SAND2011-4543C

Nanostructured Devices for Communication, Sensing, and Energy

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DSL 2011

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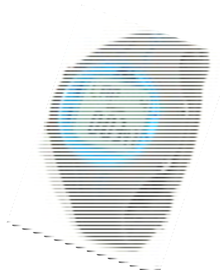
Silicon Carbide Phononic Devices and Systems

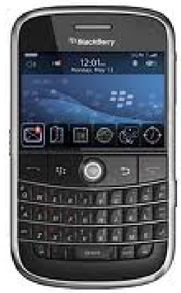
Energy
- Thermoelectric energy generation and harvesting
- On-chip cooling

Sensing
- Bio and Chemical Sensing
- Medical Diagnostics
- Inertial Sensing
- Optical Sensing

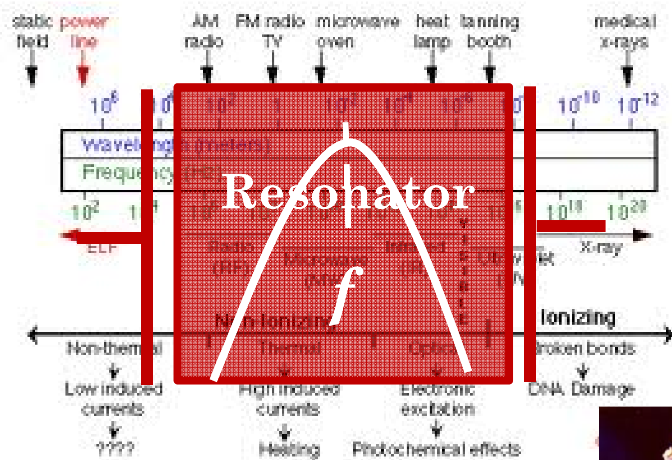
Communication
- Phononic Signal Processing and Timing
- Phononic Logic
- RF and Microwave Antennas

COMMUNICATION DEVICES ARE EVERYWHERE!










Resonators are passtive elements used in communication systems for signal generation (oscillators) and signal processing (filters)

High $f.Q$ Micromechanical Resonators for Smaller, Lighter, Lower Power, Cognitive Communication Systems

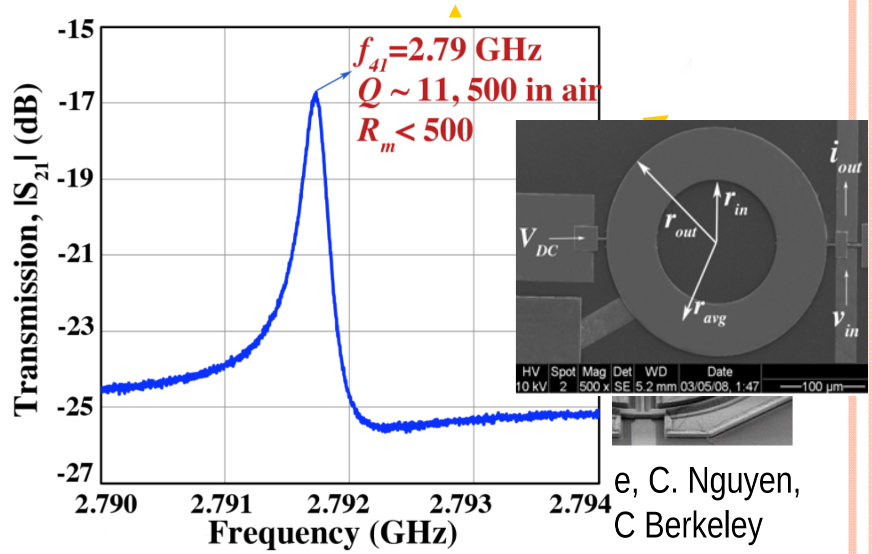
Resonator Trade Off : F.Q vs. Insertion Loss

Capacitive MEMS Resonators

✓ *Highest f.Q products for acoustics*

x *Weak electromechanical coupling leads to high motional impedance*

- Higher noise, matching problems
- Arraying and high-K dielectric transduction lead to high parasitic capacitance



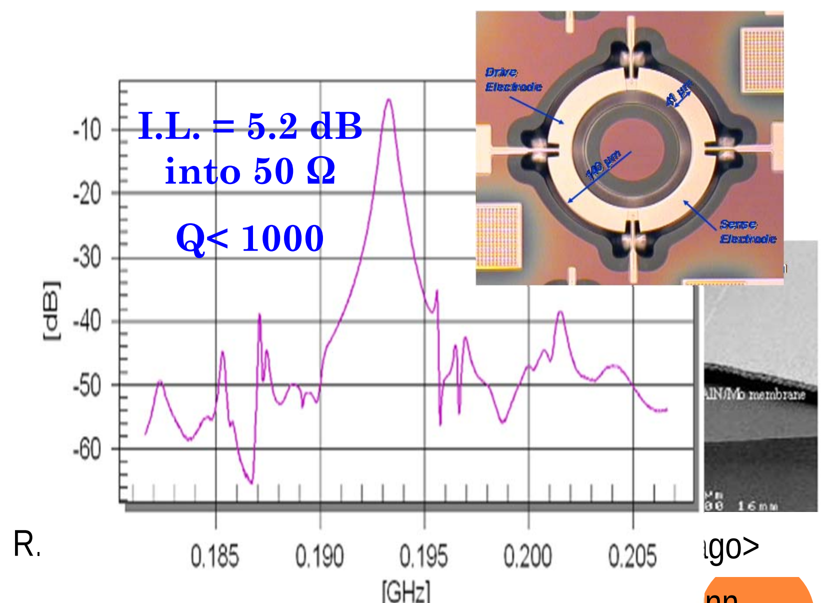
Piezoelectric MEMS Resonators

✓ *Low Insertion Loss and impedance (< 50)*

- Strong electro-acoustic transduction
- Easily matched to antenna, off-chip circuits

x *Q limited to a few thousand*

- Material damping in metal electrodes and piezoelectric films, creep, aging

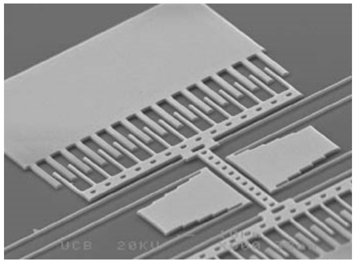


Want Highly Efficient Transduction + High f.Q in Microresonators

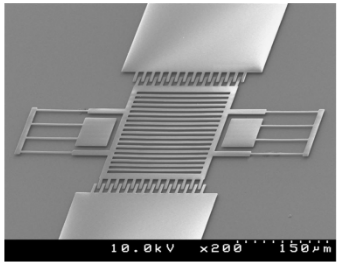
Silicon Carbide: Good Mechanical Material

Silicon Carbide is an ideal material for harsh environment micromechanical resonators, sensors, and actuators due to its

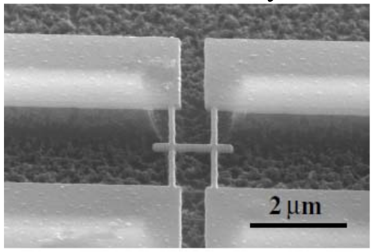
- Chemical Inertness
- Mechanical strength
- High wear resistance
- Large Young's modulus
- Low acoustic losses



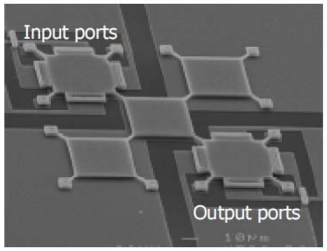
SiC resonator, Pisano Group, UC Berkeley



SiC resonator Case Western Reserve



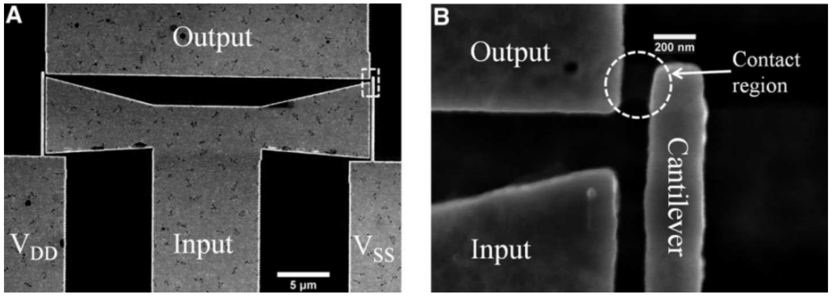
SiC nanowire resonator Case western reserve & Caltech



SiC Lamé-mode filters, UC Berkeley

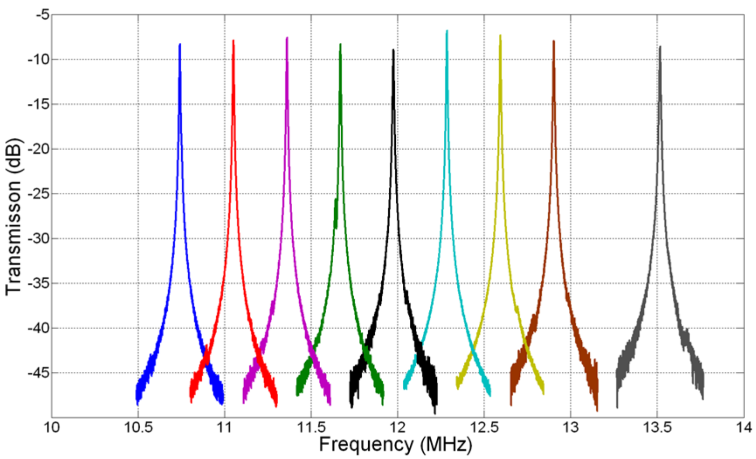
Silicon Carbide is also a candidate material for high temperature, high power, and high voltage microelectronic devices due to its

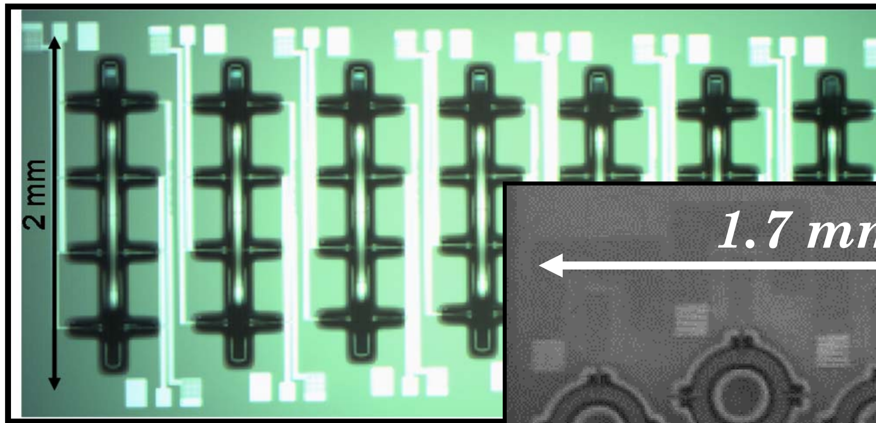
- Wide energy bandgap
- High thermal conductivity
- Large break down field
- High Saturation velocity



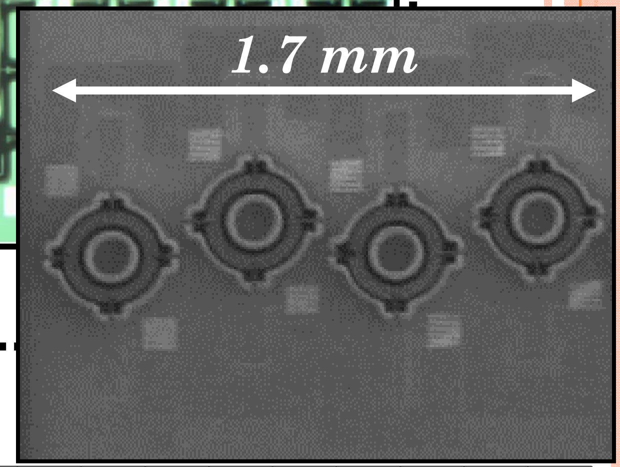
SiC high temp switch, Mehregany group, Case Western Reserve

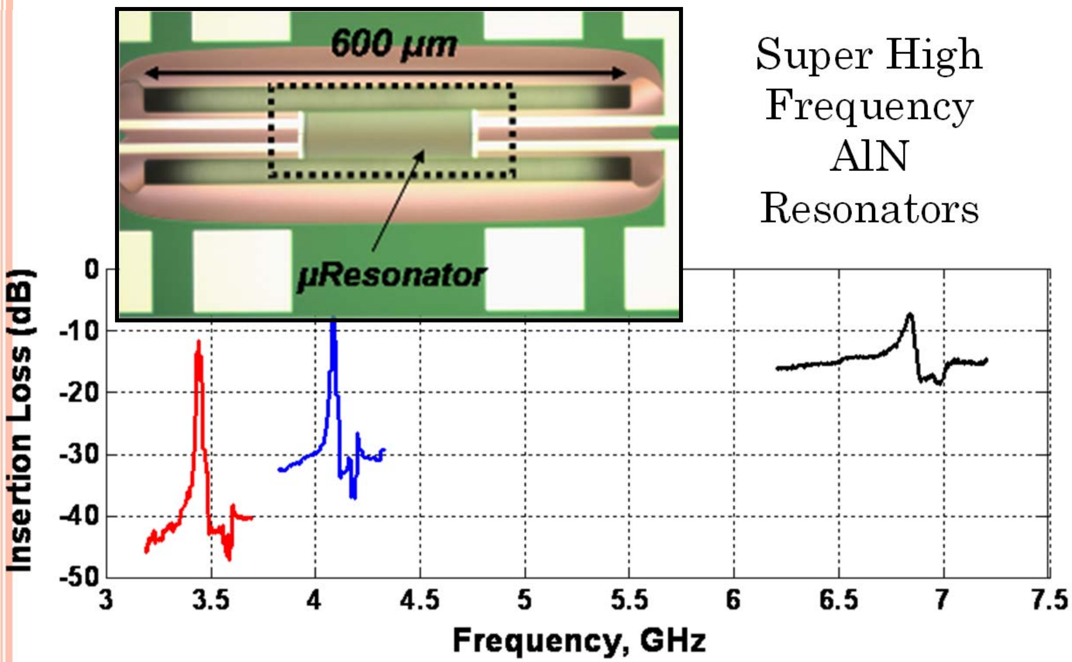
ALUMINUM NITRIDE: PIEZOELECTRIC MATERIAL



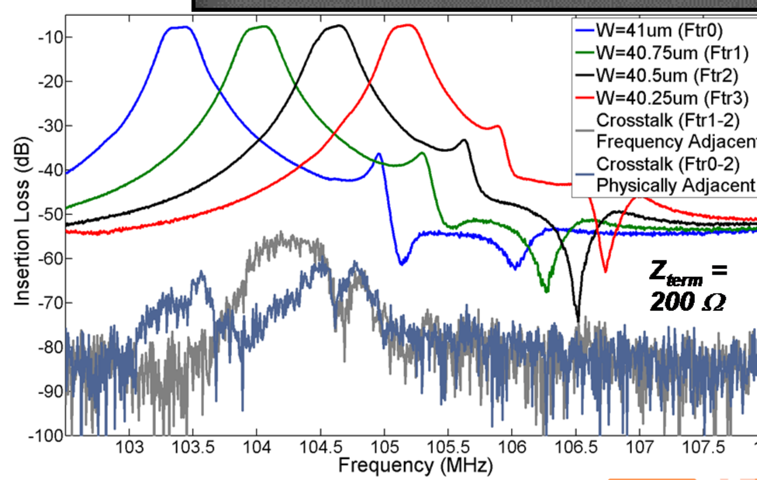


6 kHz BW AlN Filter Bank from DARPA ASP Program





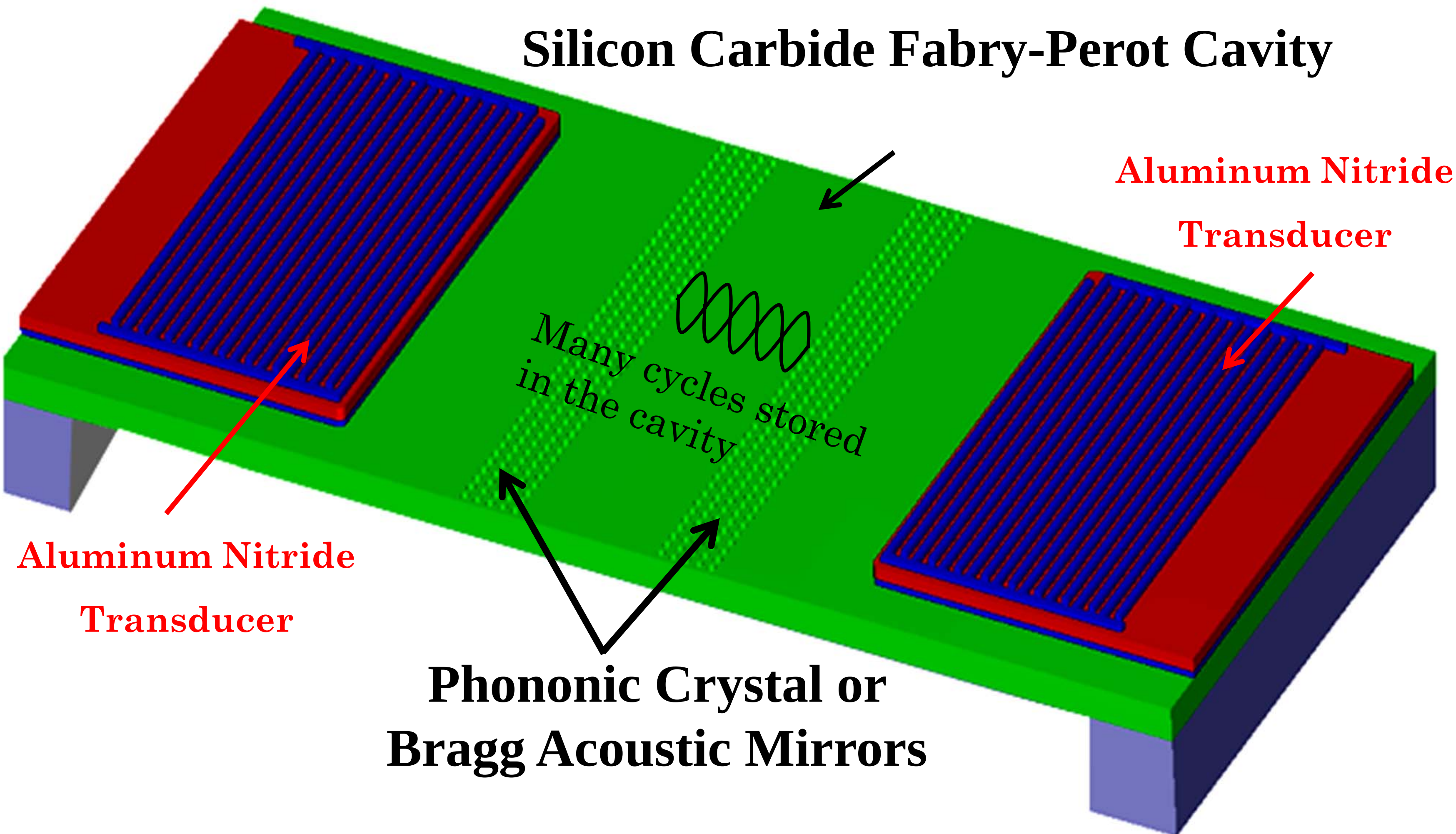
Super High Frequency AlN Resonators



100 MHz AlN Filter Bank

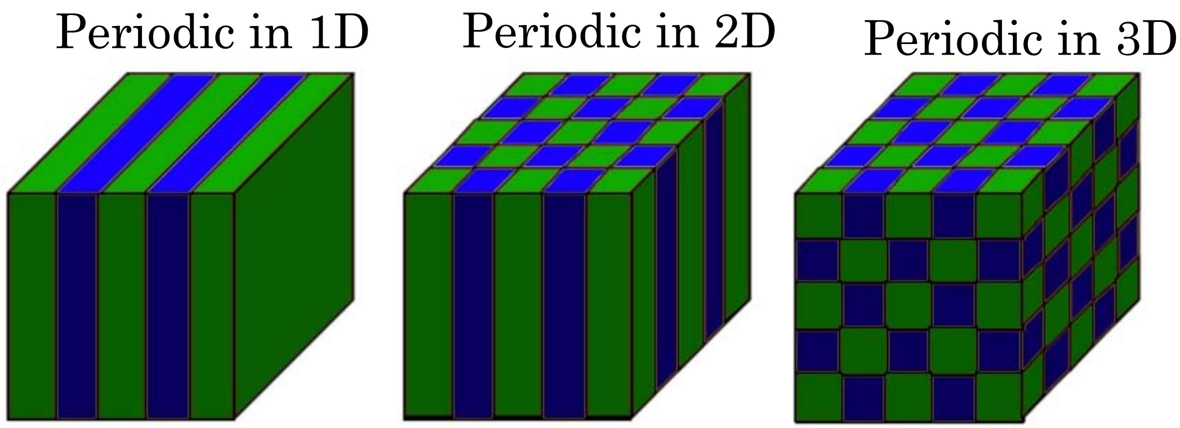
Phononic Crystal Cavity Resonators

Phononic Crystal Acoustic Mirrors decouple Fabry-Perrot Cavity from piezoelectric transducers



PHONONIC CRYSTALS (PNC)

- Periodic Arrangements of Elastic Material

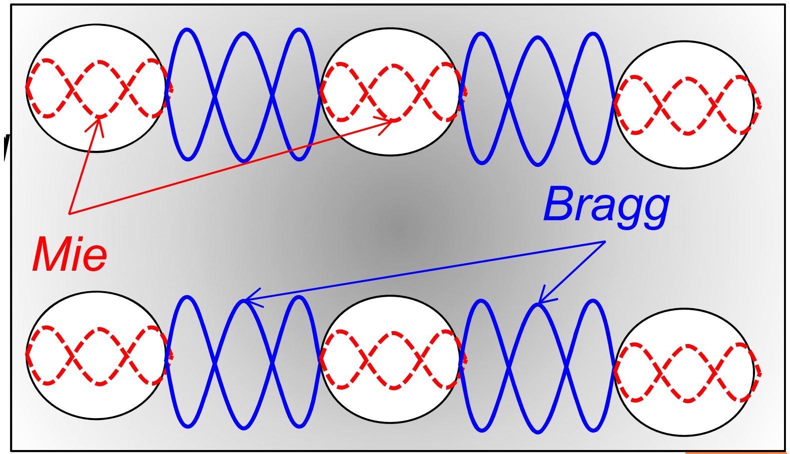


→ *Phonic Bandgap (PBG) – Frequencies where the propagation of phonons is prohibited*

→ *Engineering Anomalous dispersion (flat and negatively-sloped bands)*

Applications of PnCs

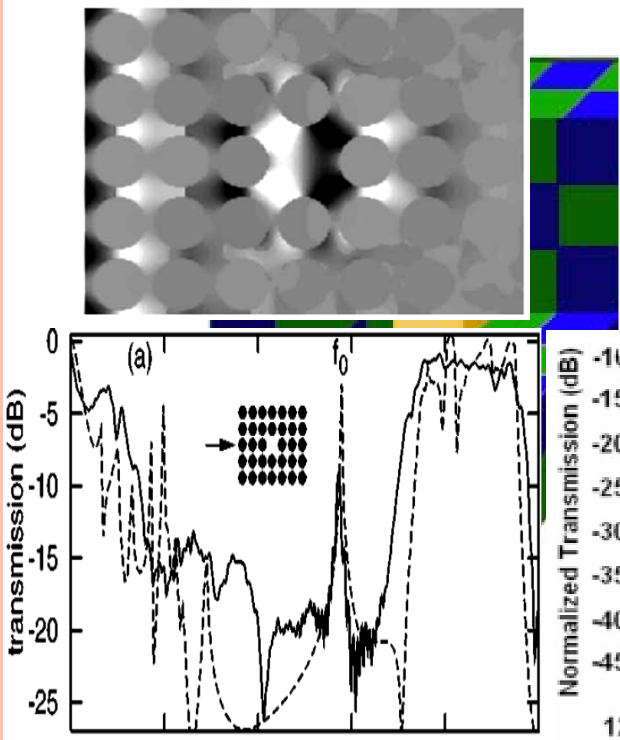
- *Acoustic isolation*
- *Signal processing/filtering*
- *Acoustic sensing*
- *Thermal isolation and energy harvesting*
- *High-resolution ultrasonics*



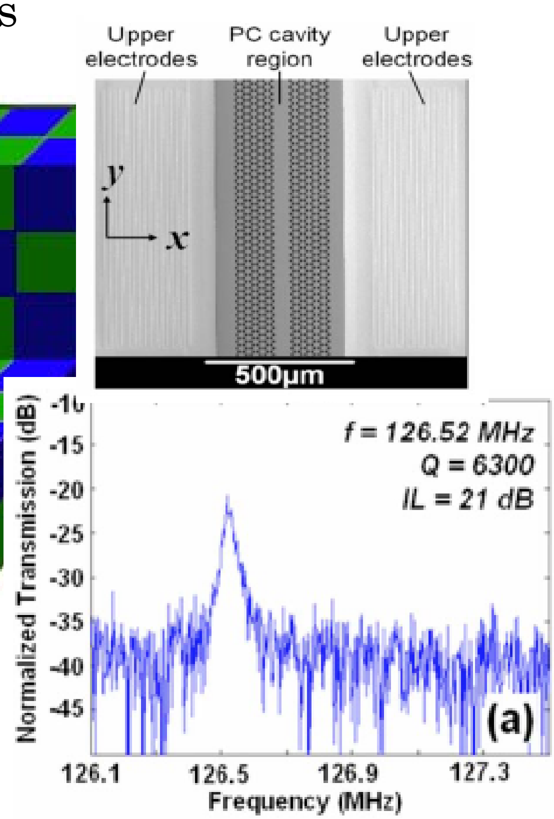
Phonic Crystals for Communication

- Defects in the Phononic Crystals can form cavities or waveguides
  - → Micromechanical timing and signal processing devices

Cavities

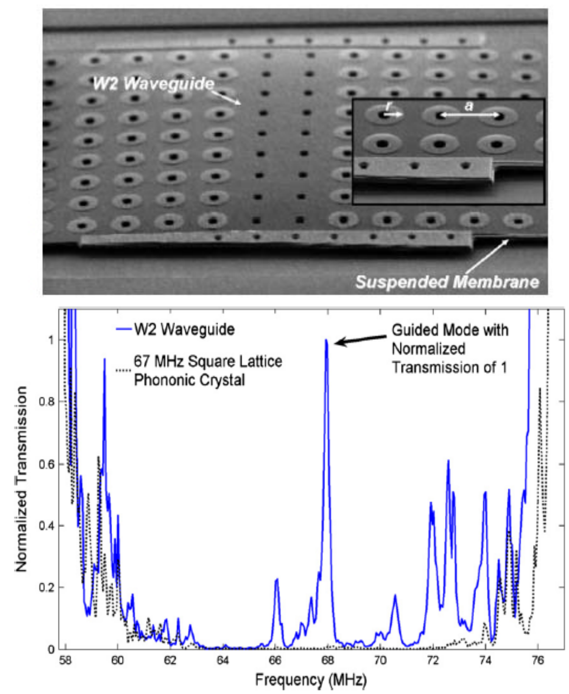


A. Khelif, et al. *Phys. Rev.* B, vol. 68, 214301,2003.



S. Mohammadi, et al. *App. Phys. Lett.* **94**, 051906

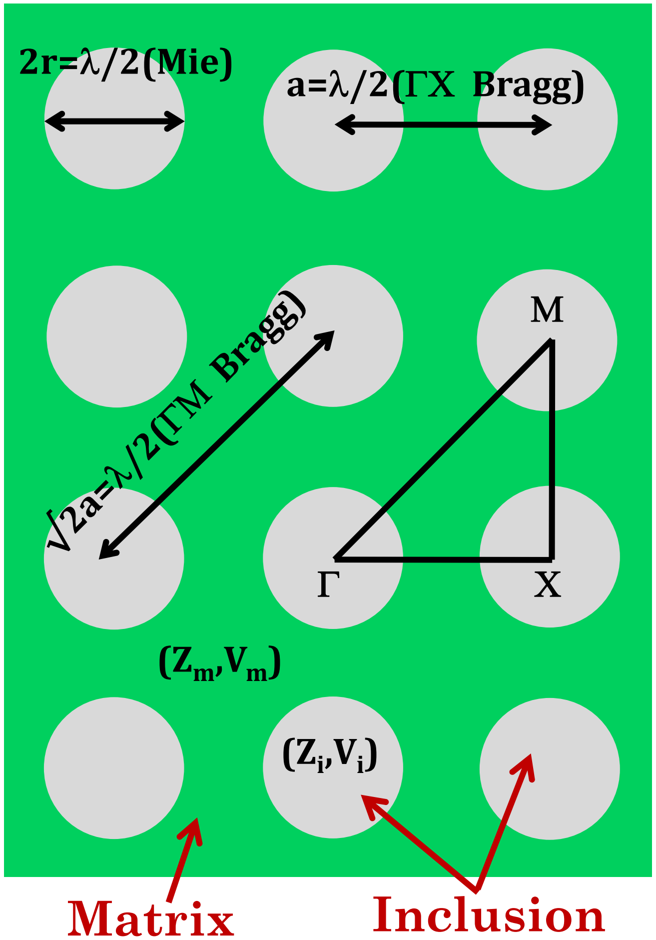
Waveguides



R. H. Olsson III, et al. *Sensors and Actuators A*: Physical **145-146**, pp.87-93

PHONONIC BAND GAPS

2D square lattice PnC



Filling fraction = r/a

Bragg and Mie resonances due to periodic scattering inclusion

$$f(Bragg)_{\Gamma X} = \frac{V_{avg}}{2a} \qquad f(Bragg)_{\Gamma M} = \frac{V_{avg}}{(2a)\sqrt{2}}$$

$$f(Mie) = \frac{V_i}{4r}$$

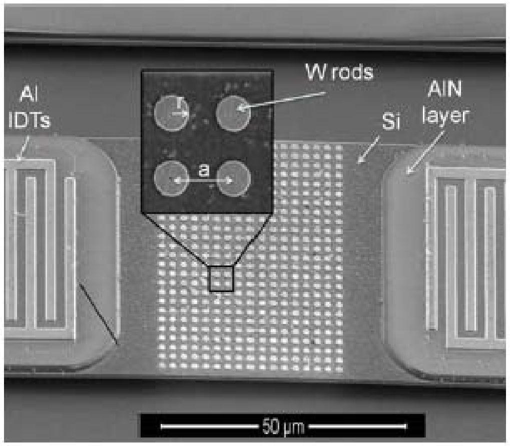
$$V_{avg} = \pi\left(\frac{r}{a}\right)^2 V_i + \left(1 - \pi\left(\frac{r}{a}\right)^2\right) V_M$$

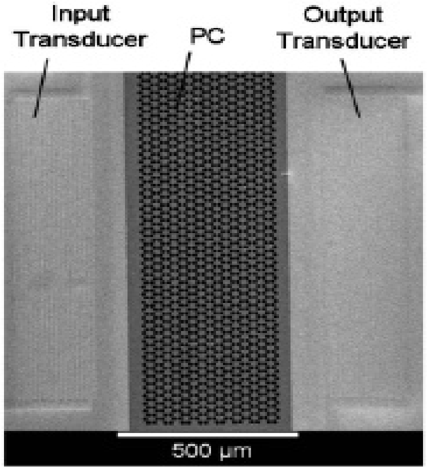
Acoustic impedance and velocity

$$Z = \rho V = \sqrt{E\rho} \qquad V = \sqrt{\frac{E}{\rho}}$$

→ Maximize band-gap width and depth by maximizing acoustic impedance, Z, mismatch

SOLID-SOLID VS. SOLID-AIR PHONONIC CRYSTALS





Si-W Square Lattice PnC by Olsson et al, Sandia Labs

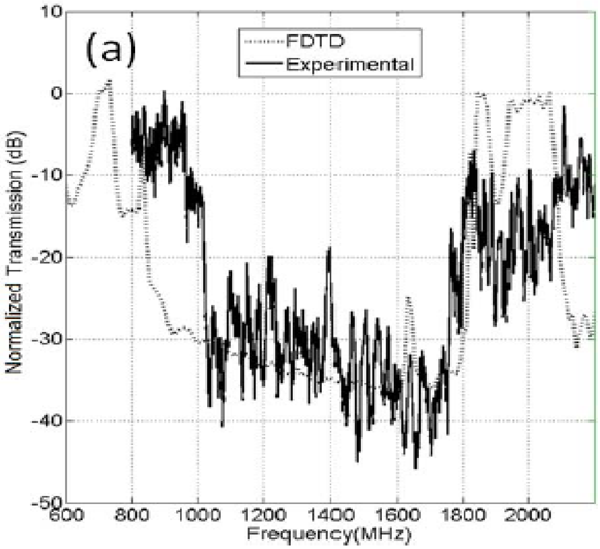
$a = 2.5\mu m,\ r/a = 0.26,\ \ t/a = 0.46$

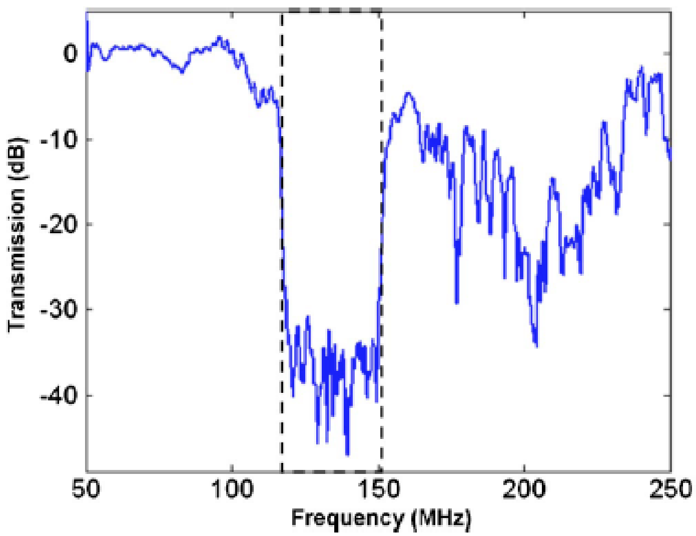
Bandgap from f = 1-1.8GHz (57%)

Si-Air Hexagonal Lattice PnC by Mohammadi et al, Georgia Tech

$a = 15\mu m,\ r/a = 0.43,\ \ t/a = 1$

Bandgap from f = 118-150MHz (25%)





Solid-Solid vs. Solid-Air Phononic Crystals

Maximum bandgap ~10%

Bandgap appears over a wide range of r/a of 0.13-0.35

-- Relaxed fabrication

Ideal thickness 1.0 ≥ t/a ≤ 1.25

– Structurally stable, reinforced by W rods

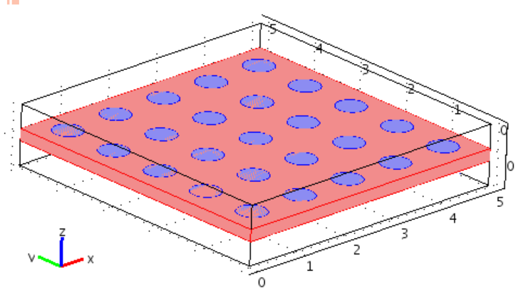
Maximum bandgap ~25%

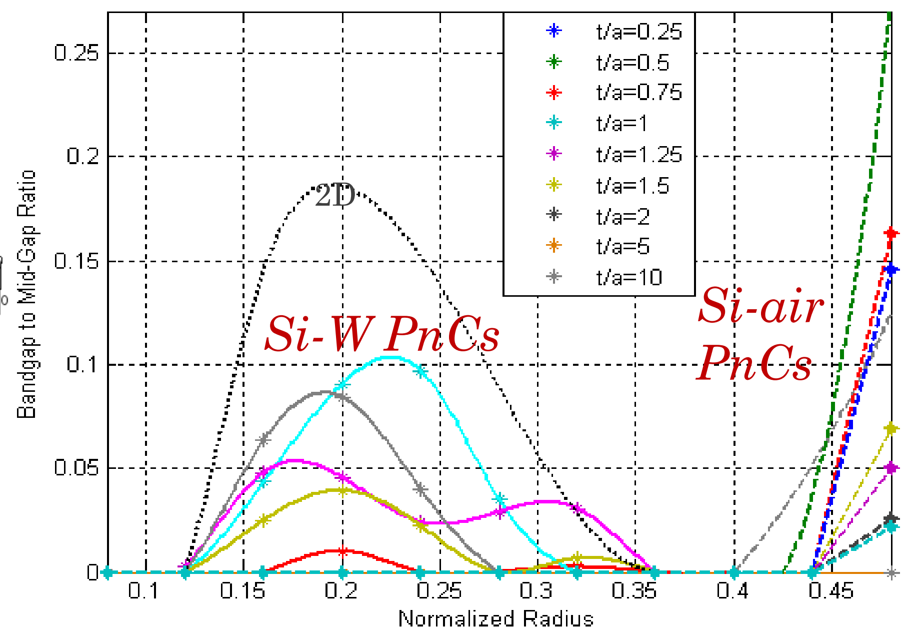
Bandgap does not appear until r/a ≥ 0.4

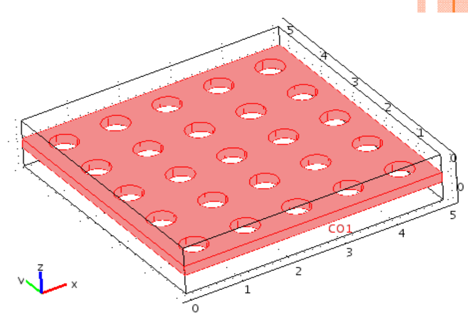
-- Difficult to fabricate

Ideal thickness 0.25 ≥ t/a ≤ 0.75

– Thin, structurally compromised



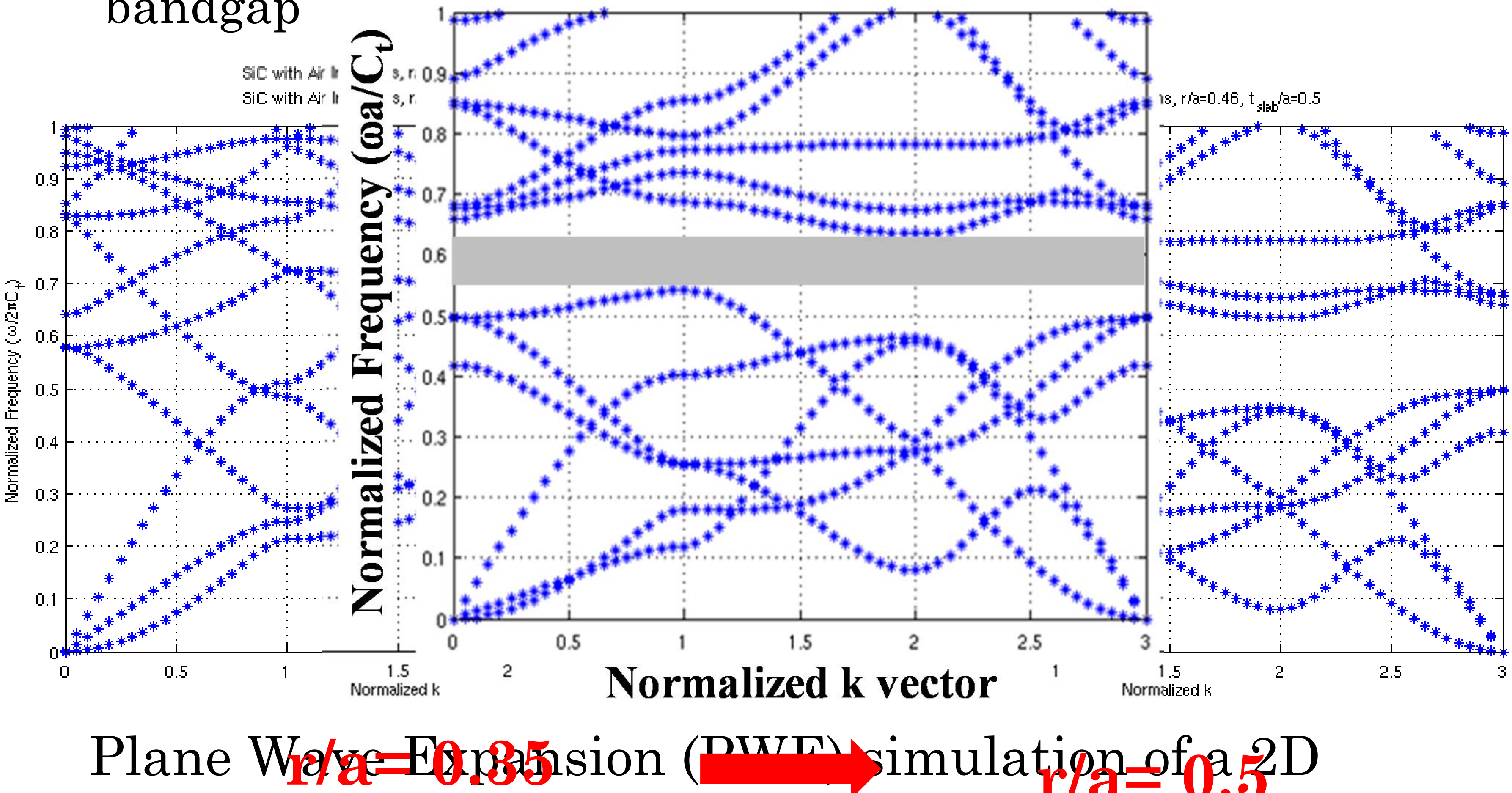




C. Reinke, M. Ziaei-Moayyed, et al, Ultrasonics 2010

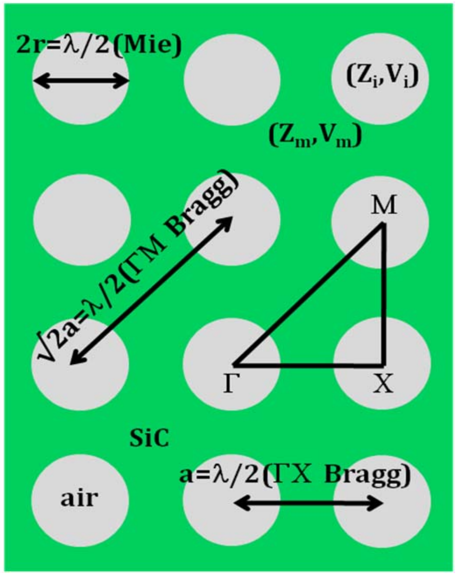
SiC Bandgap: PLANE Wave Expansion

- SiC with air inclusions filling fractions of 0.35 (Left) and 0.46(right) → higher filling fractions required complete bandgap



