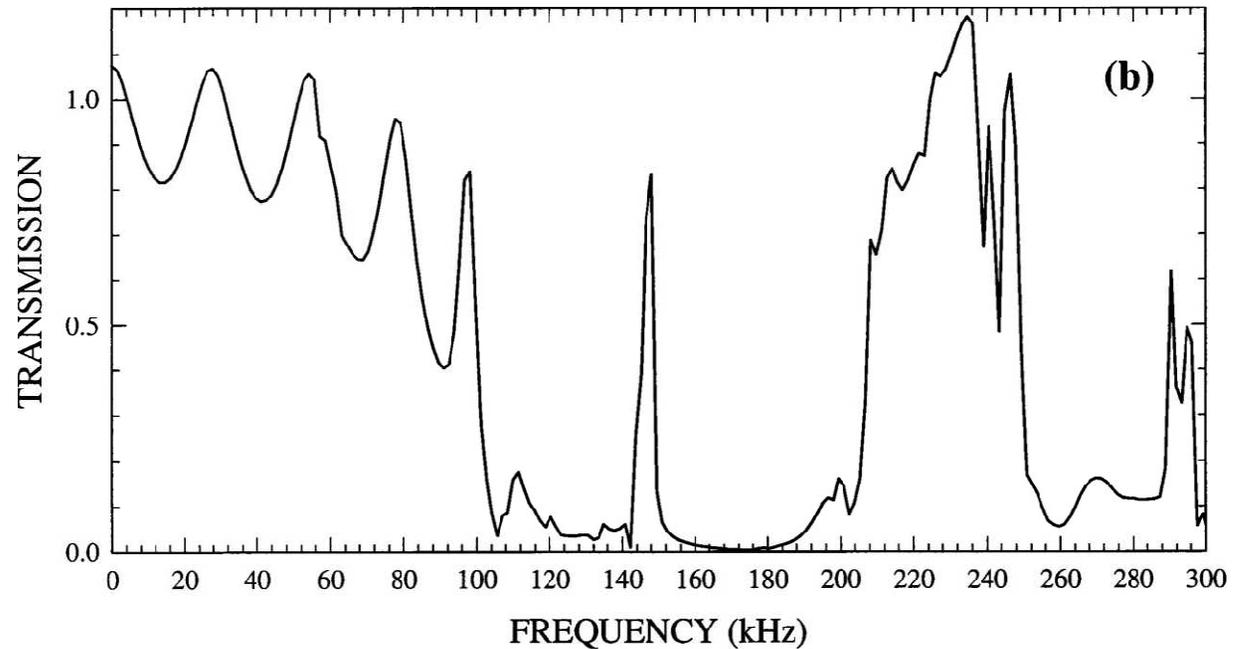
J.O. Vasseur, et. al, *Phys Rev E.* **65** (2002)

Early Work in Phononics

Waveguide Structures:

2-D structure with hollow steel rods

(a)

(b)

A. Khelif et. al, *Jour. Appl Phys,* **94,** 3. (2003)
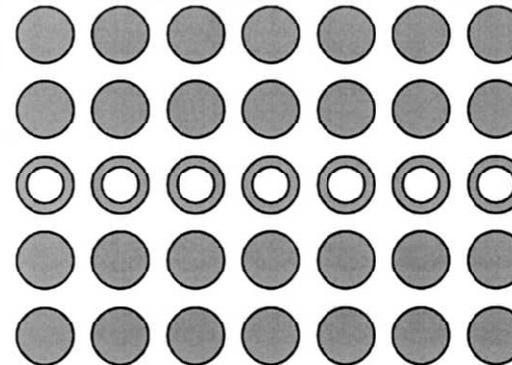
Phononic Metamaterials: Current Strategy

Novel utilization of real/k-space functionality of metamaterials
- refractive properties
- spatial scaling: macro to nano functionalities
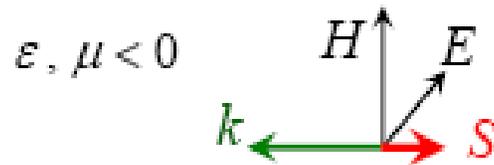- using Bragg scattering

To ensure real space control of phononic propagation over a broad spectral range (acoustic to atomic-vibrations)

➢ **Superlensing: Acoustic imaging**
➢ **Acoustic collimation**
➢ **Thermal interface materials (TIM): Ballistic phonon transport**
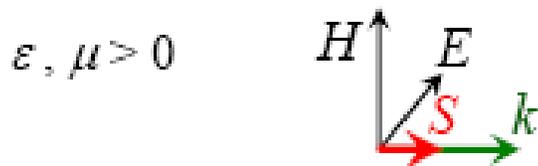➢ **Thermoelectrics (TE)**

Negative refraction-Left-handed materials

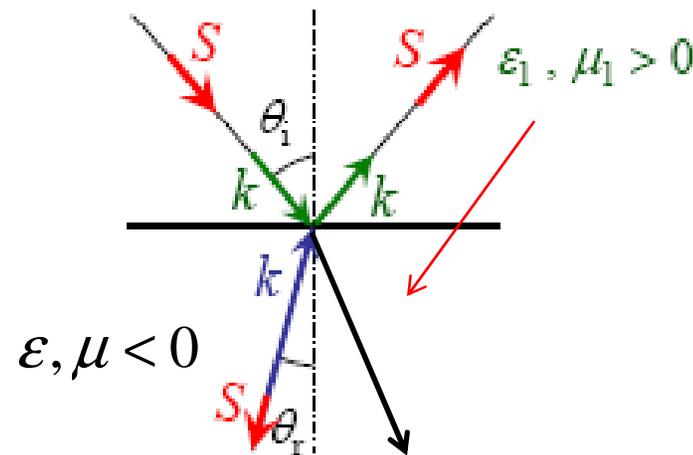Left-Handed Materials (LHMs) were considered by Veselago[1]

Left-Handed materials: k and S are in opposite directions

$\varepsilon, \mu < 0$

Right-Handed materials: k and S are in the same direction

$\varepsilon, \mu > 0$

Veselago[1] also predicted the unusual phenomenon of negative refraction:
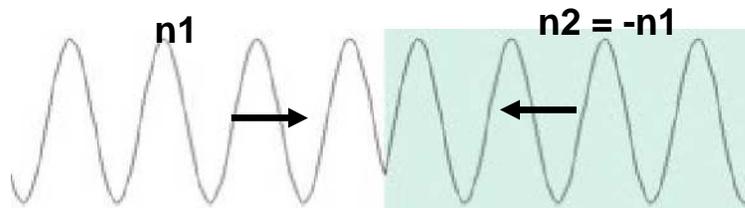
$\varepsilon_1, \mu_1 > 0$

$\varepsilon, \mu < 0$

[1] V. G. Veselago, Sov. Phys. Usp. 92, 517 (1964)

Negative refraction in phononic metamaterials:
1. Bragg scattering (phononic crystals)
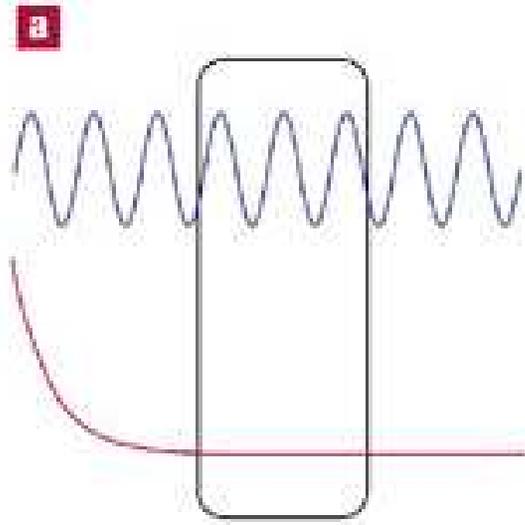2. Locally resonant materials ($\rho < 0$, $C_{ij} < 0$)

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n < 0

n > 0

Negative Refraction

Positive Refraction

continuum

dispersive
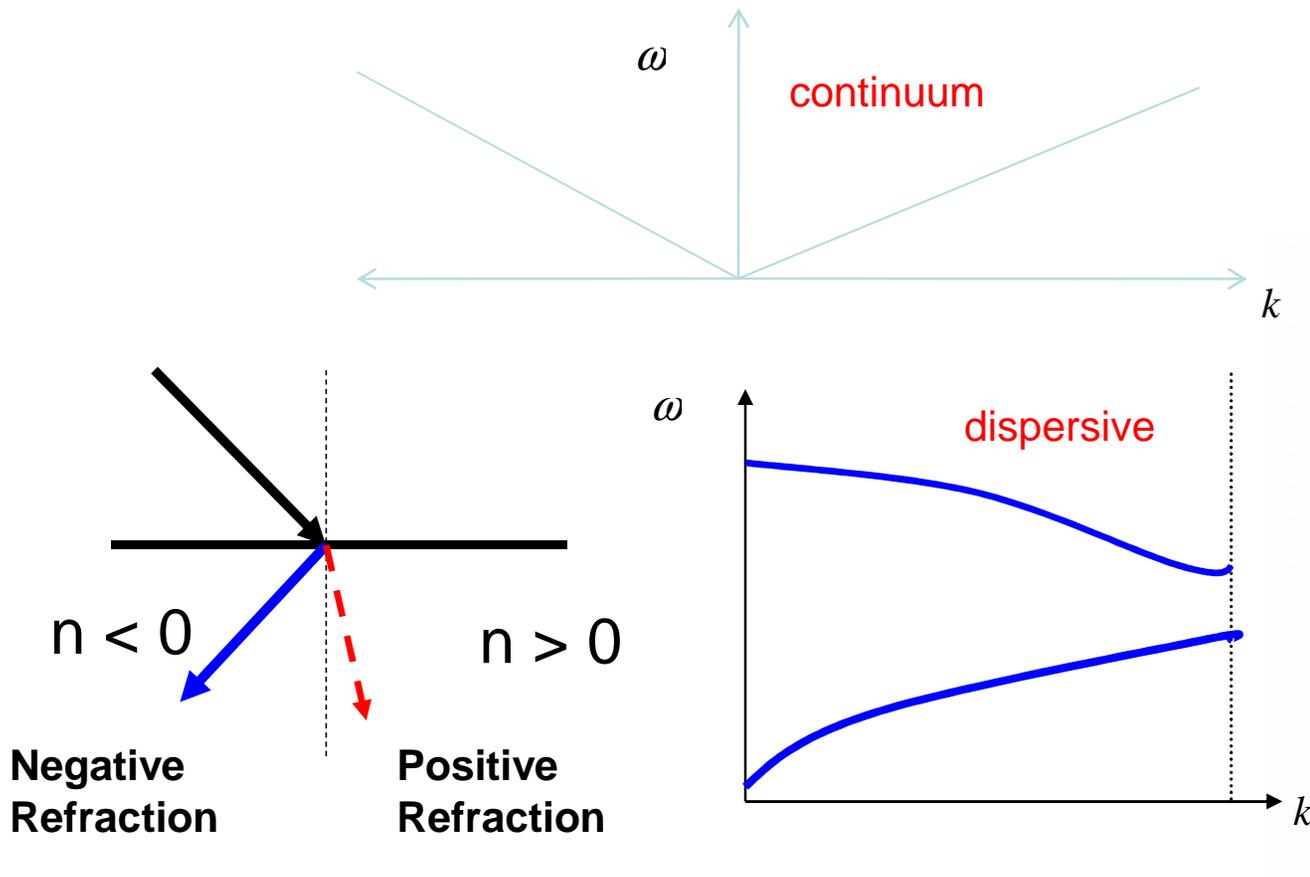
Bands of **negative slope** represent frequencies at which **negative refraction** will occur.

n1

n2 = -n1

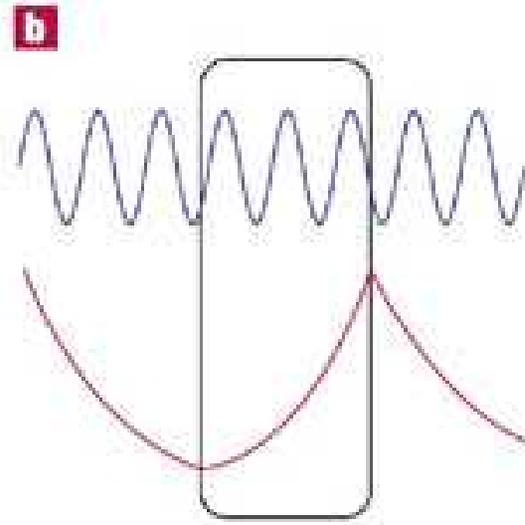*However: Energy still flows to the right.

Phononic Crystal Super Lens

Conventional Lens

(Loss of Evanescent Component)
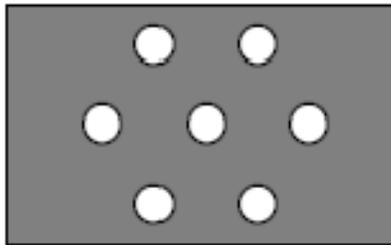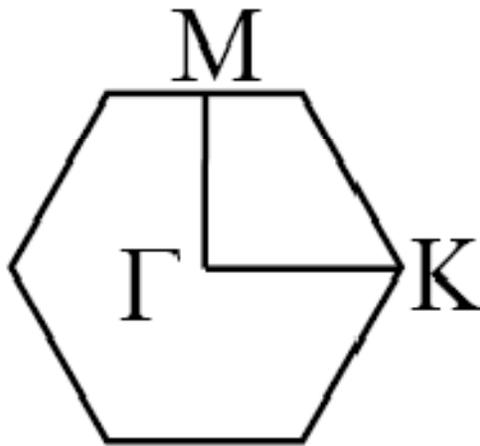
Diffraction limit = λ/2

Near-Field Super Lens

(Amplification of Evanescent Component)

Solid-fluid phononic crystal with negative refraction

Steel cylindrical inclusions in fluids (methanol)

Inter-cylinder spacing (a)=1.27mm,
Cylinder diameter=1.02mm
Steel:
Density= 7780kg/m^3
Longitudinal speed of sound=5825m/s
Transverse speed of sound=3227m/s
Methanol:
Density=790kg/m^3
Speed of sound=1138m/s

Experimental and Theoretical Evidence for Subwavelength Imaging in Phononic Crystals

A. Sukhovich,[1] B. Merheb,[2] K. Muralidharan,[2] J. O. Vasseur,[3] Y. Pennec,[3] P. A. Deymier,[2] and J. H. Page[1]
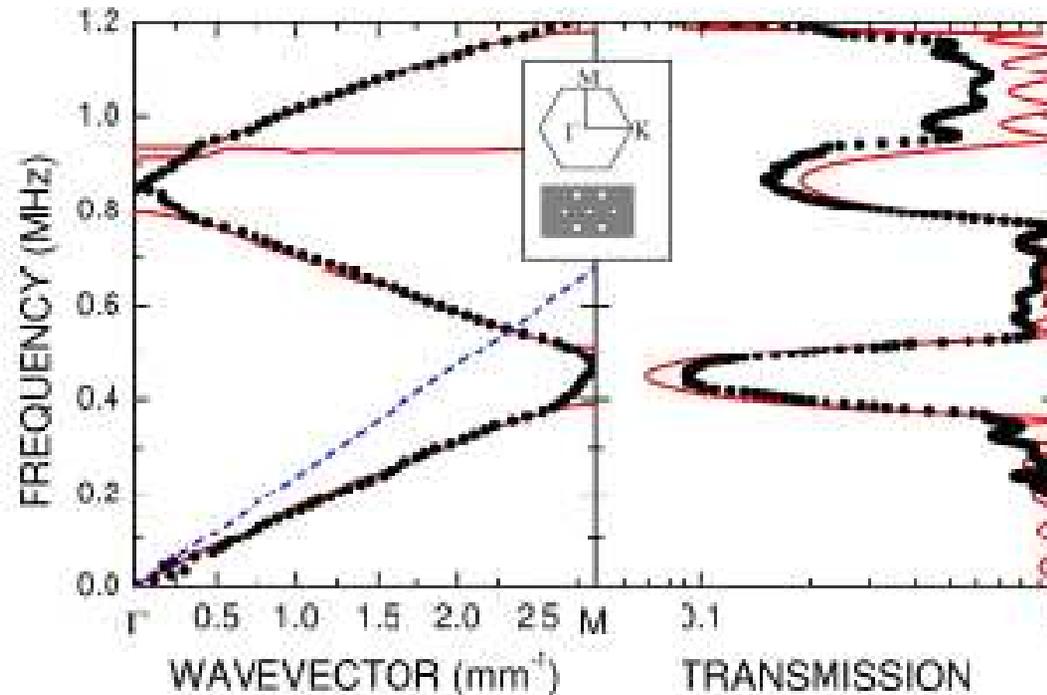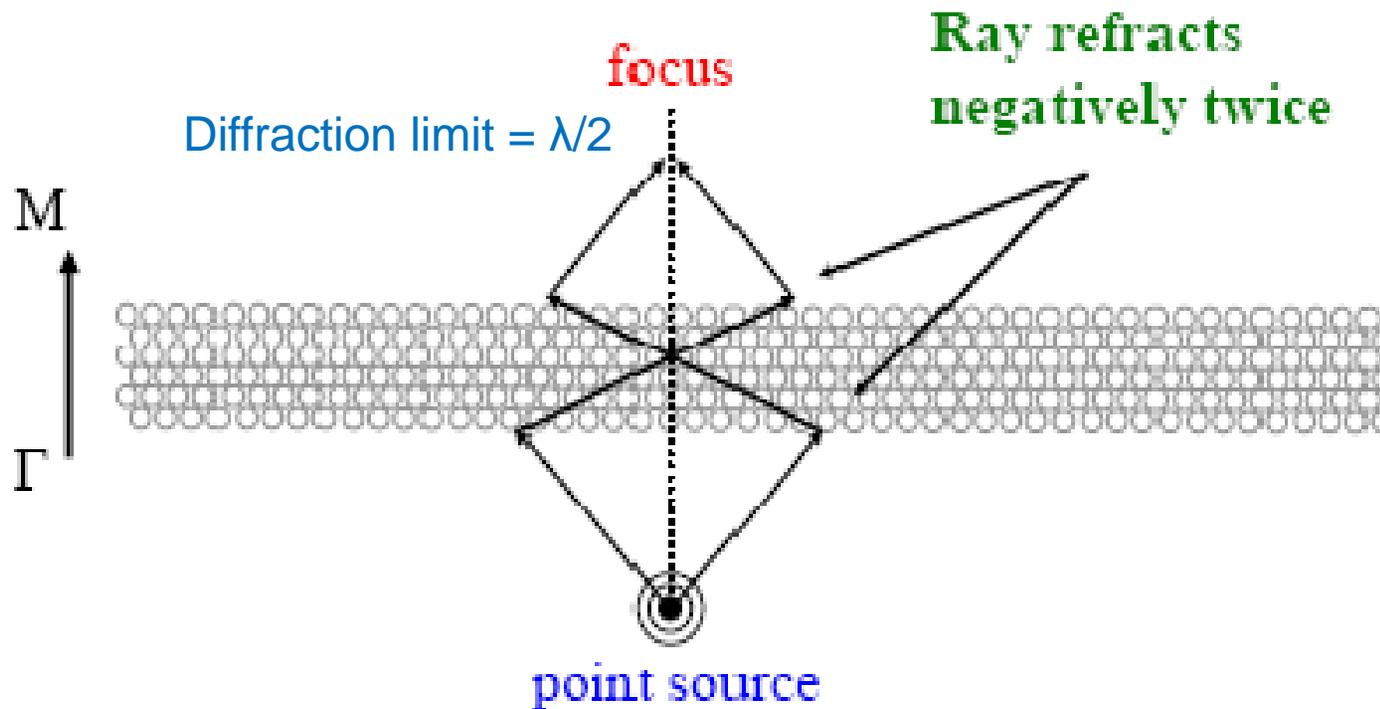
11

Methanol/Steel phononic crystal

FIG. 2: Band structure of the methanol-steel phononic crystal in the ΓM direction of the first Brillouin zone (left panel) and transmission coefficient for a 8-layer crystal along the same direction (right panel): symbols, experimental data; solid red lines, FDTD calculation; dashed blue line, homogeneous water. The inset illustrates the phononic crystal structure and the associated first Brillouin zone.

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Sound focusing in phononic crystal

Ray refracts
negatively twice

focus

Diffraction limit = $\lambda/2$

M

Γ

point source

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FDTD method

- Discretize space $dx=dy=2 \times 10^{-5}$m
- X axis parallel to flat lens
- Z axis perpendicular to flat lens
- Absorbing Boundary Conditions in all directions