Plane Wave Expansion (PWE) simulation of a 2D simple cubic SiC/Air Phononic Crystal showing a full acoustic bandgap around 2.7 GHz. r/a=0.45, t/a=0.5

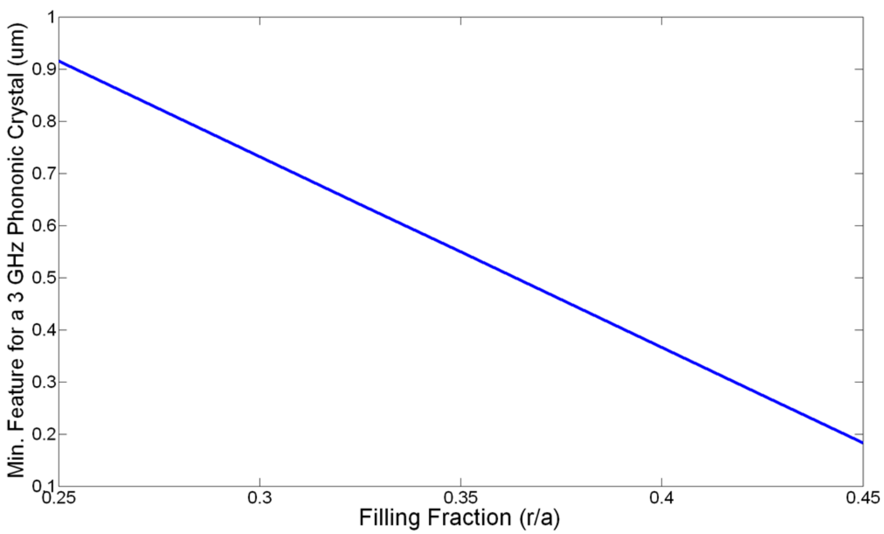
SILICON CARBIDE PHONONIC CRYSTAL

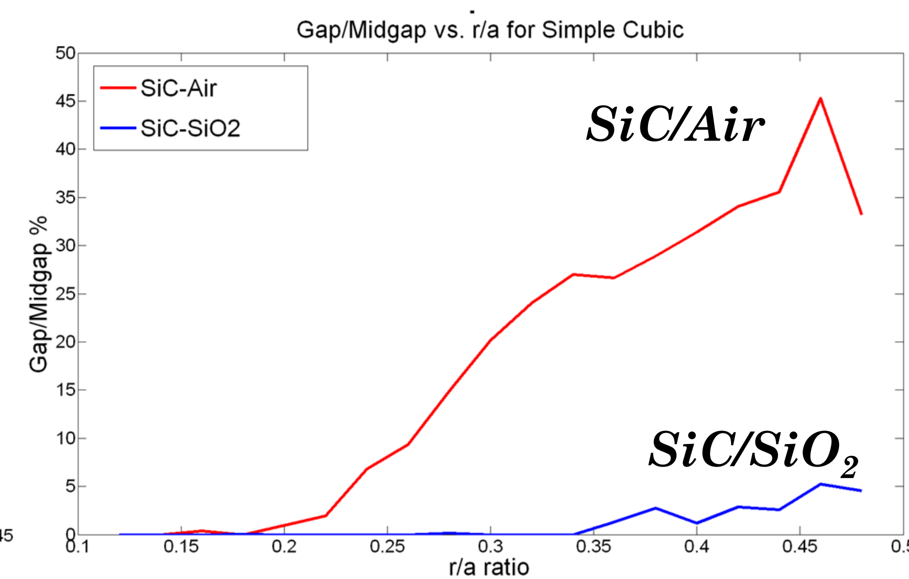


•Silicon Carbide/Air square lattice phononic crystal require a high filling fraction, r/a > 0.4, to open a phononic bandgap

•Minimum lithography feature of 350nm for a 3 GHz SiC/Air PnCwith a lattice constant of 1.83 μm

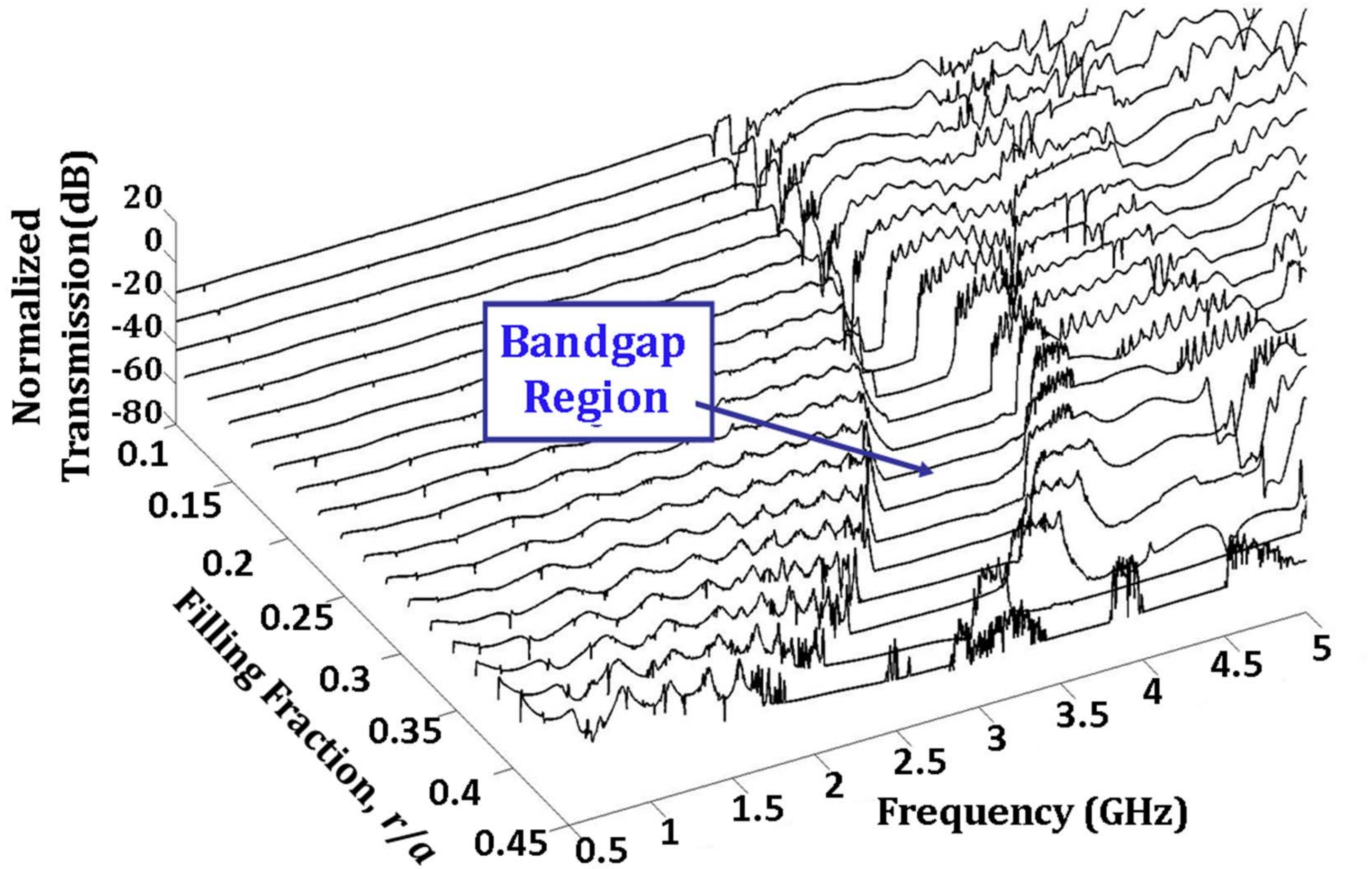
$$Z_{SiC} = \sqrt{E\rho} \approx 40M\Omega \qquad V_{SiC} \approx 12.5km/s$$





SiC-Solid vs. SiC-Air PnC

FINITE DIFFERENCE TIME DOMAIN (FDTD) MODELING OF PHONONIC CRYSTAL

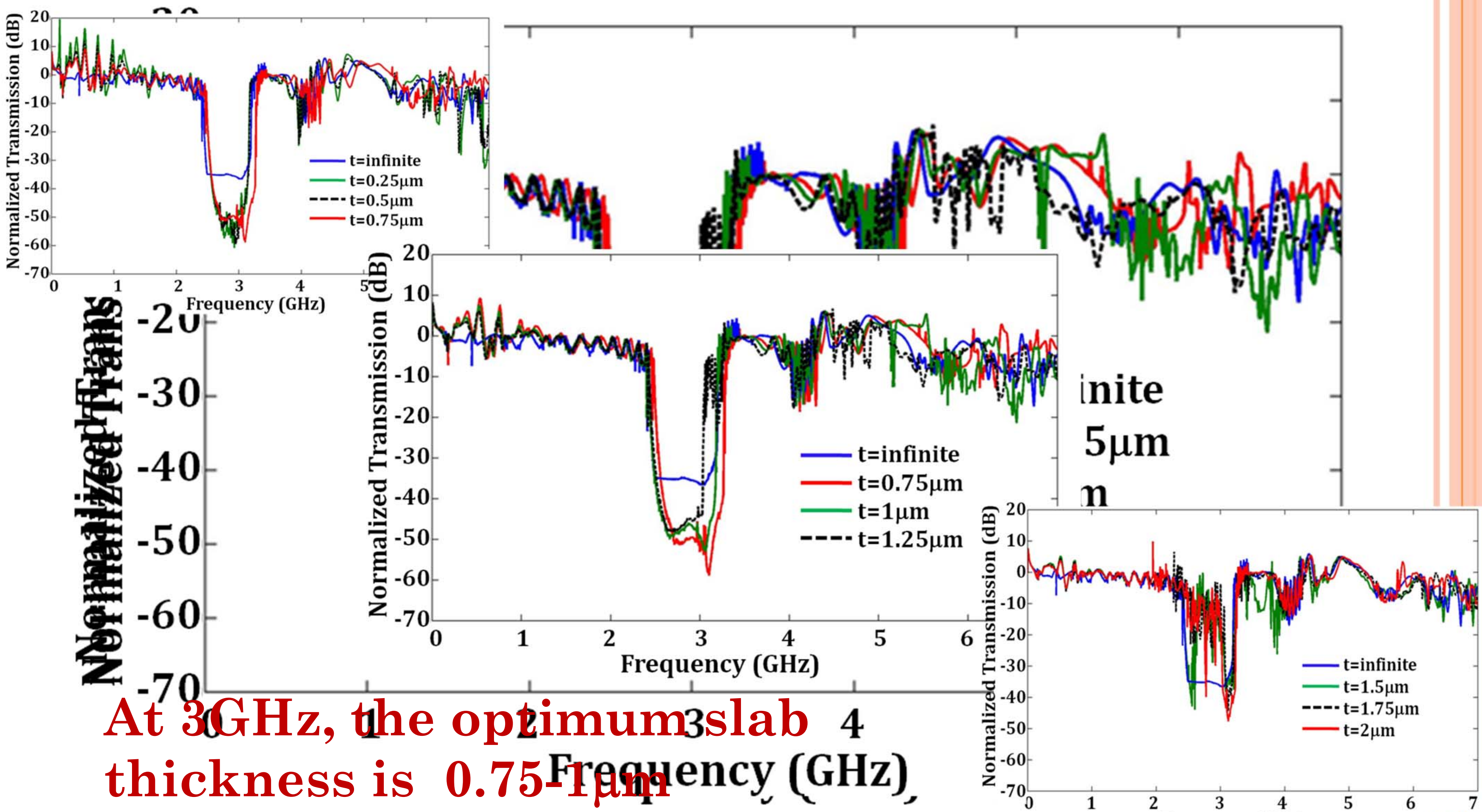


Phononic Crystal Transmission for an Infinitely Thick Membrane vs. Filling Fraction. Simple cubic lattice with 7 layers and Lattice Constant of 1.83 µm.

Filling Fraction increases → Bandgap moves to lower frequencies
Bandgap becomes wider and more reflective

M. Ziaei-Moayyed, et al, Ultrasonics 2010

TRANSMISSION VS. SLAB THICKNESS



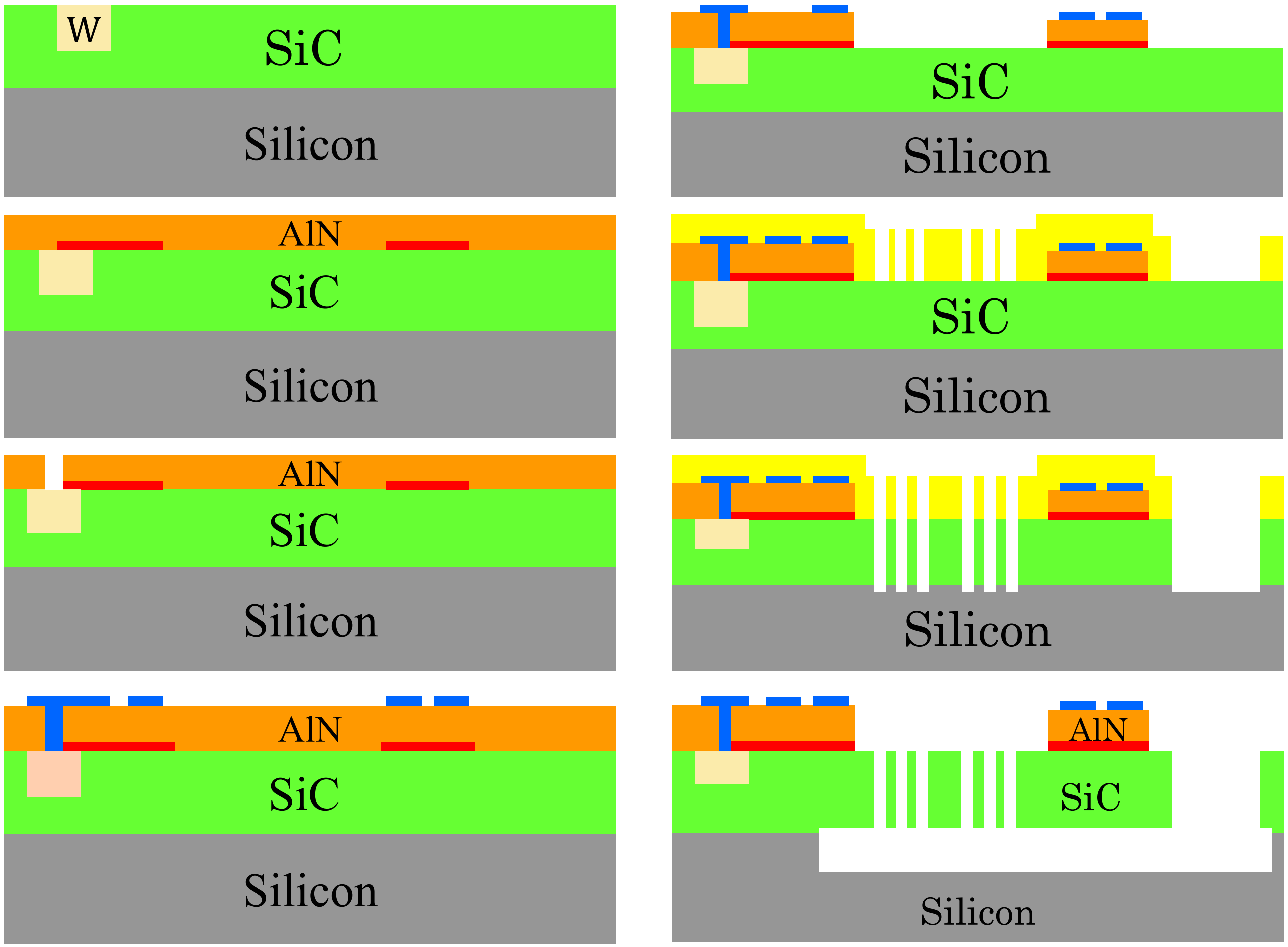
At 3GHz, the optimum slab thickness is 0.75-1µm

FDTD simulation of a 2D simple Cubic SiC/Air Phononic Crystals with 7 layers, a=1.83µm, and r/a=0.5 µm

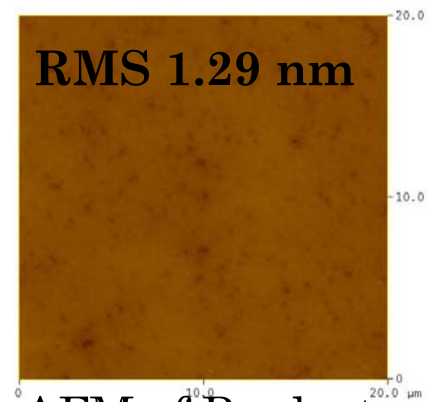
Slab thickness increases → Bandgap becomes narrorwer and less reflective

M. Ziaei-Moayyed, et al, Ultrasonics 2010

SILICON CARBIDE ON SILICON FABRICATION PROCESS



- 6 Mask Process
- Layer Thicknesses
  - *SiC = 1000 nm*
  - *Al = 100 nm*
  - *AlN = 200 nm*
  - *Al = 100 nm*



AFM of Product SiC Surface

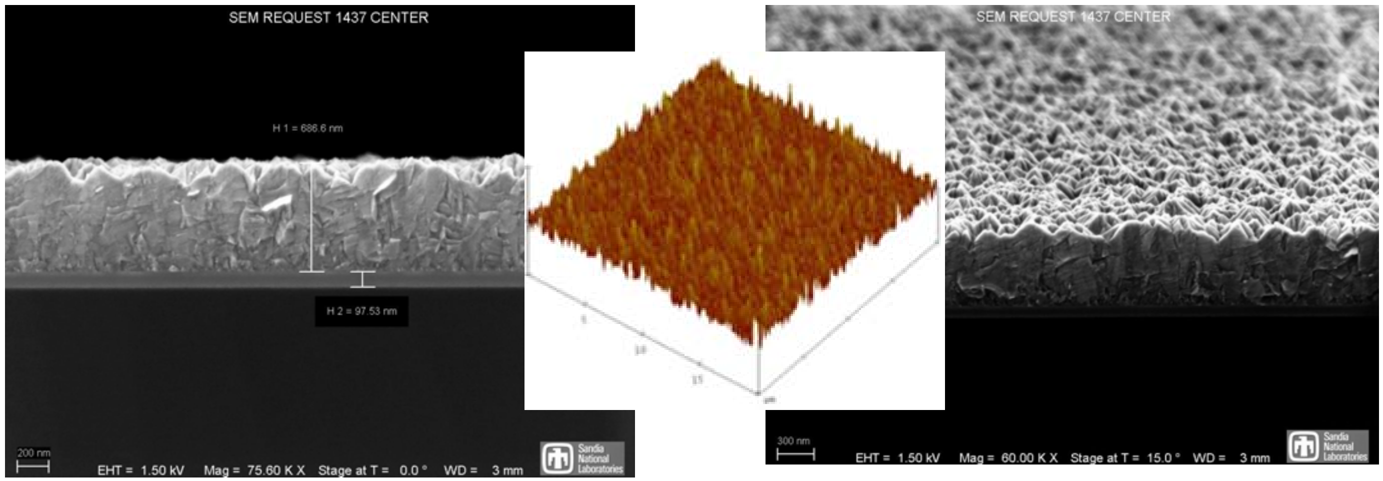
Silicon | Silicon Dioxide | Aluminum | Tungsten

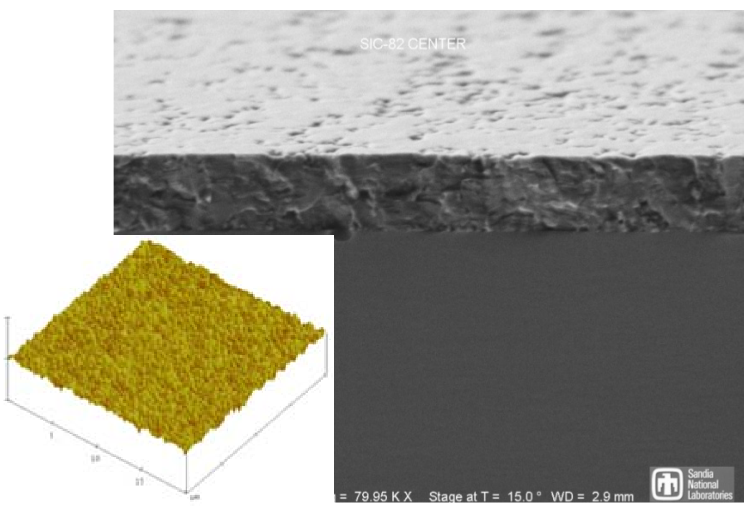
Silicon Carbide | Ti/TiN/Al | Aluminum Nitride

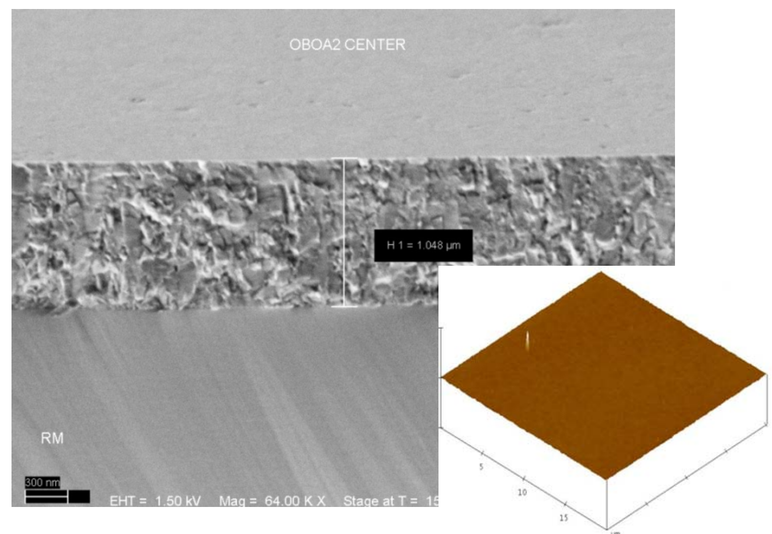
Process tailored to achieve high Q resonators in SiC

SILICON CARBIDE PLANARIZATION (CMP)

As-deposited SiC (850C) has a surface roughness of ~ 20nm







Oxide CMP: rms < 5nm

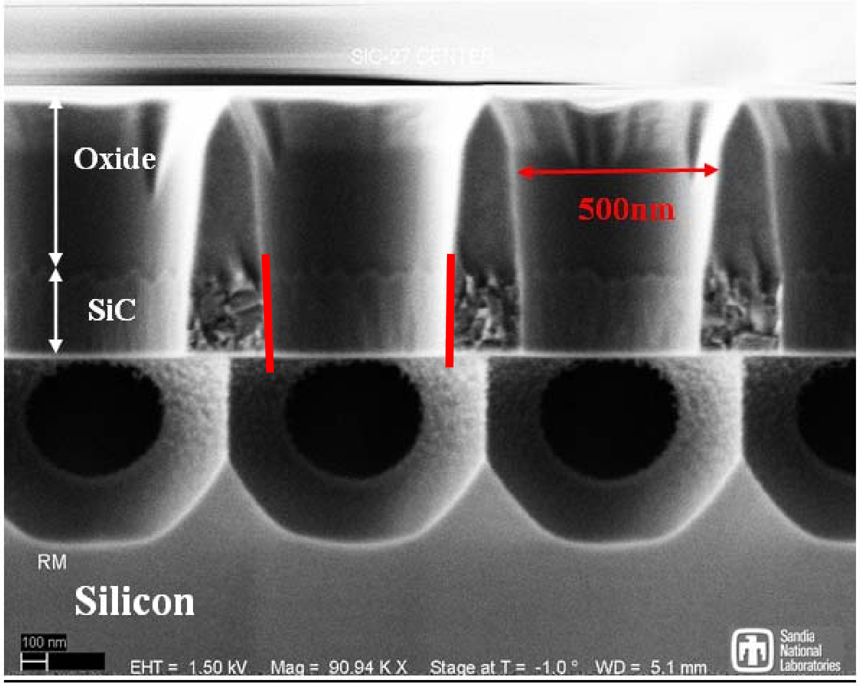
Tungsten CMP: rms < 1nm

Unpublished Data

SiC CMP: Keith Yoneshige, Scott Habermehl, Kira fishgrab

SILICON CARBIDE ETCH

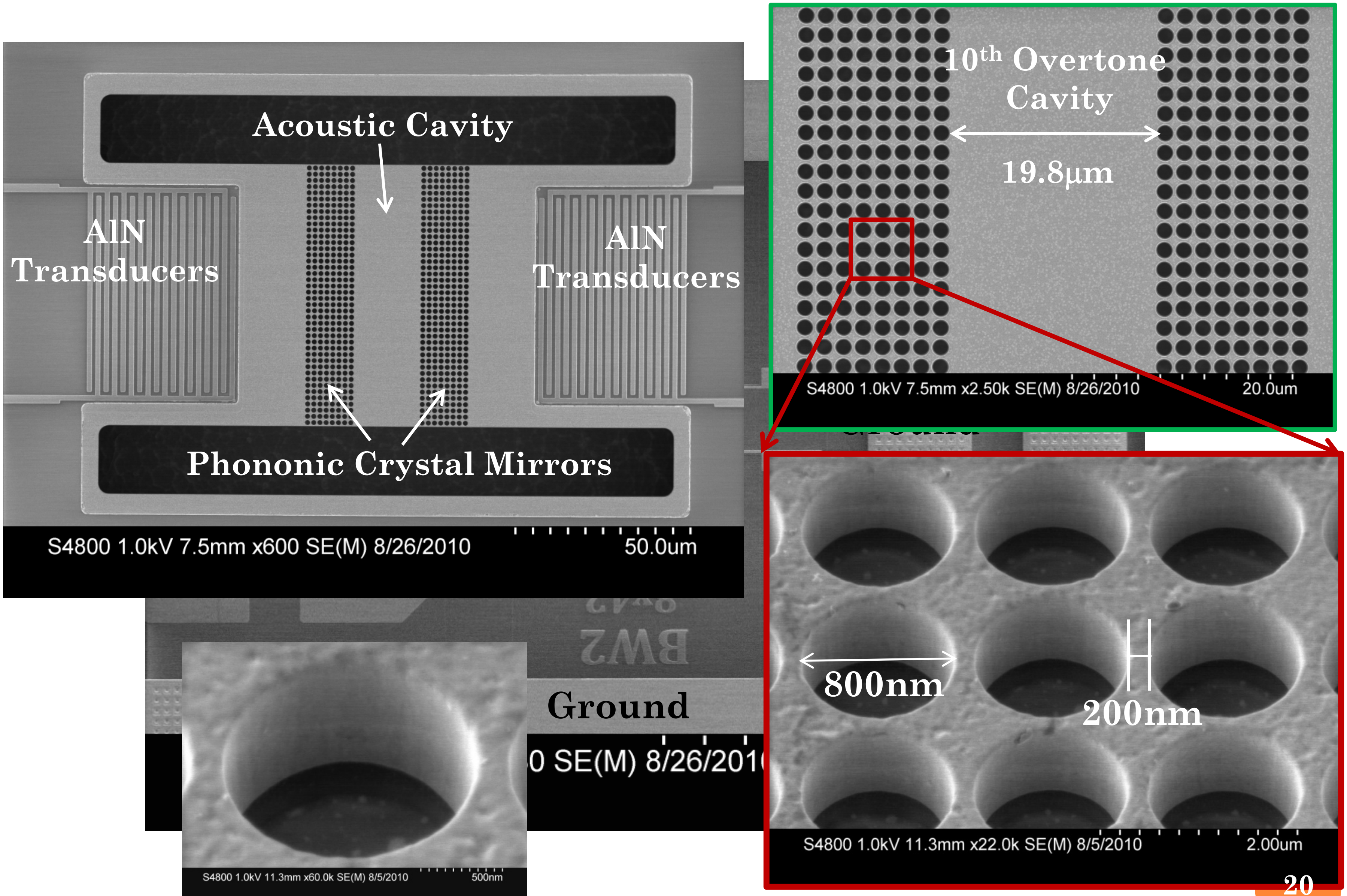
- SiC Etched Using Oxide Hard Mask
- 500 nm line and space etching demonstrated
  - *550 nm required for longitudinal wave phononic bandgap*
- Etch side wall slope is ~90 deg.
  - *important for high Q phononic crystals*
- Fluorine rich chemistry (SF_6) difficult to stop in Si
  - *Added mask to process flow to allow over etch into Si*



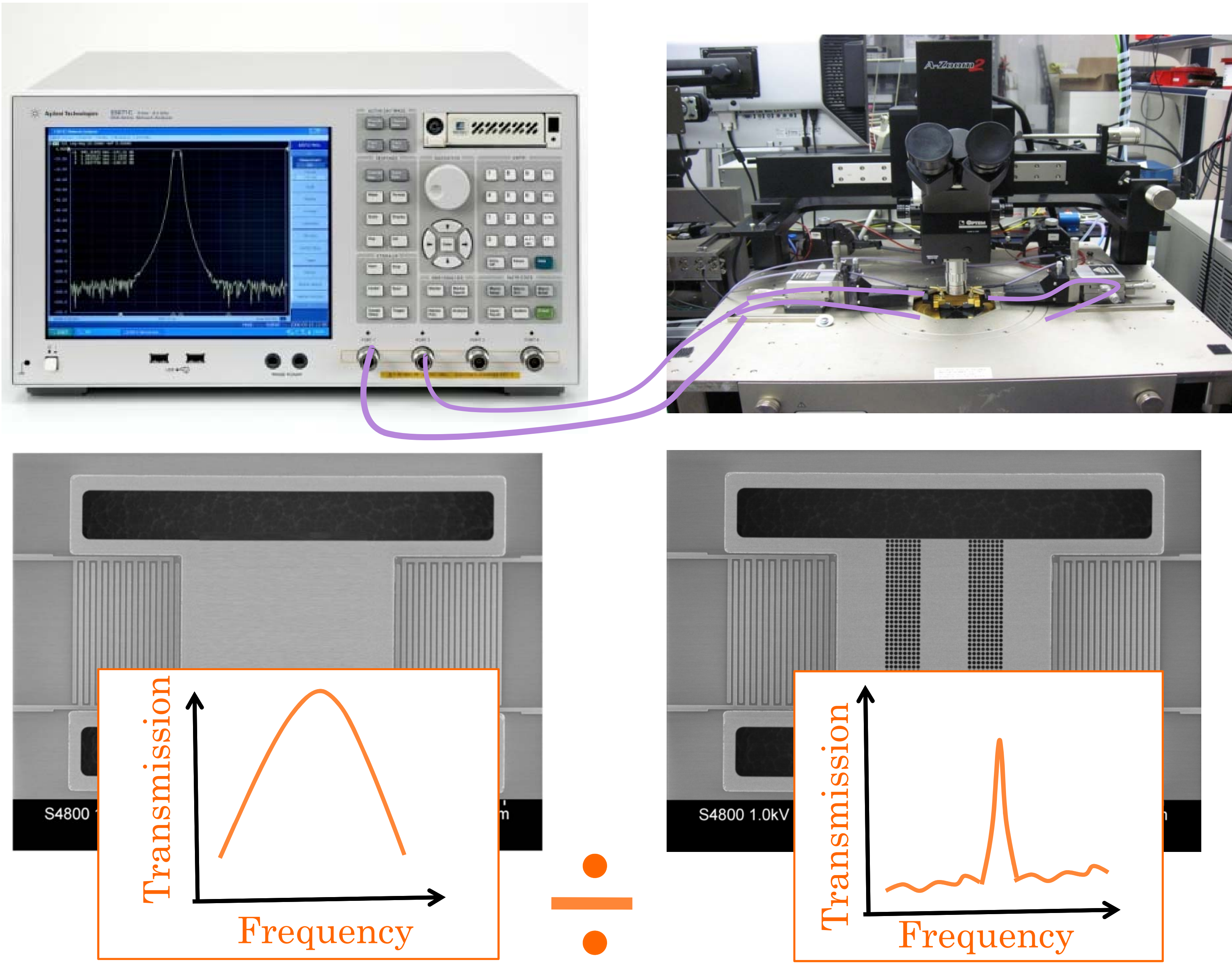
Cross section SEM of SiC etch profile

SiC Etch: Todd Bauer

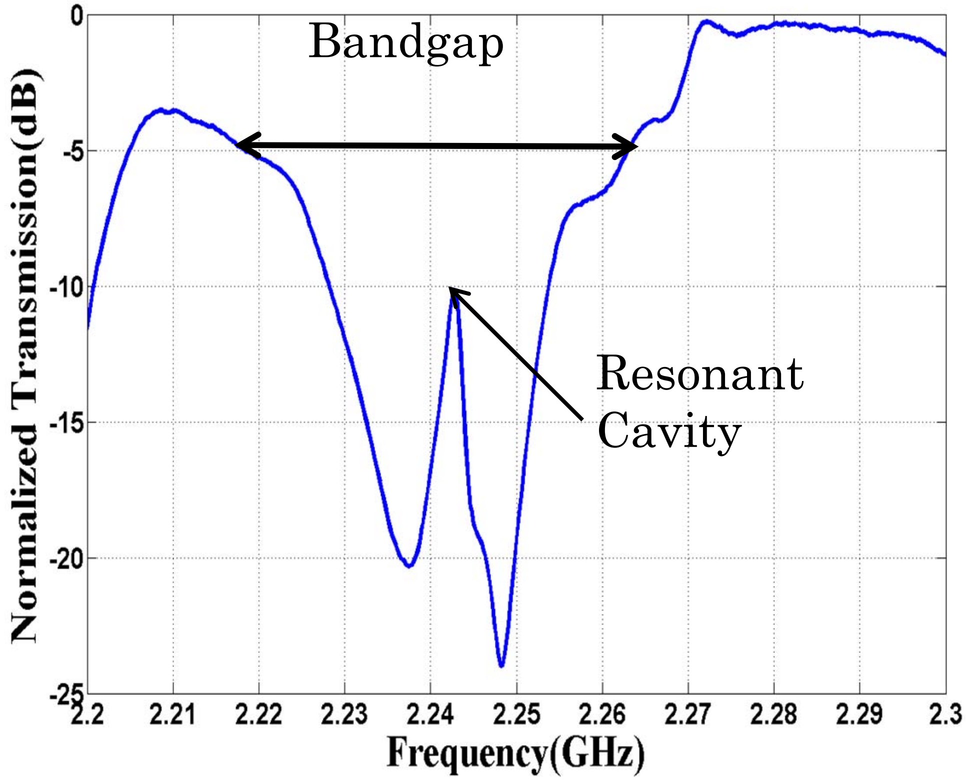
SEMs of Phononic Crystal Cavities



Measurement Setup



Phononic Crystal Overtone Cavities

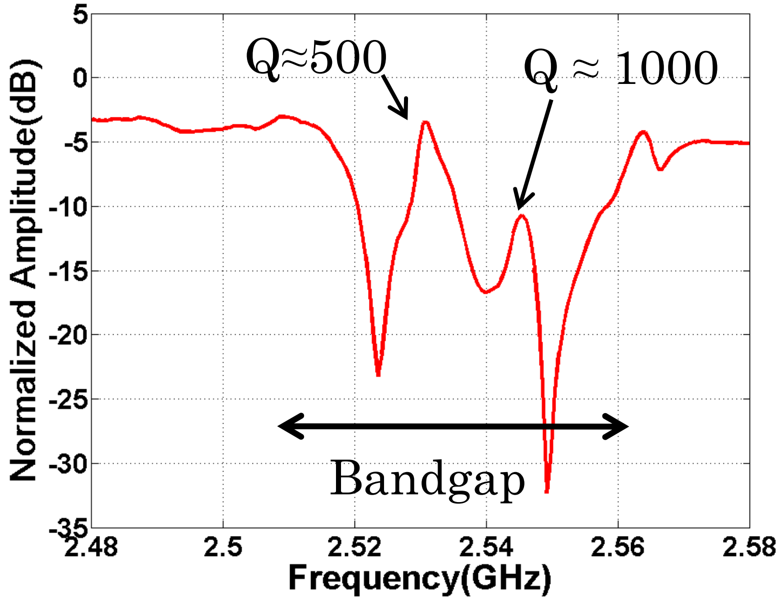


10th Overtone
5 Layer PnC
Cavity
Q~2000

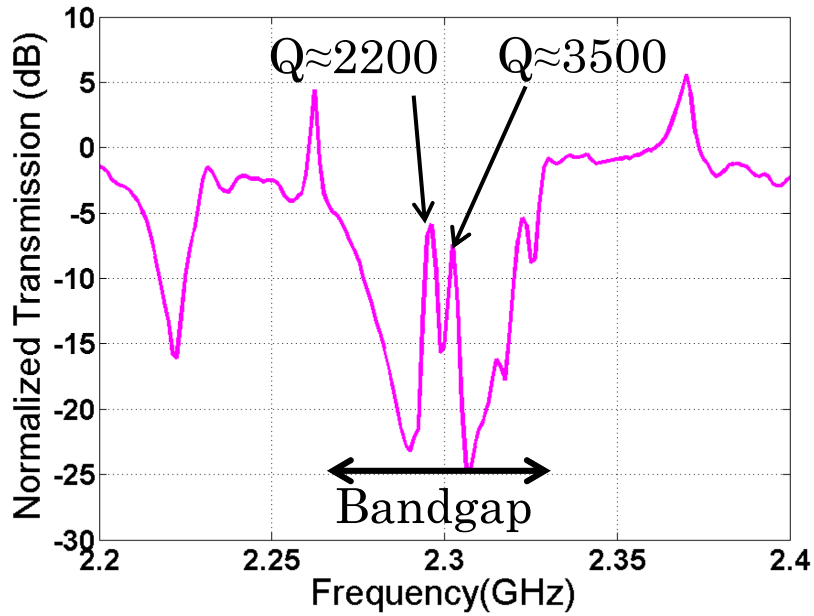
M. Ziaei-Moayyed, et al, MEMS 2011

Phononic Crystal Overtone Cavities

50th Overtone Cavity with 3 layer SiC/Air Phononic Crystals



50th Overtone Cavity with 5 layer SiC/Air Phononic Crystals



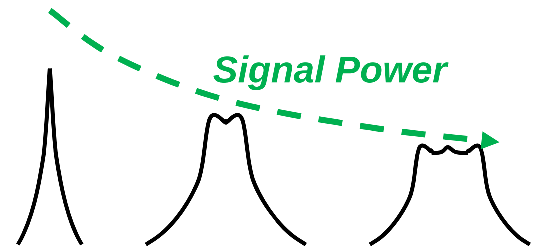
Quality Factor of Fabry-Perot Cavity is improved with higher number of Phononic Crystal Layers

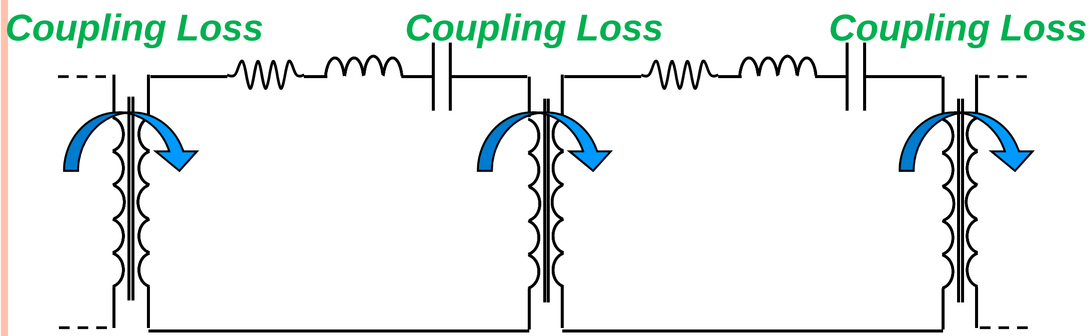
M. Ziaei-Moayyed, et al, MEMS 2011

Phononic Crystal Acoustic Signal Processing

Higher-Order Electrically Coupled Filters

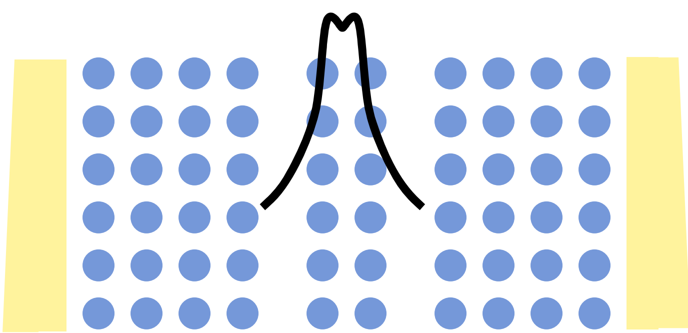
- Filter insertion loss dominated by electro-acoustic coupling losses
- Repeated conversion from electrical to acoustic domain rapidly increases insertion loss





once we are in the acoustic domain we would like to remain in it!