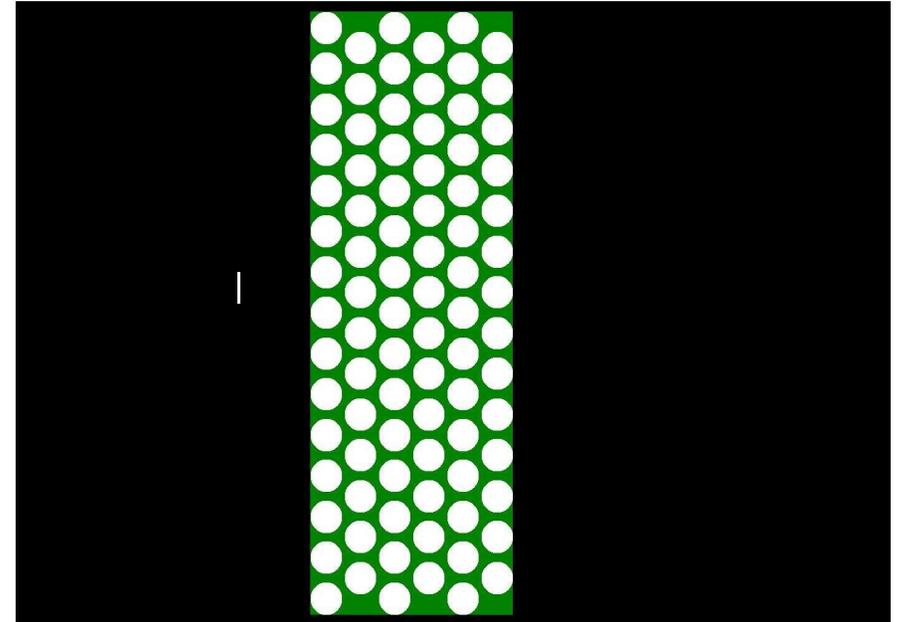Line source as a model of the pinducer:
along a line 0.55mm long // x axis:
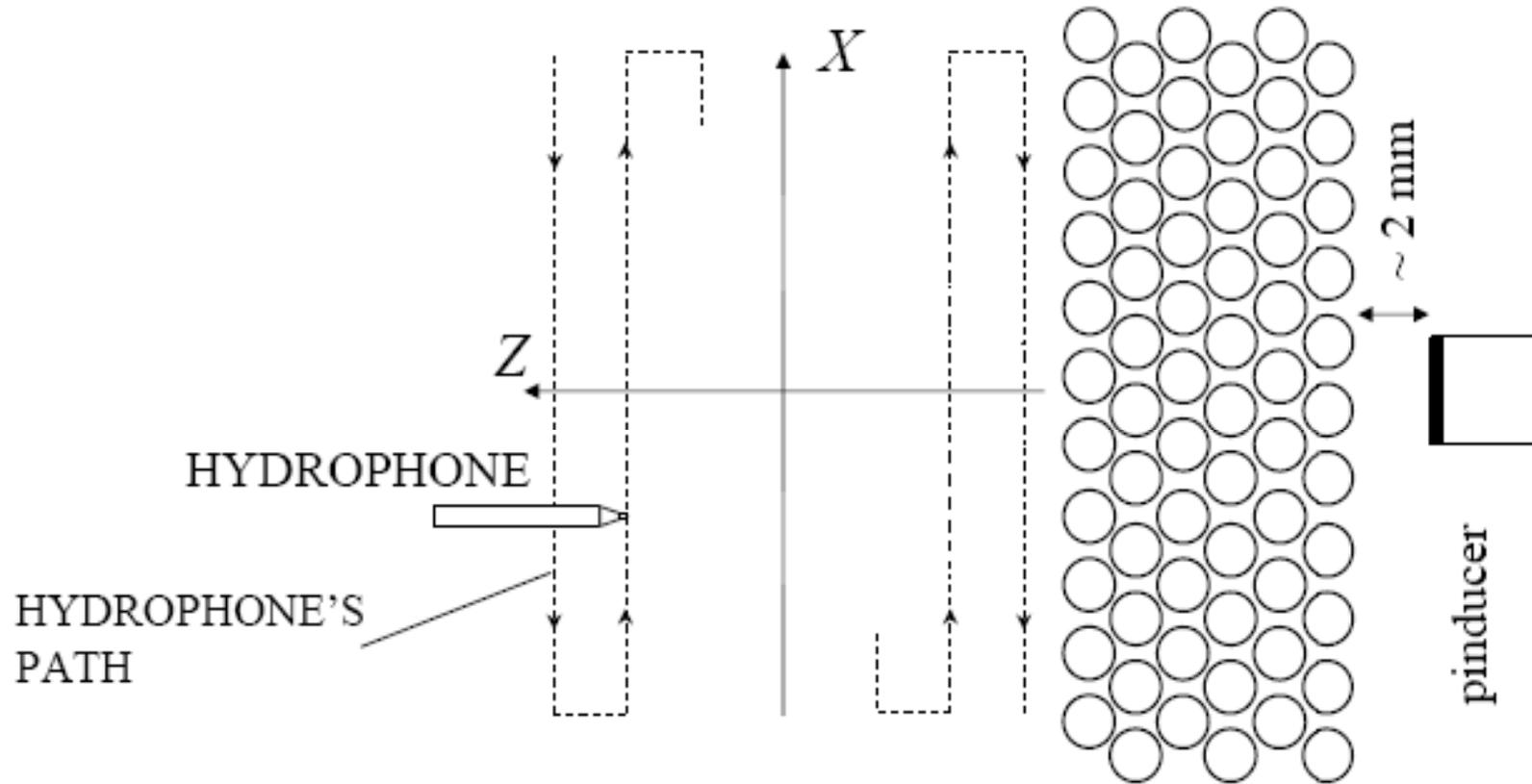
$$u_x = u_x + \cos(\omega t)$$
$$u_z = u_z + \cos(\omega t)$$

Lateral length $= 60a$

Distance of source to lens=1.6 or 0.1mm
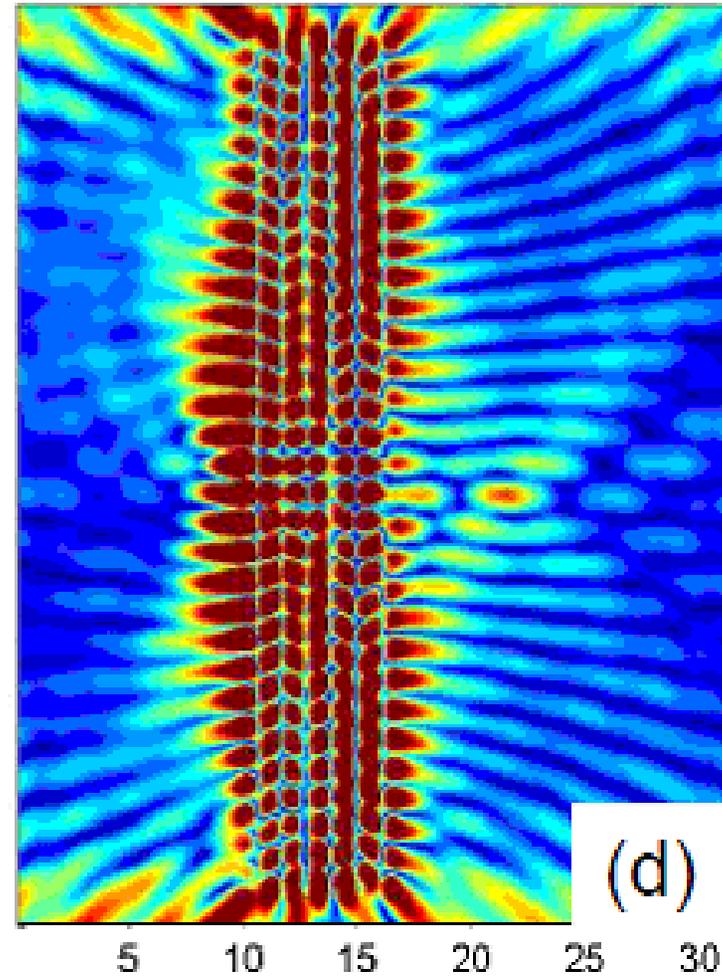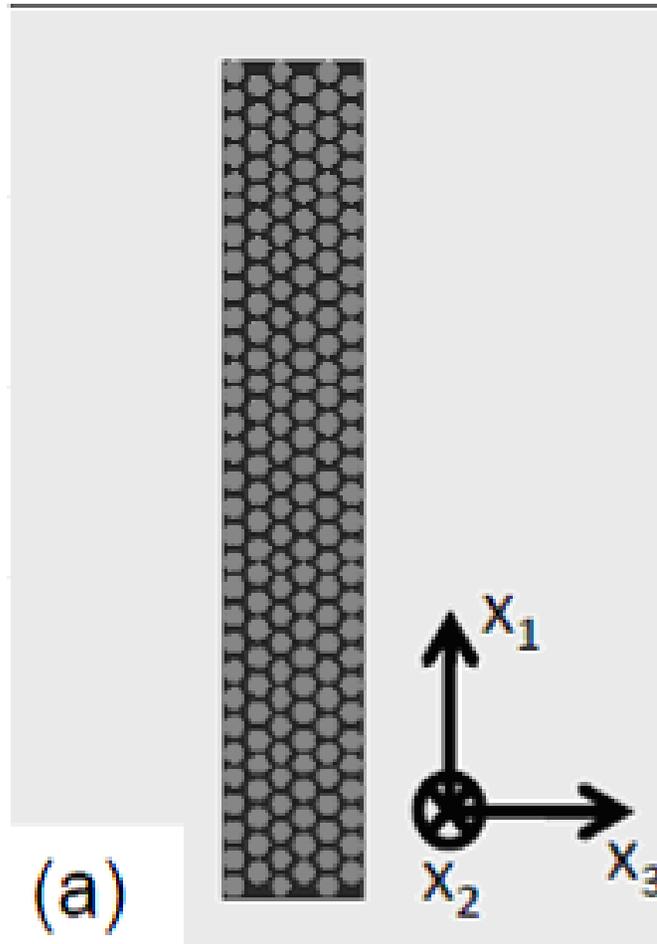
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Experimental measurements

~2 mm

pinducer

X

Z

HYDROPHONE

HYDROPHONE'S PATH

Lens immersed in water

15

Phononic Crystal Super Lens

(a)

X_1
X_2
X_3

(d)

5   10   15   20   25   30

0.35 Lambda

(b)

Amplitude (a.u.)

0.4
0.3
0.2
0.1
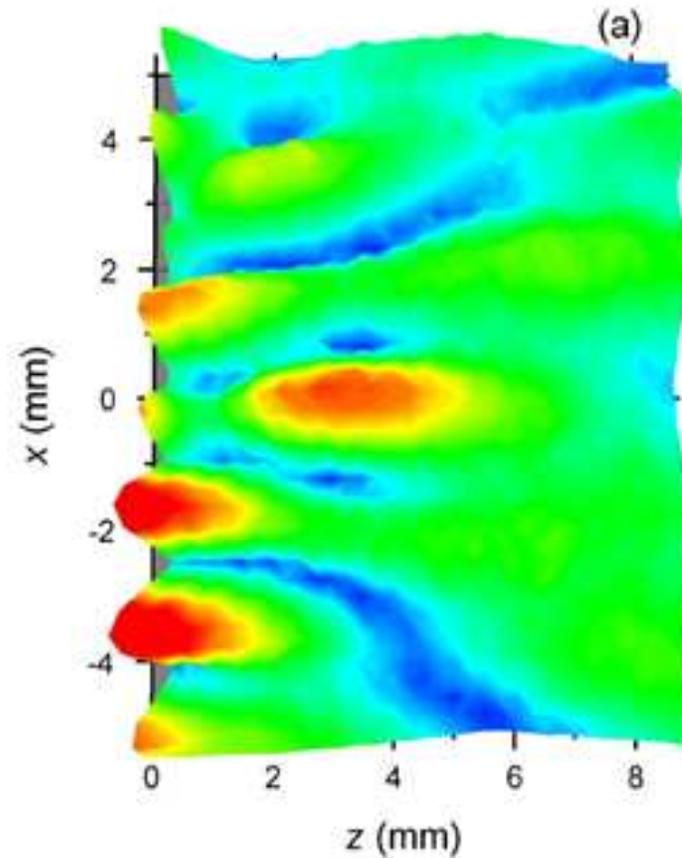0.0

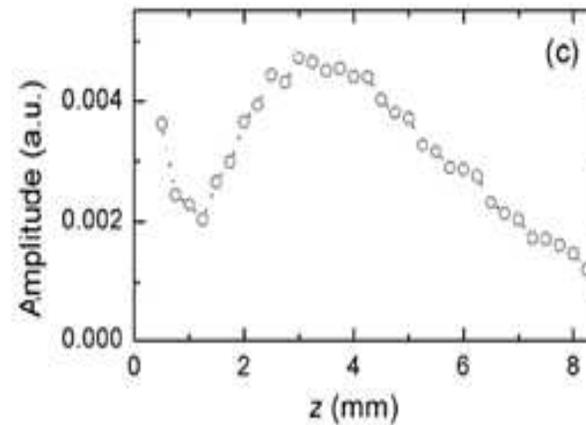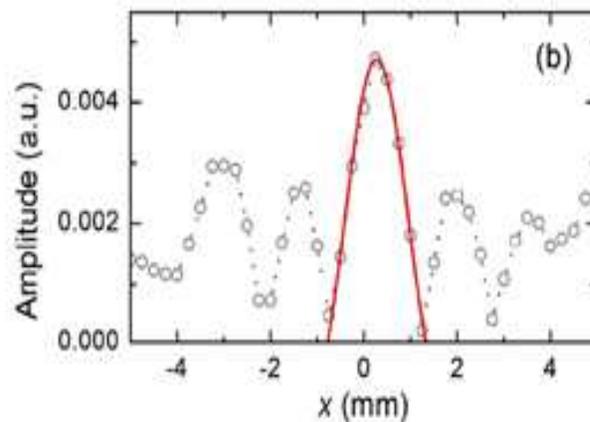-4   -2   0   2   4

x (mm)
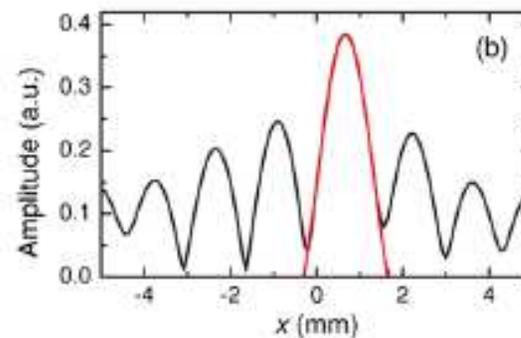
Band Structure Calculations
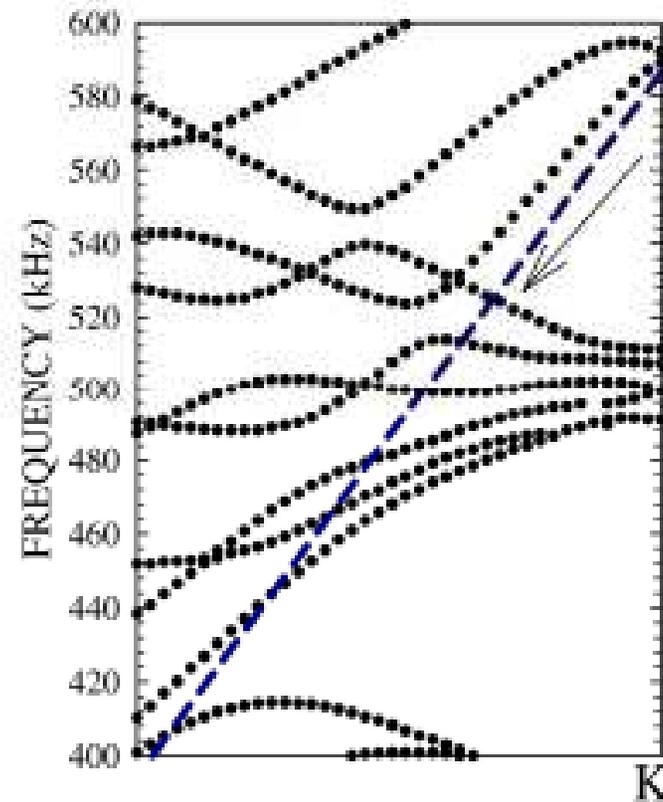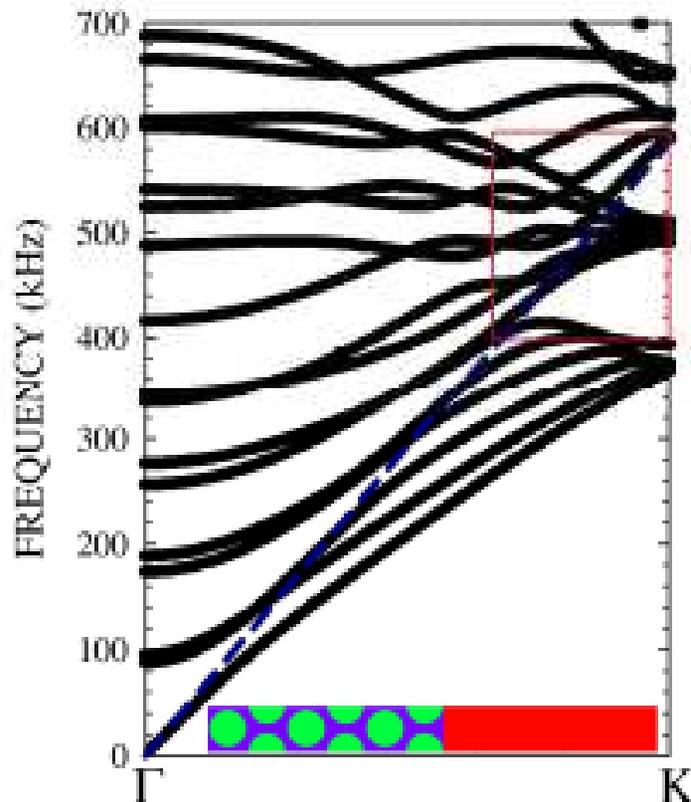
- Evanescent components excite the bound modes of the crystal, leading to its amplification.

Experimental Validation
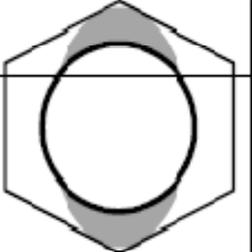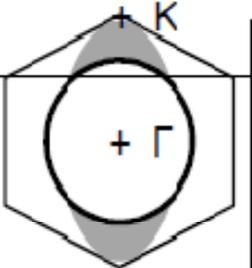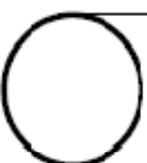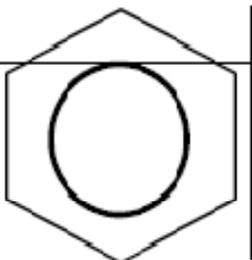

Resolution = 0.37 λ

Operation Frequency

Water	PC	Water	Freq. (kHz)	Resol.	Position (mm)
			515	0.34 λ	2.56
	+K / +Γ		530	0.35 λ	4.80
			545	0.47 λ	5.84
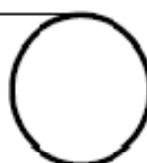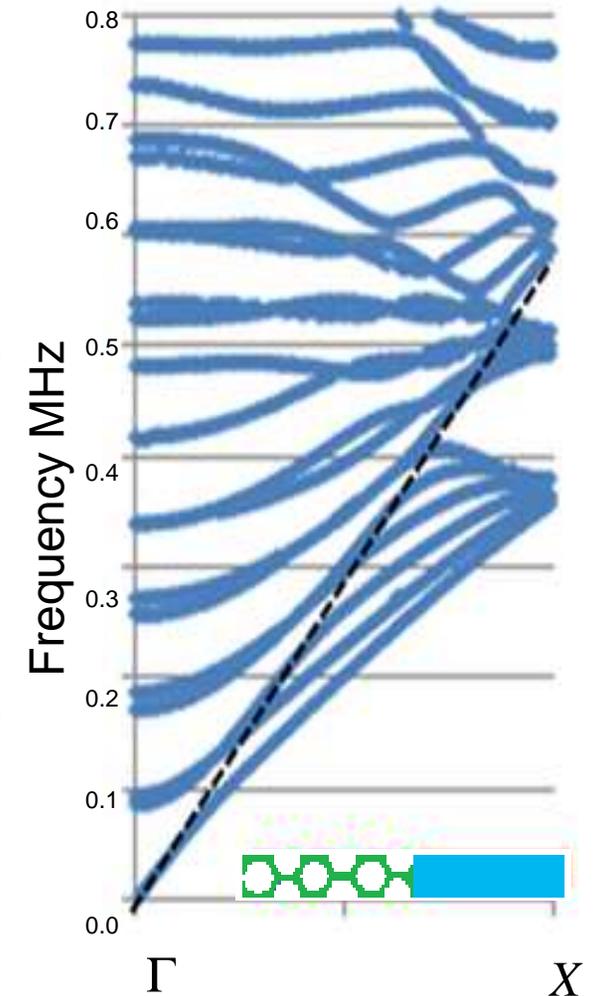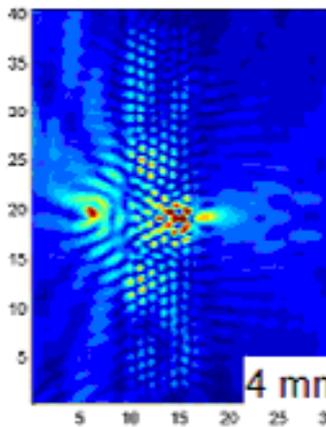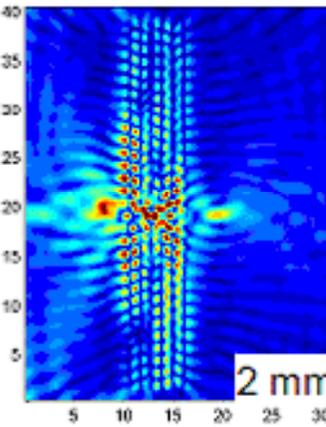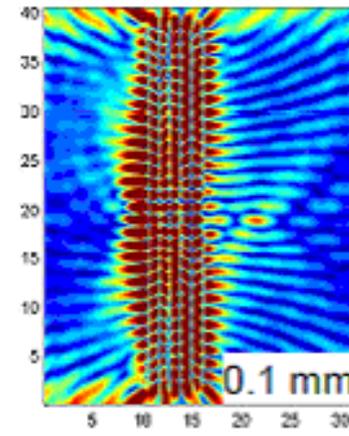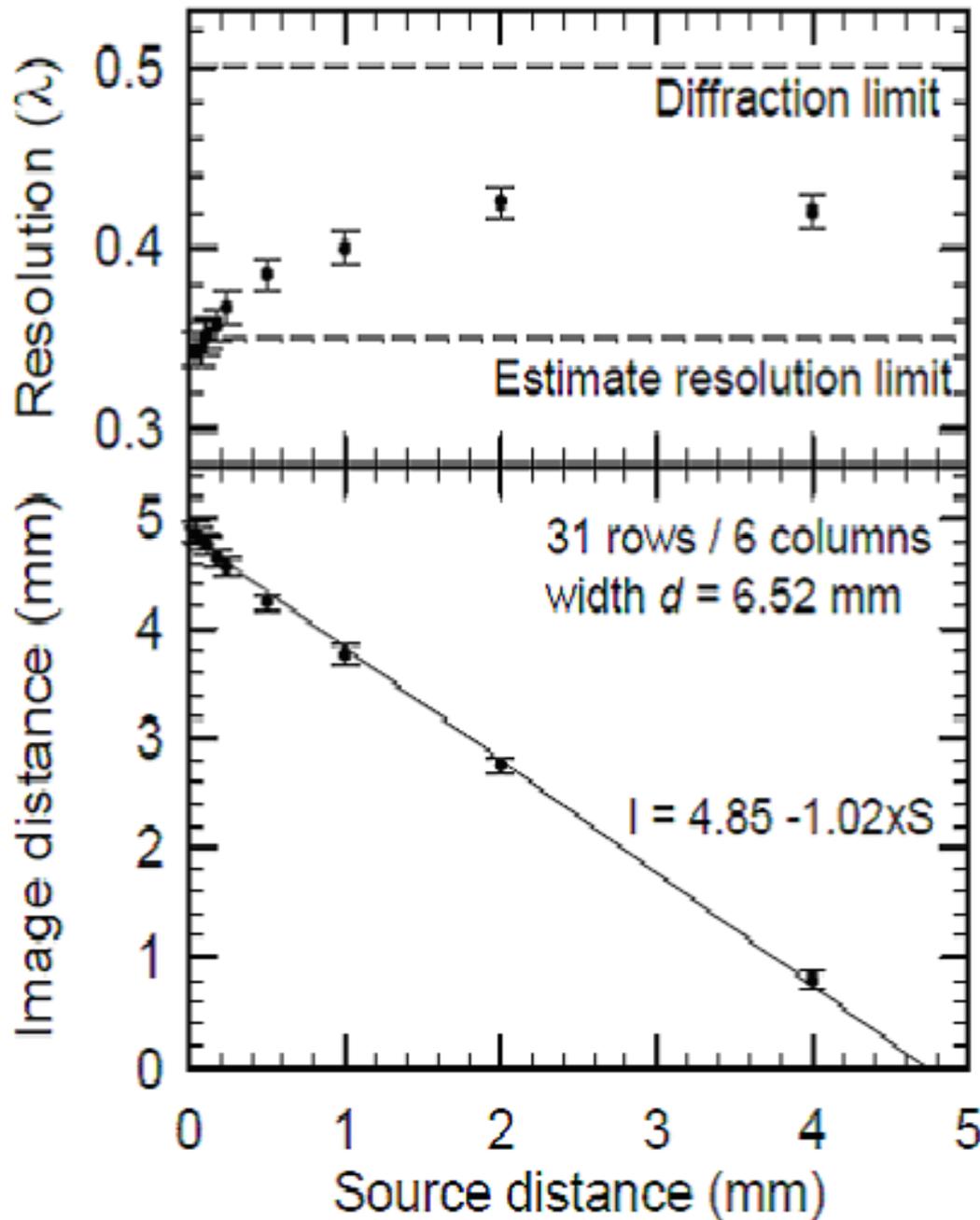
Time dependent Resolution
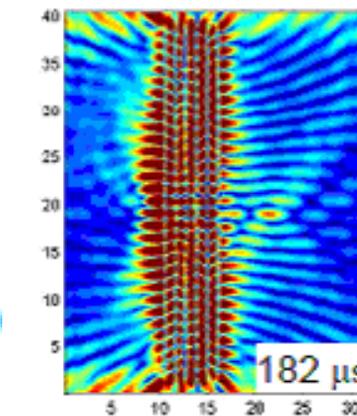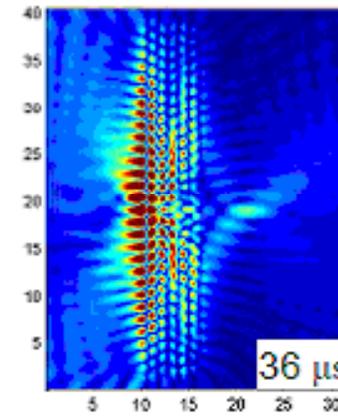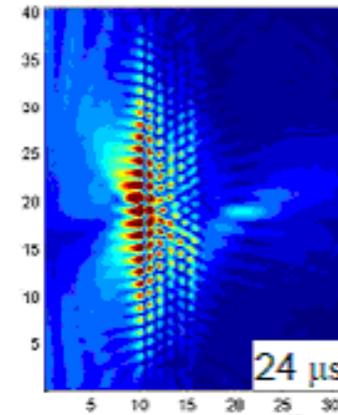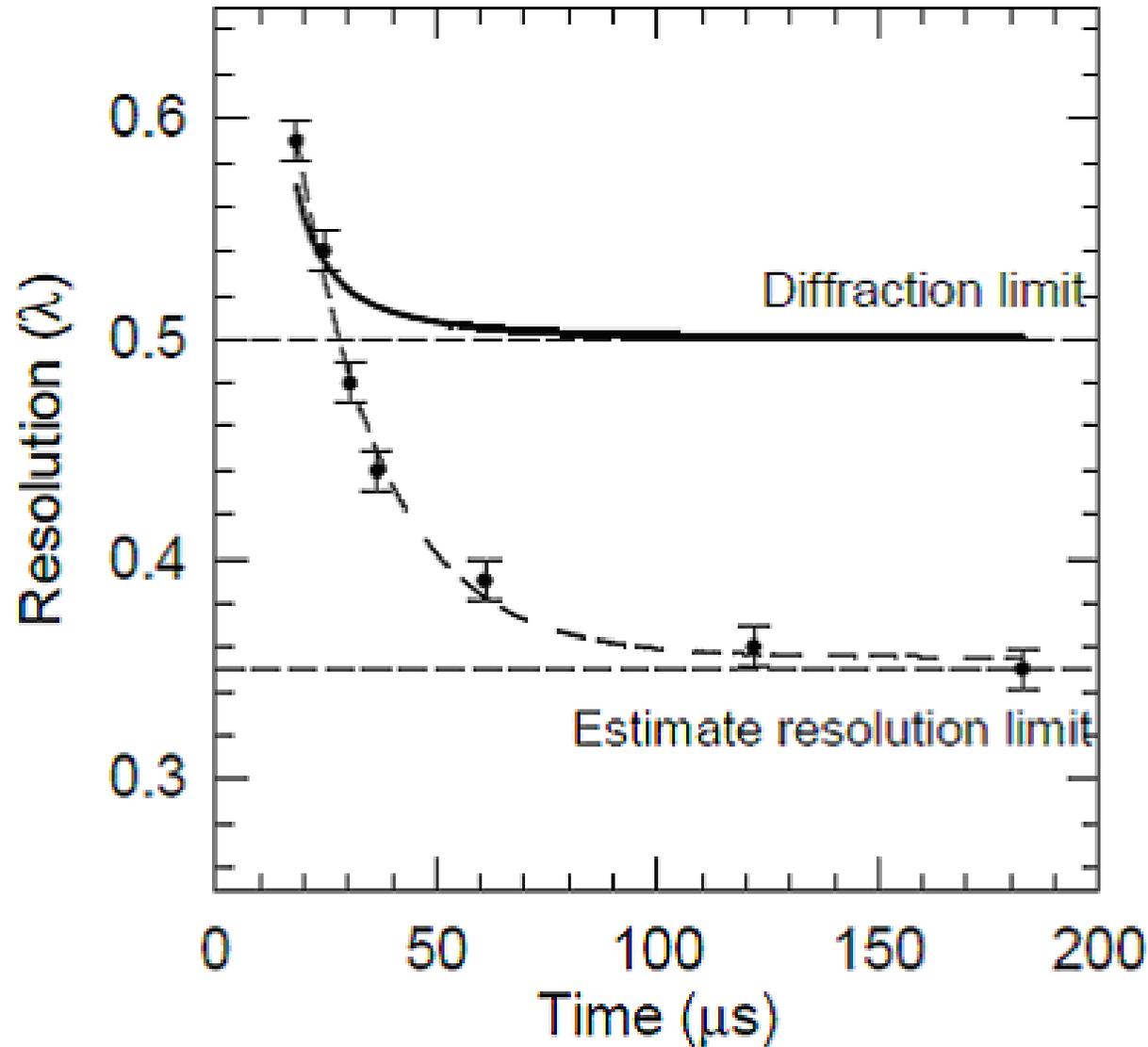
Rubber/Steel/Water Phononic Crystal