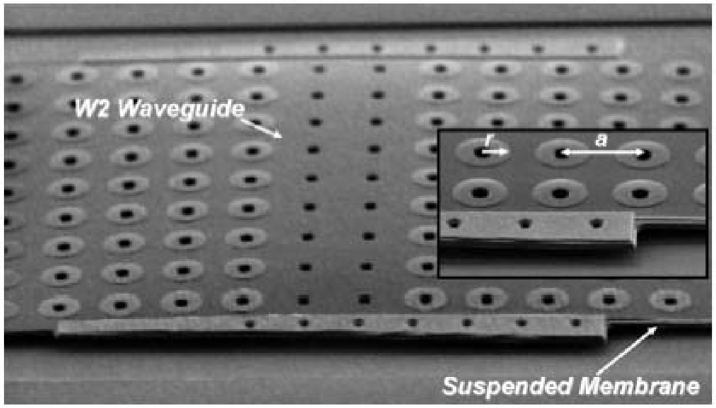
Multi-Order PnC Filters

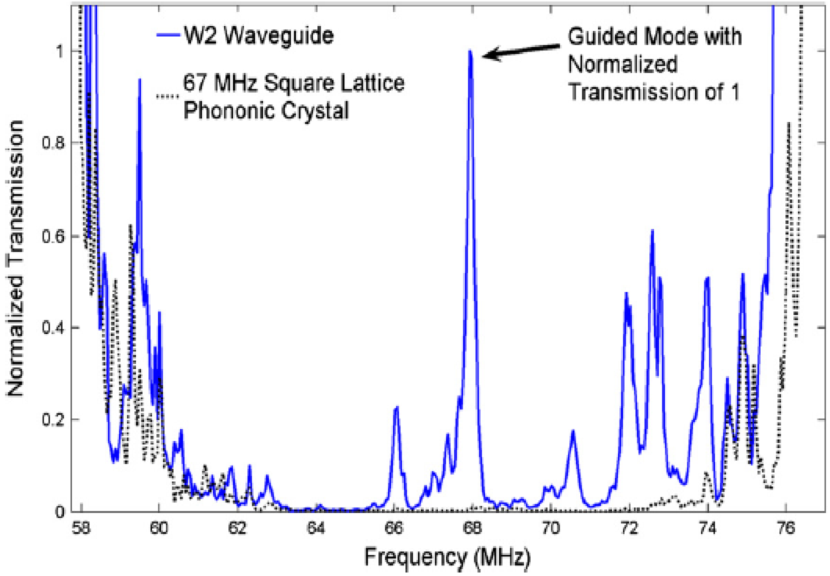


- **Insertion Loss Dictated by Single Electro-Acoustic-Electro Conversion**
- **Once in Acoustic Domain, High Order Signal Processing in Low Loss Materials**
- **Cavities based on pitch, easier to fab.**

PnC Waveguide Applications

- Multiple signal processing functions in a single compact device
- "Slow Sound" Miniature Delay Lines
  - Delay Line Signal Processing and Oscillators (Radar, Imaging)
- Acoustic Transmission Lines
  - Distributed Acoustic Circuits
- Acoustic Isolation

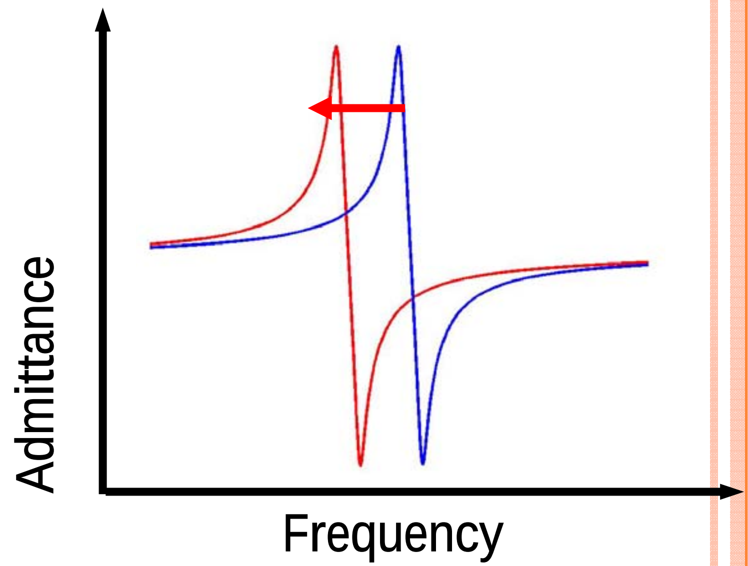




W2 waveguide and response

ACOUSTIC SENSORS

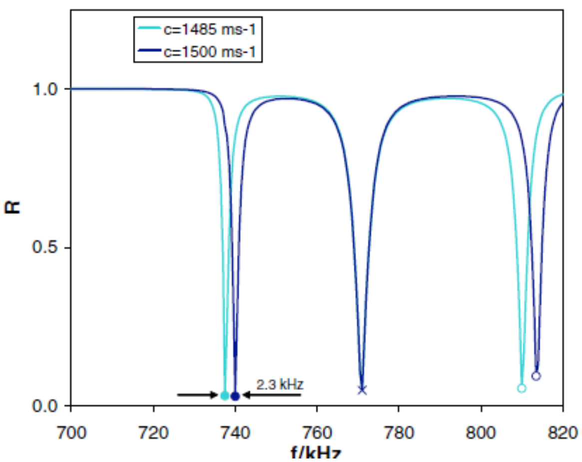
- Chemical and Biological Sensing
  - Change in the acoustic properties of medium results in a shift in the transmission response of the acoustic resonator
  - Sensitivity of the sensor depends on frequency, quality factor, and mass of the sensor

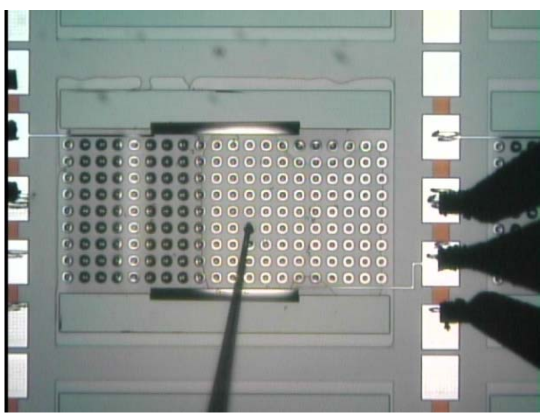


sensitivity ↑ m_{res} ↓ f_o ↑

$$\omega = \sqrt{\frac{k}{m}}$$

$$\Delta m = m_{res} \frac{\Delta f}{f_O}$$

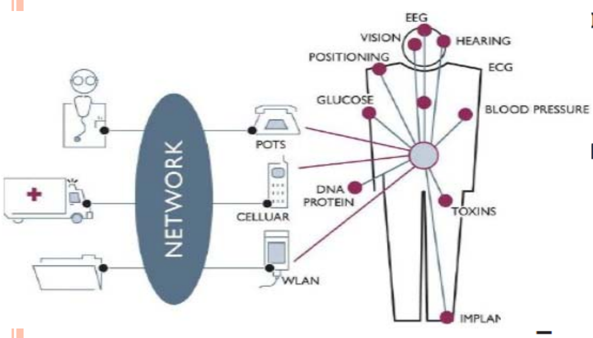


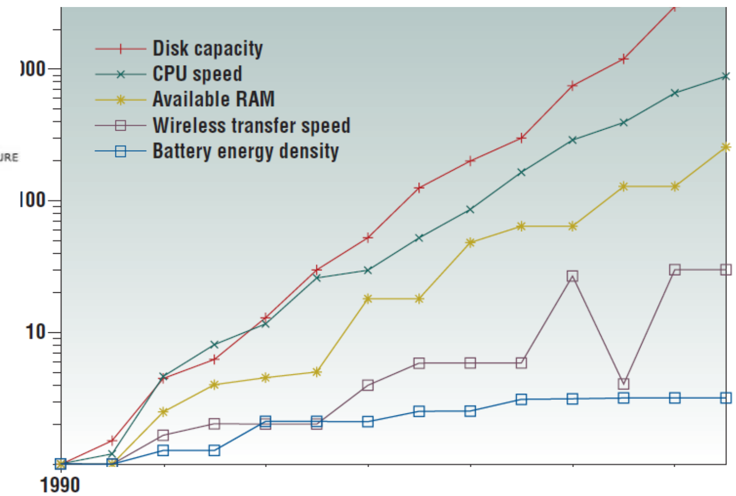


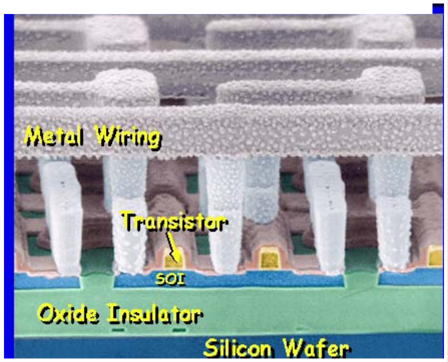
R. Luckum, et al Phononic Crystals for liquid sensor applications, Meas. Sci. Tech. 20 (2009) 124014

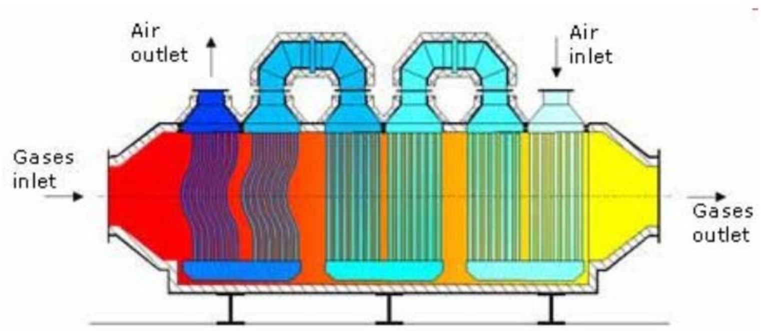
Thermal Energy Management

Removing heat in microelectronics to recovering the wasted heat in the environment, electronic devices, engines, power plant, and human body to power intelligent autonomous systems such as a wireless sensor networks and wireless implantable biomedical devices





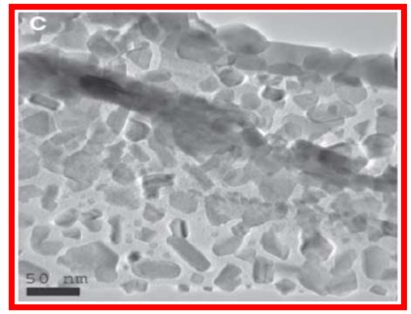




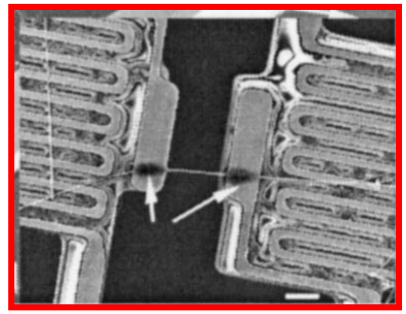
MANIPULATING THE PHONON POPULATION

- *Current Approaches*
  - *Surface Scattering: Roughening the surface to increase phonon scattering*
    - *Affects only surface propagating modes*
    - *Acts only on a narrow spectrum* $\Delta\lambda$*~roughness length scale*
    - *Non-deterministic*
  - *Nano-tubes/wires: Waveguide cutoff*
    - *Acts only on a narrow thermal spectrum* $\lambda \leq$ *diameter*
    - *Suppresses low frequency phonons, rather than THz phonons*
  - *Grain boundary Scattering:*
    - *Highly non-deterministic*

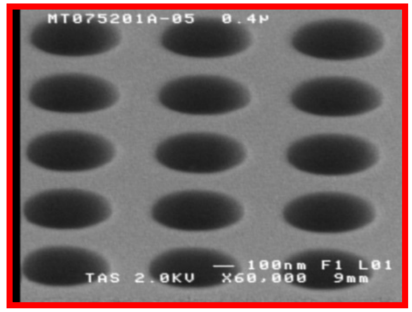
- *PnC Approach*
  - *Highly deterministic: "at-will" control*
  - *Wide spectrum: in the THz*
  - *3D control: Bulk, surface, shear, …etc.*



Poudel *et al.*, Science 320, 634 (2008)



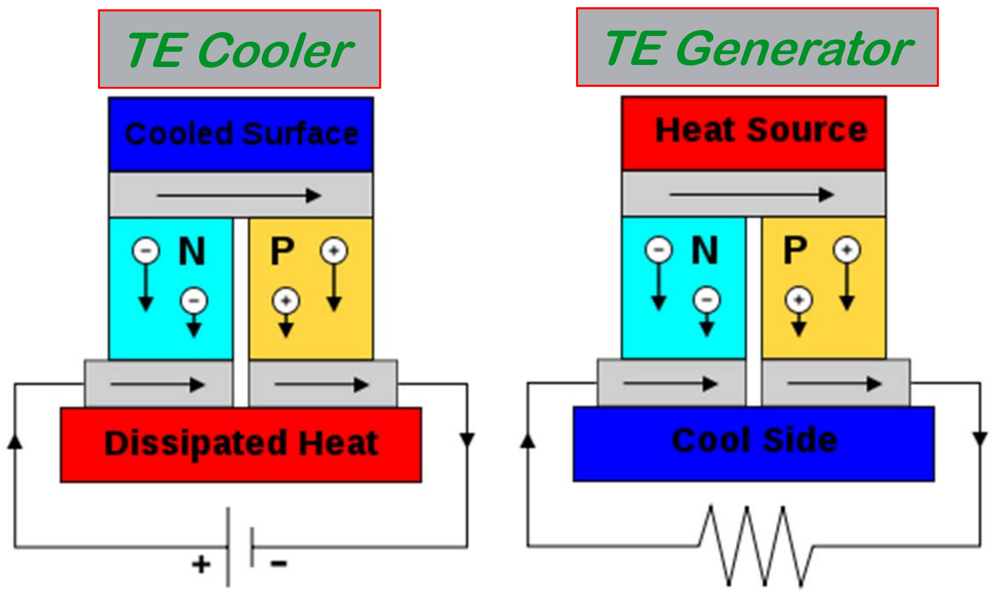
Hochbaum *et al.*, Nature 451, 163 (2008)



Hopkins *et al.* , Nano Lett. 11 (1) 2011

Manipulating Thermal Phonons

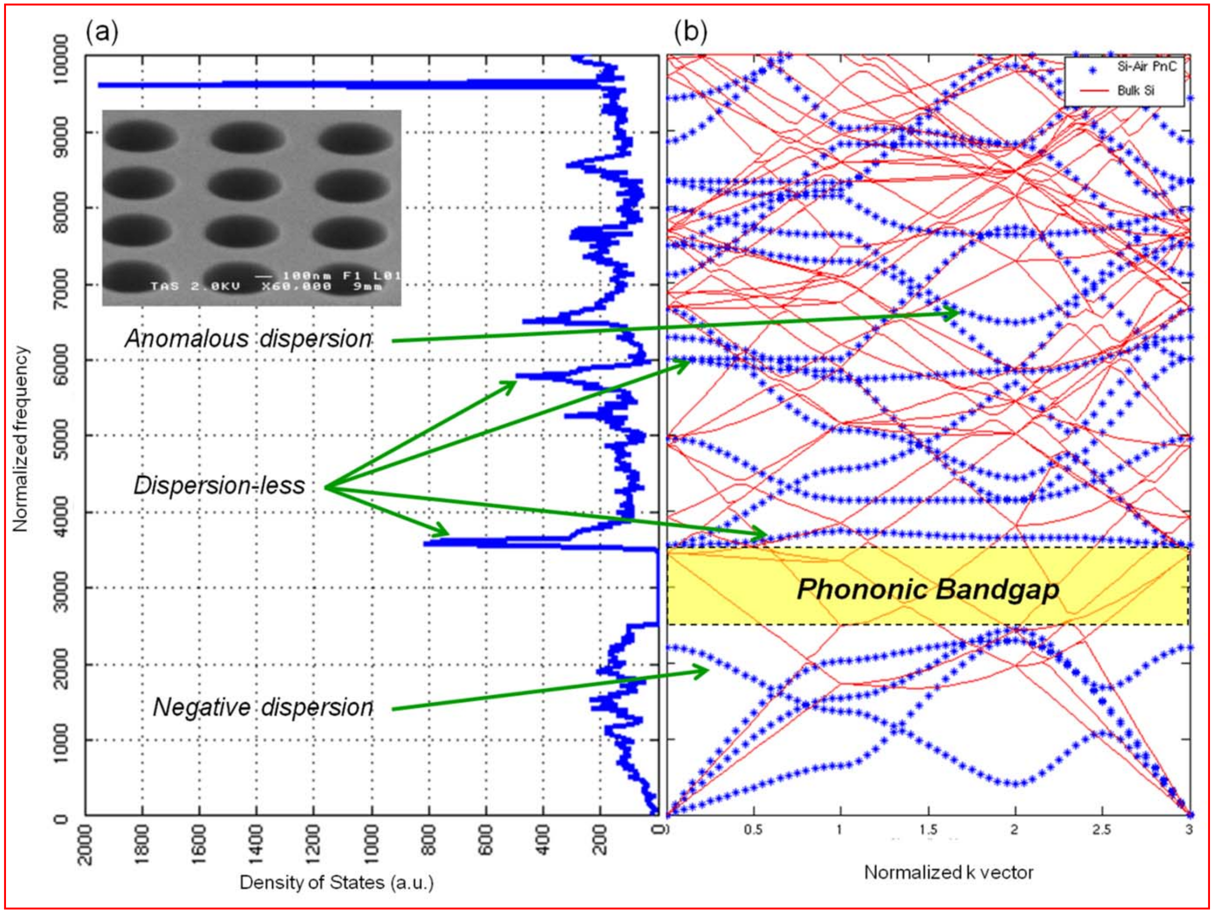
- *Electronics*
  - *Thermoelectric Energy Scavenging and Cooling*
  - *ZT Figure of merit*
- *Silicon Laser*
- *Nonradiative relaxation in QW's*
  - *Cap on SS-laser efficiency*
  - *Cap on SSL device efficiency*
- *Spin wave relaxation*
  - *Stability of Spintronics*
  - *Quantum Computing*
- *Superconductivity*
  - *Binding of Cooper pairs*
  - *Phonon Bottleneck*
  - *Hi-TC*
- *Quantum Friction*

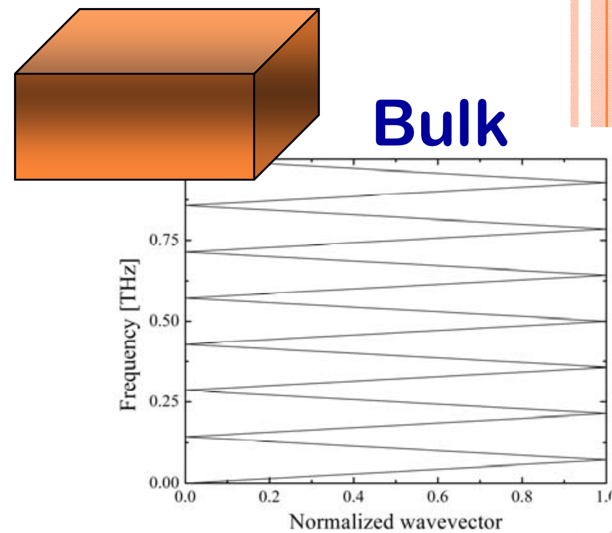


TE Seebeck and Peltier Effects:

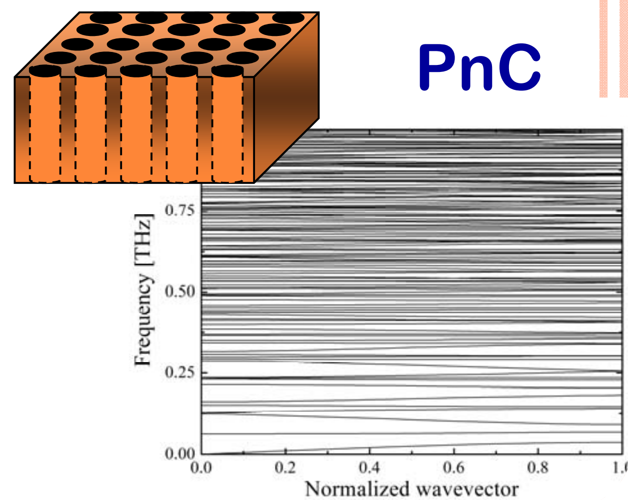
- *Cooler:* *Apply DC voltage* ➔ *heat moves from cold-side to hot-side*
- *Generator:* *Heat gradient* ➔ *current flow*
- *Efficiency:* *Quantified by the dimensionless quantity ZT*
- *Figure of merit :* $Z = S^2\sigma/K$
- *S:* *Seebeck Coefficient* $(\Delta V/\Delta T)$
- *σ:* *Electrical conductivity*
- *K:* *Thermal conductivity* $(= K_e + K_{ph})$

Harmonic and Anharmonic Effects



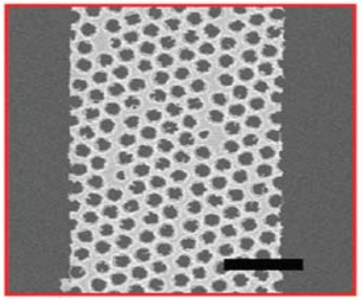


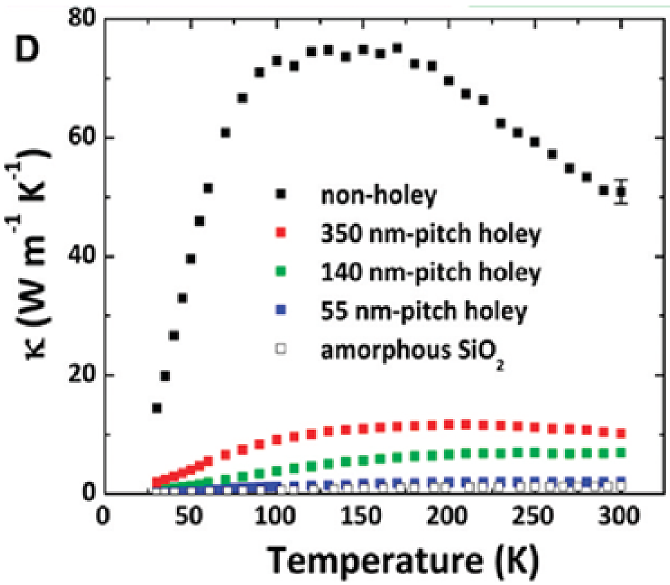
$$\rho(\vec{r})\frac{\partial^2 u_i(\vec{r},t)}{\partial t^2} = \sum_{j,m,n} \frac{\partial}{\partial x_j}\left[C_{i,j,m,n}(\vec{r})\frac{\partial u_n(\vec{r},t)}{\partial x_m}\right],$$

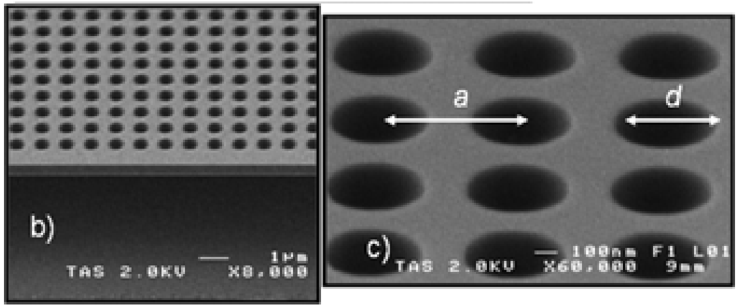


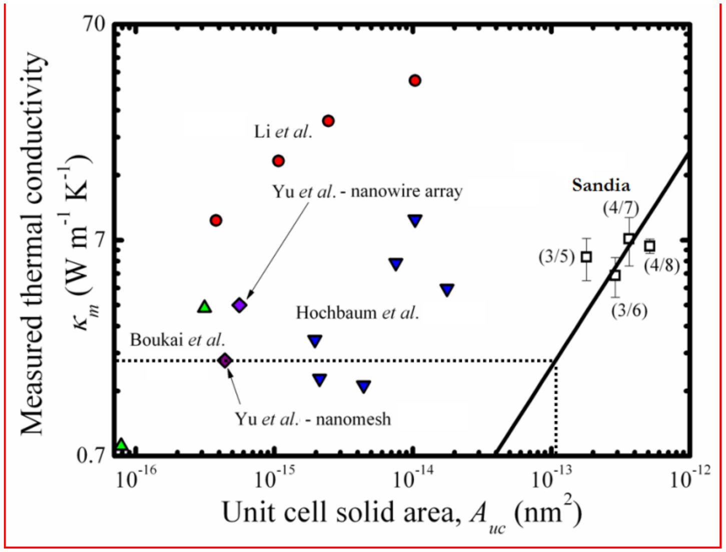
- Harmonic (coherent) Reflections ➔ Creation of gap
- Anharmonic Effects ➔ Anomalous dispersion
- Flat Bands ➔ Reduced Group Velocity
- Negative Bands ➔ Backward propagation (backward scattering)

AN ORDER OF MAGNITUDE LOWER κ DEMONSTRATED









Nanowires: φ= 0
Microporous Si: φ ~ 25%
PnC: φ < 20%

PnC outperforms nanowires @ 2 orders of magnitude larger limiting dimension (L)!

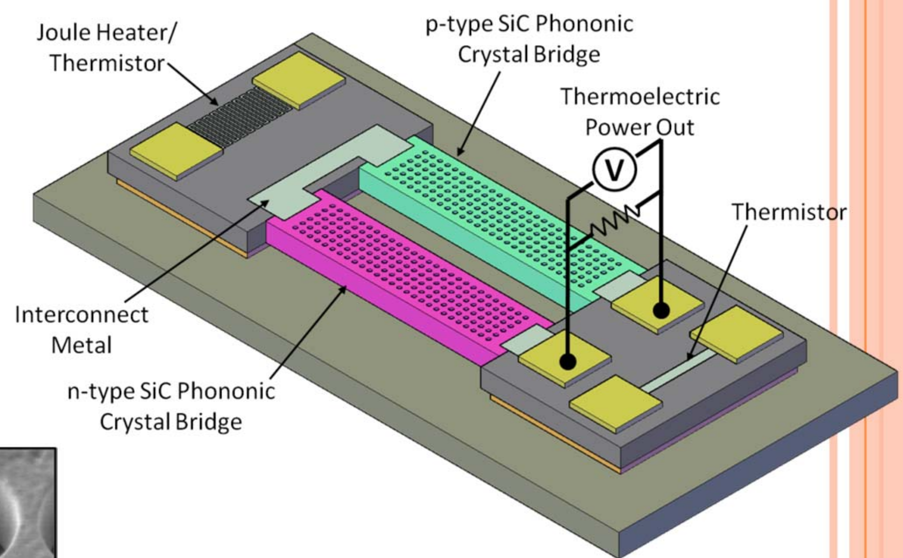
Since the mean free path of electrons is an order of magnitude lower than that of phonons, ➔ Based solely on phonon thermal conductivity reduction, ZT of greater than 1 can be achieved

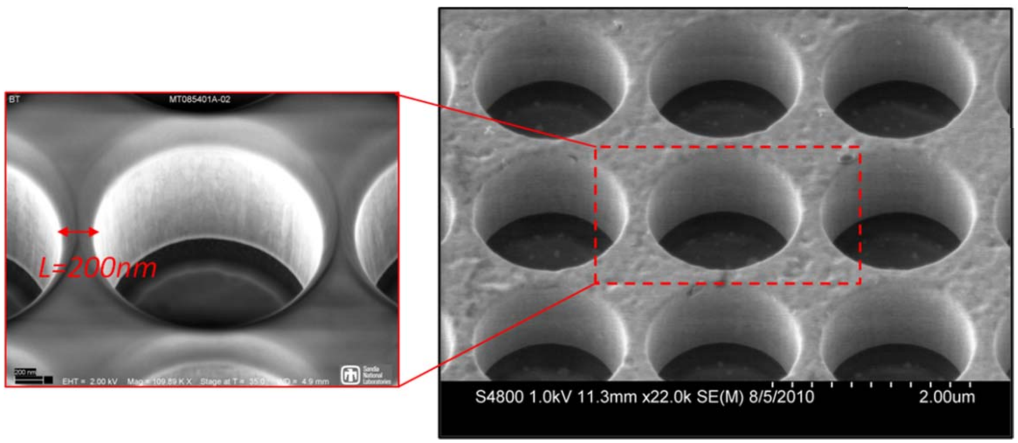
Silicon Carbide PNC Thermoelectric Devices

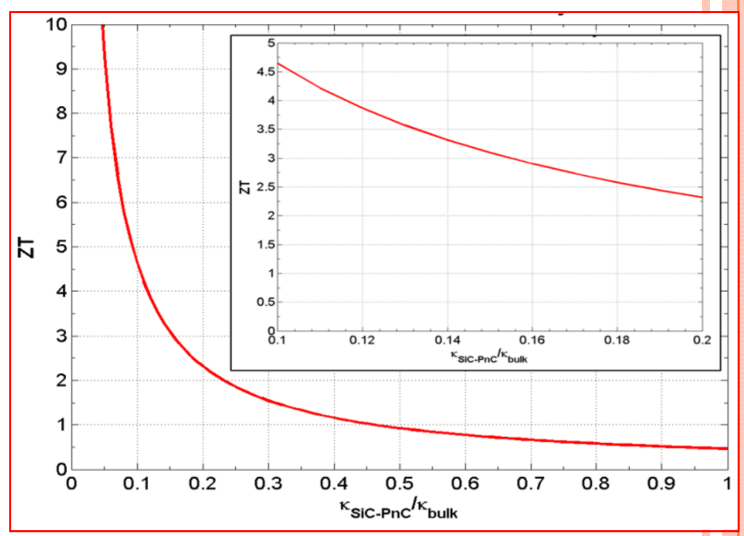
Silicon Carbide is a target material for harsh environment applications

Silicon Carbide has high Seebeck Coefficent (S) but also high thermal conductivity (κ)

→Silicon Carbide Phononic Crystal Thermoelectric Devices



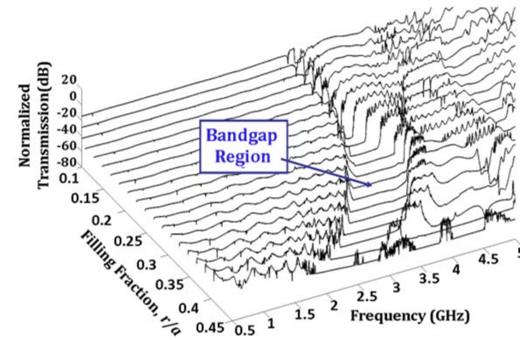


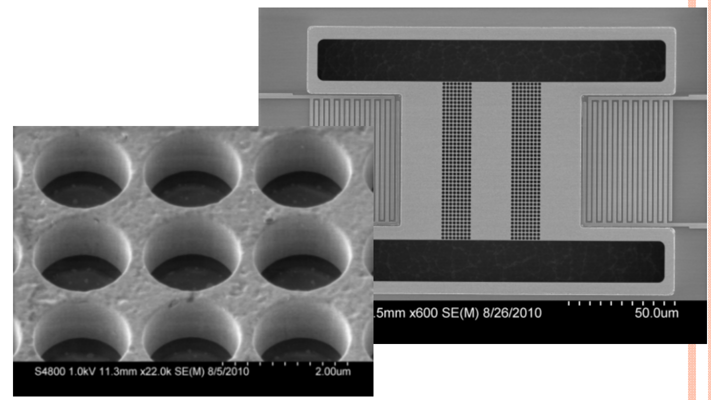


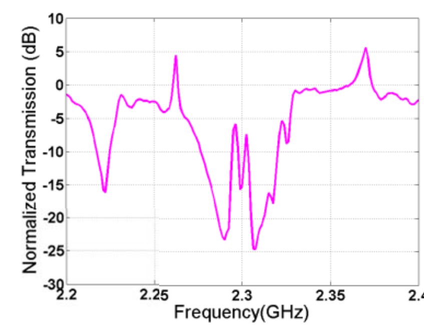
SiC TE property	n-type	p-type
Doping level, N	$2.4*10^{20}/cm^3$ [1]	$10^{21}/cm^3$ [4]
Seebeck coefficient, S	-2000 μV/K [1]	600μV/K [6, 7]
Electrical resistivity, ρ	5mΩ·cm [1, 7, 8]	10mΩ·cm [4]
Thermal conductivity, κ	50W/mK [10, 13]	50W/mK [10, 13]

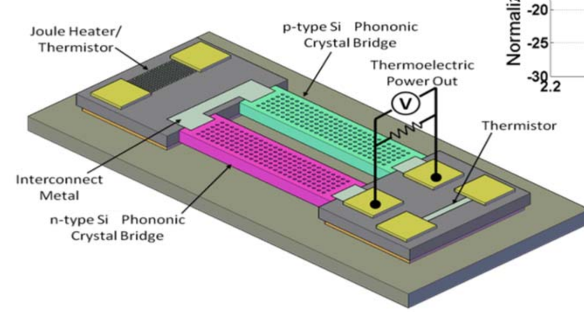
CONCLUSIONS

- We have developed a highly oriented SiC thin film with
  - ***Low Stress <150MPa***
  - ***Low Surface Roughness <1nm***
  - ***Micromachined with Near Vertical Sidewalls***
- Modeling and Design
  - Design and modeling of phononic crystals
  - Fabry perot cavity resonators with phononic crystals have been designed and modele
- Fabricated SiC phononic crystal-based cavities with integrated piezoelectric transducers
- Demonstrated phononic crystal cavities with quality factors greater than >5,000 at ~2.5GHz
- Silicon Carbide phononic crystal devices for harsh environment/high temperature thermoelectric energy management









Acknowledgments

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- Amy Duwel, Draper Labs

Funding Sources

DARPA MTO CSSA pogram (Dr. Dennis Polla and Dr. Sanjay Ramab)
Sandia LDRD program

Key Contributors

Fabrication: Tracy Peterson, Scott Habermehl, Peggy Clews, Melanie Tuck, Keith Yoneshige, Todd Bauer, Kira Fishgrab, Mark Loviza, Ross Hanold, Doug Greth, Dana Pulliam

Design and Modeling: Maryam Ziaei-Moayyed, Troy Olsson, Ihab El-Kady, Darren Branch, Mehmet Su, Charles Reinke, Chris Nordquist.