	$\rho(kg/m^3)$	$C_l(m/s)$	$C_t(m/s)$
Rubber	1000	1200	20
Water	1000	1490	0
Steel	7780	5825	3227
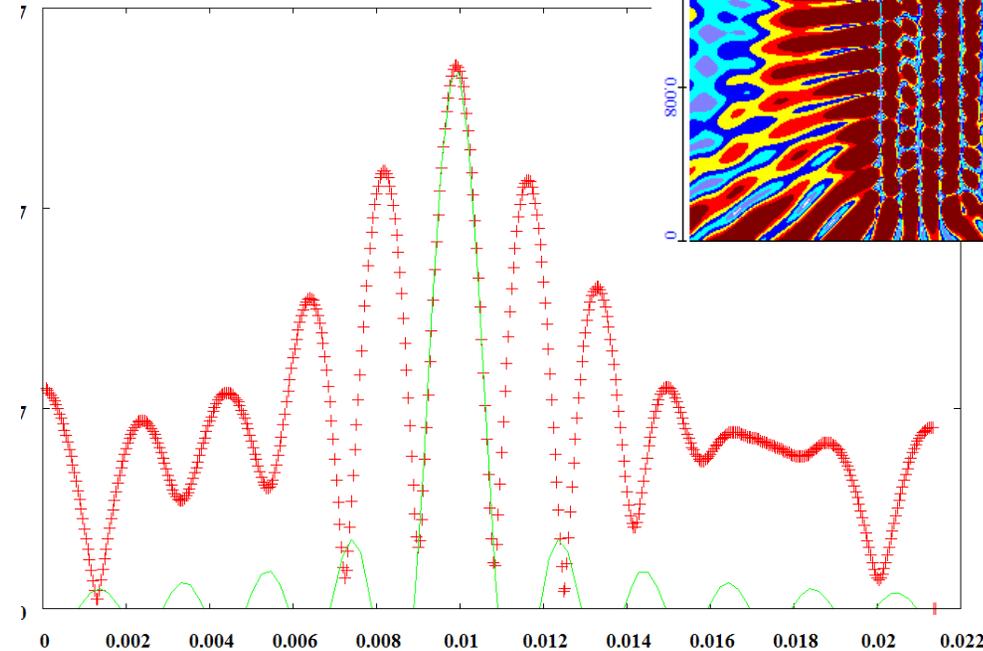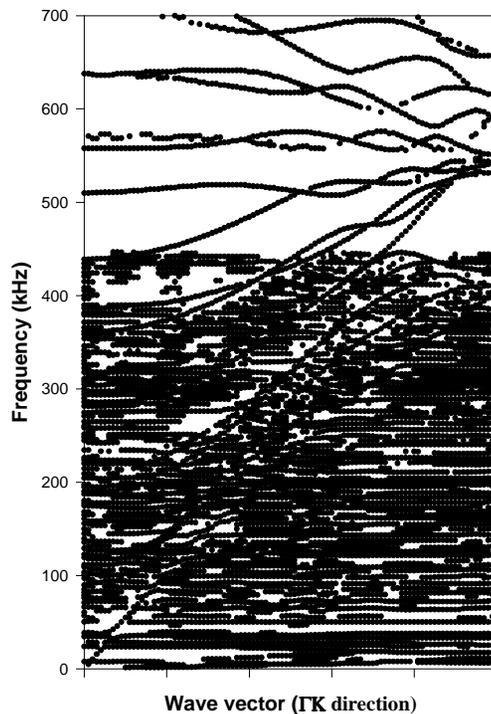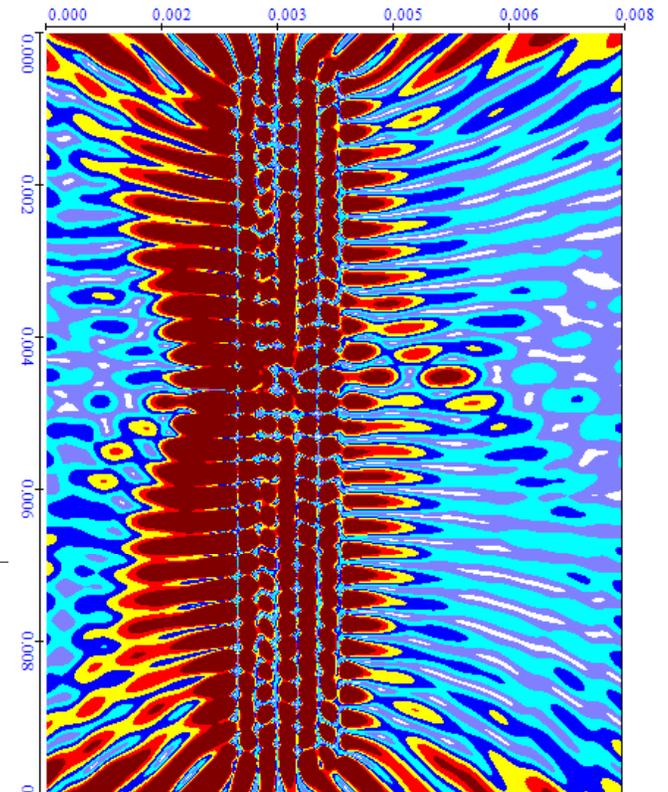
Resolution = 0.35 λ

PVC-Air crystal

- PVC cylindrical inclusions (r=12.9mm)
- Air Matrix
- Square lattice (a = 27mm)
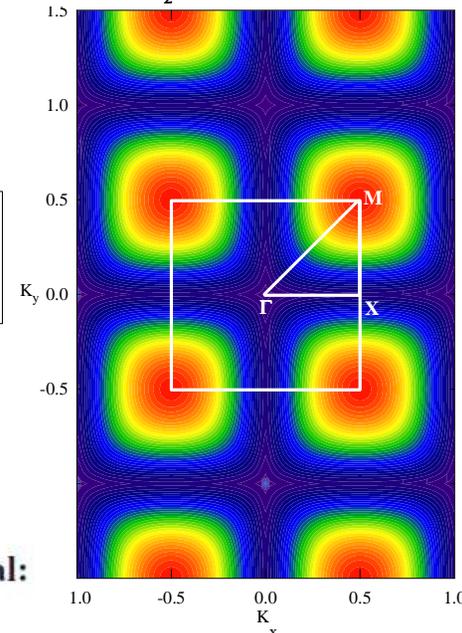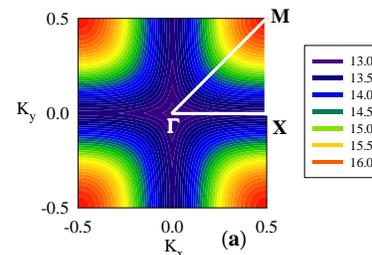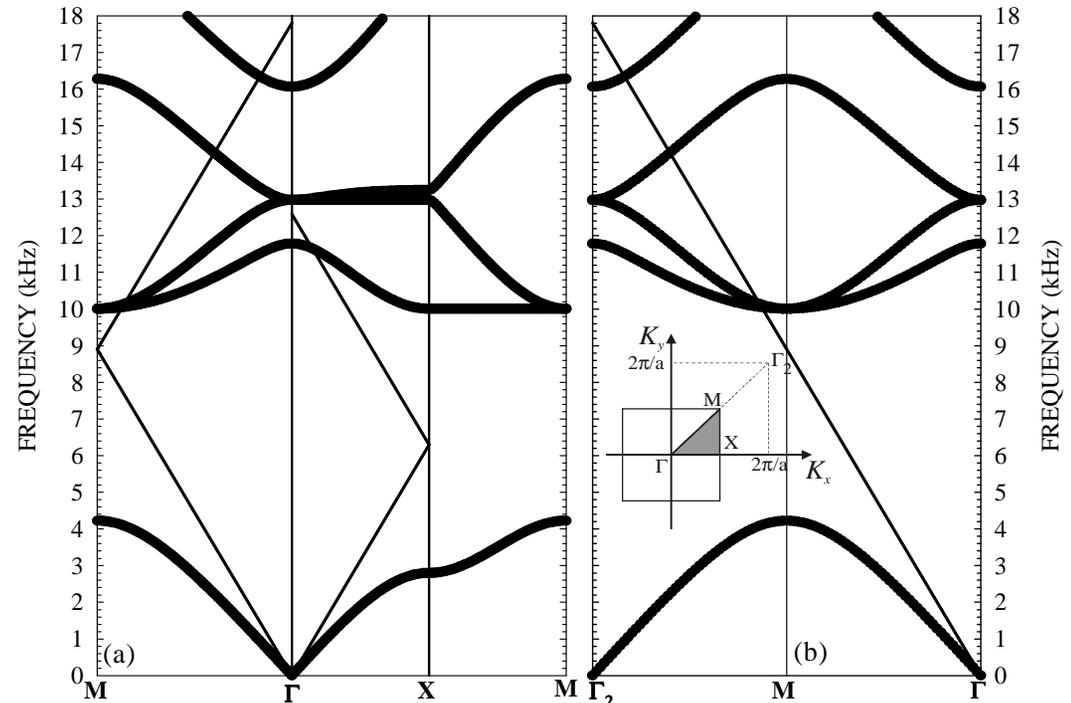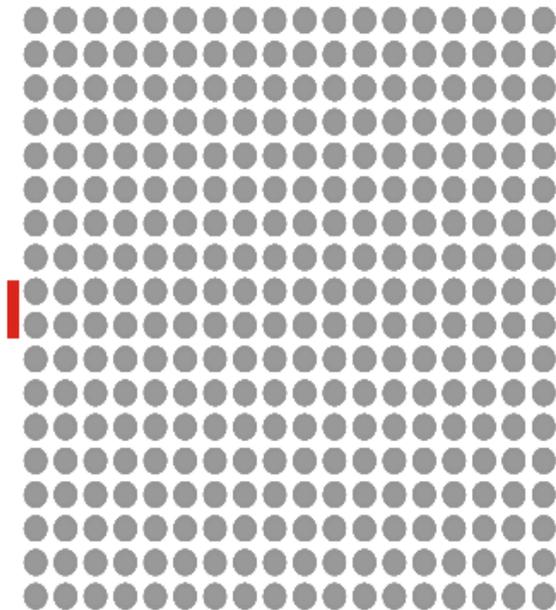
Positive, negative, zero refraction, and beam splitting in a solid/air phononic crystal: Theoretical and experimental study

J. Bucay,[1] E. Roussel,[2] J. O. Vasseur,[2] P. A. Deymier,[1] A-C. Hladky-Hennion,[2] Y. Pennec,[2] K. Muralidharan,[1]

Frequency contours: 4th band
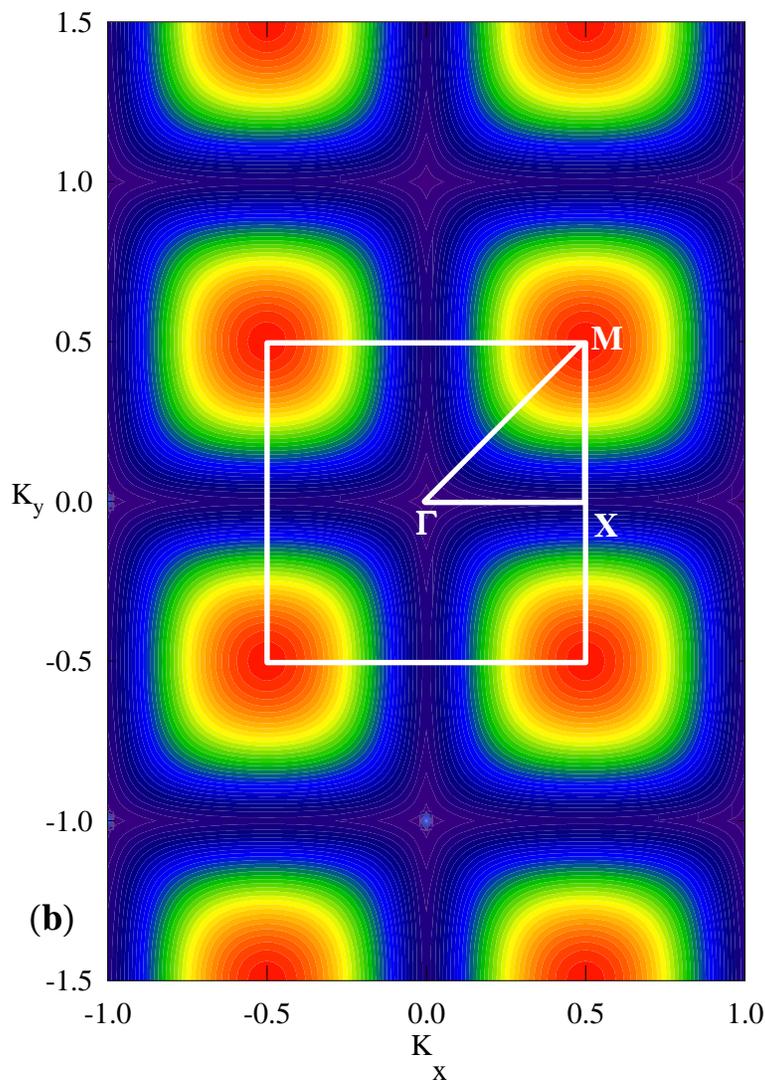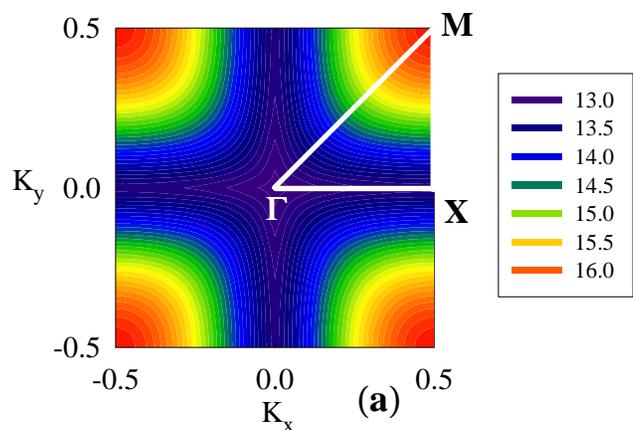
Figure : Equifrequency surface corresponding to the fourth band in the first Brillouin zone (a) and in an extended zone scheme (b). The EFS of the PC calculated inside the first Brillouin zone (a) has been repeated by a large number of translations of the reciprocal vectors. One notes that in the extended zone scheme, the EFS are centered on the M point and are of square shape except at their corners.

Positive, Negative, and Zero-angle Refraction
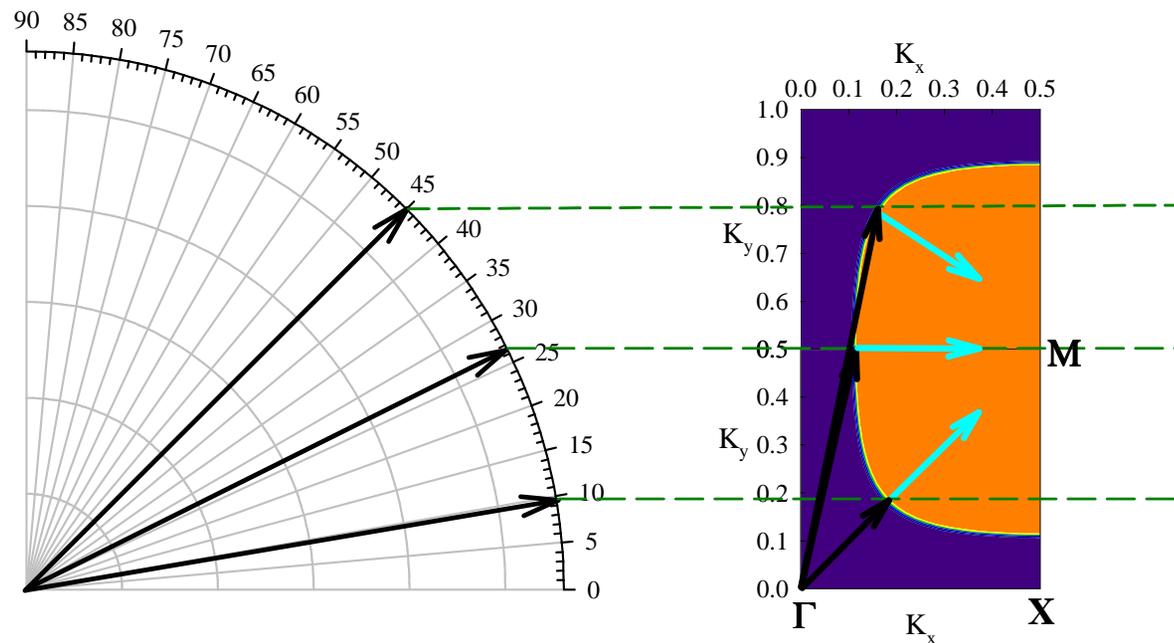
✓ **Collimation of waves**