Contact Information

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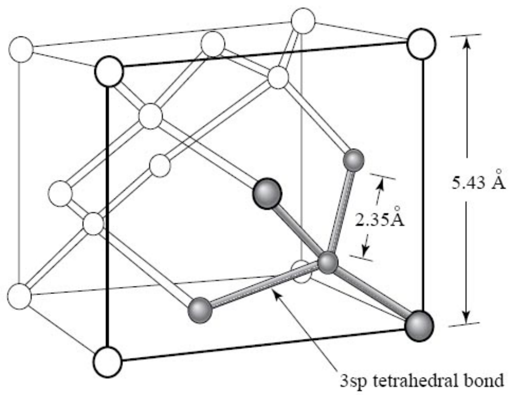
Questions???

mziaeim@sandia.gov

BACKUP SLDIES

Band-Gaps Formed Through Scattering

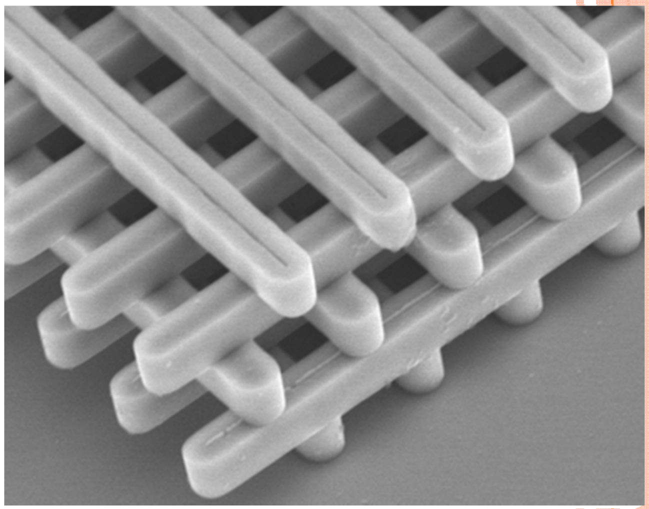


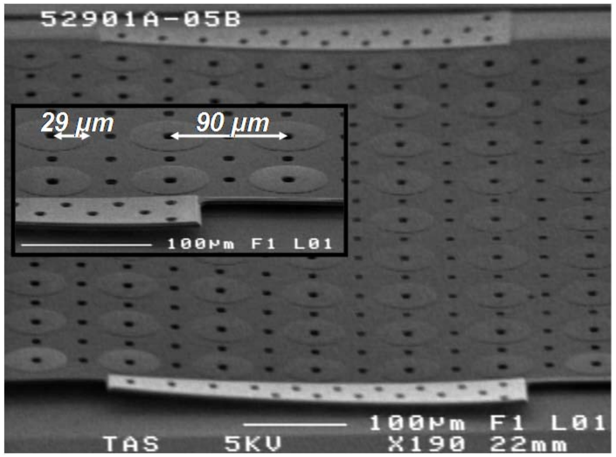
Semiconductor Band-Gap Crystal

Bragg Scattering of Electrons in a Crystal Lattice Based on Bloch's Theorem Results in the Well Known Semiconductor Band-gap

Photonic Band-Gap Crystal (PtC)

Bragg Scattering of Photons Opens Frequency Ranges Where Photons Can Not Propagate Within the Crystal





Phononic Band-Gap Crystal (PnC)

Bragg and Mie Scattering of Phonons Opens Frequency Ranges Where Phonons Can Not Propagate Within the Crystal

Fundamental Loss Mechanisms in Resonators with Small Damping

Thermoelastic Damping:

$$Q_{TED} = \frac{9C^2}{\kappa T \alpha^2 \rho \omega}$$

ω = angular frequency
T = temperature
ρ = density
C = heat capacity/volume
α = thermal expansion coefficient
κ = thermal conductivity
ν = sound velocity
γ = Gruneisen constant
ν_l = longitudinal sound velocity
ν_t = transverse sound velocity

Phonon-Phonon Damping:

$$Q_{phph} = \frac{\rho \nu^2}{CT\hat{\gamma}^2} \frac{1 + (\omega \tau_{ph})^2}{\omega \tau_{ph}}$$

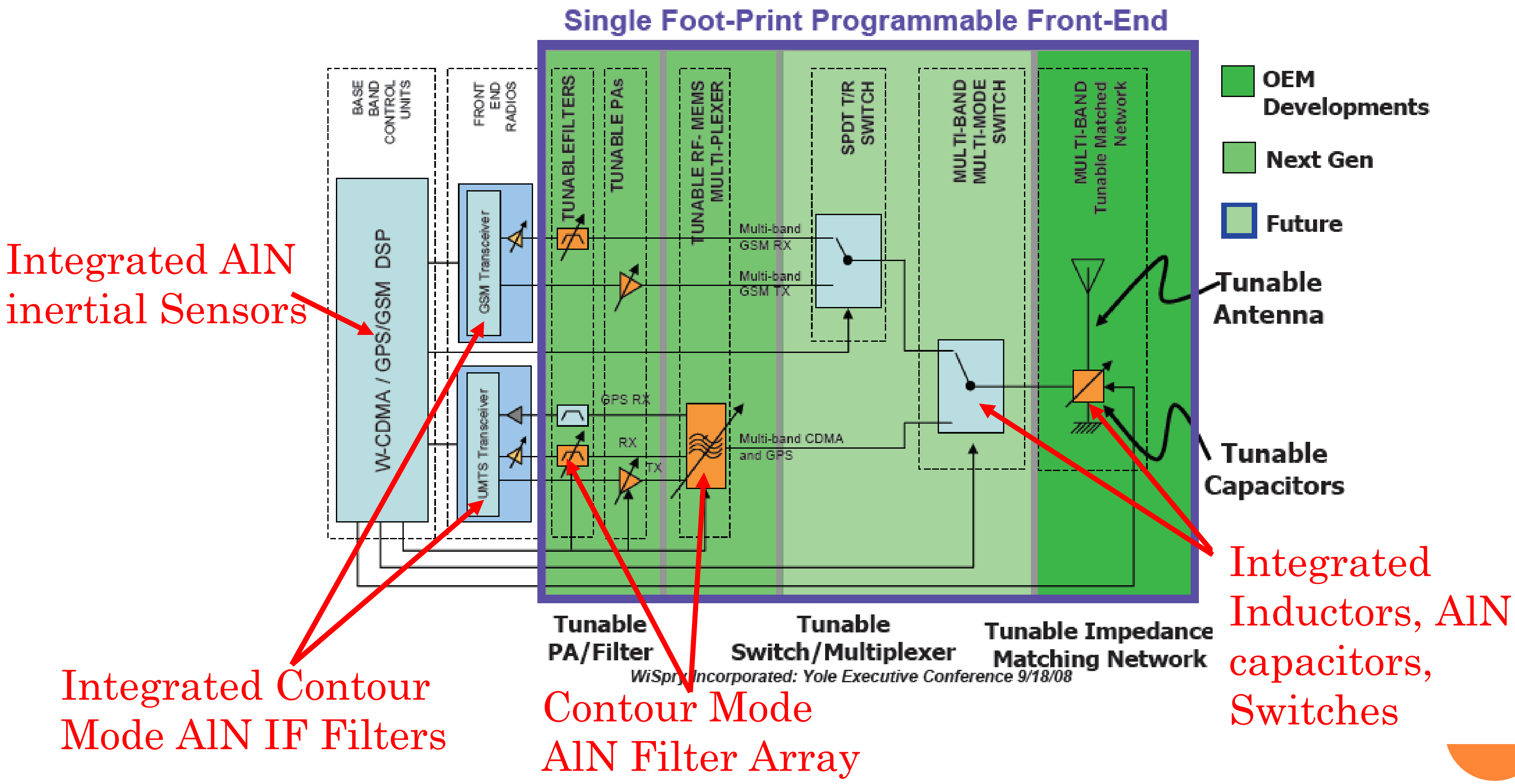
$$\tau_{ph} = \frac{3\kappa}{C \nu_D^2}$$

$$\nu_D = \left(\frac{1}{\frac{1}{3\nu_l^3} + \frac{2}{3\nu_t^3}} \right)^{1/3}$$

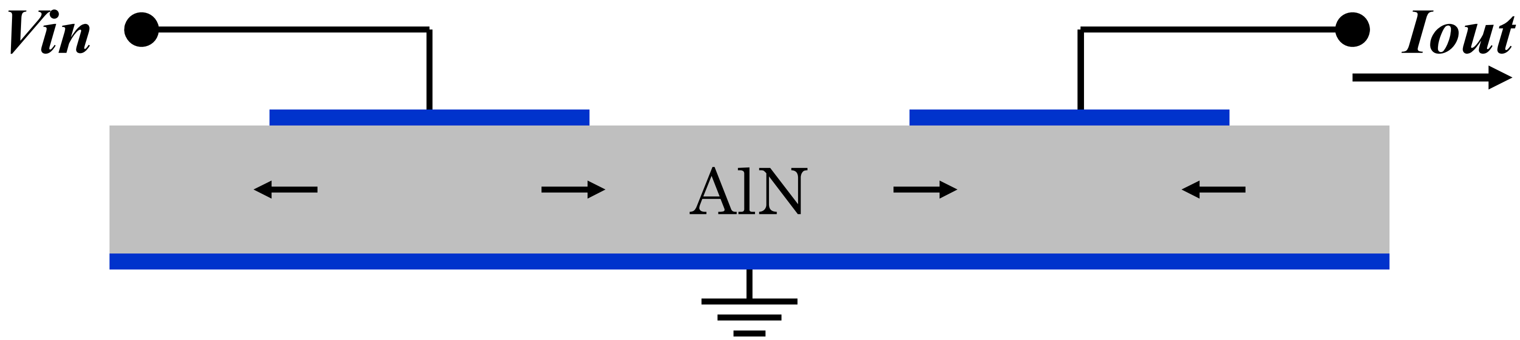
Aluminum Nitride Resonators and Filters

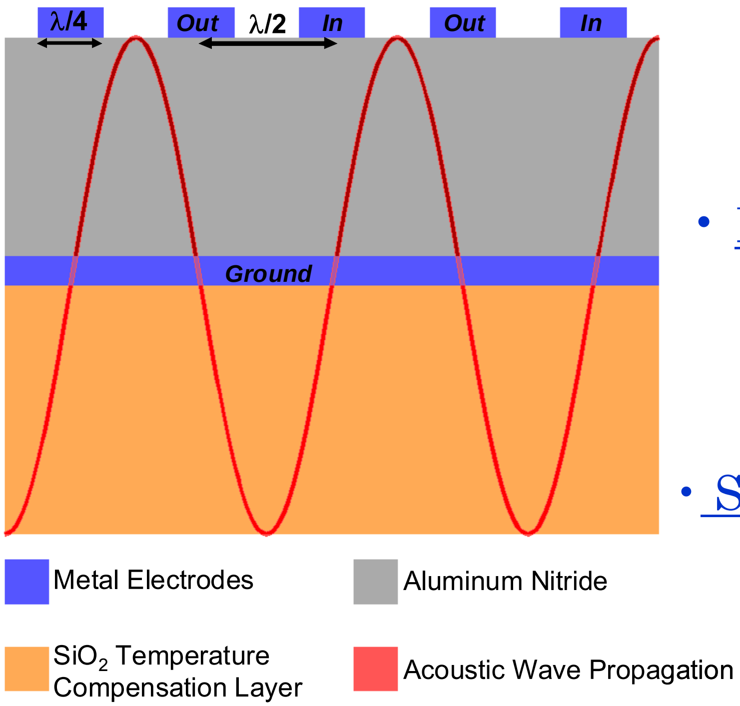
FILTERS BANKS FOR RF COMMUNICATIONS

- Next Generation Handset Require > 20 Filters Operating in Different Bands: CDMA, GSM, GPS, WiFi, WiMax, BlueTooth, etc.
- Typically Large Foot Print (1-2 Acoustic Filters per Package)
- Microresonator Technology Can Potentially Address Many of These Filters on a Single Chip, Reducing Size, Cost, and Power.



PIEZOELECTRIC TRANSDUCTION



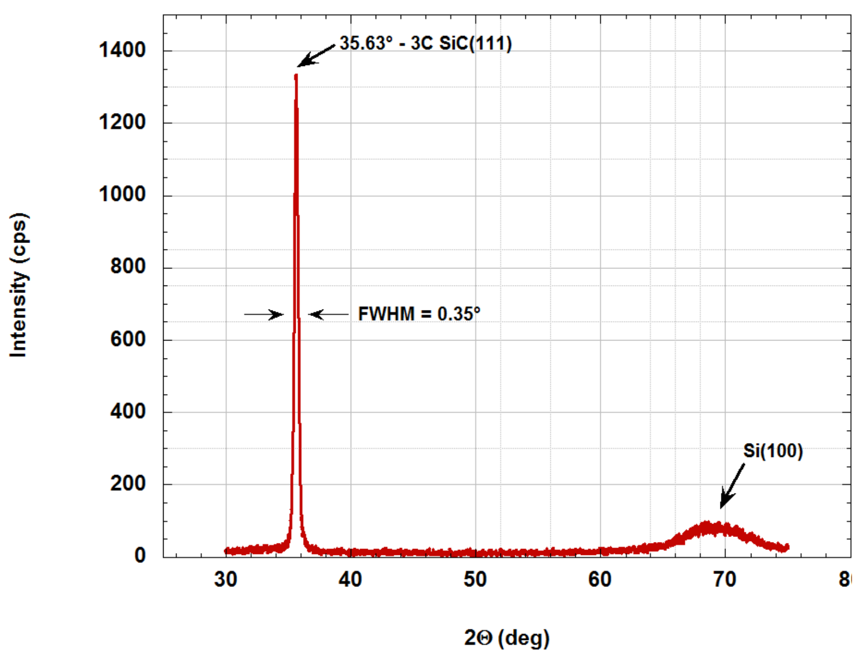


- Microresonators
  - *Constant Film Thickness vs. Frequency*
  - *I.L./Area Constant Over Frequency*
  - *Substrate Isolation and Etched Sidewall*
- FBAR or BAW (Bulk Acoustic Wave)
  - *Resonant Freq. Set By Film Thickness*
  - *I.L./Area Varies With Frequency*
  - *Resonators Become Large at Low UHF*
- SAW (Surface Acoustic Wave)
  - *Transduced Via Lateral Fringe Field*
  - *Spacing Between Electrode Large at Lower Frequencies (High I.L./Area)*
  - *Lithography Too Expensive Above a Few GHz*
  - *Narrow-Band Requires Many Finger Pairs*

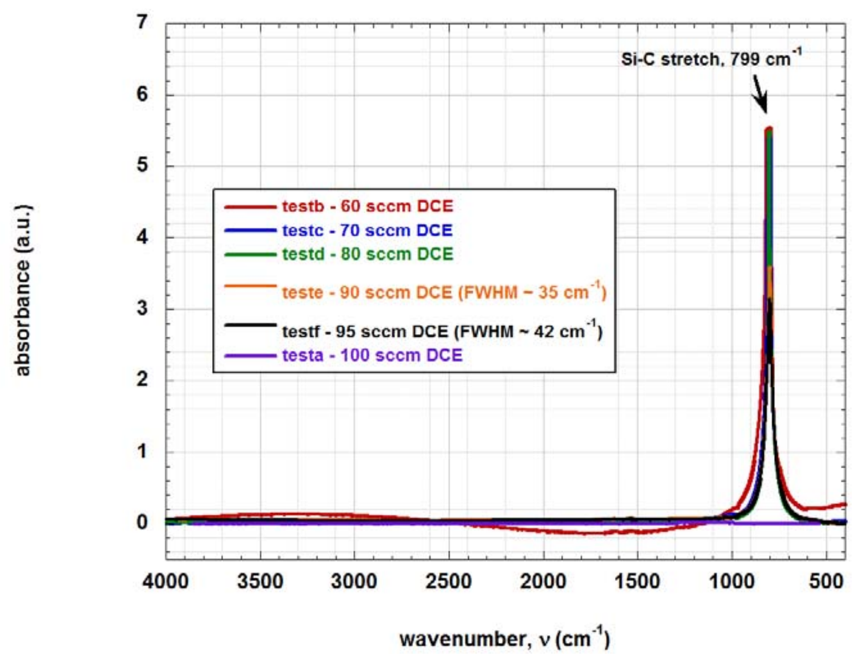
THIN FILM SILICON CARBIDE DEVELOPMENT

- The quality of the silicon carbide film determines the highest possible f.Q
- Novel Silicon Carbide LPCVD process developed at Sandia
- As deposited stress of less than 150 Mpa Tensile

X-Ray Diffraction



FTIR



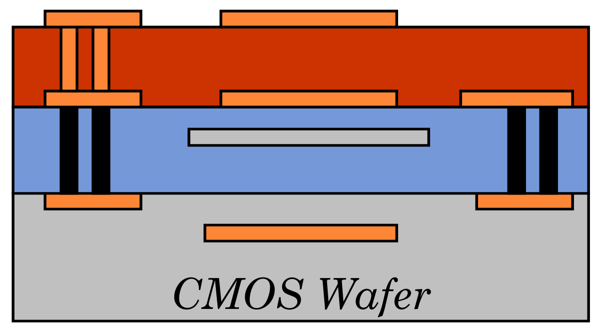
Highly oriented and textured Poly-crystalline Cubic SiC

SiC film development: Scott Habermehl

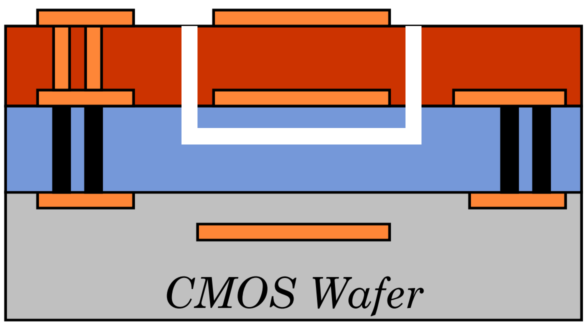
Post-CMOS μResonator Integration

Start: Deposit oxide and low temperature custom Si release layer over foundry CMOS

Pattern Si release layer, deposit planar SiO_2 temperature compensation film and form W contacts to CMOS



Deposit and pattern bottom Al electrode, AlN piezoelectric layer and top Al electrode



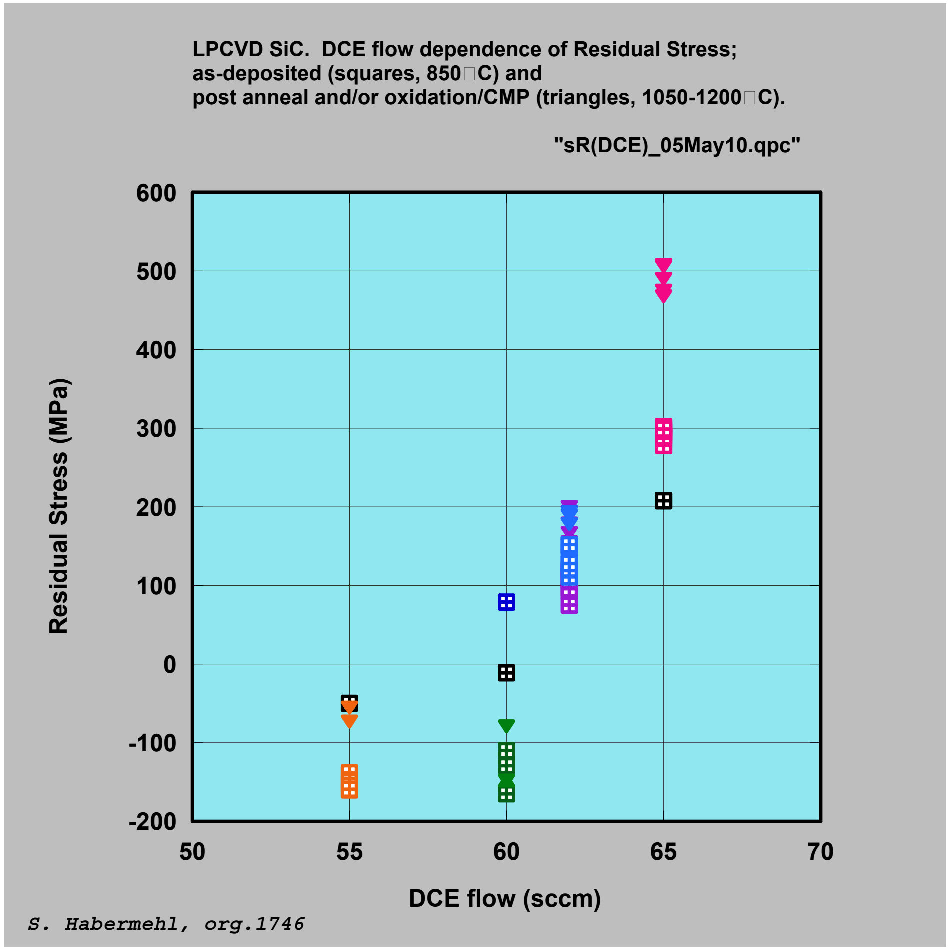
Finish: Etch trenches to Si release layer and suspend the accelerometer using dry SF_6

Process Backup

SiC As Deposited Stress

Residual Stress in LPCVD SiC films for different DCE flows

Residual Stress in LPCVD SiC from DCE, continued



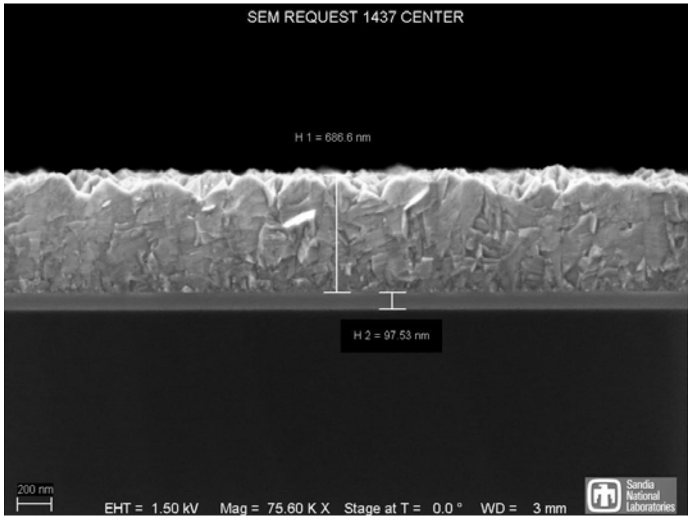
Key:
squares = as-deposited
triangles = post oxidation/CMP

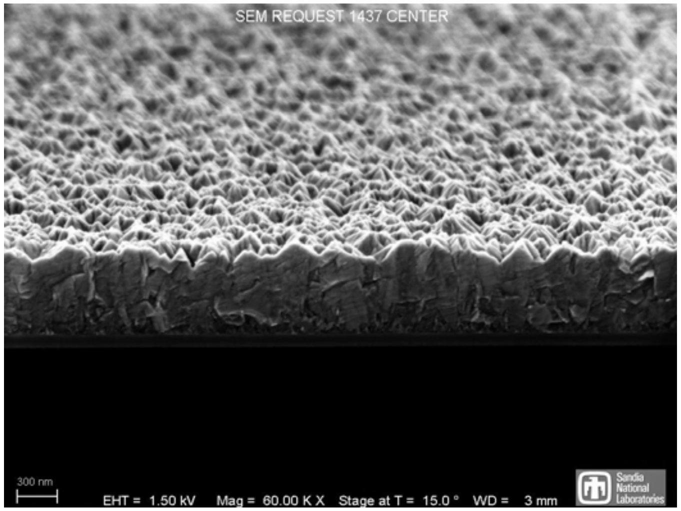
- **⇒ 55-60 sccm films are compressive,**
- **⇒ film stress increases 50-100 MPa after oxidation/CMP cycles for 55-62 sccm films and ~ 200 MPa for 65 sccm films.**
- **⇒ variations in σ_R at a given flow are actually related to wafer position in the reactor (i.e., local DCS/DCE ratio).**

SILICON CARBIDE PLANARIZATION (CMP)

SiC Surface Planarization CMP Development

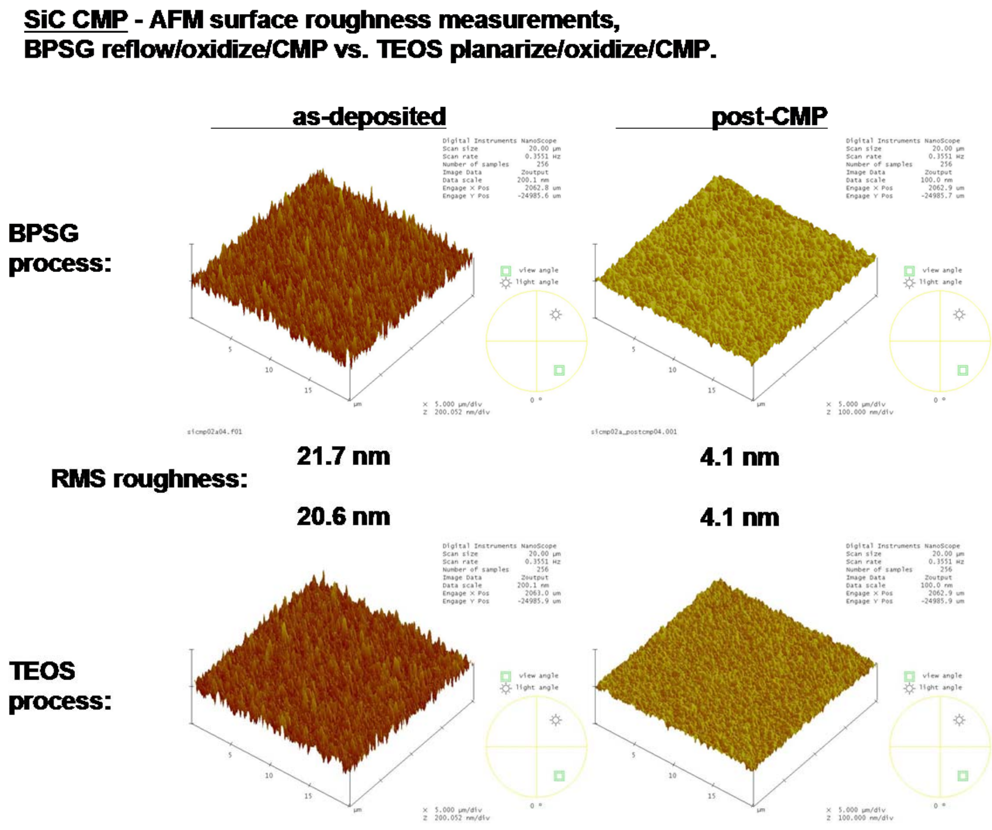
Methods tested		typical Rms roughness	
1)	as-deposited, 850°C (no smoothing)	20-22	
2)	Thermal oxidation/oxide CMP	4-5	**First Process Run**
3)	BPSG deposit/reflow/oxidize/oxide CMP	3.6-5.2	
4)	a-Si deposit/CMP planarize/oxidation/oxide CMP	7.7-10.2	
5)	W slurry CMP, direct SiC polish	< 1	**Future Process Runs**
6)	as-deposited, 950°C (no smoothing)	~ 6.5	





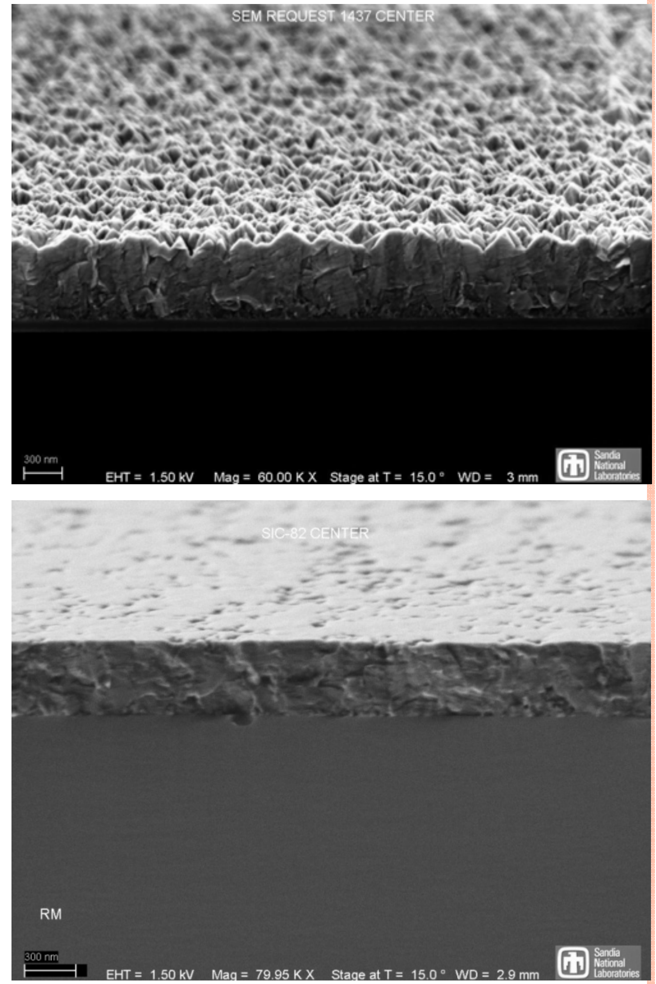
SEM images of as deposited SiC

OXIDATION AND CMP



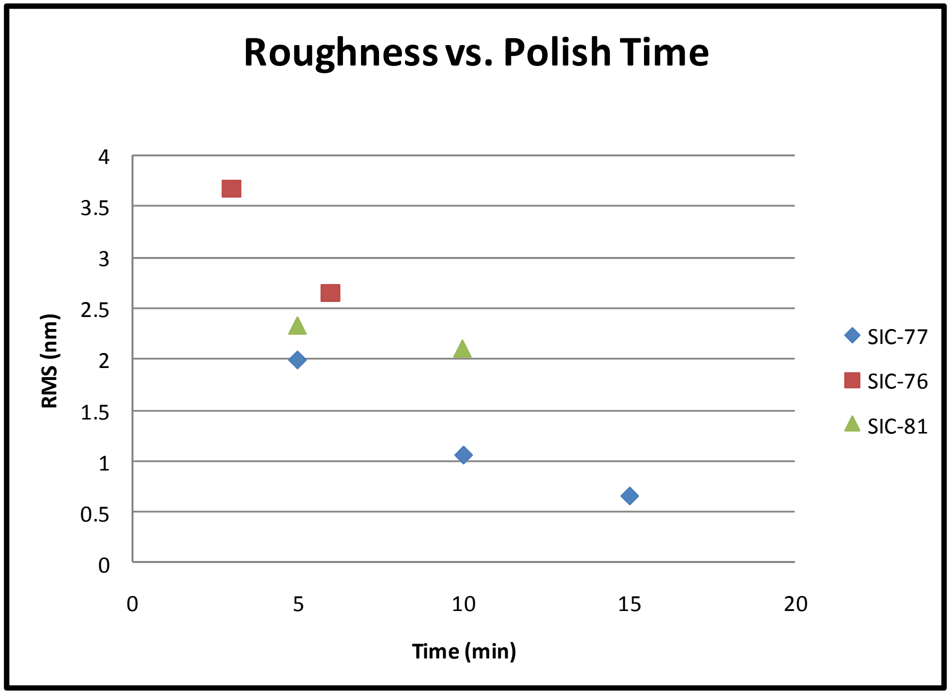
• SiC oxidation then CMP is a significant improvement but

- *Roughness limited to 4 nm*
- *Actually smoother but pitting in surface*
- *This is used in the 1st fabrication of devices*

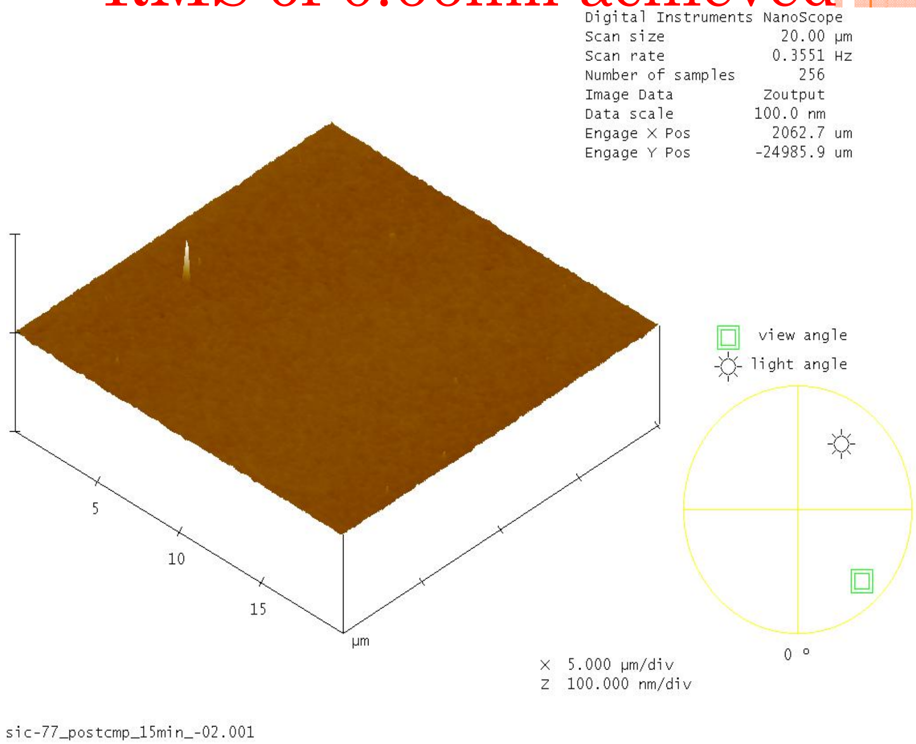


SEM images of as deposited and oxidation/smoothed SiC

CMP Using W Slurry



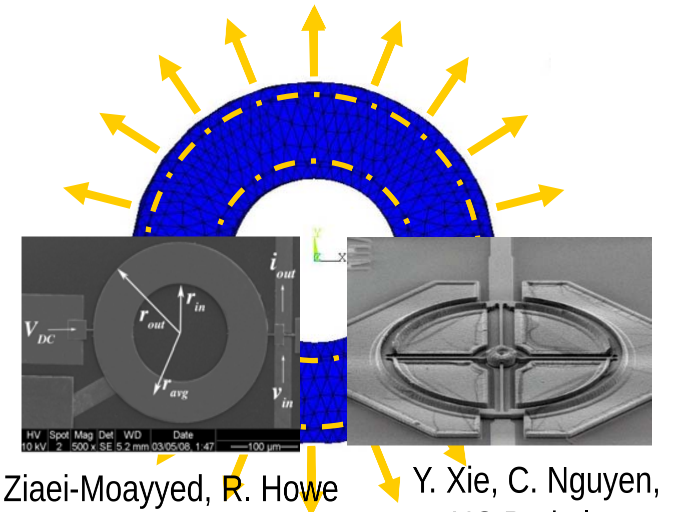
RMS of 0.66nm achieved



- Direct CMP of SiC Using W Slurry
  - *Roughness less than 1 nm*
  - *Eliminates oxidation for lower stress*
  - *Drastically reduces surface pitting*
  - *Will be used in future lots*

THE ULTIMATE TRADE OFF : F.Q VS. INSERTION LOSS

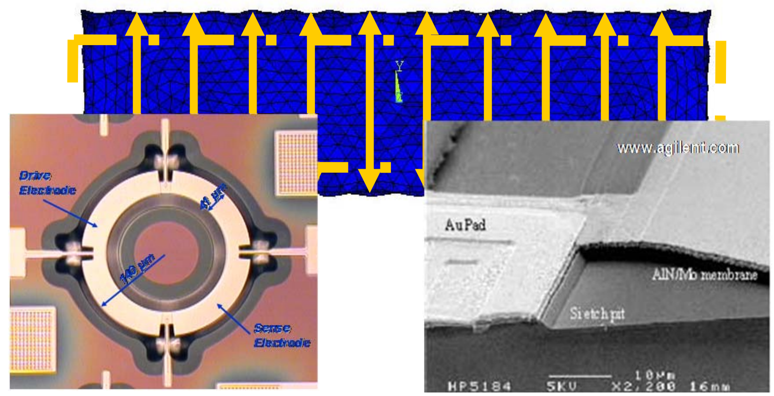
- **Capacitive MEMS Resonators**
  - ✓ *Highest f.Q products for acoustics*
  - x *Weak electromechanical coupling leads to high motional impedance*
    - Higher noise, matching problems
    - Arraying and high-K dielectric transduction lead to high parasitic capacitance



M. Ziaei-Moayyed, R. Howe
Stanford U.

Y. Xie, C. Nguyen,
UC Berkeley

- **Piezoelectric MEMS Resonators**
  - ✓ *Low Insertion Loss and impedance (< 50)*
    - Strong electro-acoustic transduction
    - Easily matched to antenna, off-chip circuits
  - x *Q limited to a few thousand*
    - Material damping in metal electrodes and piezoelectric films, creep, aging



R. Olsson et. Al, Sandia

<R. Ruby, et. al, Avago>

Al Pisano UC Berkeley, Piazza Group, U Penn

Want Highly Efficient Transduction + High f.Q in Microresonators

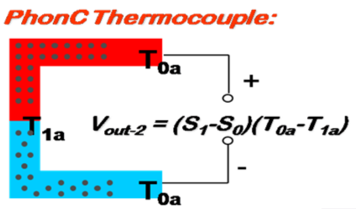
Phonon Manipulation with Phononic Crystals (130777)

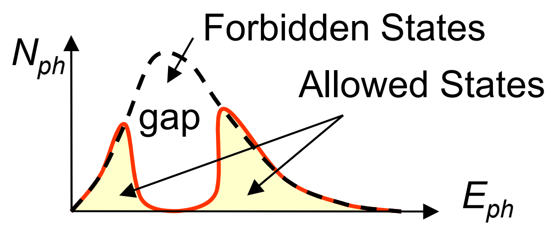
PI: Ihab El-Kady (1725), PM: Rick McCormick (1727), FY09-11, Total Costs: $1735K

Project Purpose and Approach

"We seek to demonstrate the at-will control of thermal (THz) phonons using phononic crystals"

- Thermal conductivity manipulation
- Thermal noise control and suppression
- Thermal energy scavenging
- TE cooling
- Modify electron-phonon, photon-photon interactions
- High ZT



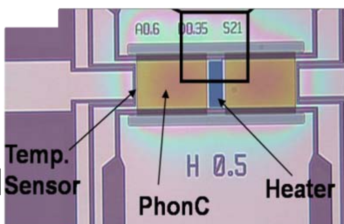


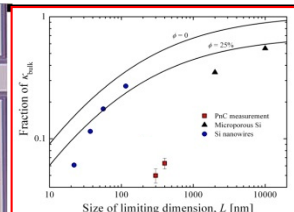
R&D Goals & Milestones

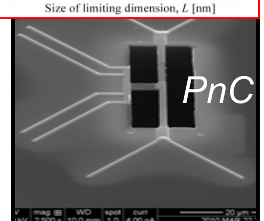
- Demonstrate~10 GHz (0.5K) phononic crystal
  - Continuum Wave Mechanics regime *100%*
  - Standard MDL lithography *100%*
  - Modification of the thermal noise spectrum *80%*
- Demonstrate ~100 GHz (5K) phononic crystal
  - Semi-Classical regime *100%*
  - Current FIB technology *90%*
  - Brillouin Light Scattering Exp. *On Schedule*
- Demonstrate ~0.5THz (25K) Phononic crystal
  - Lattice dynamics model
  - State of the art FIB technology *Ahead of Schd*
  - Full TE with var. T charact. . *Ahead of Schd*

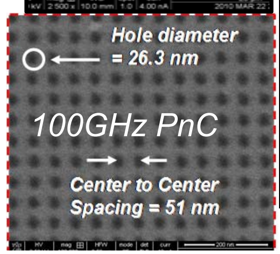
Relationship to Other Work

- Ended "*ABG*" LDRD
- CSSA-Darpa Funded









Key Accomplishments:

- Measured κ <predicted by porosity by 20
- World record on FIB UHAR vias.
- World record on UHF PnCs
- Self consistent CWM/Latt. dynam. κ model.
- Dev. of Nano-Characterization κ aparatus.
- BLS SNR model.
- Chair and host of 1st Int. Conf. (PMCO)
- 2 Invited talks to International Conferences
- 4 Nature Journal papers in prep.+ 2Journal

Significance of Results

- Enable a new class of thermal materials and devices
  - directional cooling of integrated circuits
  - thermo-electric cooling/power generation
  - thermal noise filtering/suppression
- Explore the crossover between continuum and quantum regimes
- Uncover new physical phenomena
  - modified electron-phonon interaction
  - Photon-Phonon interactions in simultaneous *phononic-photonic* structures

WHY PHONONIC CRYSTALS?