Beam Splitting

Air

PC

Air
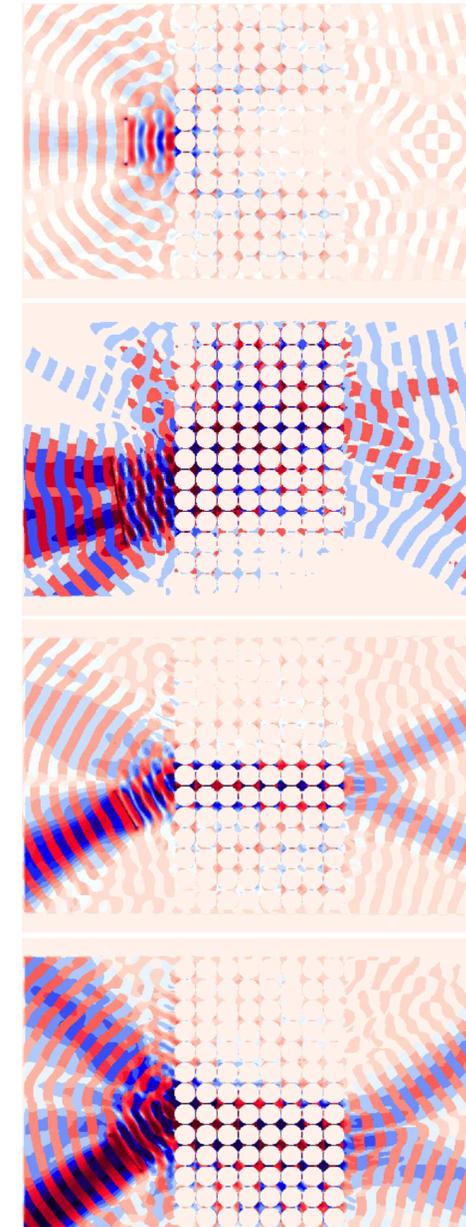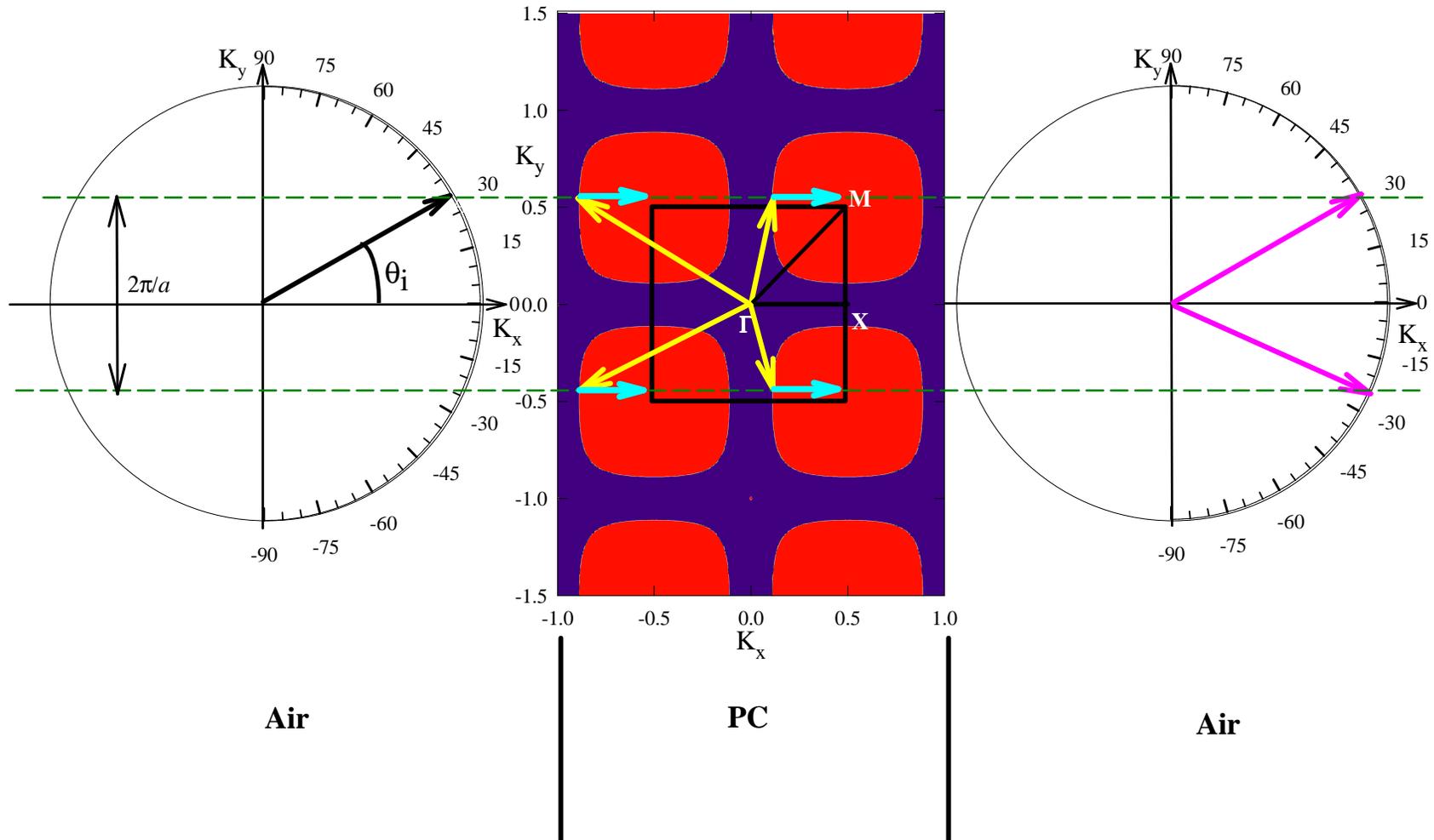
Validation of Beam Splitting
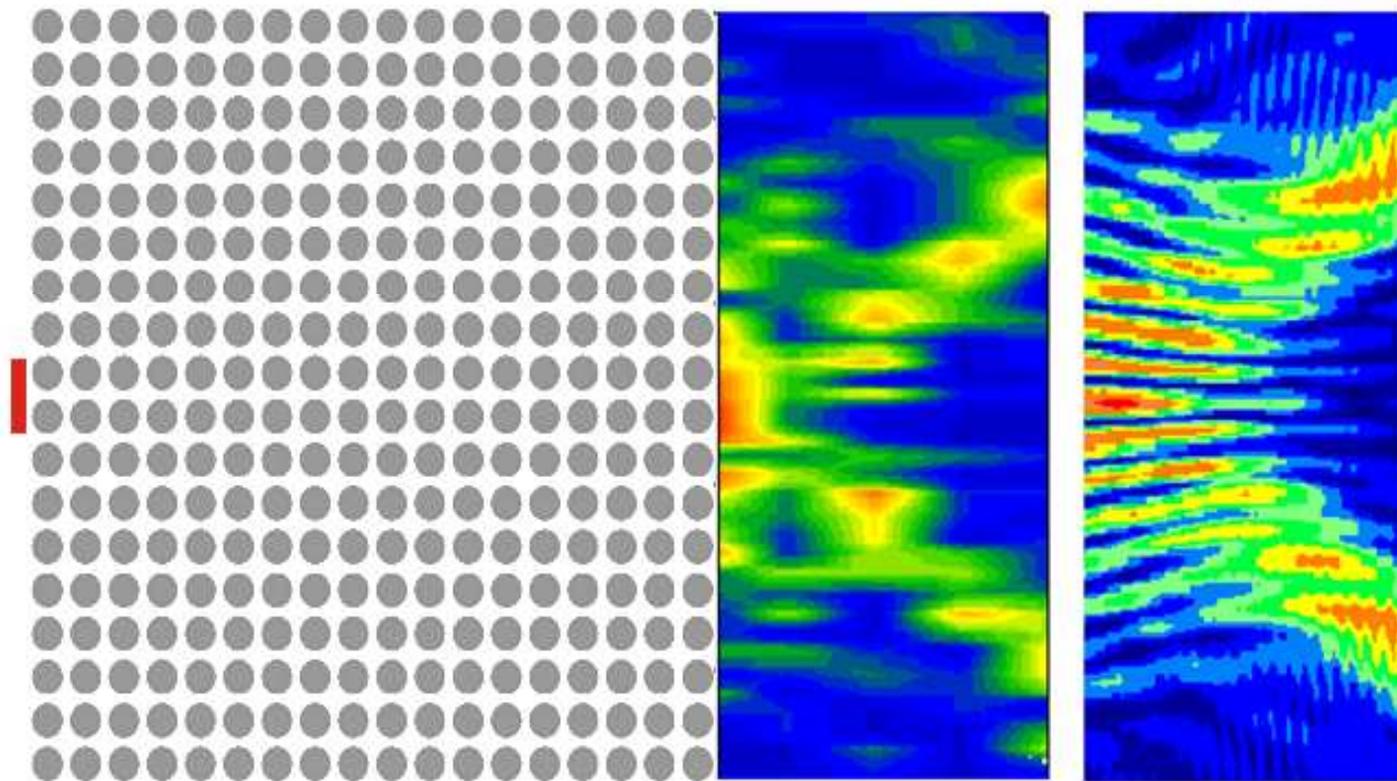
Experiment   Simulation

Thermal Management

- Heat harvesting offers tremendous potential for energy management during chip operation

  ➢ Thermoelectrics (TE)

- Thermal screening is critical to ensure safety and security in many areas (e.g. thermal barrier films)

- Heat dissipation methods: reduce hot spots in chips

  ➢ Thermal Interface Materials (TIM)
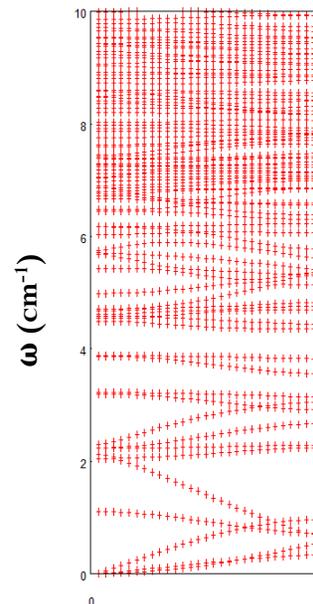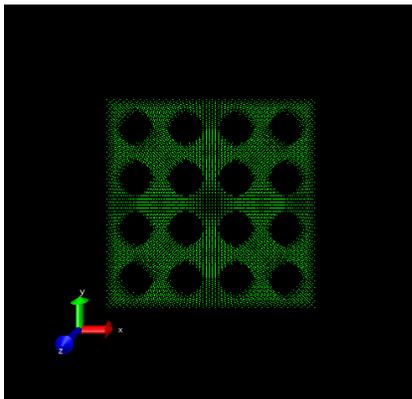
Thermal Conductivity

Fourier law defines thermal conductivity
Coefficient heat flux / thermal gradient

$$J = -\bar{k} \cdot \vec{\nabla} T$$

tensor

Most heat is carried by:
- electrons ⟶ Main heat carriers in metals
- phonons ⟶ In the low frequency regime phonons are equivalent to sound waves
  ⟶ Only heat carriers in insulators
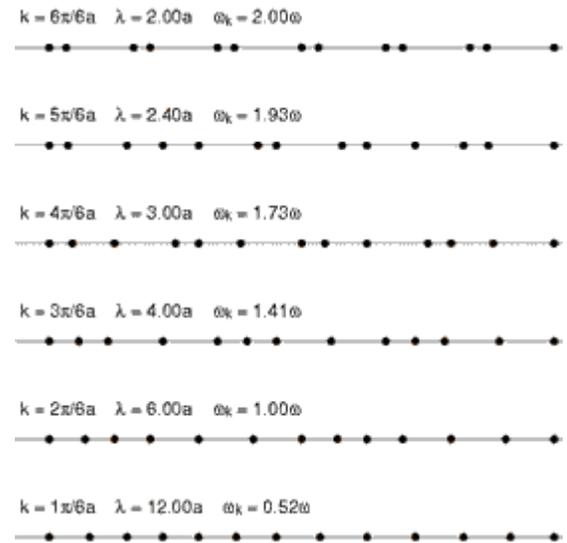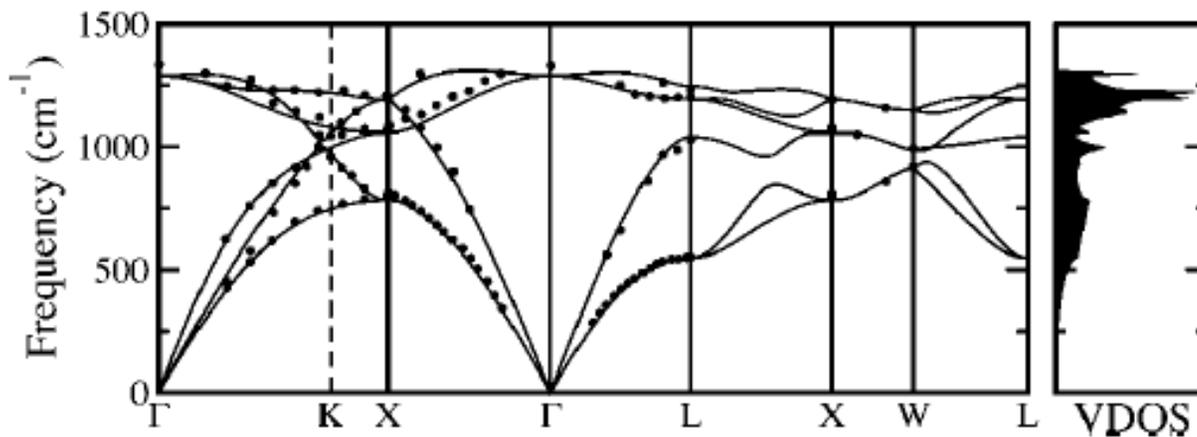
$$\bar{k} = \sum_{\omega}\sum_{\vec{q}} c(\omega, q)\vec{V}_g(\omega, q)\vec{V}_g(\omega, q)\tau(\omega, q)$$

heat capacity   group velocity   phonon mean life-time

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Thermoelectric materials for energy harvesting

The ability to harvest the heat produced and recycle it back as DC electric power is an invaluable method of reducing power consumption during semiconductor chip operation

THERMOELECTRICS (TE):
• Transformative technology for energy conversion (heat to electricity)

• Based on Seebeck effect: A temperature difference (ΔT) across a material gives rise to a corresponding electrochemical potential (ΔV); the Seebeck coefficient (S) equals ΔV generated per unit temperature gradient.

• Typical TE devices consist of alternating n-type and p-type materials, such that

$$\Delta V = (S_p - S_n) \times \Delta T$$

semiconductors have intrinsically higher Seebeck coefficients (are 10^3 greater than metals)
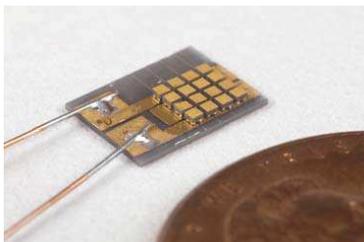
*Venkatasubramanian et al.,
IEEE ,(2007)*

Hot side

n-type   p-type

Cold side

ΔV
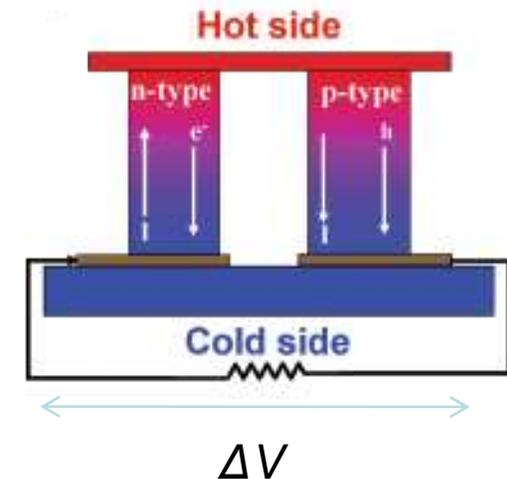
Thermoelectric materials for energy harvesting

A defining characteristic of an efficient TE material is its *ZT* (figure of merit)
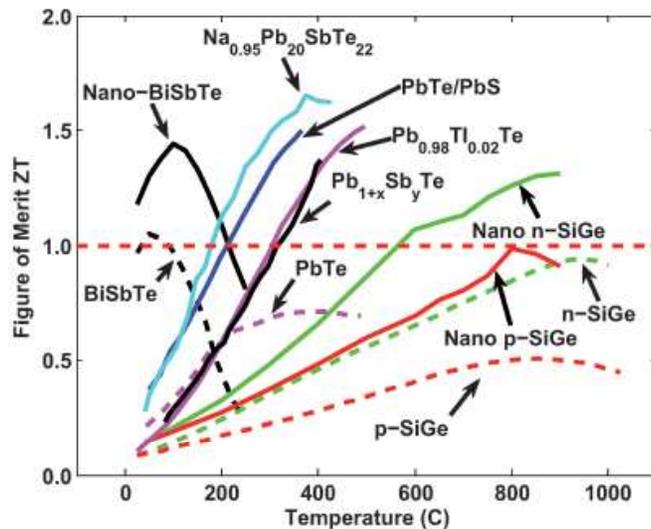
$$ZT = \frac{S^2 \sigma}{k} T$$

S = Seebeck coefficient
σ = electrical conductivity
k = thermal conductivity
T = absolute temperature

Traditional high ZT materials

Maximum power output: *1-2 mW/mm²*)

Minnich et al. (Energy Environ. Sci, 2, 2009)

Future Direction:

• Next generation high *ZT* materials can be realized by **significantly reducing thermal conductivity** while enhancing/maintaining electrical conductivity of existing systems

• *Heat energy harvesting in semiconductor chips*- explore **newer TE systems** compatible with IC fabrication requirements that have optimal *S, k, σ.*

• Work at a range of operating temperatures compatible with semiconductor chips, and characterized by high power densities (> 10's mW/mm²).
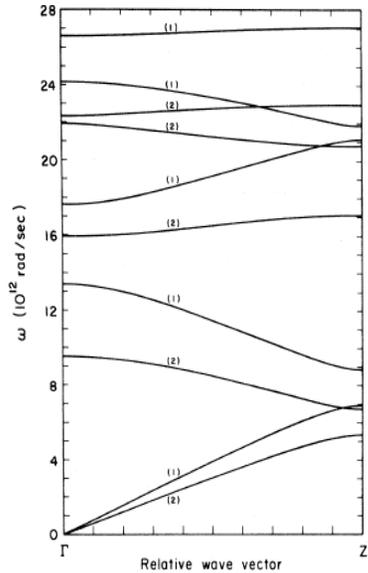
→ **Phononic band structure of Bi$_2$Te$_3$**

- High frequency 'non-thermal' phonons scatter charge carriers (electrons/holes)

- Acoustic (low frequency) phonons: responsible for thermal propagation (nanometric wavelengths)

ZT can be greatly enhanced if
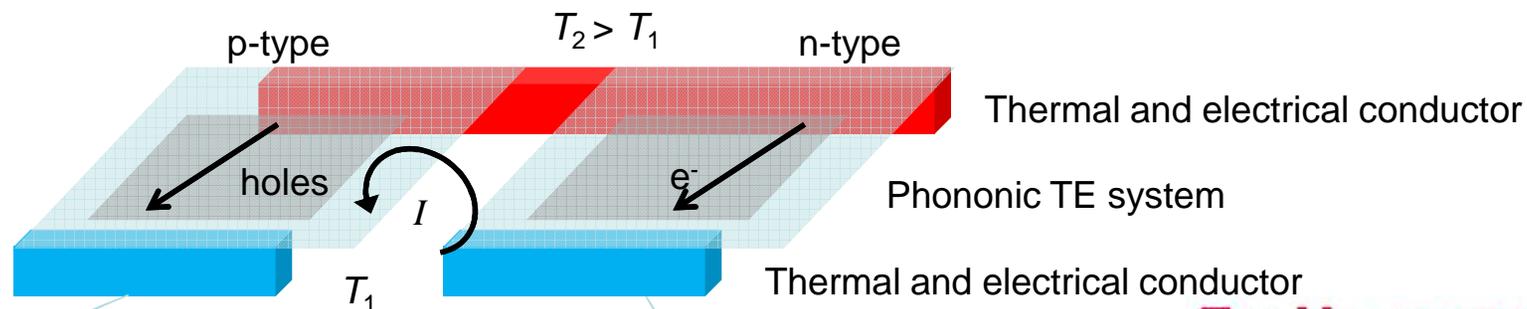-thermal phonon transport is reduced (via introduction of band-gaps), without affecting electrical conductivity
- electron/hole transport is increased (by non-thermal phonon drag)

Phononic band structures of metamaterials can be modified based on **size, periodicity and properties of the secondary phase** (*inclusions, pores*)- the inclusions /pores should be of 10's of nanometers to achieve low-frequency bad-gaps.

Non-thermal, high-frequency phonon transport (leading to phonon-drag), is achieved by introducing negative bands at high frequencies (*Bucay et al.*, *Phys. Rev. B, 2009*)


p-type $T_2 > T_1$ n-type

Thermal and electrical conductor

holes I e$^-$

Phononic TE system

T_1

Thermal and electrical conductor

➢ **SiGe: superlattices, 3D nanostructures**: computational work by Gillet et al. (*J. heat transfer, 131, 2009*) has shown that the thermal conductivity can be reduced by two orders of magnitude for 3D nanostructure given below

$d = Na =$ $Ma =$
(a) 2.7155 nm   1.6293 nm
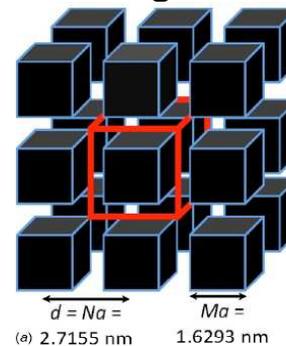
Nanoscale Ge inclusions in a Si matrix.

➢ **Single layer and multilayer patterned graphene**: preliminary work has shown that low-frequency band-gaps are introduced in graphene nano-antidots
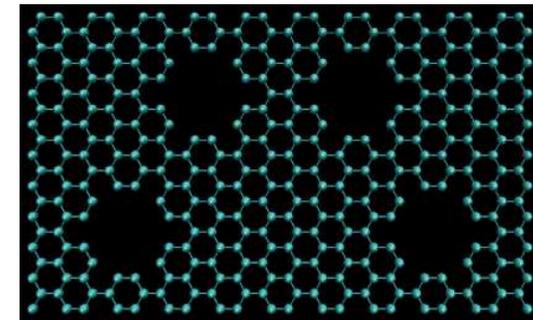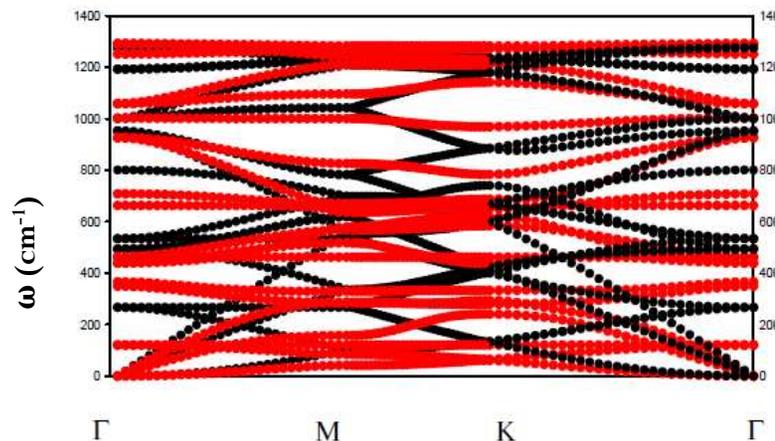
Other systems examined:
➢ **Nanoporous silicon**
➢ **GaAs**

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