Capacitive MEMS Resonators

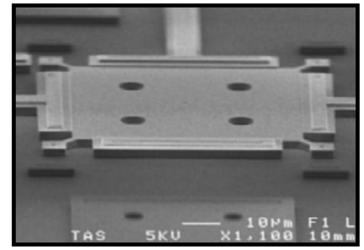
- *High fQ product for acoustics (2x10^{13}), but …*
- *Weak transduction; high impedance/insertion loss*
  - *Noise, hard to match to antennas or off-chip components*
  - *Arraying and high-K dielectric transduction lead to unmanageable parasitic capacitance*
- *Force ≈ V^2 (Low Power Handling)*
  - *Unsuitable for transmit filters, limits oscillator phase noise and sensor resolution*

Piezoelectric MEMS Resonators

- *Low impedance (< 50)/ Insertion Loss*
  - *Strong electro-acoustic transduction*
  - *Easily matched to antenna, off-chip circuits*
- *Force ≈ V (High Power Handling), but …*
- *Q limited to a few thousand*
  - *Material damping in metal electrodes and piezoelectric films, creep, aging*

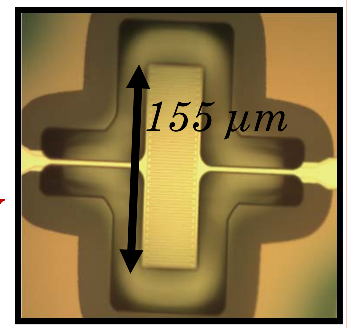
52MHz Capacitive Poly-Si Resonator

$Q = 100k$
$I.L. = 45dB$
$f_0 = 52.2MHz$
$P_{max} = 0.18\mu W$
$V_{bias} = 5V$



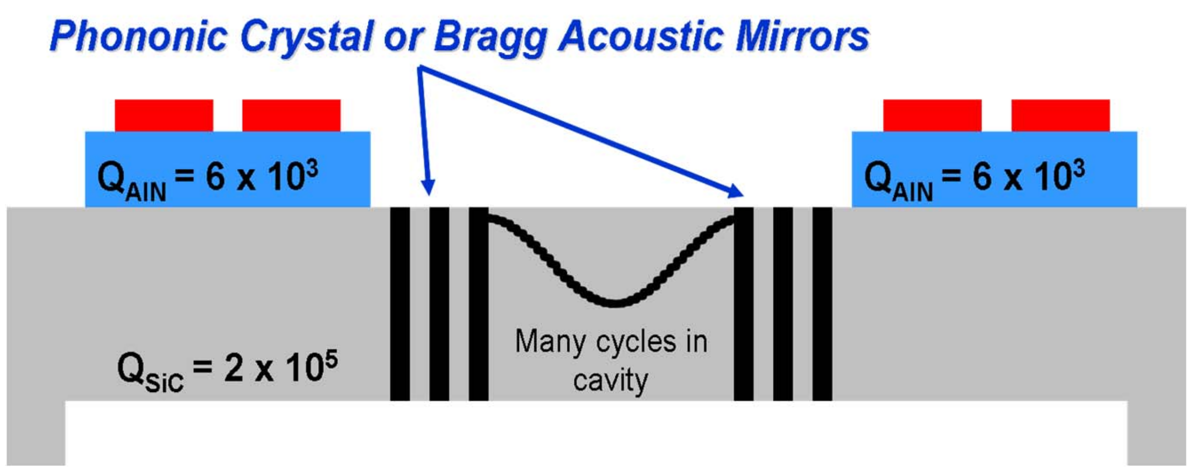
2.1GHz Piezoelectric AlN MEMS Resonator

$Q = 1000$
$I.L. = 20dB$
$f_0 = 2.1GHz$
$P_{max} = 50\mu W$
$V_{bias} = 0V$



Phononic Crystal Advantages

- *≈ 100x smaller size, more scalable to arrays*
- *Lithographically controlled frequency and bandwidth*
- *Si IC processing/packaging compatible*
- *Low Impedance, High dynamic range, High isolation*
- *Co-fabrication with traditional lateral resonator approach*



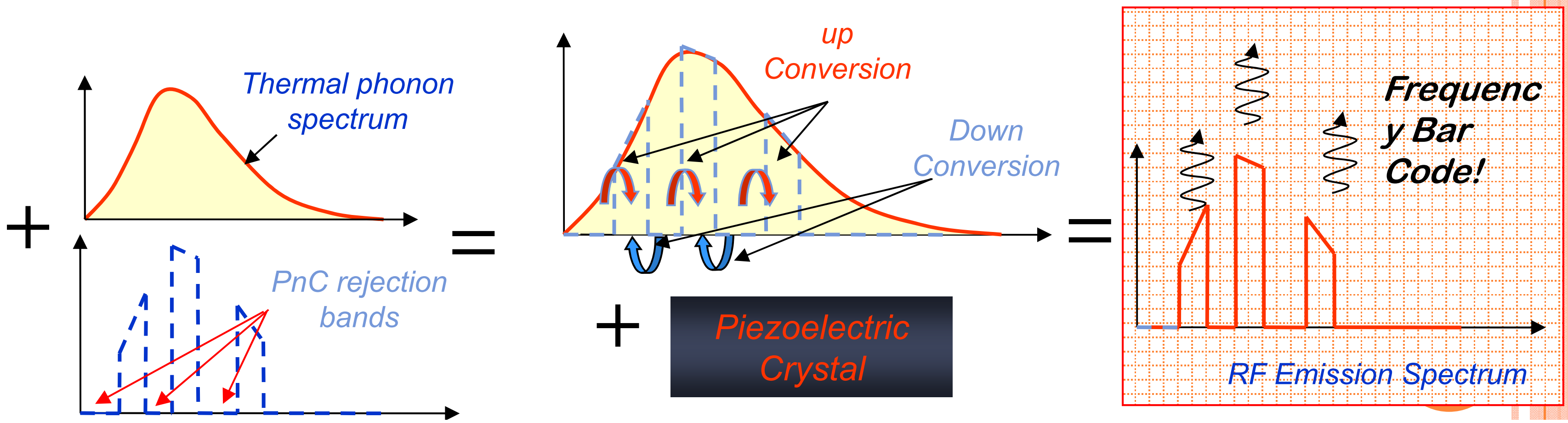
Programmatic Objectives

"Demonstrate the at-will control of thermal (THz) phonons using PnCs"

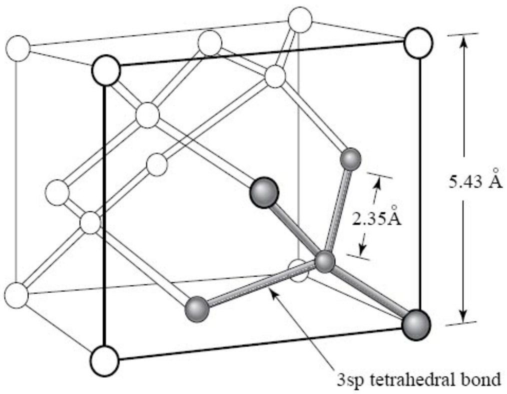
- *FY09-Milestones:*
  - *Demonstrate the molding and redistribution of the inherent thermal phonon density of states*
  - *Design, fabrication and characterization of 10 GHz (0.5K) phononic crystal.*

Freq	Radius "r"	Pitch "a"	Phonon Temp "T"
10GHz	250nm	500nm	0.5K
100GHz	25nm	50nm	5K
0.5 THz	5nm	10nm	25K
1THz	2.5nm	5nm	50K

- *Approach:*
  - *Theory: Continuum wave-mechanics 100% complete (iteration phase)*
    - *(CWM): bulk based elastic properties (Lame` coefficients).*
    - *FDTD-full elastic wave equation*
    - *Tailor the phononic bands to achieve spectrally narrow, high Q-bands.*
    - *Multi-phonon (nonlinear) processes: system resonates in the high-Q mode*
  - *Fab: Standard MDL-Fab (W-rods/Si-Matrix ➔ Air-rods/SiC-matrix) In fab 80% Comp.!*
  - *Experiment: Modification of the thermal noise Spectrum On FY10 schedule*



Band-Gaps Formed Through Scattering

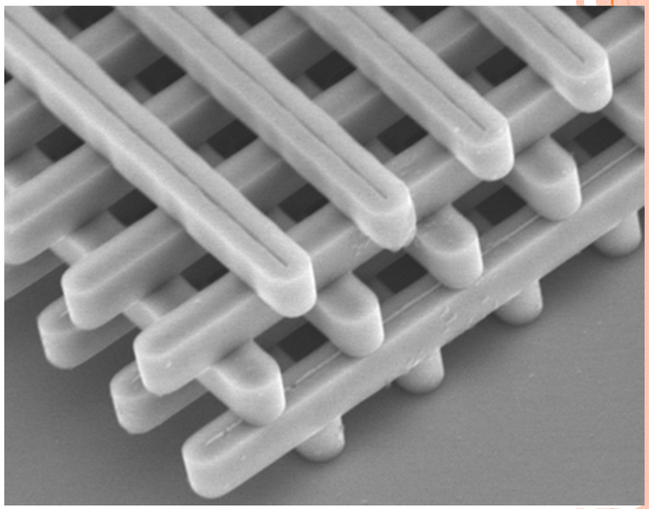


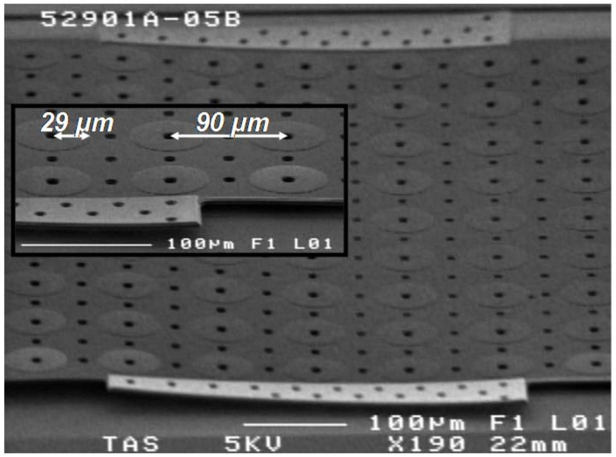
Semiconductor Band-Gap Crystal

Bragg Scattering of Electrons in a Crystal Lattice Based on Bloch's Theorem Results in the Well Known Semiconductor Band-gap

Photonic Band-Gap Crystal (PtC)

Bragg Scattering of Photons Opens Frequency Ranges Where Photons Can Not Propagate Within the Crystal





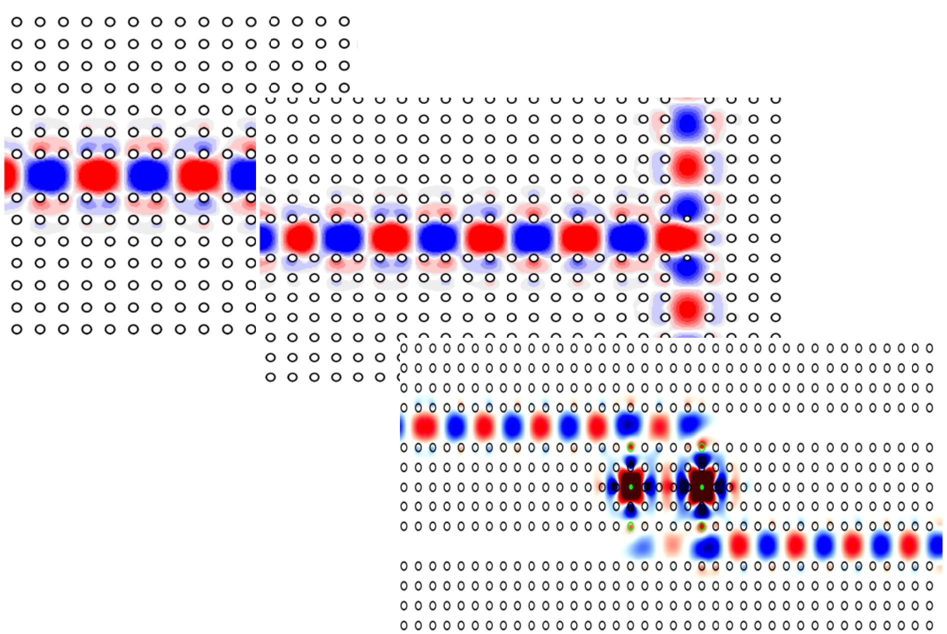
Phononic Band-Gap Crystal (PnC)

Bragg and Mie Scattering of Phonons Opens Frequency Ranges Where Phonons Can Not Propagate Within the Crystal

Why Phononic Crystals?

Why are we interested in the PnC—PhC analogy?

- *Wealth of literature on PhCs that can be used as a first iteration for the design and study of PnC applications*



Photonic Crystals (PnC)	Phononic Crystals (PhC)
Refractive index mismatch	Velocity and density mismatch
Integration of lasers and photodetectors problematic	Micromachined integration of piezoelectric or capacitive couplers
3D required for full control	2D (+vacuum) required for full control
Inherently linear	Inherently non-linear
2nd order coupled vector equations with 2 polarizations	2nd order coupled vector equations with 3 polarizations
Usually isotropic constitutive parameters	Usually anisotropic constitutive parameters

What materials should we use?

- *Ideal photonic materials may not work for phononics!*

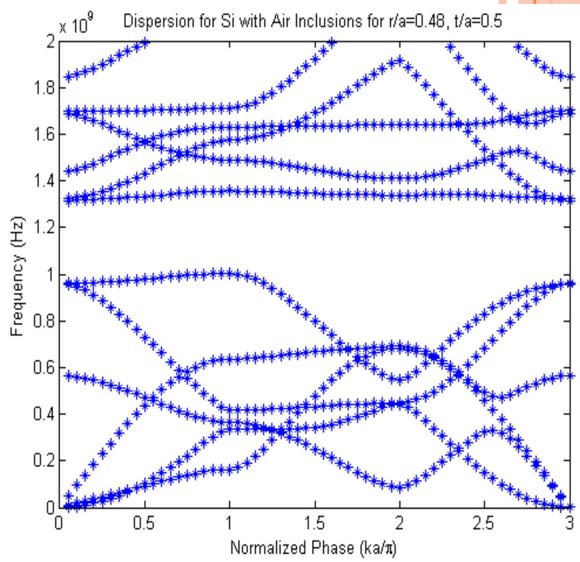
Why Phononic Crystals?

Properties of Phononic Crystals (PnCs)

- *Engineered phononic dispersion*
- *Phononic bandgap*
- *Anomolous dispersion (flat and negatively-sloped bands)*

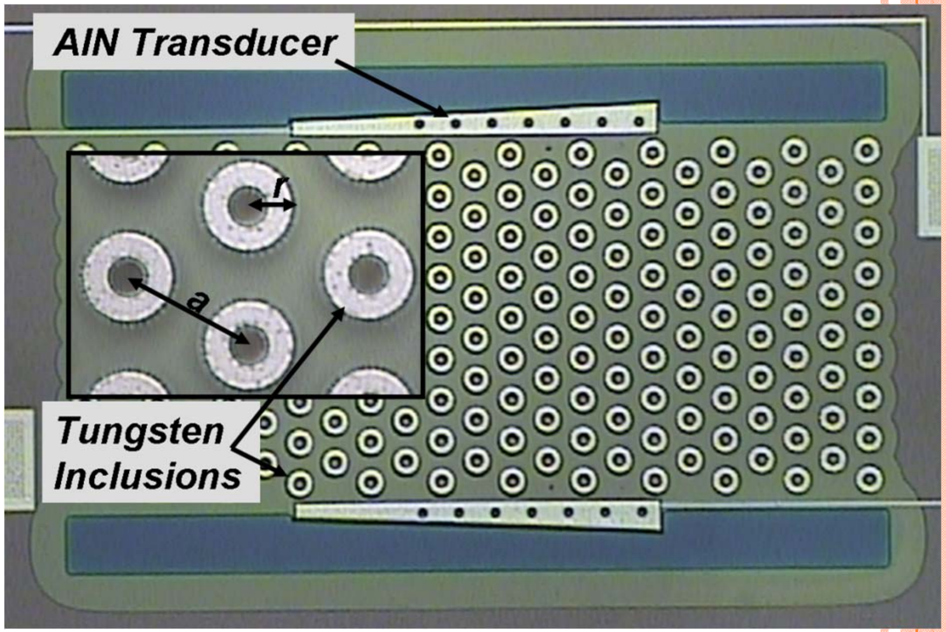
Applications of PnCs

- *Acoustic isolation*
- *Signal processing/filtering*
- *Thermal isolation and energy harvesting*
- *High-resolution ultrasonics*



Micro-Phononic Crystal Outline

- Background
  - Semiconductor, Photonic and Phononic Band-gaps
- Theory and Modeling
  - Origins of Phononic Band-gaps
  - Modeling Techniques
- Measured Performance
  - Measurement Techniques and Coupler Design
  - VHF and UHF Micro-Phononic Crystals
- Devices and Applications
  - Waveguides
  - Sensors
  - Cavities and Filters
  - Acoustic Imaging
  - Thermal Phonon Control

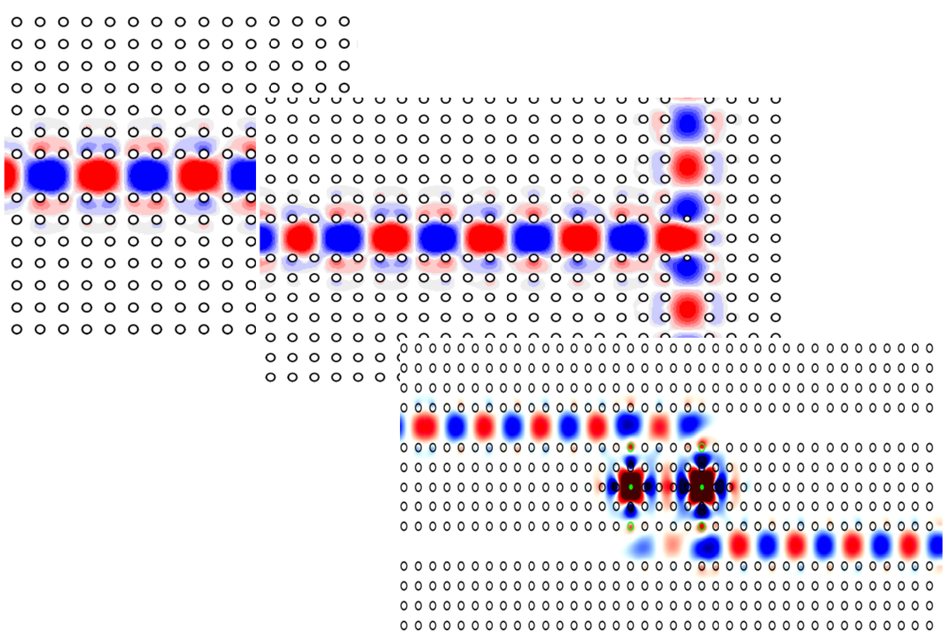


Hexagonal lattice phononic crystal operating at 67 MHz

Why Phononic Crystals?

Why are we interested in the PnC—PhC analogy?

- *Wealth of literature on PhCs that can be used as a first iteration for the design and study of PnC applications*



Photonic Crystals (PnC)	***Phononic Crystals (PhC)***
Refractive index mismatch	***Velocity and density mismatch***
Integration of lasers and photodetectors problematic	***Micromachined integration of piezoelectric or capacitive couplers***
3D required for full control	***2D (+vacuum) required for full control***
Inherently linear	***Inherently non-linear***
2nd order coupled vector equations with 2 polarizations	***2nd order coupled vector equations with 3 polarizations***
Usually isotropic constitutive parameters	***Usually anisotropic constitutive parameters***

What materials should we use?

- *Ideal photonic materials may not work for phononics!*

PhonC Material Systems

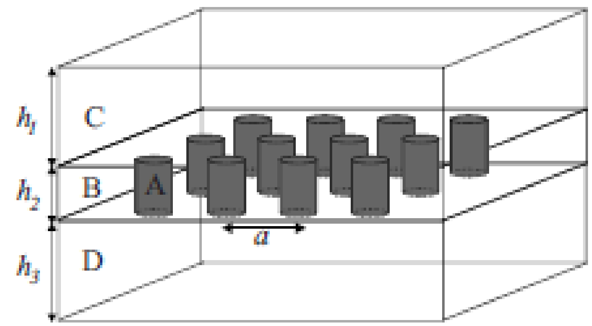
Matrix	*Inclusion*	*Topology*	*Reflection Coefficient (Γ^2)*	*Velocity Mismatch (V_m/V_i)*
Elastic Solid	air	Network	~1	> 10
SiO_2	W	Cermet	0.58	1.3
SiO_2	Pt	Cermet	0.42	2.1
SiO_2	Mo	Cermet	0.41	1.0
Poly-Si	W	Cermet	0.4	1.9
Poly-Si	Pt	Cermet	0.25	3.0
Diamond	SiO_2	Network	0.45	3.2

Plane Wave Expansion

- Plane wave expansion (PWE) solves an eigenvalue problem for the modes of a periodic structure
  - *FFT algorithm used to calculate structure factors*

$$\rho(\vec{r})\frac{\partial^2 u_i(\vec{r},t)}{\partial t^2} = \sum_{j,k,l}\frac{\partial}{\partial x_j}\left(C_{ijkl}(\vec{r})\frac{\partial u_l(\vec{r},t)}{\partial x_k}\right)$$

- Densities
  - *Silicon: 2332 kg/m³*
  - *Air: 10^{-4} kg/m³*
  - *Tungsten: 19250 kg/m³*



$$C_{air} = \begin{bmatrix} 10^6 & -10^6 & -10^6 & 0 & 0 & 0 \\ -10^6 & 10^6 & -10^6 & 0 & 0 & 0 \\ -10^6 & -10^6 & 10^6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 10^6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 10^6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10^6 \end{bmatrix}$$

$$C_{Si} = \begin{bmatrix} 16.7\cdot10^{10} & 6.39\cdot10^{10} & 6.39\cdot10^{10} & 0 & 0 & 0 \\ 6.39\cdot10^{10} & 16.7\cdot10^{10} & 6.39\cdot10^{10} & 0 & 0 & 0 \\ 6.39\cdot10^{10} & 6.39\cdot10^{10} & 16.7\cdot10^{10} & 0 & 0 & 0 \\ 0 & 0 & 0 & 7.956\cdot10^{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 7.956\cdot10^{10} & 0 \\ 0 & 0 & 0 & 0 & 0 & 7.956\cdot10^{10} \end{bmatrix}$$

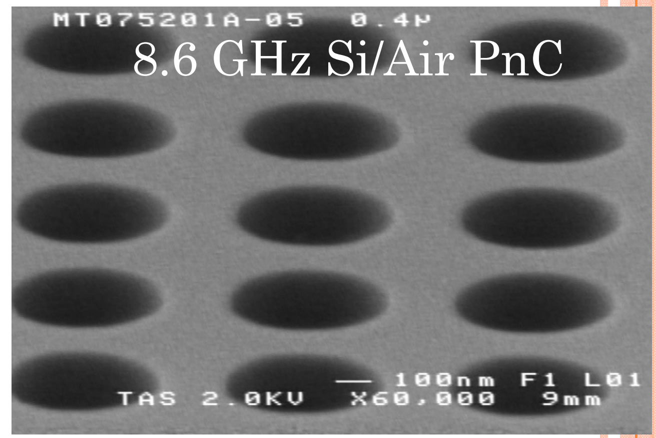
$$C_{W} = \begin{bmatrix} 40.9\cdot10^{10} & 17.1\cdot10^{10} & 17.1\cdot10^{10} & 0 & 0 & 0 \\ 17.1\cdot10^{10} & 40.9\cdot10^{10} & 17.1\cdot10^{10} & 0 & 0 & 0 \\ 17.1\cdot10^{10} & 17.1\cdot10^{10} & 40.9\cdot10^{10} & 0 & 0 & 0 \\ 0 & 0 & 0 & 6.74\cdot10^{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 6.74\cdot10^{10} & 0 \\ 0 & 0 & 0 & 0 & 0 & 6.74\cdot10^{10} \end{bmatrix}$$

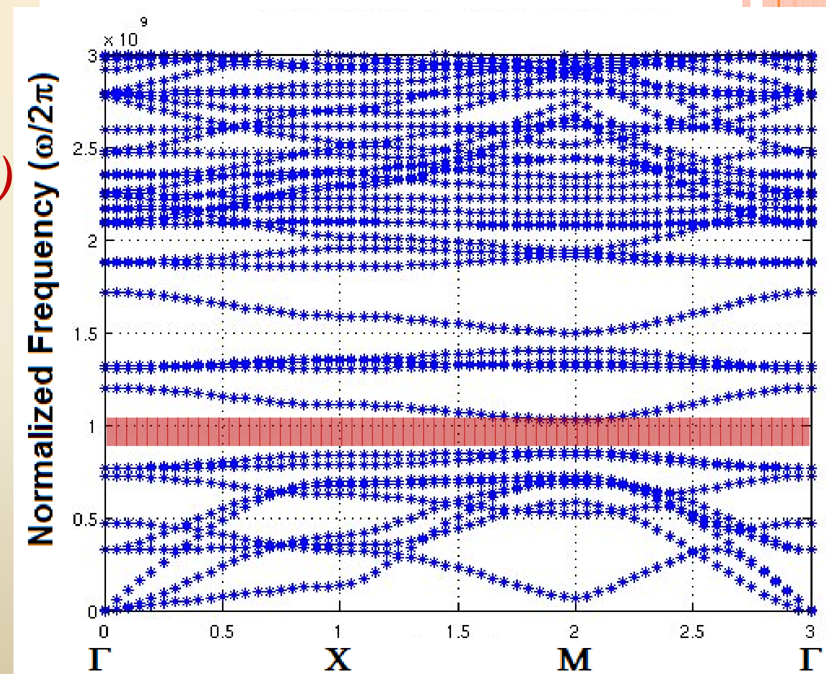
Vasseur, *et al.*, *Phys. Rev. B*, 77, 085415 (2008)

SOLID-AIR VS. SOLID-SOLID

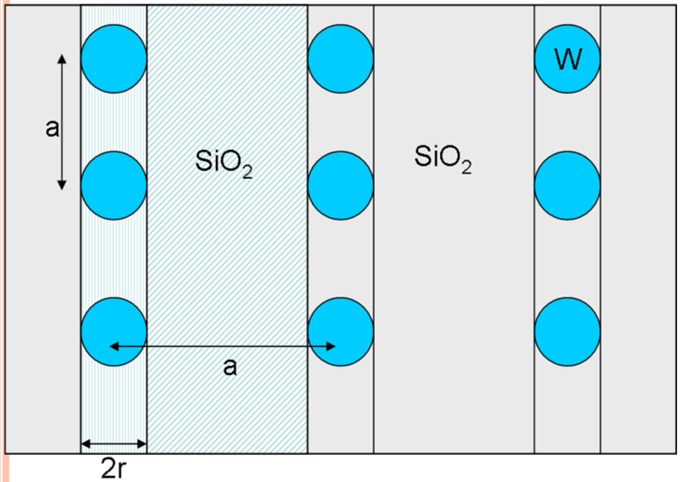
How can we compare these devices?

- *Different lattices*
  - *Square lattice only*
- *Bandgap in some/all directions*
  - *Full bandgap (Γ-X, X-M, and Γ-M)*
- *Exclusion of certain modes*
  - *All possible modes considered*
- *Multiple bandgaps*
  - *Only first (lowest frequency) bandgap considered for all parameters*

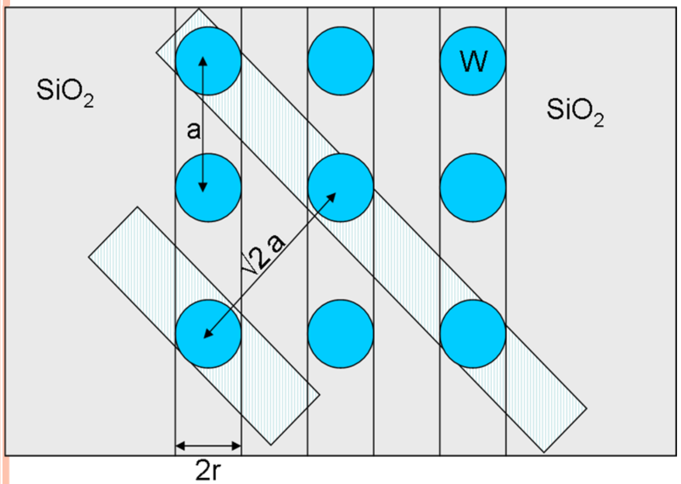




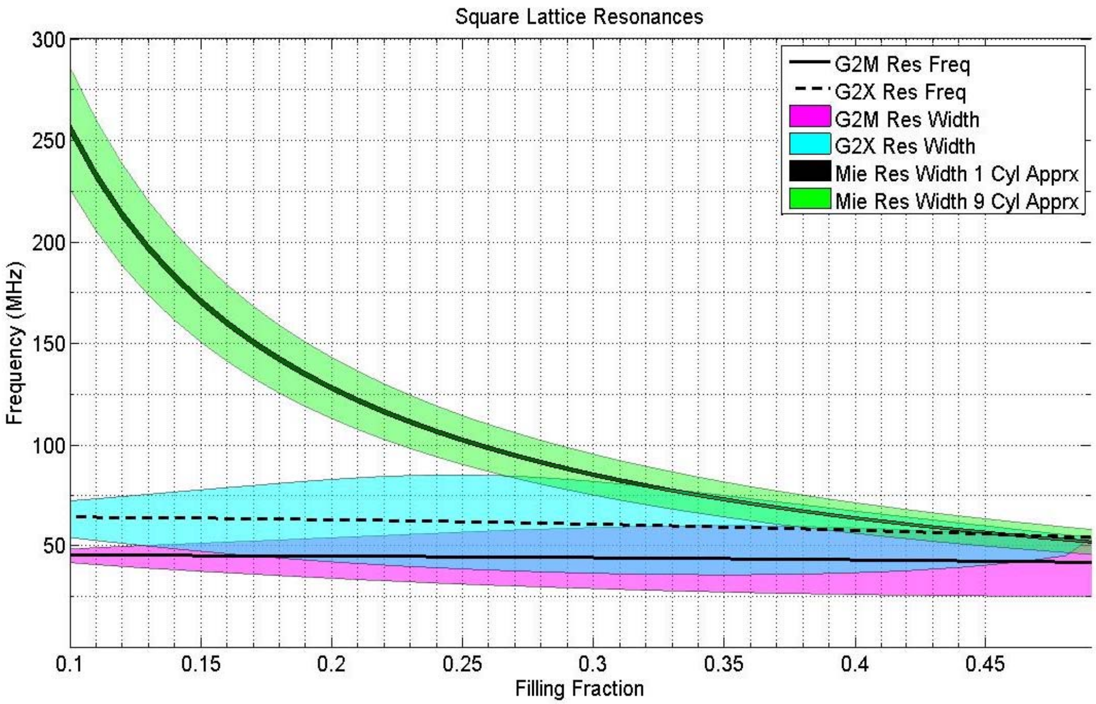
PhonC 1D Planes Approximation



ΓX 1D Approximation Model



ΓM 1D Approximation Model

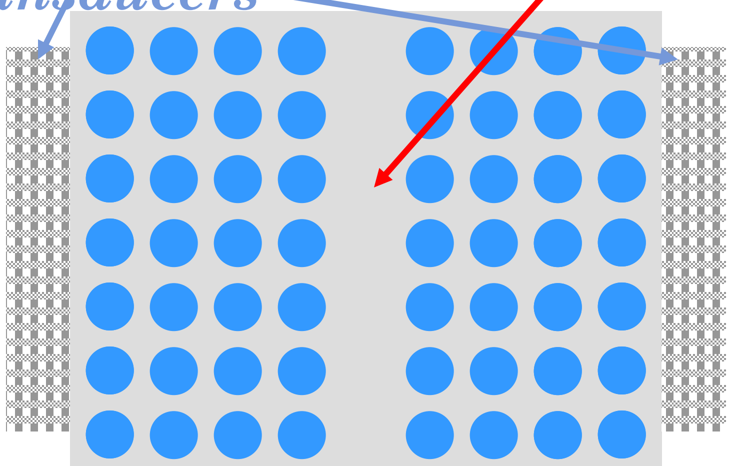


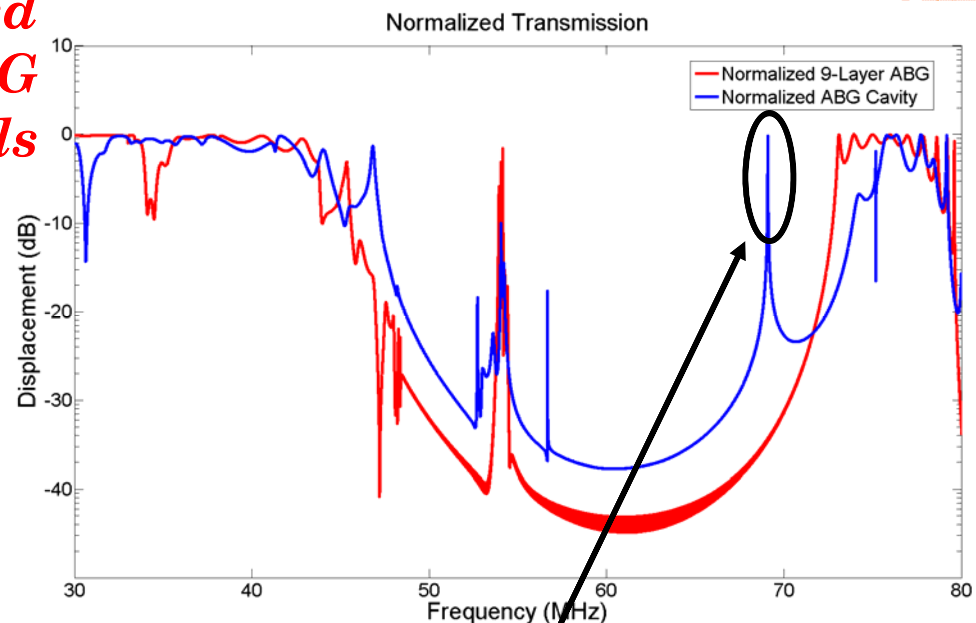
- ❖ Analytically approximate resonance widths using recursion
- ❖ Mie is direction independent (cylinder)
- ❖ Resonance overlap indicates a full band-gap

High fQ Product PhonC Cavities

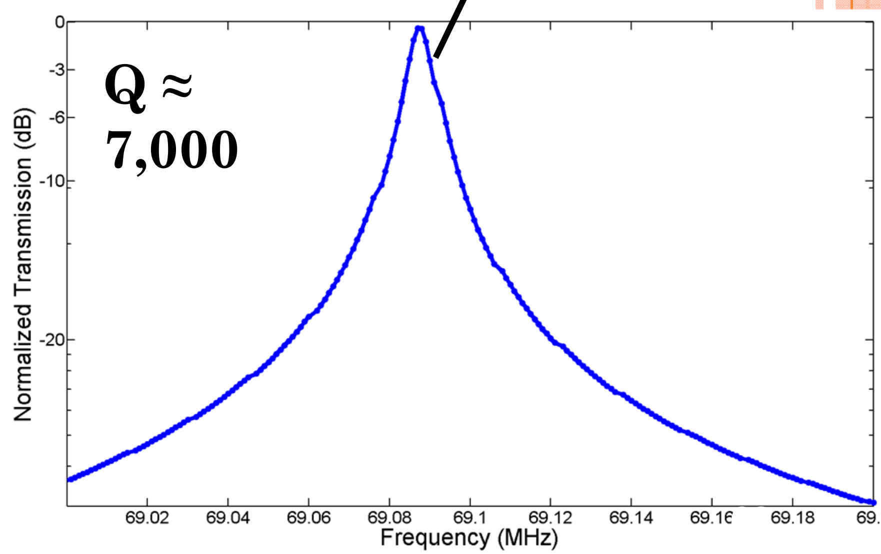
Highly Efficient, Linear Piezoelectric Transducers

Cavity Realized in High-Q ABG Materials





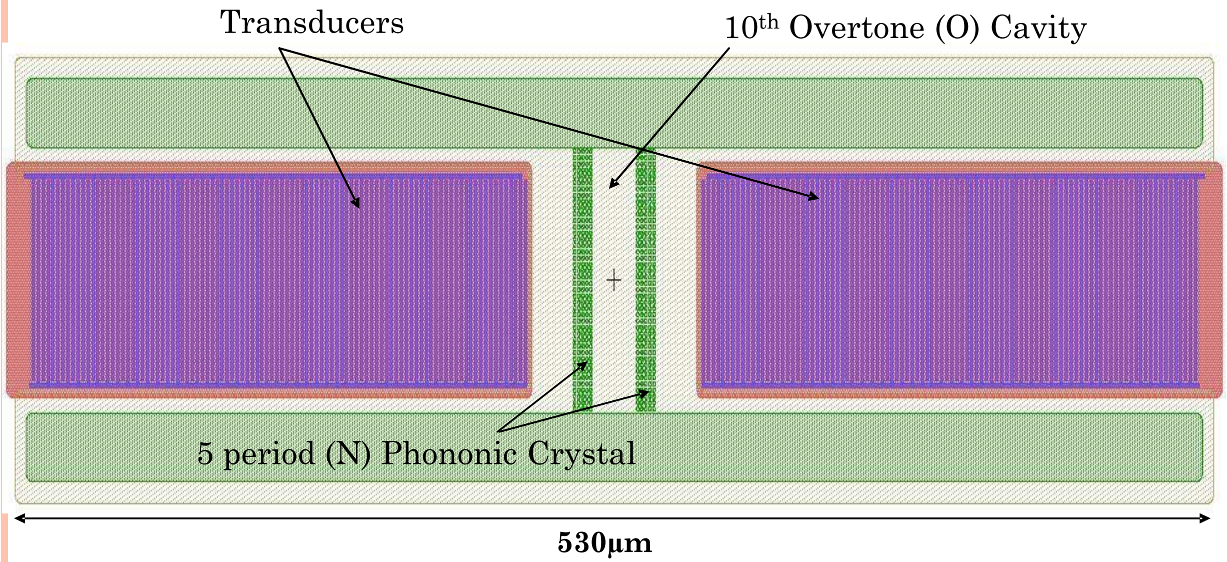
PhonC Cavity Schematic (Top) and FDTD Simulation (Left) with 4 Mirror Layers Isolating the Resonator

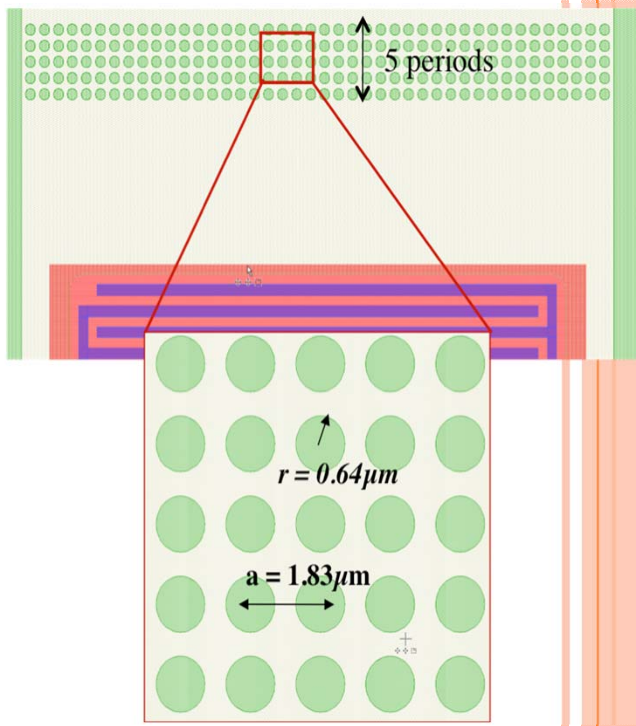


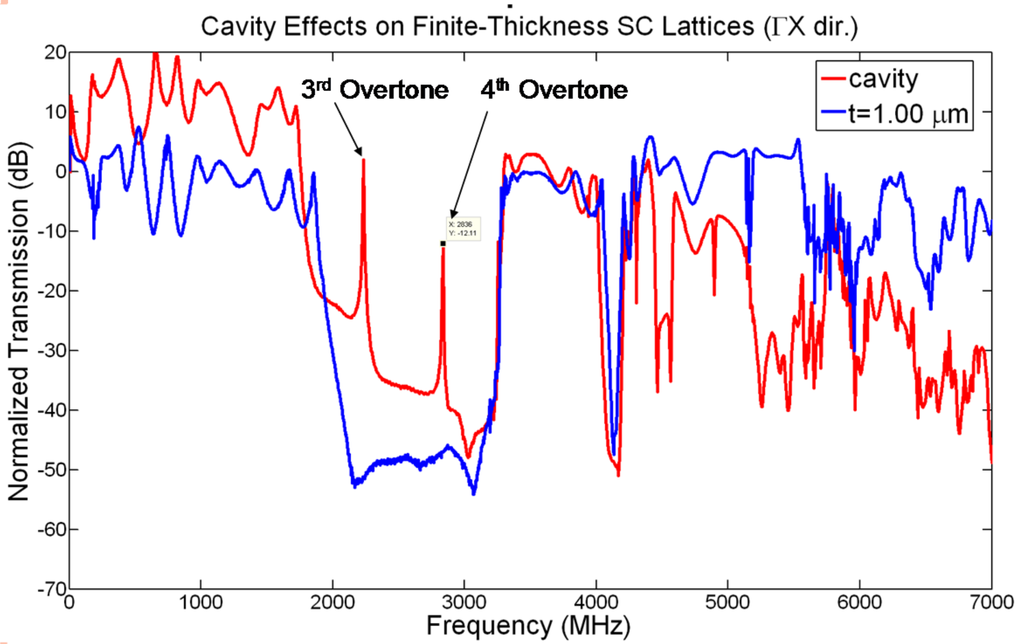
PhonC Allows Highly Efficient Piezoelectric Transduction + Cavities in High-Q PhonC Materials

Low Insertion Loss + Record fQ Products

Example Phononic Crystal Cavity Design







(Top) Example Phononic Crystal Cavity Layout

(Left) FDTD Simulation of an 8 µm wide phononic crystal cavity placed between identical, 3-period SiC/vacuum phononic crystal plates

TE Backup

Manipulating the Thermal Conductivity of Silicon

- *Spectral thermal conductivity is given by:*

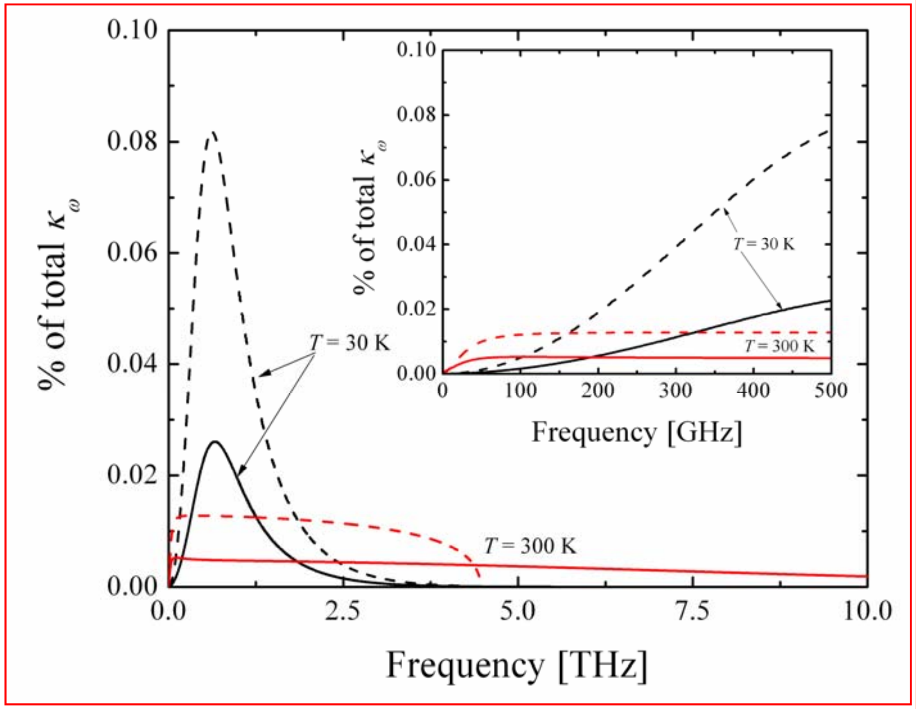
$$\kappa_{\omega,j} = \frac{1}{6\pi}\frac{\hbar^2\omega_j^2(q)}{k_B T^2}\frac{\exp\left[\frac{\hbar\omega(q)}{k_B T}\right]}{\left(\exp\left[\frac{\hbar\omega(q)}{k_B T}\right]-1\right)^2}\upsilon_j(q)\tau_j(q)q^2$$

- *The fractional contribution to κ is given by:*

$$\frac{\kappa_{\omega,j}}{\sum_j\sum_\omega \kappa_{\omega,j}}$$

- *Fraction of the total spectral thermal conductivity for 30 and 300 K. The longitudinal (solid lines) and transverse (dashed lines)* contribution
- *(inset) Spectral phonon contribution over the range from 0 to 500 GHz.*

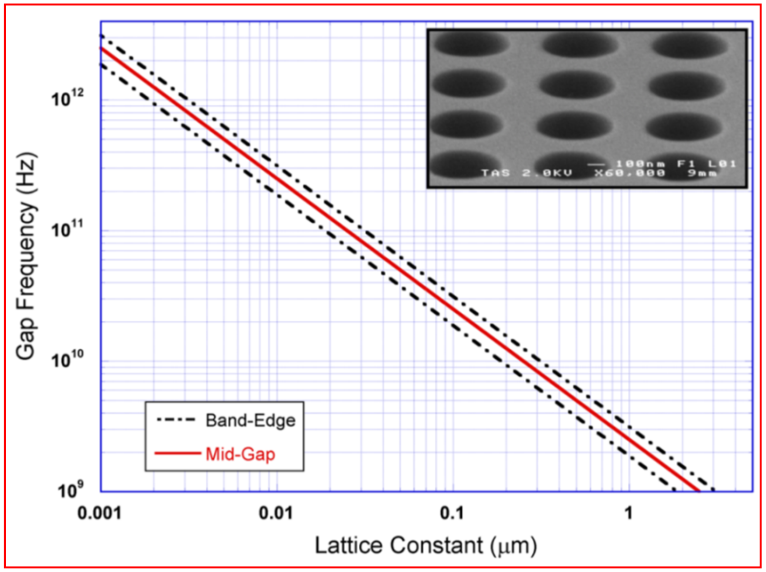
- *Transverse spectral thermal conductivity is multiplied by 2 since we assume degenerate transverse branches.*

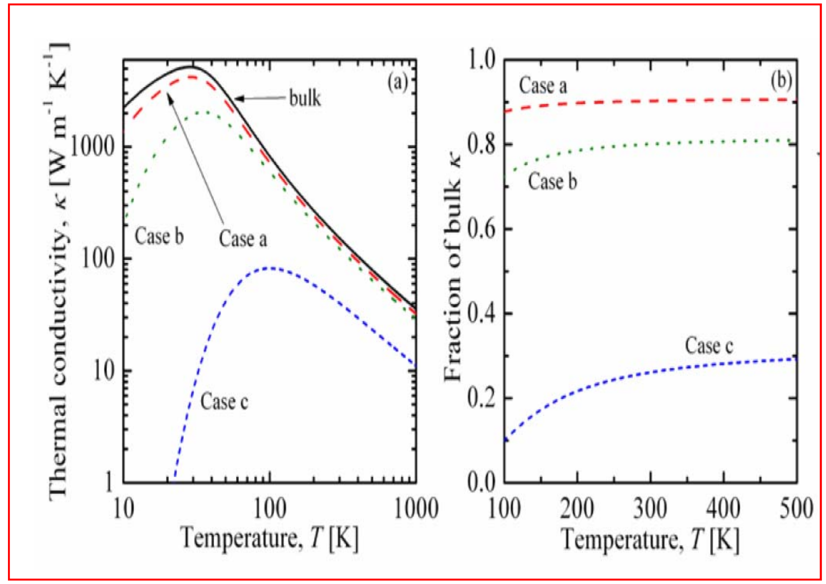


- *The major contribution to κ is from 10GHz-to-4THz phonons given by:*

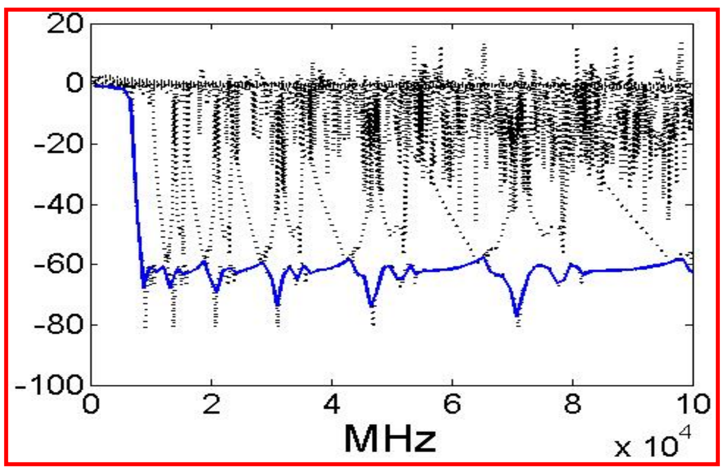
MANIPULATING κ OF SILICON

Modified Spectral thermal conductivity in Silicon





➢*Cascaded PnC gaps 10GHz-to-1THz: Normalized Transmission (dB)*



Thermal conductivity of Si assuming unmodified bulk dispersion with:

- ➢*Case a: Suppression of 10GHz-to-0.5THz Phonon*
- ➢*Case b: Suppression of 10GHz-to-1THz Phonons*
- ➢*Case c: Suppression of 10GHz-to-4THz Phonons*

1- Hopkins, Rakich, Olsson III, El-kady, and Phinney, "Origin of the reduction in phonon thermal conductivity of microporous solids," Applied Physics Letters 95, 161902 (2009).

2- Hopkins, Phinney, Rakich, Olsson III, El-kady, "Phonon considerations in the reduction of thermal conductivity in phononic crystals," currently under review JAPA.

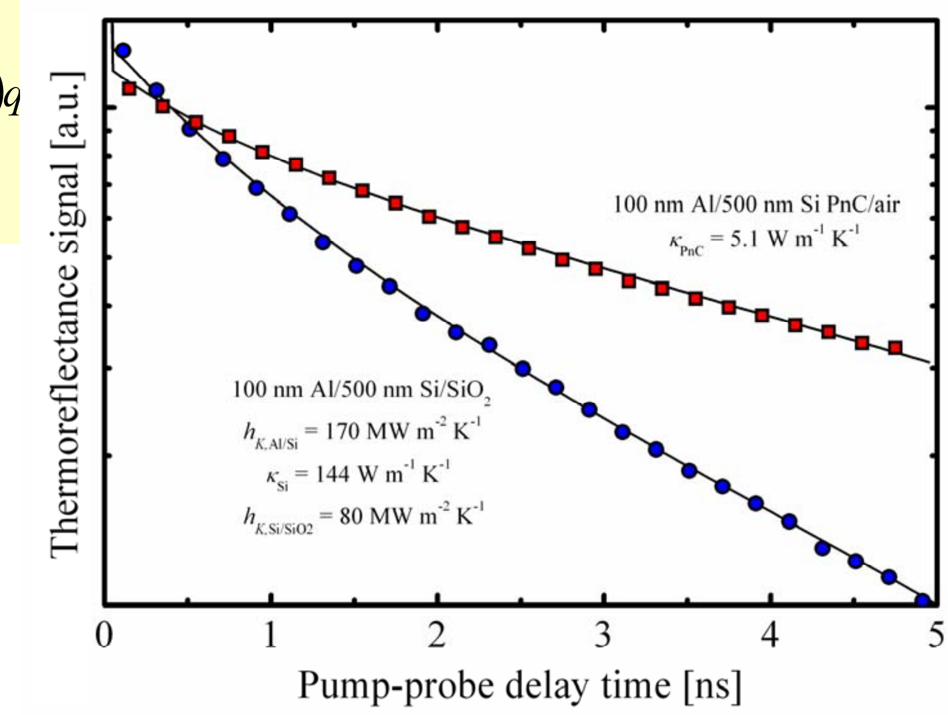
MEASURED κ OF SILICON PNC

Thermal conductivity measurements on a 500 nm thick suspended PnC structure

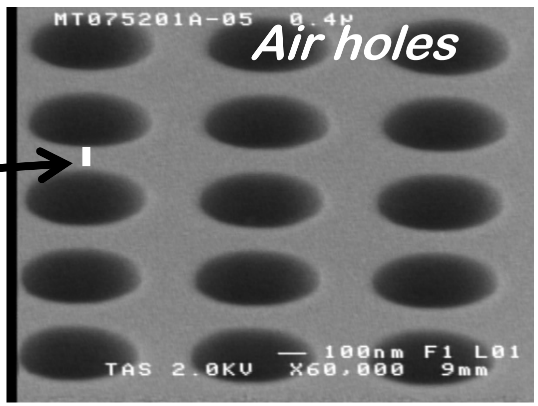
$$\kappa_{\omega,j} = \frac{1}{6\pi}\frac{\hbar^2\omega_j^2(q)}{k_B T^2}\frac{\exp\left[\frac{\hbar\omega(q)}{k_B T}\right]}{\left(\exp\left[\frac{\hbar\omega(q)}{k_B T}\right]-1\right)^2}\upsilon_j(q)\tau_j(q)q$$

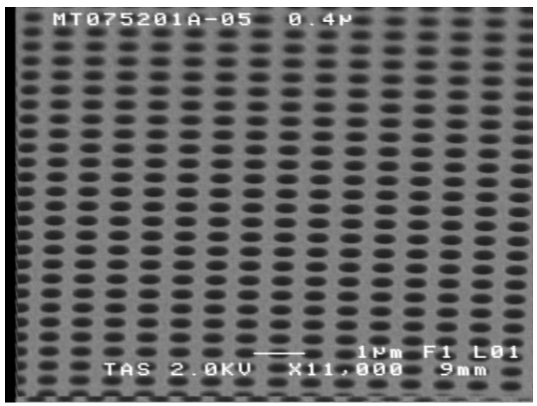
$$\frac{1}{\tau_j(q)} = \frac{1}{\tau_{Umklapp,j}} + \frac{1}{\tau_{impurity,j}} + \frac{1}{\tau_{boundary,j}}$$

$$\frac{1}{\tau_{Boundary,j}} = \frac{\partial\omega_j(q)}{\partial q}\frac{1}{L}$$



L
Limiting Dimension
(Min Feature size)





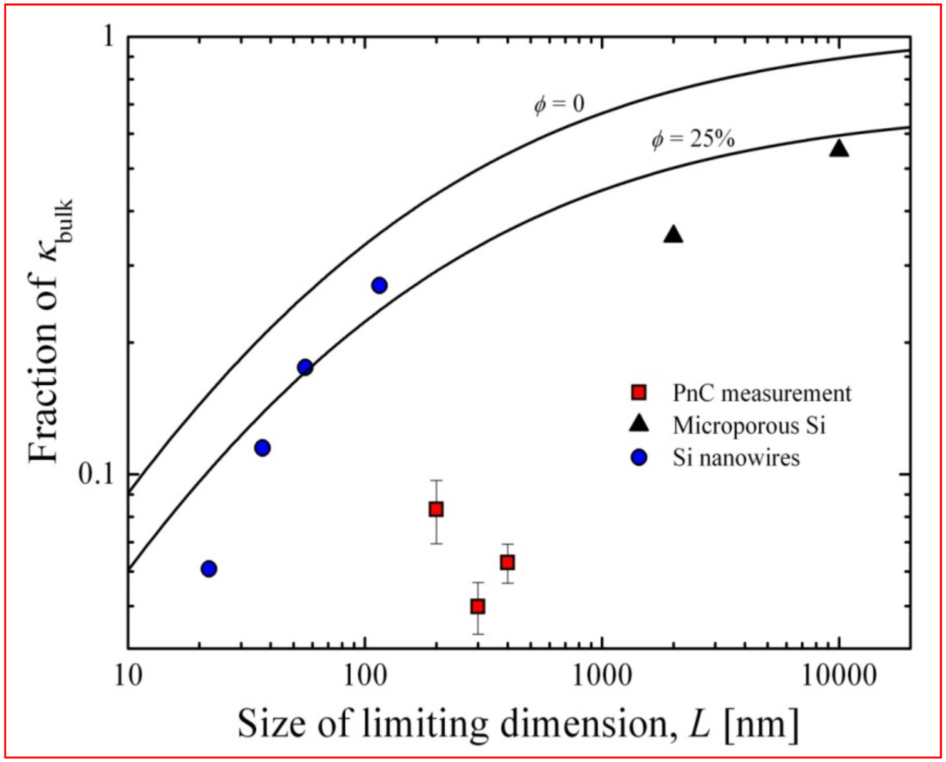
$$\frac{\kappa_{PnC}}{\kappa_{bulk}} = 0.035$$

An order of magnitude lower !

Nanowires: φ= 0
Microporous Si: φ ~ 25%
PnC: φ < 20%

PnC outperforms nanowires @ an order of magnitude larger limiting dimension (L)!
➔ Consider PnC with a = 60 nm and r/a = 0.46 (L = 4.8 nm)

$$\Rightarrow \frac{1}{\left(\dfrac{\kappa_{PnC}}{\kappa_{bulk}}\right)} = 500\,!$$



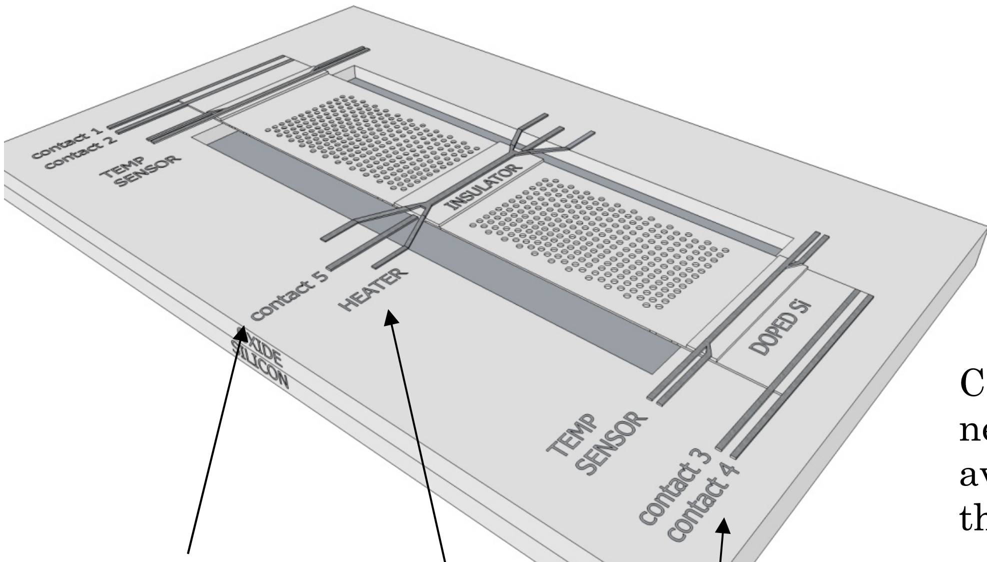
Since the mean free path of electrons is an order of magnitude lower than that of phonons, ➔ Based solely on phonon thermal conductivity reduction, predicted room Temp. ZT enhancement in Si by factor is 500!

This would increase ZT in Si to ~5!

Full TE characterization

(*Originally an FY11 goal on cold FIB samples only!*)

To do this right, in the end we need to measure all parameters in a single sample: thermal conductivity, Seebeck, and electrical conductivity

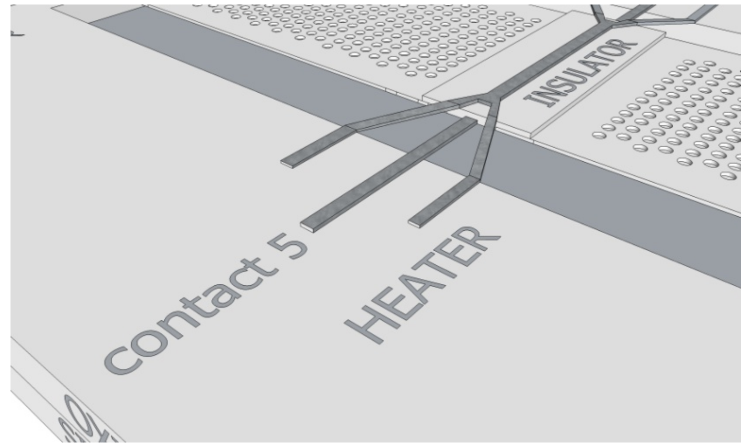


Central electrical contact needed for measuring open circuit voltage (Seebeck)

Heater will likely be serpentine, our measurements on next MDL run will be instructive

Electrical contacts needed for 4pt electrical resistance measurement

Detailed center view



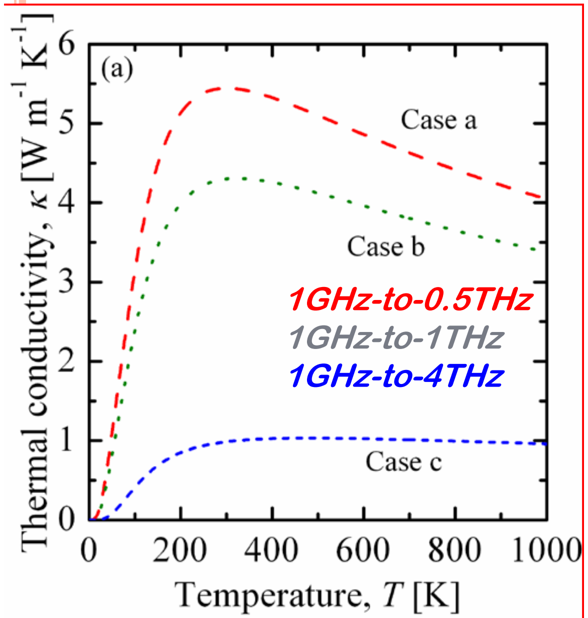
Center contact 5 is Ohmic to silicon. The heater needs to be electrically isolated from material to avoid current spreading into silicon (which would throw off all measurements)

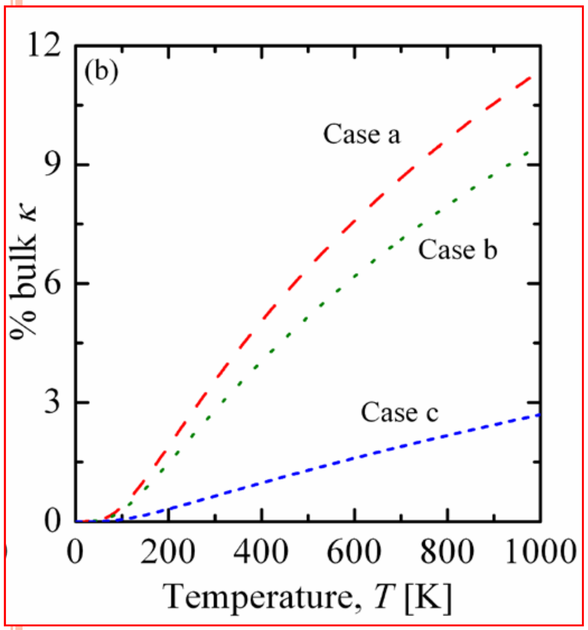
Electrical conductivity: Measure 4pt sourcing current from c1-c4 and measuring voltage from c2-c3.

Seebeck: Apply heater to create temperature difference between center and end, measure open circuit voltage between contact 5, and any other contact

Thermal conductivity: Same procedure as previously outlined

Si κ with modified PnC Dispersion

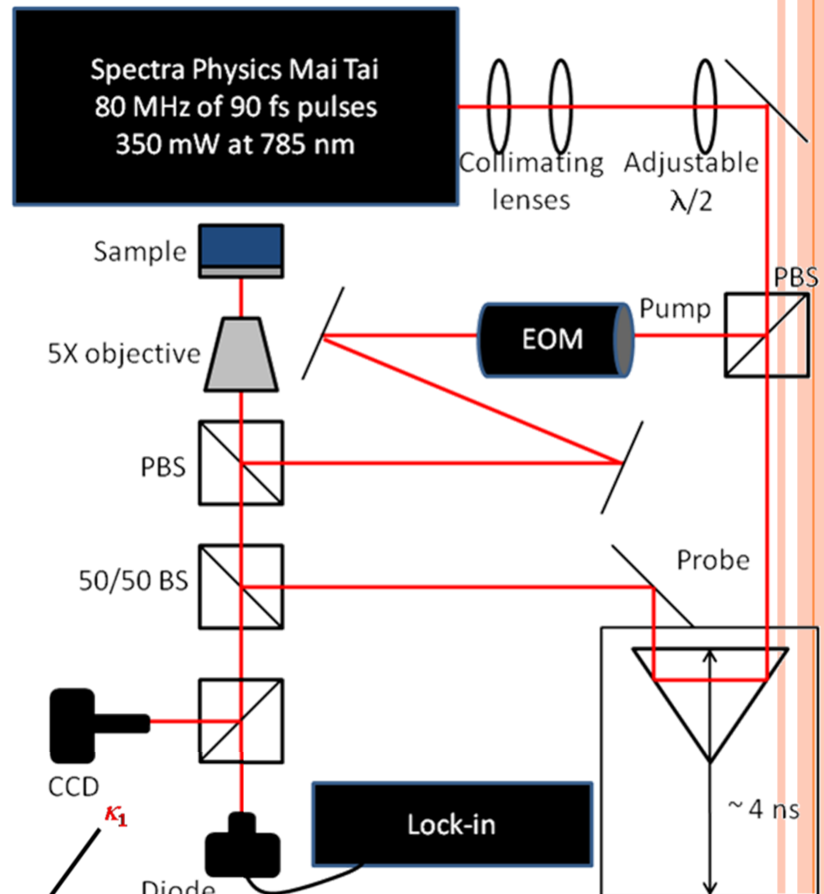


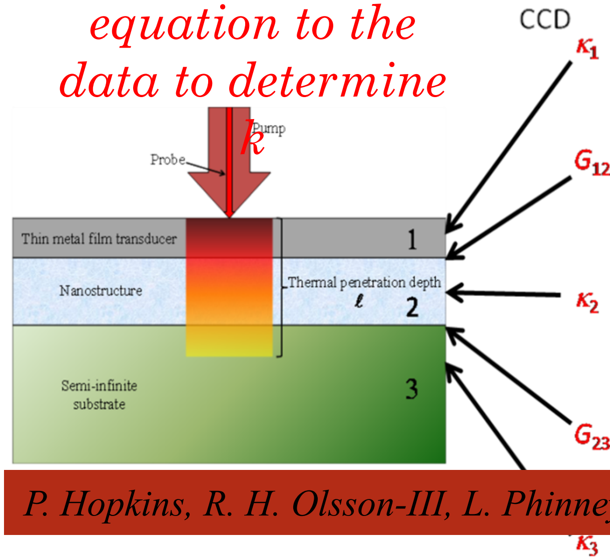


Thermoreflectance signal directly proportional to temperature change

$$C\frac{\partial T}{\partial x} = -\kappa\frac{\partial^2 T}{\partial x^2}$$

Given temperature change with time, we fit the heat equation to the data to determine κ



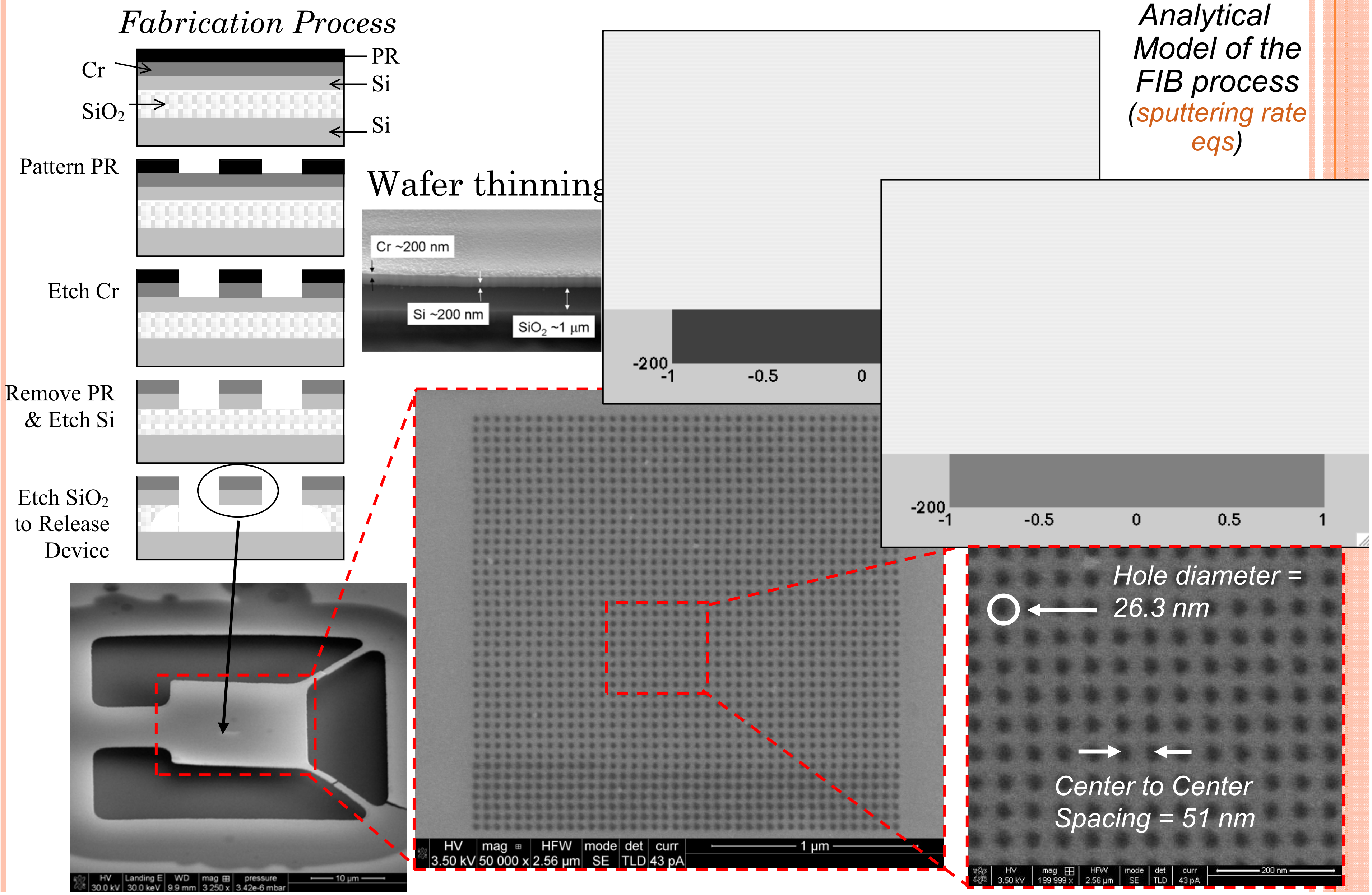


➔ *Deposit Al on top surface and Measure off shelf GHz lattice!*

P. Hopkins, R. H. Olsson-III, L. Phinney and I. El-kady, App. Phys. A (2010)

FIB PnCs: Towards the T=5K sample

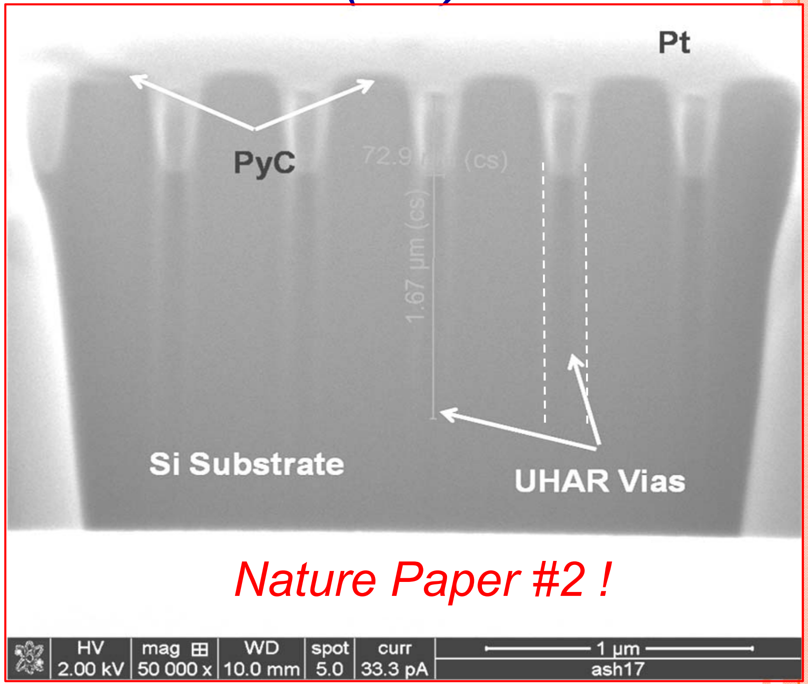
Allows for T dialing of harmonic/anharmonic effects (On Schedule!)



UHAR FIB VIAS: HARD (PYC) ON SOFT (SI)

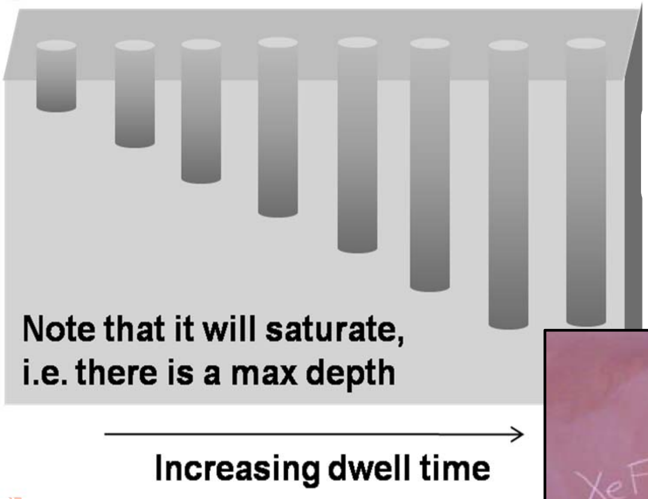
- *73 nm diameter & >1.67 μm deep*
- *Best Literature value: 10:1*
- *We have a Record: 22:1*
- *Nature Paper #2*
- *NOT optimized yet*

IMPACT
Resolves Structural rigidity issues and allows us to go t >10a

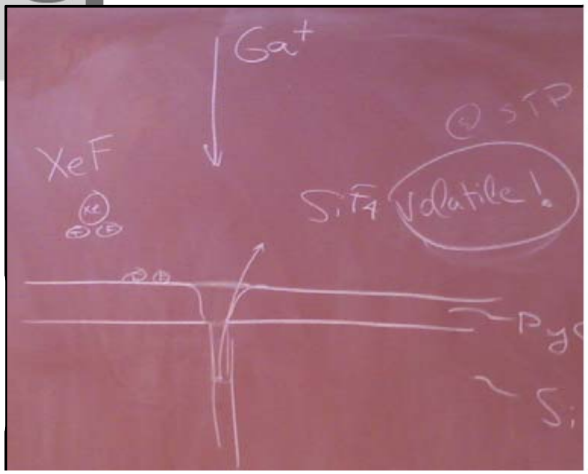


Next step (Max of "hard" on "soft"):

- *Will systematically increase dwell time of FIB then perform cross-section of vias*

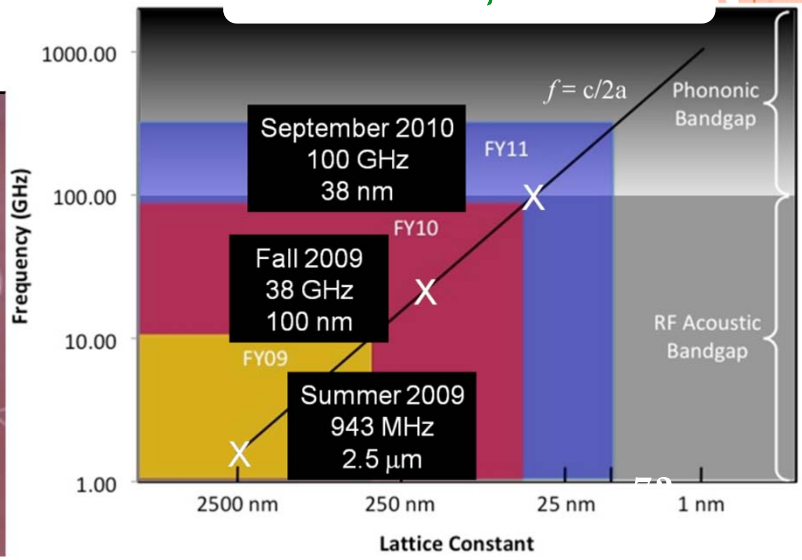


Will get us to over 50:1



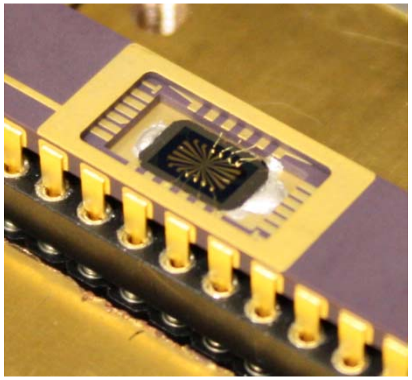
With XF_2
Will get us over 100:1
Need + $35K

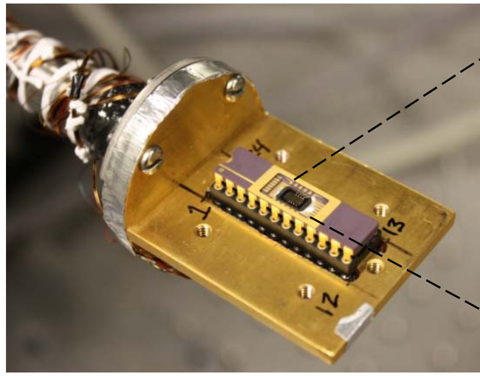
Moor's Law for PNC's

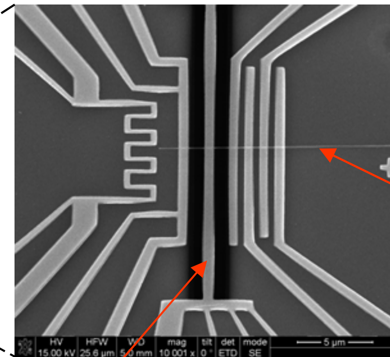


MEASURING κ IN FIB SAMPLES (AN FY11 GOAL ON TRACK!):

SUSPENDED WIRE TECHNIQUE





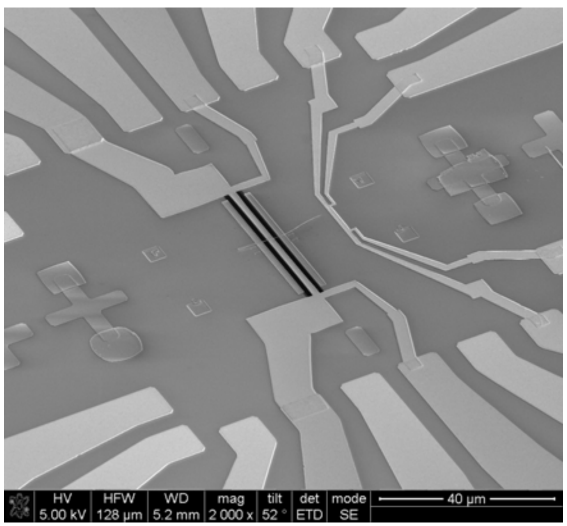


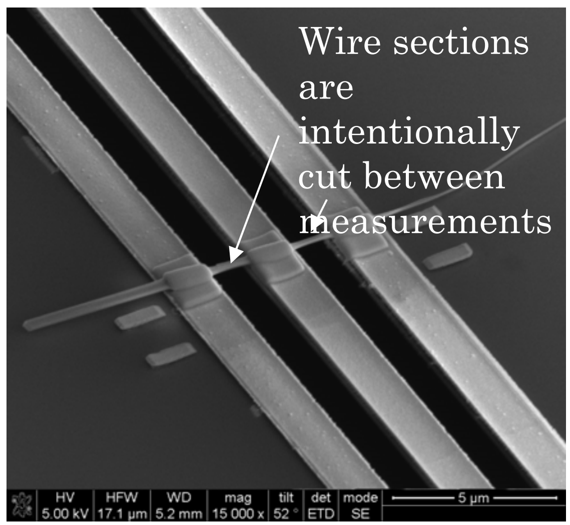
Method partly developed under this LDRD

Nanowire placed across electrical leads, suspended heater line, and temp sensor

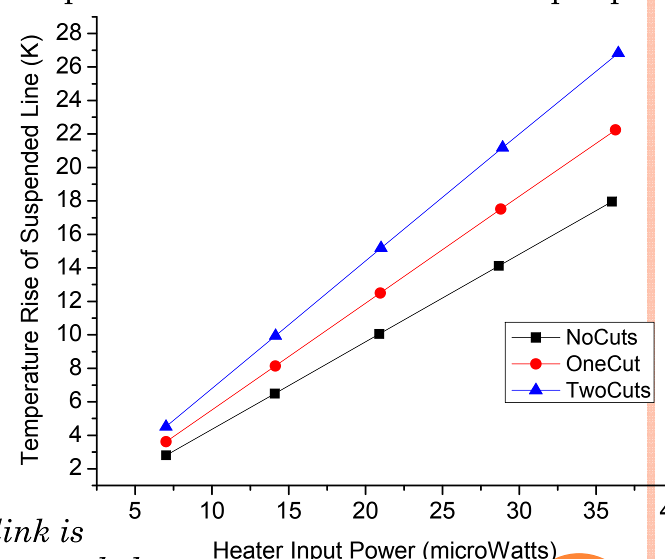
Suspended heater line

First successful measurement using this technique on GaN wires





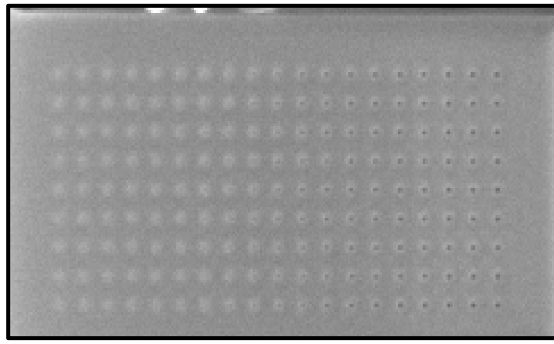
Temperature rise of heater line vs. input power

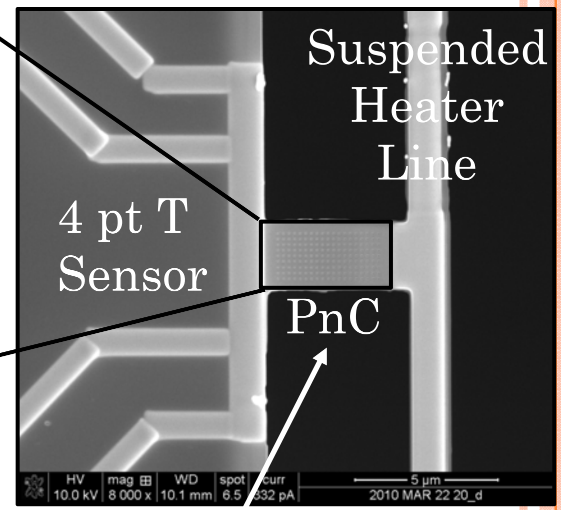


The material between the heater line and substrate allows heat to flow. As the link is broken, by cutting the GaN wire, a greater temperature rise is observed for the suspended line. From the data, a thermal conductivity of 20W/mK is measured @ 300K consistent with the increased boundary scattering caused by the size of the nanowire.

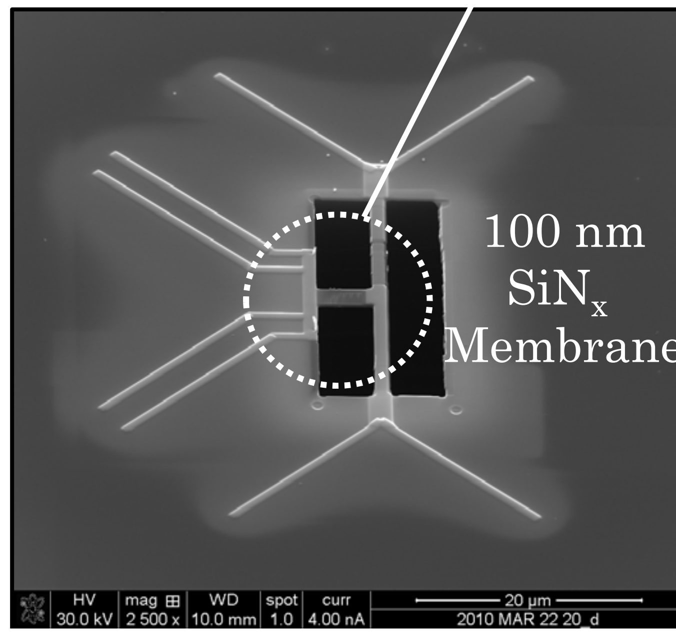
Pre-measurement Fab "Mock-up" of Thermal Characterization Layout

Ahead of Schedule!





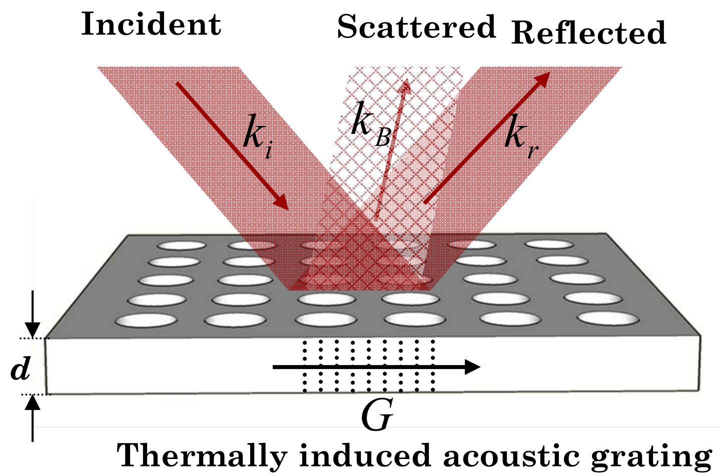
- *Currently only a mock-up.*
- *Real device to fab'd Summer '10*
- *PnC will be co-fabricated as an integral part of suspended membrane*
- *Measurement procedure*
  - *Slab*
  - *Air-hole*
  - *W filled*
  - *Removal of PnC for baseline measurement*



Optical Measurement Progress & Approac

Brillouin Light-Scattering (BLS):

Probes vibrational states of system.



BLS Scattering Efficiency (η)

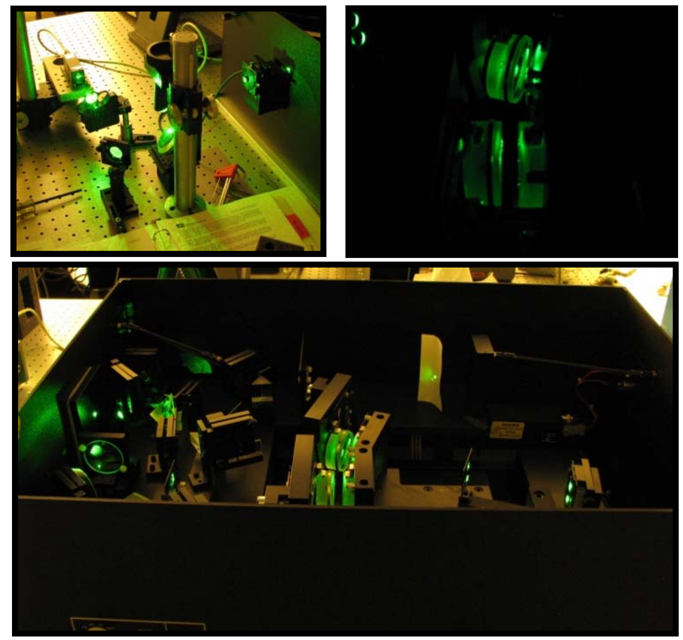
Elasto-optic coef.

Refractive index

$$\eta = \left(\frac{I_{scatt}}{I_{inc}}\right) \propto \frac{d \cdot n^2 p_{12}^2}{\lambda^2}$$

Optical Wavelength

Status of Sandia's BLS Capabilities:



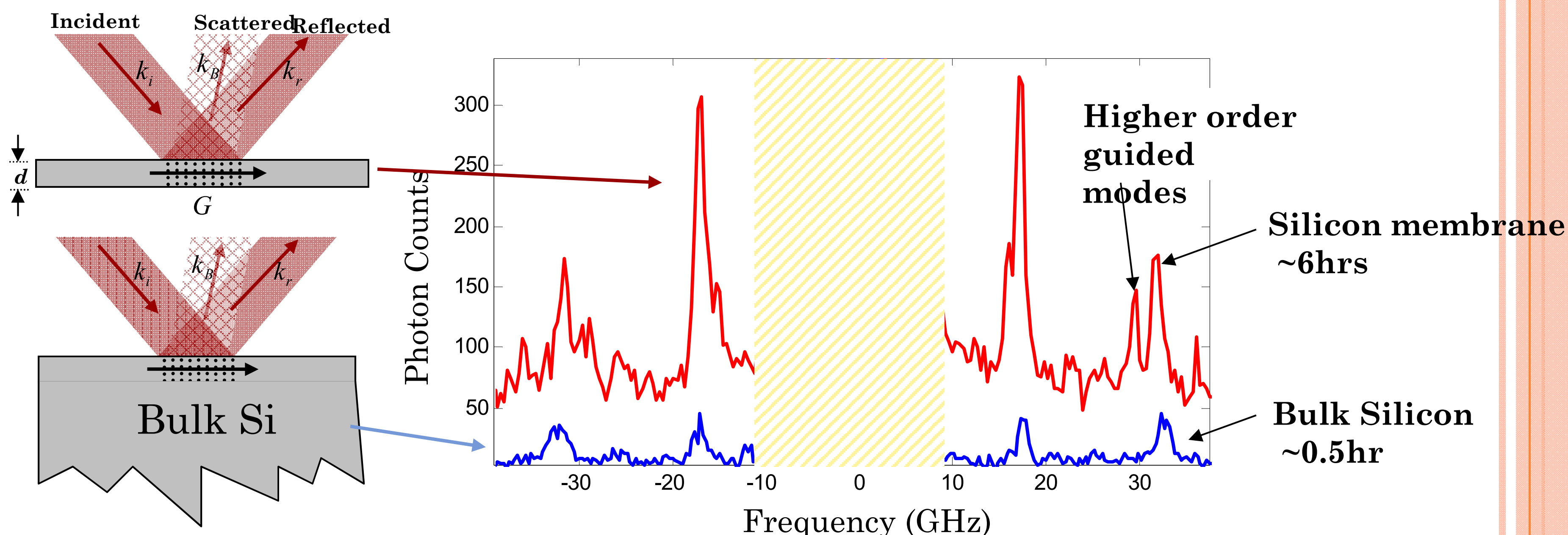
BLS Status:

1) Completed Training for assembly/operation.
2) Installed and aligned & tested BLS system.
3) Currently completing calibration.

Important next steps:

1) Stabilize room temperature to <1Deg C.

BLS Measurements Performed in Switzerland



Experiments Performed with Sandercock

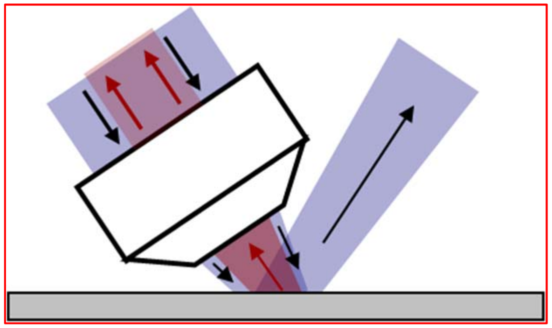
Performed BLS on:

1) **Bulk silicon**
2) **Unpatented Si membrane (thickness 500nm).**
3) **Suspended Si 2D phononic crystal.**

Conclusions:

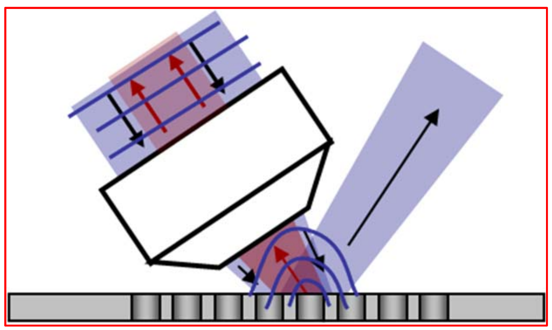
- **BLS signals are large enough to measure in thin samples of this type through surface displacements**
  - ➔ **Observed structure from guided elastic waves**
- **Large elastic scattering from holes makes it difficult to measure Phononic band structure.**
  - ➔ **Further work required to improve rejection**

The Challenge Associated with the Application of Conventional BLS Measurements to PnCs:



Ideal BLS sample:

- ***Ultra-smooth sample***
- ***Generates little elastically scattered light***



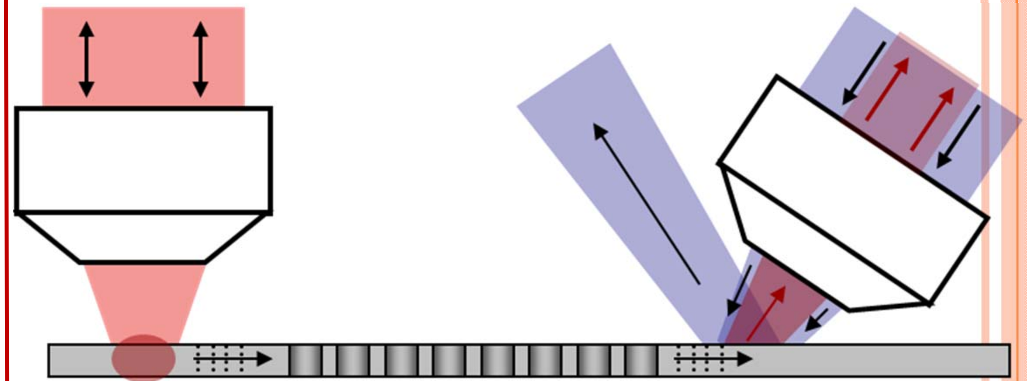
Challenge of ABG sample:

- ***Lithographic pattern ➔ "Roughness"***
- ***Tremendous elastic/specular scattering***
- ***Difficult for BLS spectrometer to reject unwanted elastically scattered light.***

Incident laser signal (ω)

Brillouin Scattered signal (ω - Ω)

New Approach for BLS-based approach for excitation and detection of GHz-0.5THz phonons.



Nature Paper #3 ?

How it will work:

1) **Generate coherent elastic waves in membrane through electrostrictively generated forces (frequencies from 1GHz-0.5THz).**

2) **Elastic waves transmit through PnC.**

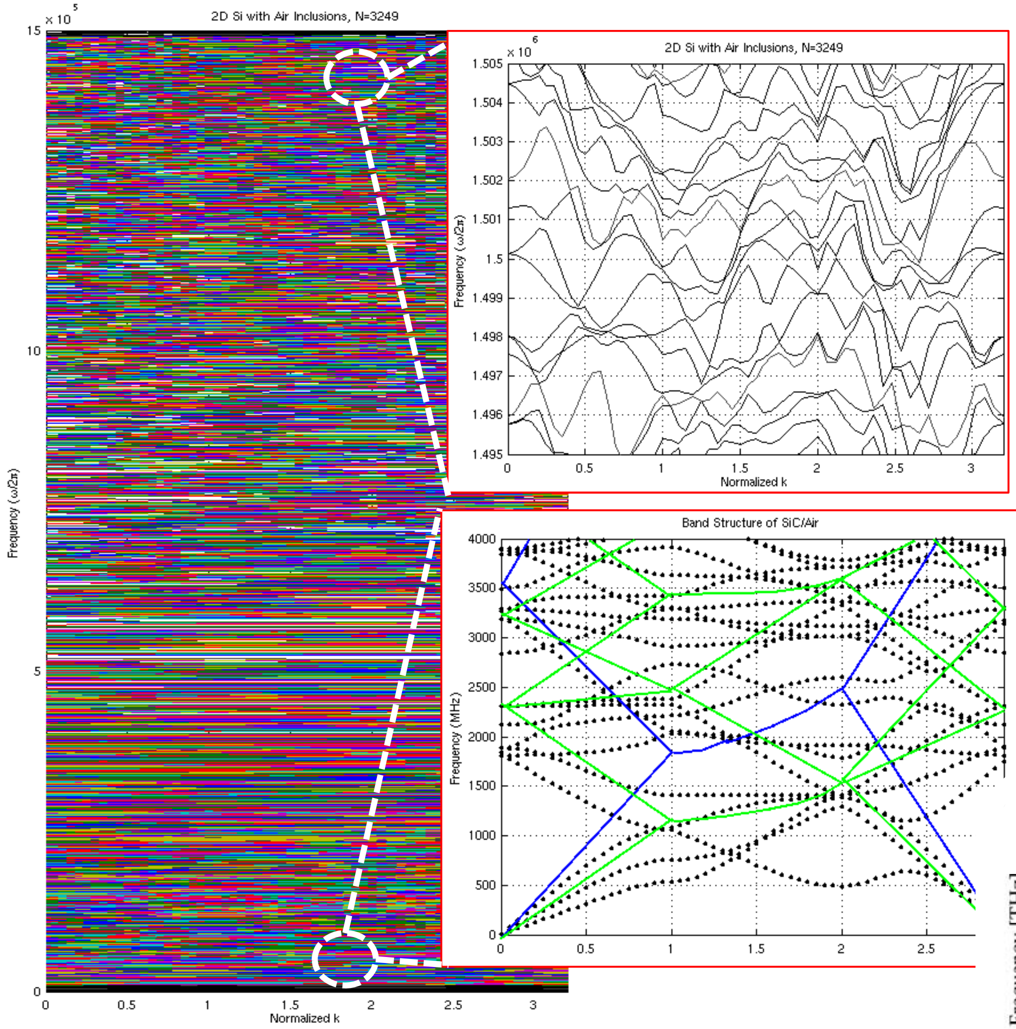
3) **Detect elastic waves on unpatterned portion of the membrane through Brillouin Light Scattering (BLS).**

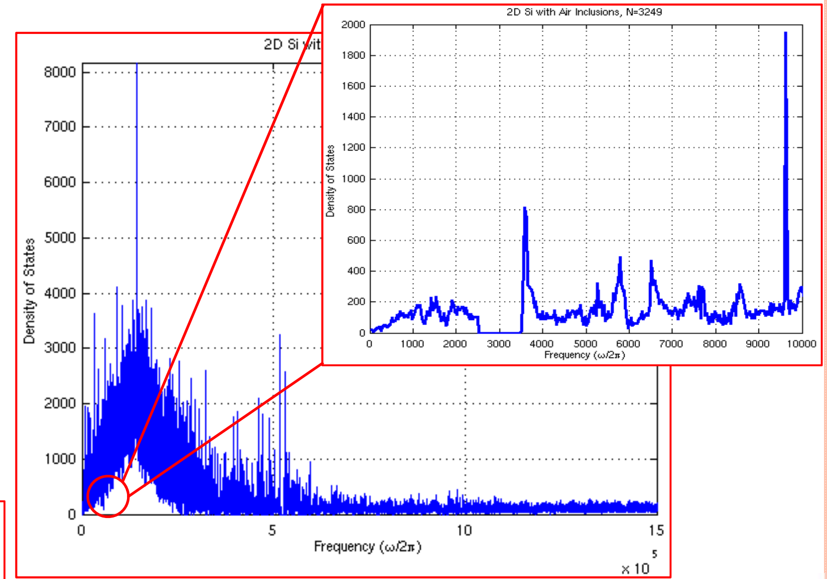
The Result: 0.5THz phononic transmission measurement

Measurement Technique Alone Would Warrant a Nature Paper!

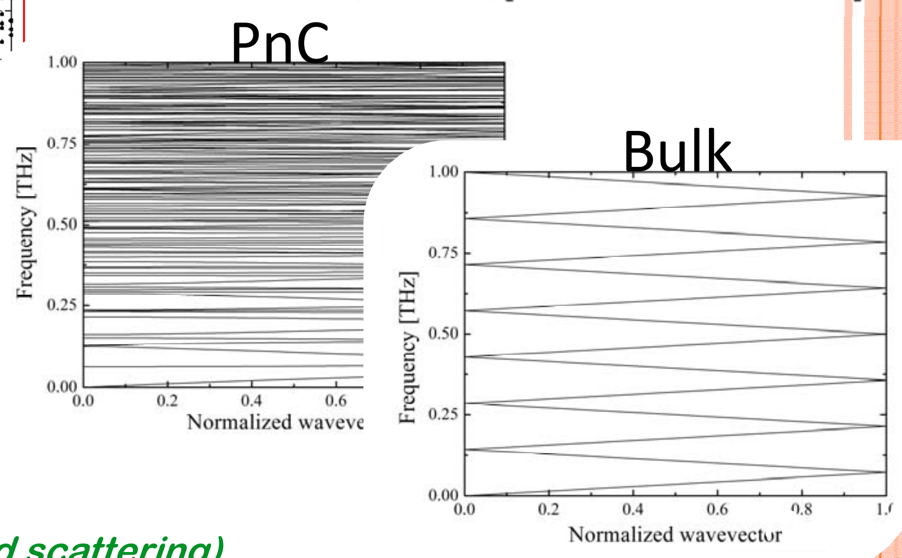
On track to report by end of FY10

Harmonic and Anharmonic Effects Combined



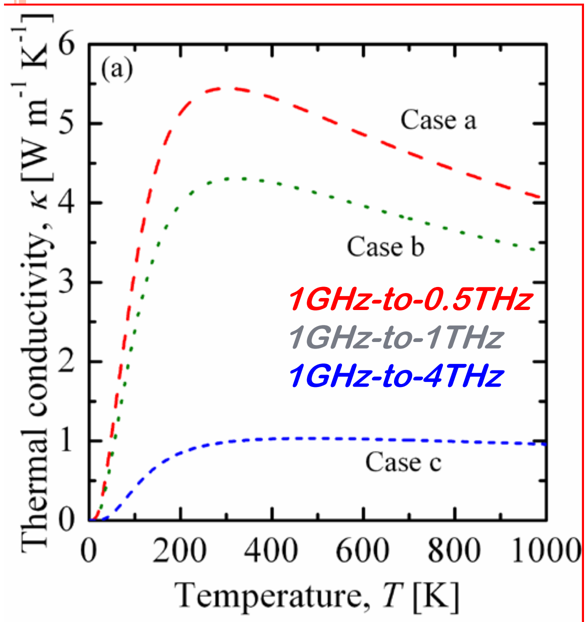


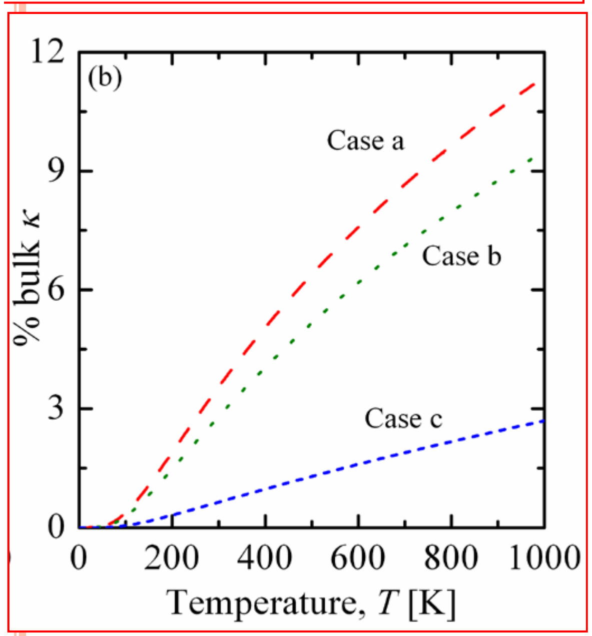
$$\rho(\vec{r})\frac{\partial^2 u_i(\vec{r},t)}{\partial t^2} = \sum_{j,m,n}\frac{\partial}{\partial x_j}\left[C_{i,j,m,n}(\vec{r})\frac{\partial u_n(\vec{r},t)}{\partial x_m}\right],$$



- ***Harmonic (coherent) Reflections → Creation of gap***
- ***Anharmonic Effects → Anomalous dispersion***
- ***Flat Bands → Reduced Group Velocity***
- ***Negative Bands → Backward propagation (backward scattering)***

Si κ with modified PnC Dispersion

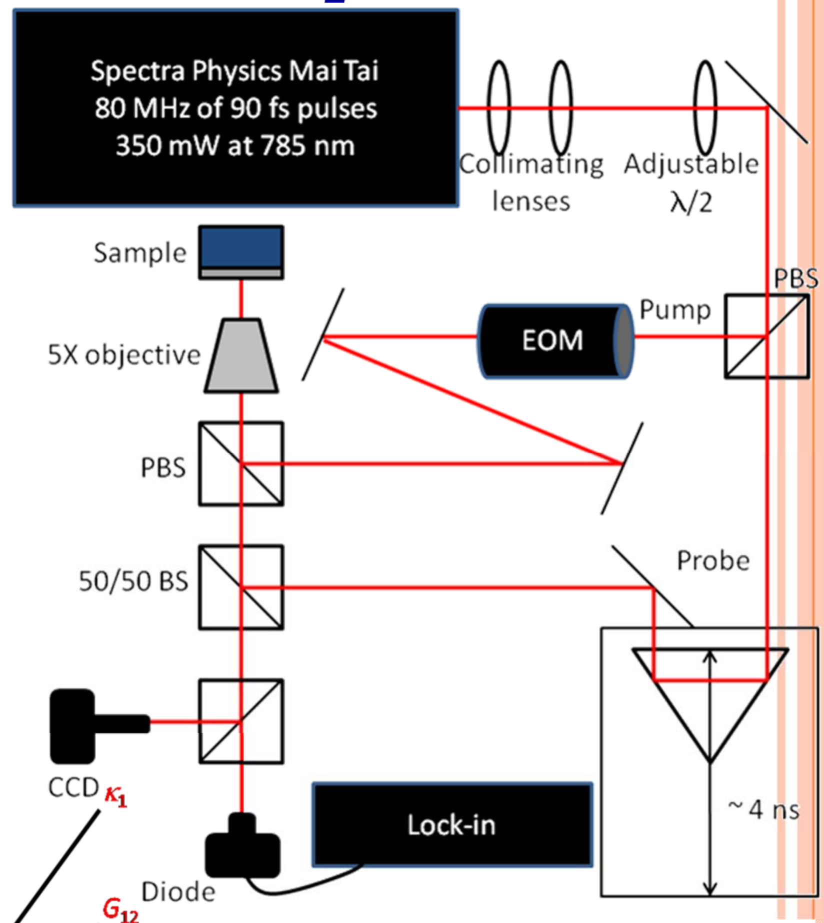


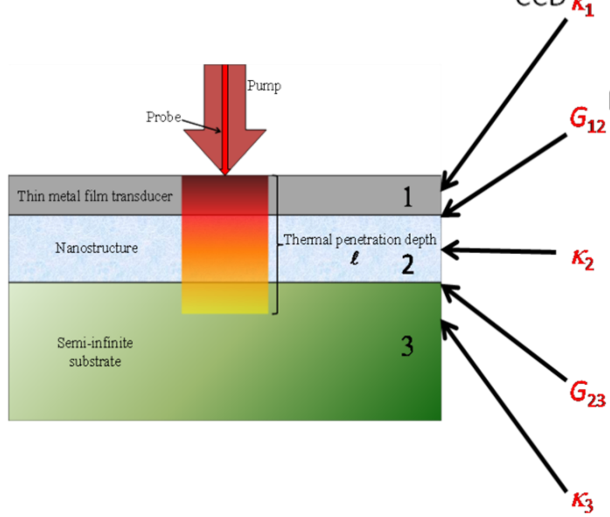


Thermoreflectance signal directly proportional to temperature change

$$C\frac{\partial T}{\partial x} = -\kappa\frac{\partial^2 T}{\partial x^2}$$

Given temperature change with time, we fit the heat equation to the data to determine k





➔*Deposit Al on top surface and Measure off shelf GHz lattice!*

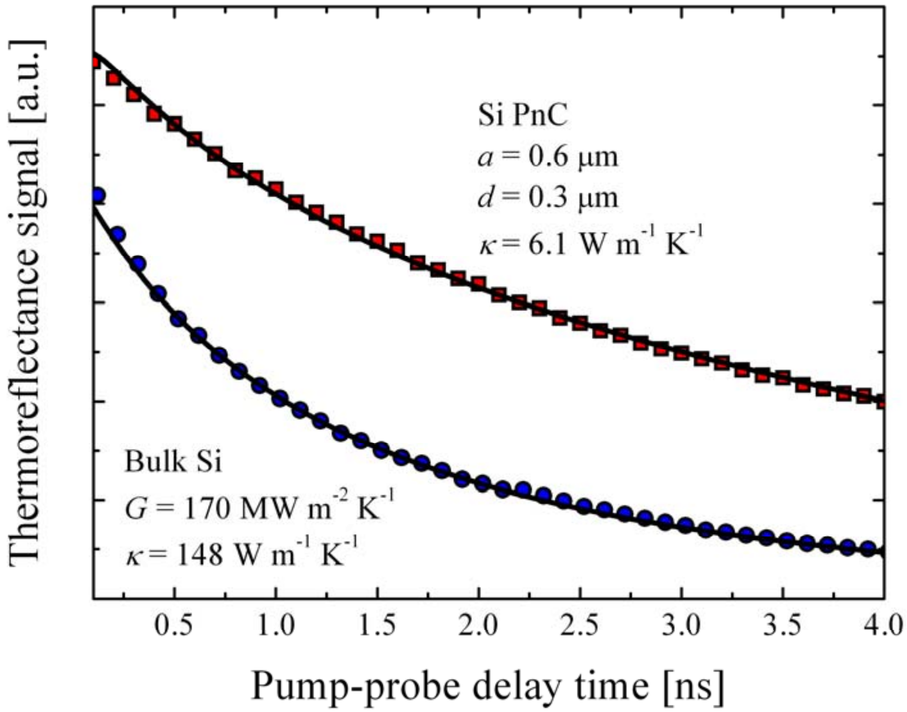
MEASURED κ OF SILICON PNC

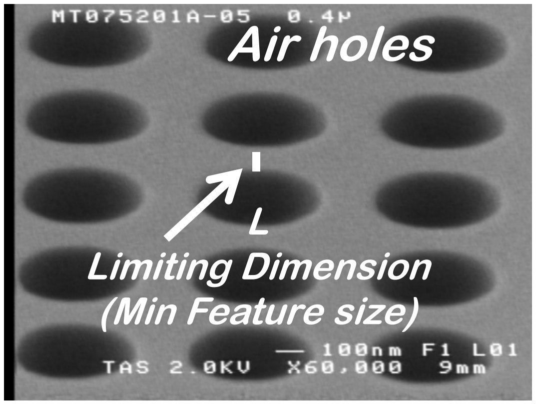
Thermal conductivity measurements on a 500 nm thick suspended PnC structure

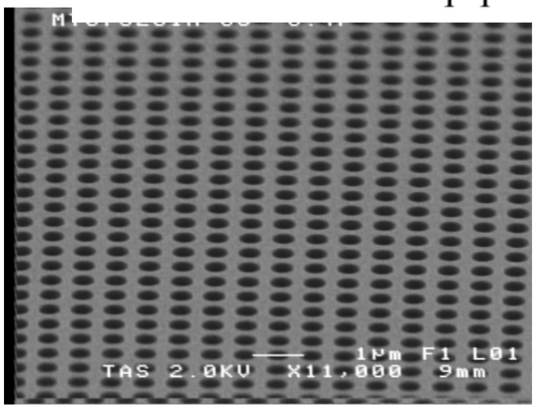
$$\kappa_{\omega,j} = \frac{1}{6\pi}\frac{\hbar^2\omega_j^2(q)}{k_B T^2}\frac{\exp\left[\frac{\hbar\omega(q)}{k_B T}\right]}{\left(\exp\left[\frac{\hbar\omega(q)}{k_B T}\right]-1\right)^2}\upsilon_j(q)\tau_j(q)q^2$$

$$\frac{1}{\tau_j(q)} = \frac{1}{\tau_{Umklapp,j}} + \frac{1}{\tau_{impurity,j}} + \frac{1}{\tau_{boundary,j}}$$

$$\frac{1}{\tau_{Boundary,j}} = \frac{\partial\omega_j(q)}{\partial q}\frac{1}{L}$$

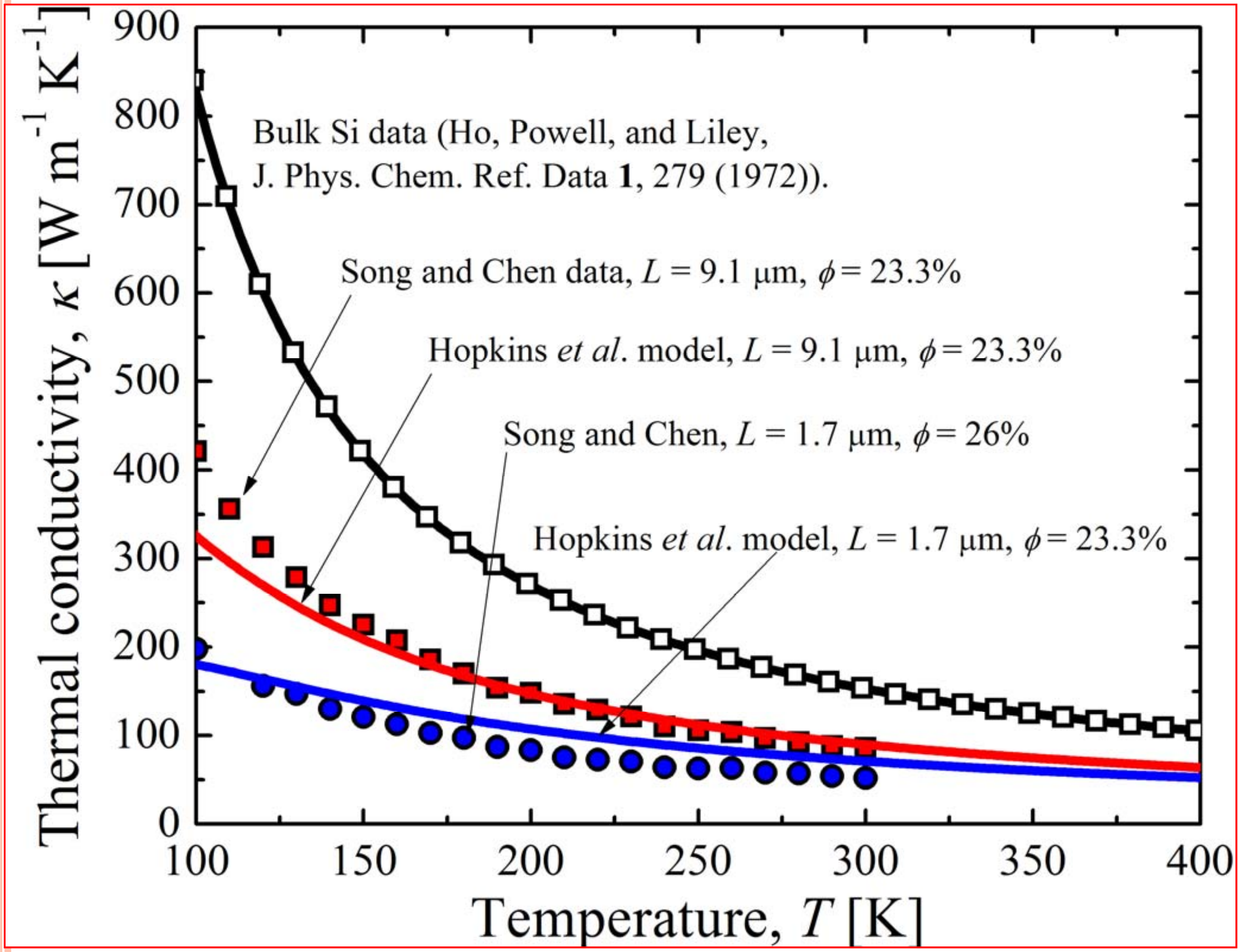






$$\frac{\kappa_{PnC}}{\kappa_{bulk}} = 0.002$$

Understanding the Effect of porosity:
Did we simply remove too much material?



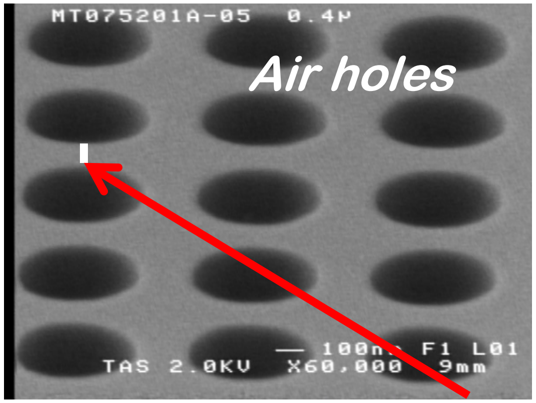
Porosity accounted for by "Eucken" model

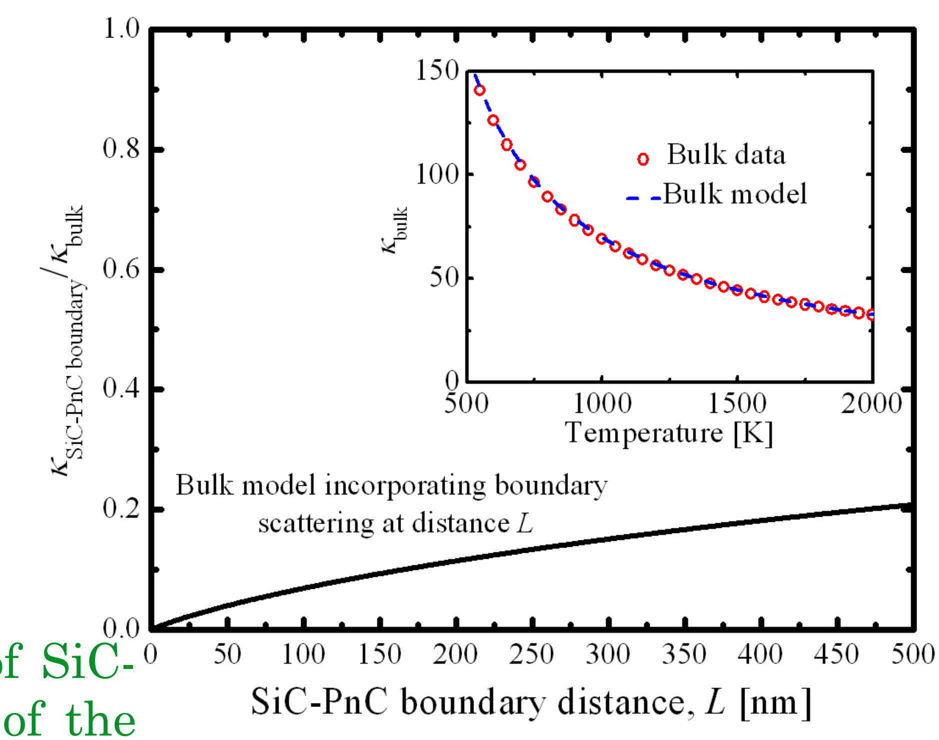
$$\frac{\kappa_{porous}}{\kappa_{solid}} = \frac{1-\phi}{1+\frac{\phi}{2}}$$

Eucken, Forschung auf dem Gebiete des Ingenieurwesens Ausgabe B(Band 3): 3/4 VDI Forschungsheft 353 (1932).

Hopkins, Rakich, Olsson, El-kady, and Phinney, APL 95, 161902 (2009)

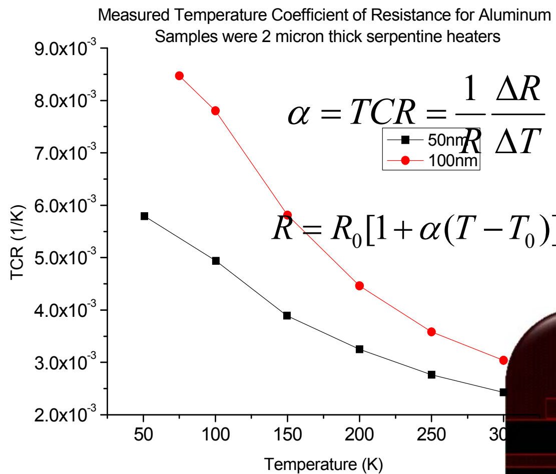
Can micron size holes affect nm wavelets like phonons?





Ratio of the thermal conductivity of SiC-PnC to that of bulk as a function of the minimum feature size, L, of the SiC-PnC. Inset shows the accuracy with which the model predicts bulk behavior. Red is actual experimental data, and the dashed blue line is the result of model.

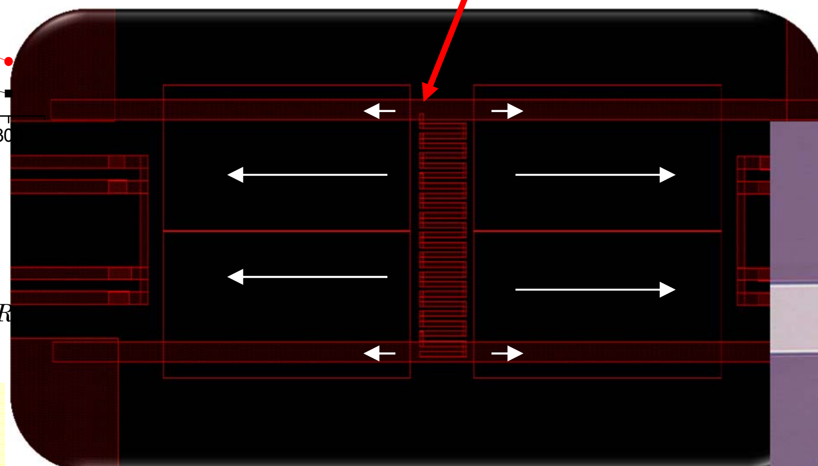
Direct Room T Electrical & Thermal Conductivity Measurement

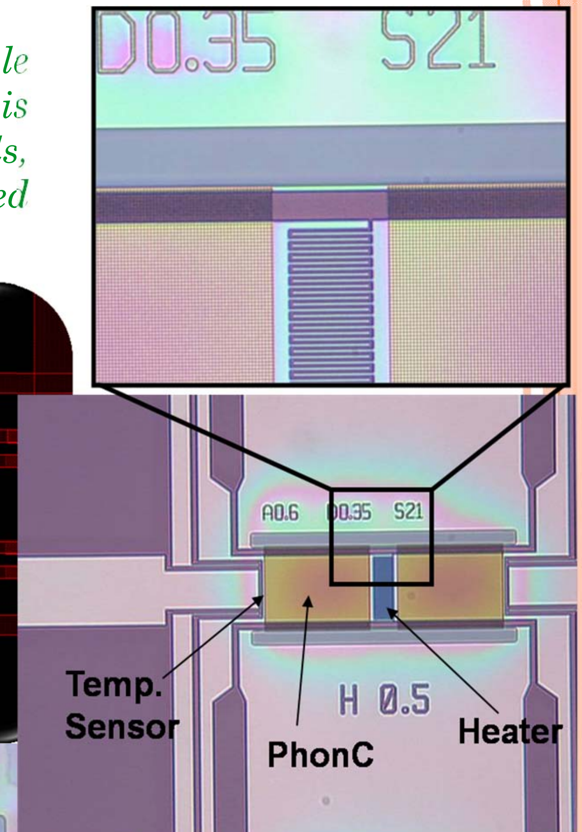


$$\alpha = TCR = \frac{1}{R}\frac{\Delta R}{\Delta T}$$

$$R = R_0[1+\alpha(T-T_0)]$$

The serpentine heater element is Joule heated to provide thermal current. This current can flow both through the leads, and through the membrane isolated sample.





As you make a film thinner, the TCR decreases. This is often done with 'thin film resistors' to keep resistance values constant with temperature. In our case, we want to be well outside this limit as we need to leverage the TCR of a material for resistance thermometry.

Thermal Ohm's law V=IR. $\Delta T = \dot{Q} R_{th}$

1) Input power to serpentine heater:

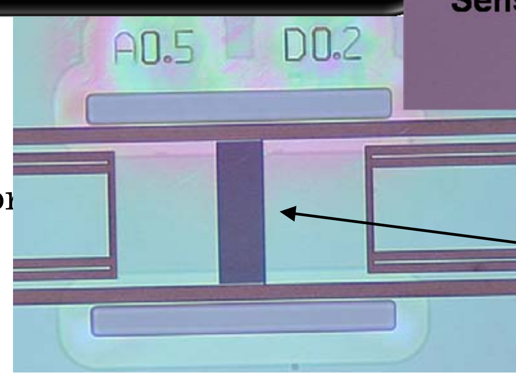
$$\dot{Q} = IV$$

2) Use serpentine as a temp sensor, and edge sensor to measure temperature difference:

$$\Delta T = T_H - T_C$$

3) Obtain the thermal conductivity:

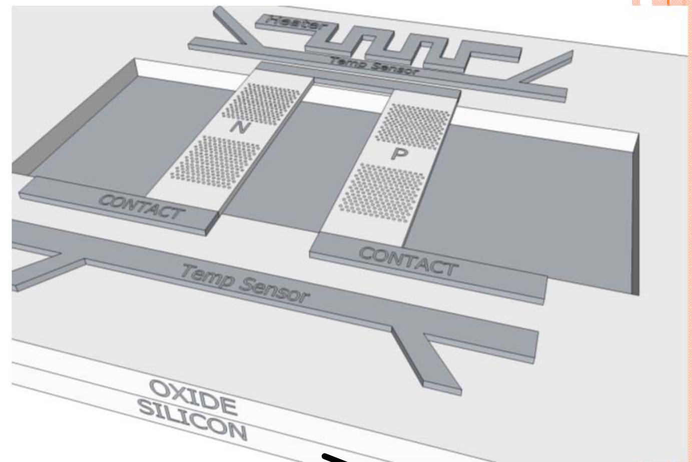
$$k = \frac{L}{R_{th} A}$$



Matrix (Reference) Device with Heaters and Temp. Sensors

In reality, uncertainty in geometry is an issue, but we use reference slabs with no holes to alleviate this problem.

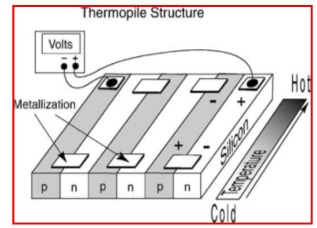
1. *Thermal Dialing of harmonic/anharmonic effects*
2. *Device Demos:*
   1. *TE Cooler*
   2. *Thermopile Stack for Thermal Energy Scavenging.*



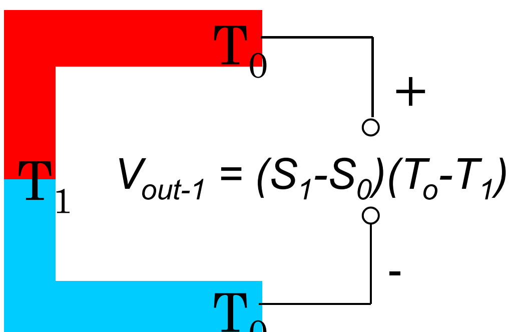
➢*A planar 2 leg structure will be developed to test true TE enhancement (compared to unpatented silicon on same chip).*

➢*A resistive heater and thermometry will be applied to evaluate performance.*

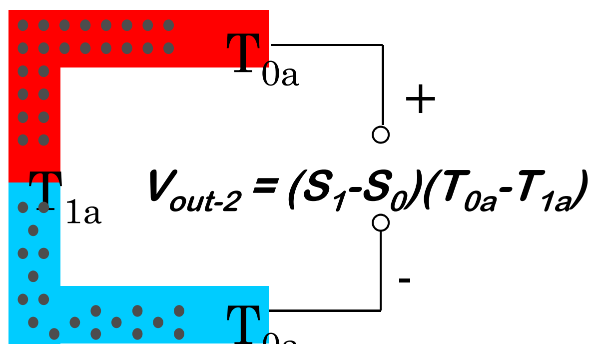
➢*The basic experiment will be to apply power to the heater, and pass a current through the n-p leg structure to transport heat from the hot to cold side of the device.*



Generic Thermocouple:



PhonC Thermocouple:



$T_{0a}-T_{1a} > T_0-T_1 \Rightarrow V_{out-2} > V_{out-1}$

Phononic bandgap allows for simultaneous low thermopile series resistance (low losses) and high thermal isolation (high ΔT and ΔV)

Seebeck coefficients of metals relative to platinum

Material	Seebeck coefficient (μV/°C)
Antimony	+48.9
Chromel	+29.8
Tungsten	+11.2
Gold	+7.4
Copper	+7.6
Silver	+7.4
Aluminum	+4.2
p-Silicon, ρ = 0.0035 Ω cm	+450
p-Germanium, ρ = 0.0083 Ω cm	+420
Platinum	0.00
Calcium	−5.1
Alumel	−10.85
Cobalt	−13.3
Nickel	−14.5
Constantan	−37.25
Bismuth	−73.4
n-Silicon, ρ = 0.0035 Ω cm	−450
n-Germanium, ρ = 0.69 Ω cm	−548

Future Work

Reduce Impedance: AlN has demonstrated low motional resistance

→ ***Mitigate the parasitic coupling and loading issues by orienting AlN directly on SiC or patterning the bottom electrode.***

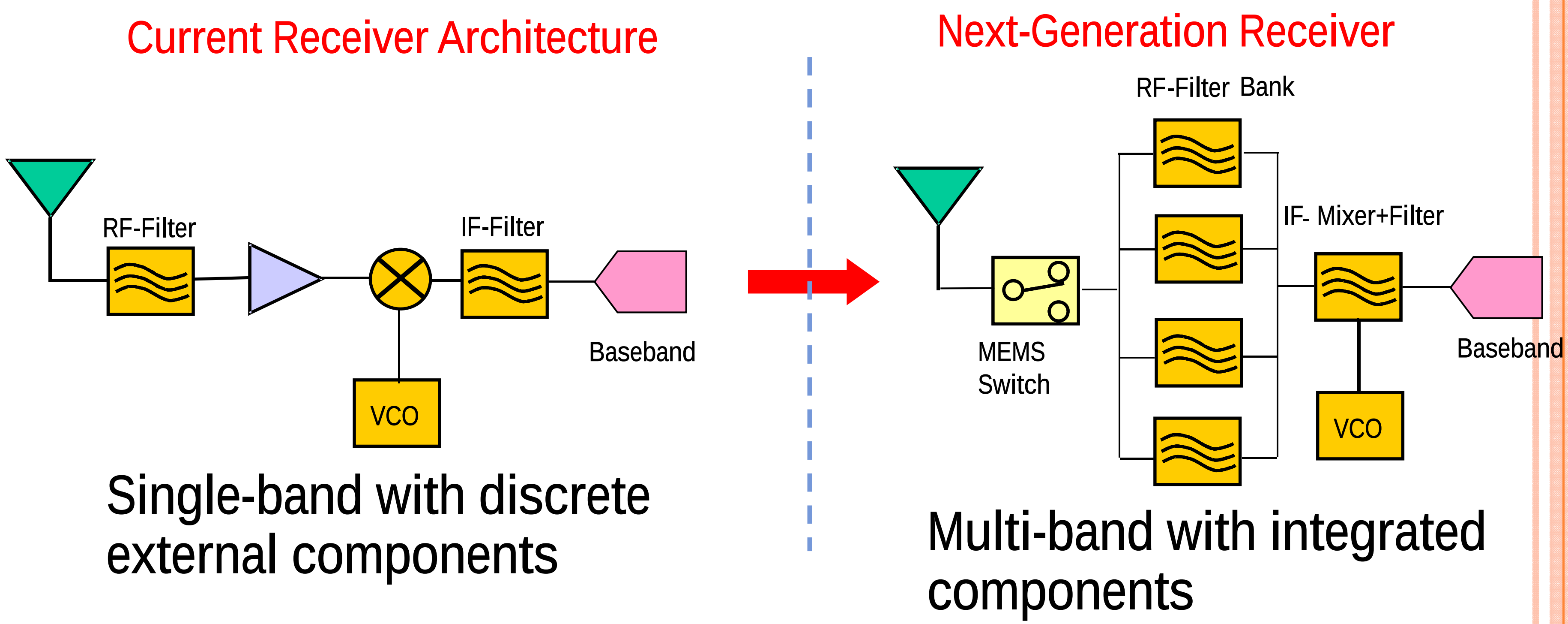
Characterization and modeling of Lateral Overtone Resonators and Phononic Crystal Cavity resonators

Optimize design of phononic crystal for better coupling to the cavity

Design Thermoelectric devices for thermoelectric energy scavenging

"Next-Generation" NEMS Cognitive Radio

- Envision a fully integrated radio, with multiple RF channels, reduced power consumption, and minimum number of electronic components

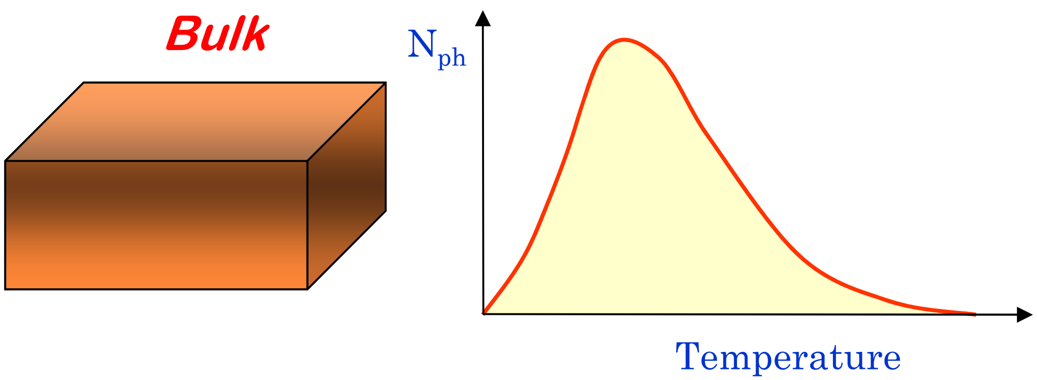


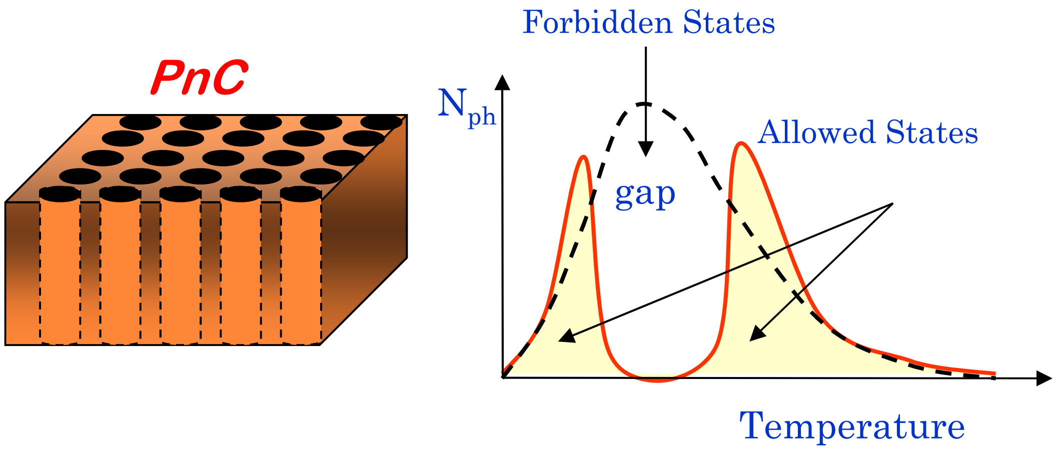
low power, ultra-small size, multi-channel, multi-band

Phononic Crystals :Thermal Phonon Control

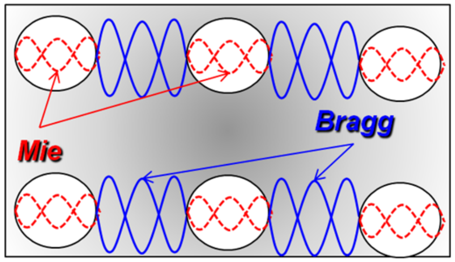
Mold and shape the thermal phonon distribution by artificially changing the density of states

$$n(\omega_{k,s}) = \frac{1}{\exp(\hbar\omega_{k,s}/k_B T) - 1}$$





Freq	Radius "r"	Pitch "a"	Phonon Temp "T"
50MHz	50µm	100µm	2.5mK
5GHz	0.5µm	1µm	0.25K
10GHz	250nm	500nm	0.5K
100GHz	25nm	50nm	5K
1THz	2.5nm	5nm	50K
2.5THz	1nm	2nm	125K



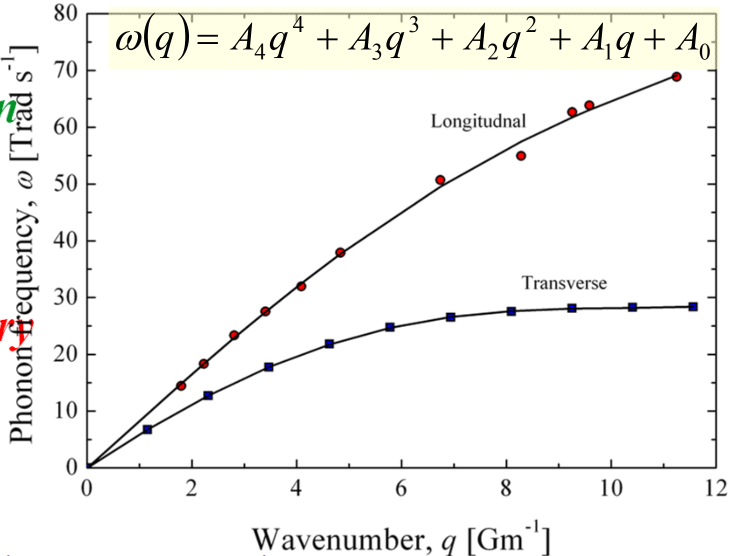
MANIPULATING THE THERMAL CONDUCTIVITY

- *The thermal conductivity is given by*

$$\kappa = \frac{1}{6\pi}\sum_j \int_q \frac{\hbar^2 \omega_j^2(q)}{k_B T^2} \frac{\exp\left[\frac{\hbar\omega(q)}{k_B T}\right]}{\left(\exp\left[\frac{\hbar\omega(q)}{k_B T}\right]-1\right)^2} \upsilon_j^2(q)\tau_j(q) q^2 dq$$

$\omega(q)$ is the phonon dispersion.
$\upsilon(q) = \partial\omega(q)/\partial q$ is the phonon group velocity,
$\tau(q)$ is the scattering time of the phonons,
q is the wavevector, and the thermal conductivity,
$j = 1,\ 2,\ 3$ (1 longitudinal, and 2 transverse).

- ***We use measured Si dispersion data and fit the data to a 4th degree polynomial for an analytical expression of the phonon dispersion***



- ***In bulk Si, phonon scattering is dominated by Umklapp scattering, impurity scattering, and boundary scattering.***

$$\frac{1}{\tau_{Umklapp,j}} = BT\omega_j^2(q)\exp\left[\frac{C}{T}\right]$$

$$\frac{1}{\tau_{impurity,j}} = D\omega_j^4(q)$$

$$\frac{1}{\tau_{boundary,j}} = \frac{\upsilon_j(q)}{E}$$

- ***Mattheissen's Rule:***

$$\frac{1}{\tau_j(q)} = \frac{1}{\tau_{Umklapp,j}} + \frac{1}{\tau_{impurity,j}} + \frac{1}{\tau_{boundary,j}}$$

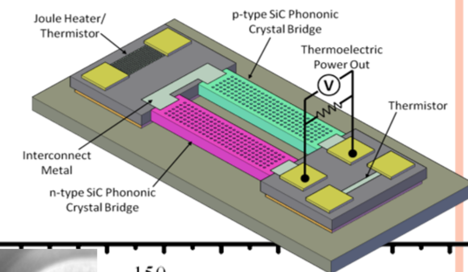
- ***where B, C, D, and E are constants determined by fitting κ to data.***

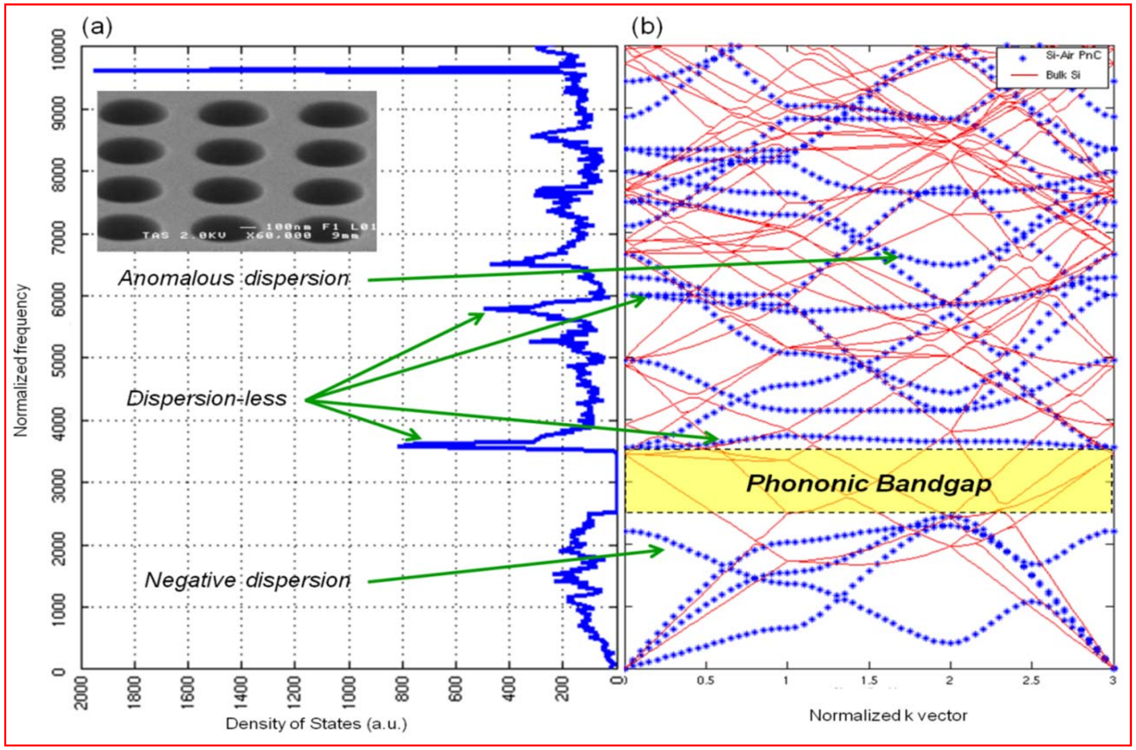
Nanostructures PnC Approach

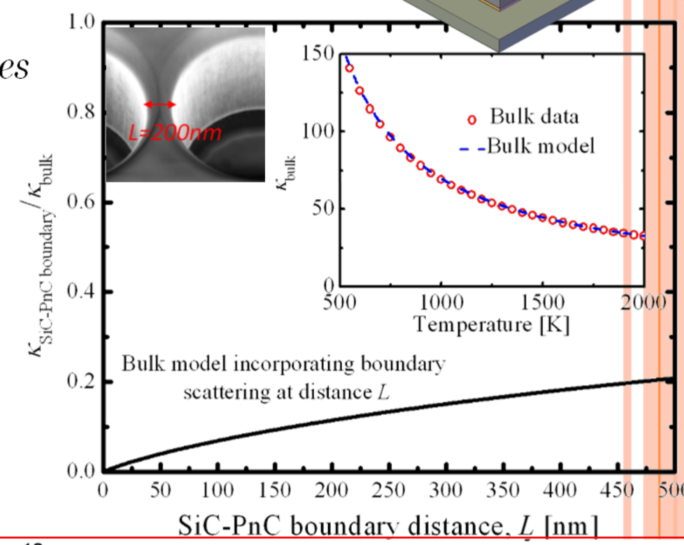
PnC Reduction of thermal Conductivity & Planar Integration

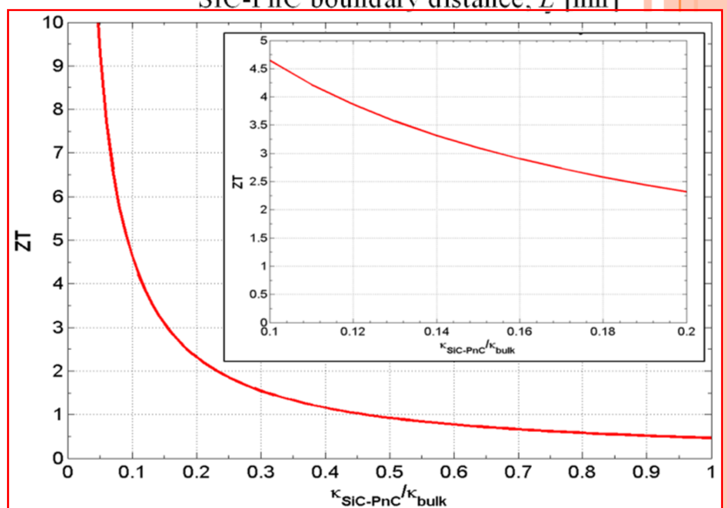
Phonic Crystals:

- *Coherent Scattering of Phonons*
  - *affect high laying frequency phonons with relatively large dimensions*
- *Minimal effect on electrons:*
  - *Mean free path is 1-to-2 orders of magnitude lower*
- *Planar integration ➔ large separation between hot and cold sides*



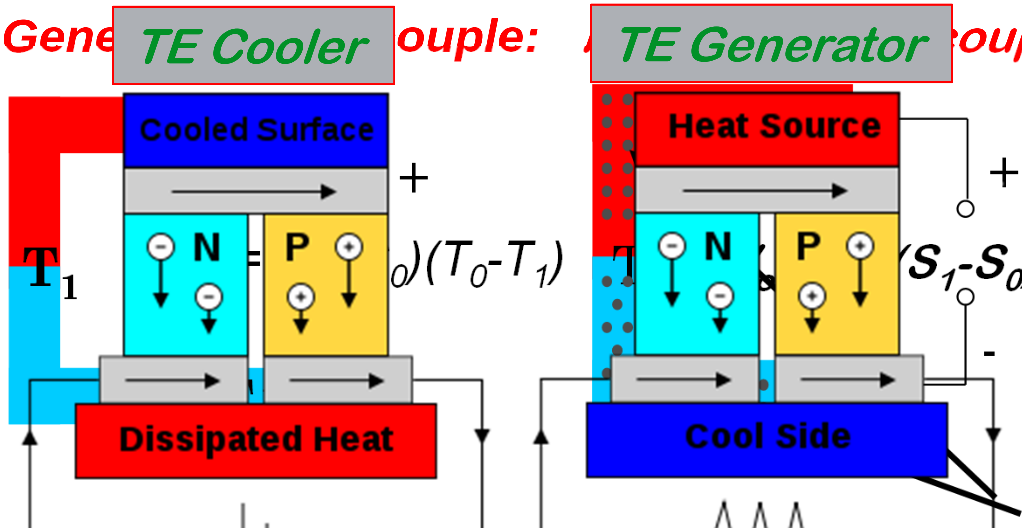






- *Harmonic (coherent) Reflections ➔Creation of gap*
- *Anharmonic Effects ➔Anomalous dispersion*
- *Flat Bands ➔ Reduced Group Velocity*
- *Negative Bands ➔ Backward propagation (backward scattering)*

THERMAL ENERGY SCAVENGING: THERMOPILES



$T_{0a}-T_{1a} > T_0-T_1 \Rightarrow V_{out-2} > V_{out-1}$

Thermal Conduction:

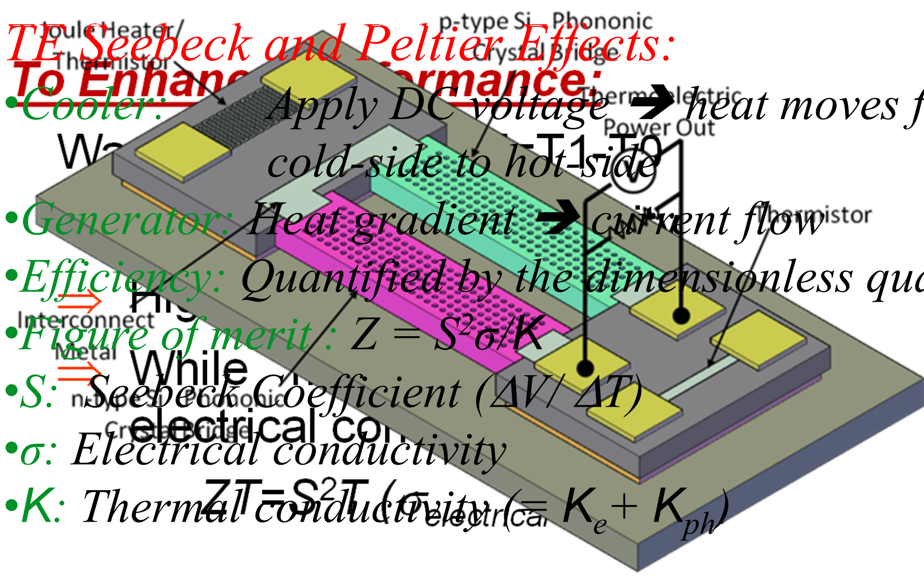
- *Semi-Conductors and Conductors*
  - *Both Electron and Phonon*
- *Dielectrics*
  - *Primarily Phonon*

Phononic bandgap allows for simultaneous low thermopile series resistance and high thermal isolation

Silicon Carbide is a target material for harsh environment applications

Silicon Carbide has high Seebeck Coefficent (S) but also high thermal conductivity (κ)

→Silicon Carbide Phononic Crystal Thermoelectric Devices



TE Seebeck and Peltier Effects:

To Enhance Performance:

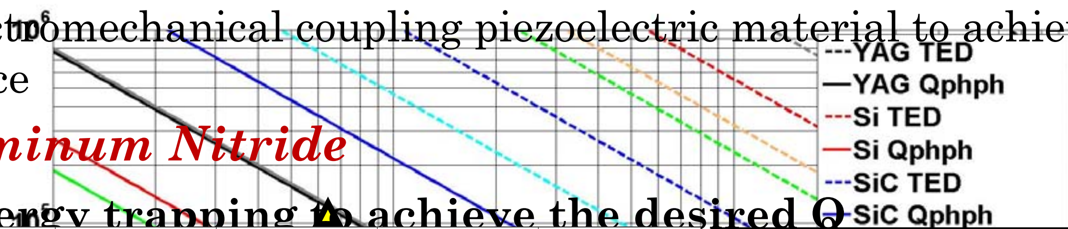
- *Cooler: Apply DC voltage → heat moves from cold-side to hot-side*
- *Generator: Heat gradient → current flow*
- *Efficiency: Quantified by the dimensionless quantity ZT*
- *Figure of merit : $Z = S^2\sigma/K$*
- *S: Seebeck Coefficient ($\Delta V/\Delta T$)*
- *σ: Electrical conductivity*
- *K: Thermal conductivity ($= K_e + K_{ph}$)*

HIGH F.Q, LOW IL RESONATORS

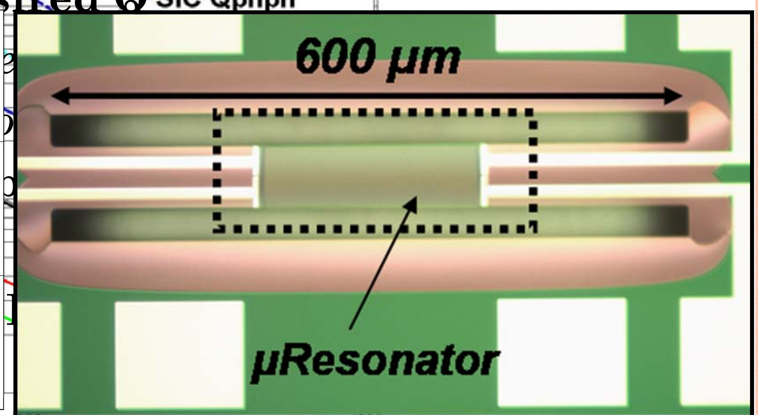
- **Materials**
  - Must have low phonon-phonon and thermoelastic damping to support the f.Q product

    → ***Silicon Carbide***
  - High electromechanical coupling piezoelectric material to achieve the low impedance

    → ***Aluminum Nitride***



- **Design : Energy trapping to achieve the desired Q**



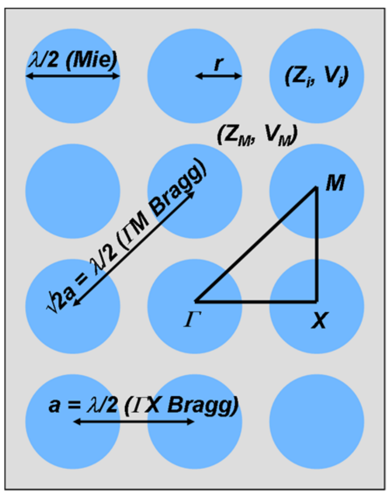
-
  - Vertical sidewall etching to support the as designed quality factor
  - Low surface roughness to support the as designed quality factor
  - Low, tensile film stress to allow for mm scale suspended structures

$$Q_{TED} = \frac{9C^2}{\kappa T \alpha^2 \rho \omega} \qquad Q_{phph} = \frac{\rho v^2}{CT\hat{\gamma}^2} \frac{1+(\omega\tau_{ph})^2}{\omega\tau_{ph}}$$

Plane Approximation Method (PAM): Origin of the Phononic Crystal Bandgap

2D PnC can be approximated by a 1D stack of alternating layers

- *Bandgap formation depends on the ratio of the acoustic impedance Z of these two layers*
  - $Z_{P2}/Z_{P1} = 2.68$ *for Si-air as compared to* $Z_{P1}/Z_{P2} = 3.11$ *for Si-W*

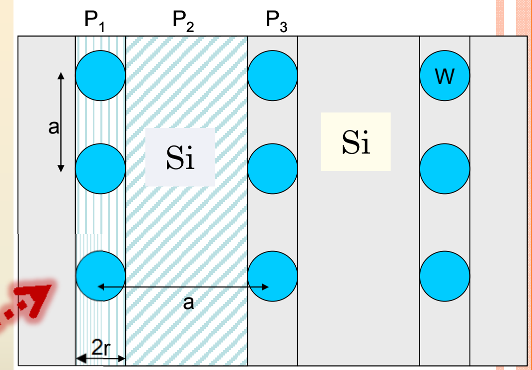


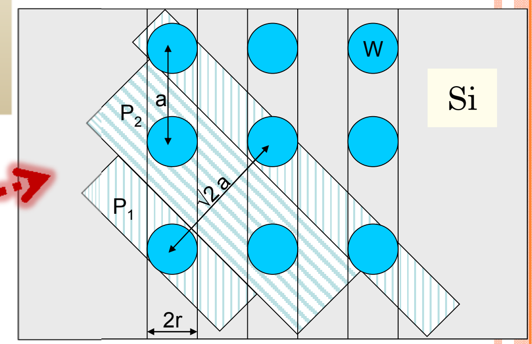
$$f(Bragg)_{\Gamma X} = \frac{V_{avg}}{2a}$$

$$f(Bragg)_{\Gamma M} = \frac{V_{avg}}{(2a)\sqrt{2}}$$

$$f(Mie) = \frac{V_i}{4r} \qquad V = \sqrt{\frac{E}{\rho}}$$

$$V_{avg} = \pi\left(\frac{r}{a}\right)^2 V_i + \left(1 - \pi\left(\frac{r}{a}\right)^2\right) V_M$$





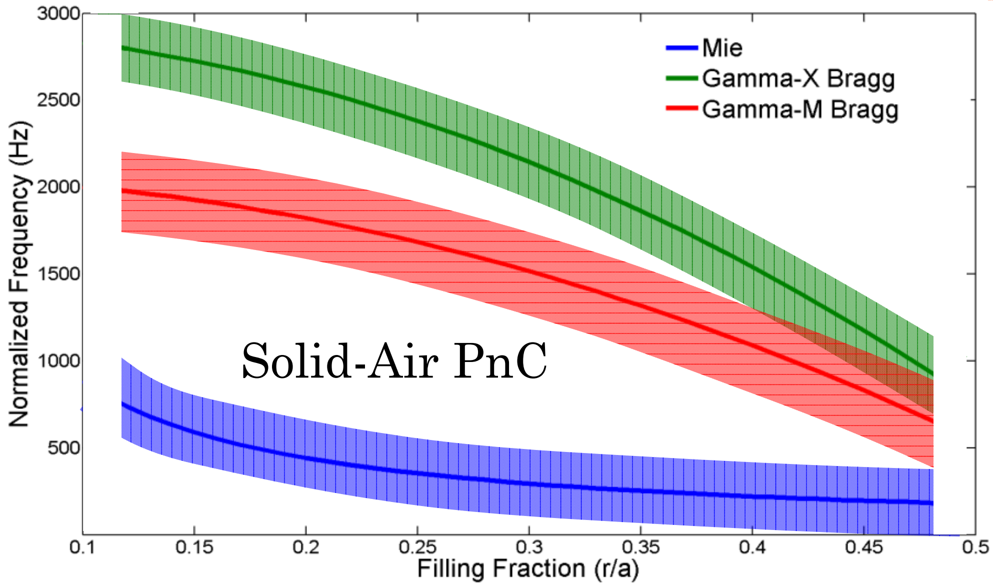
$$Z_{eff\,1} = ff_1 \cdot Z_{air,W} + (1\text{-}ff_1) \cdot Z_{Si},$$

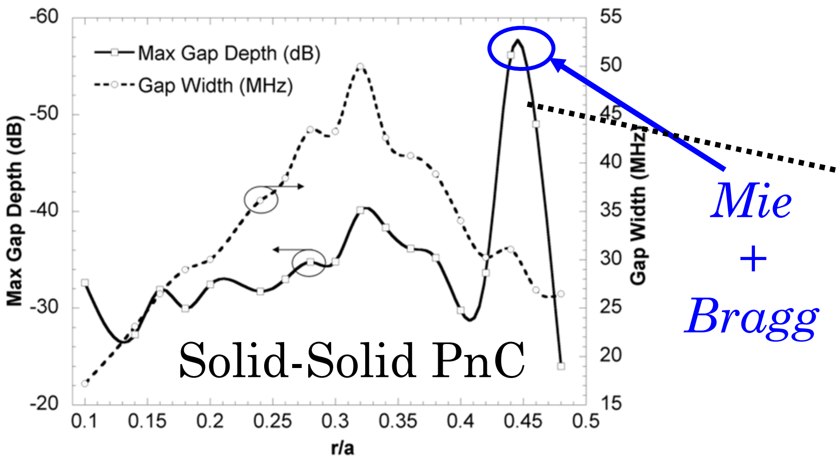
$$where \quad ff_1 = \frac{\pi r}{2a}$$

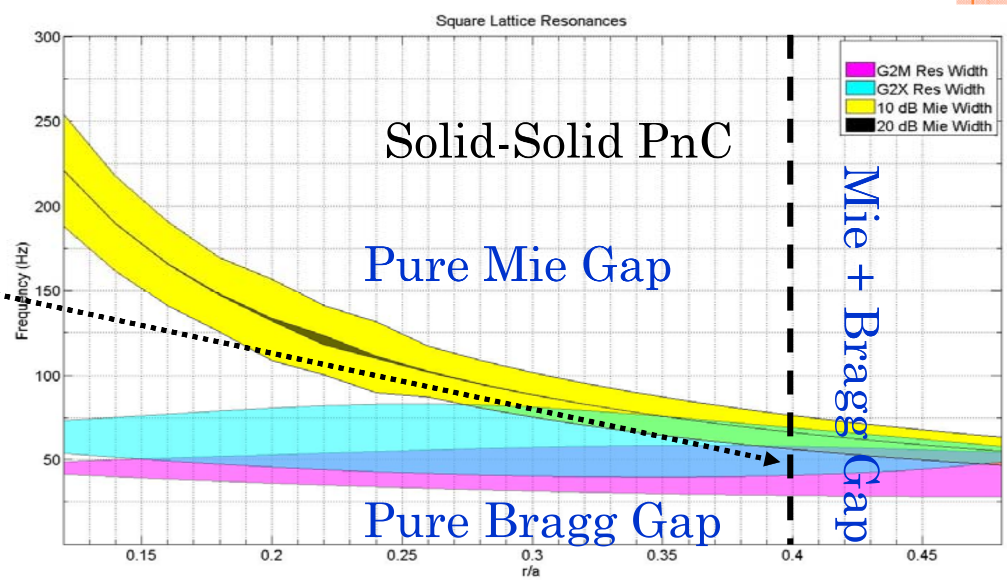
I. elkady, et al, Phyiscal Review B, under review

ORIGIN OF THE PHONONIC CRYSTAL BANDGAP

- *Solid-air PnC only has Bragg resonance overlap*
  - *–Large r/a values agree with PWE!*
- *Solid-solid PnC has greater overlap of Bragg, Mie resonances*







M. Ziaei-Moayyed, et al, Phyiscal Review B, under review