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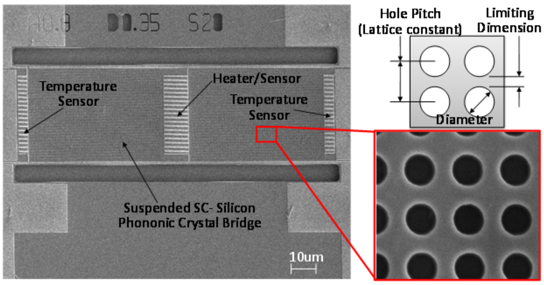
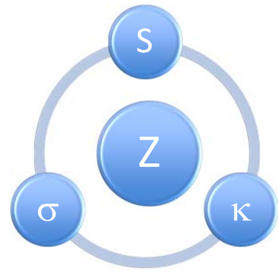
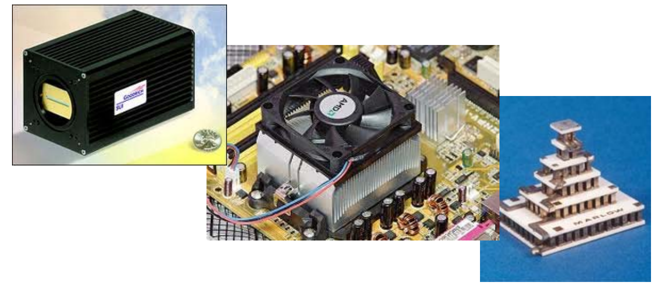






Nano-Structured Silicon Phononic Crystals with Metal Inclusions for ZT Enhancement

Charles Reinke (PI, 1712) and Ihab El-Kady (1712) — Early Career LDRD Program

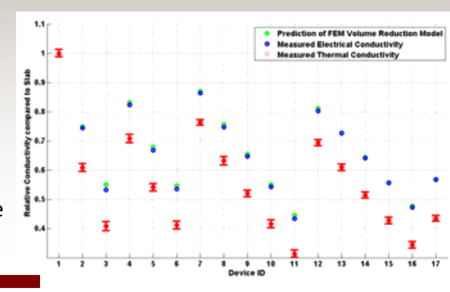
Project Purpose and Approach

*"**We propose to address all three parameters of ZT simultaneously using nano-structured phononic crystals (PnCs) with metallic inclusions**"*

- PnCs for Engineered κ Reduction
- Metallic PnC Inclusions to Engineer κ and σ Concurrently
- Full ZT Measurement of PnCs
- Metallic Nano-Shells to Enhance Seebeck

Key Accomplishments

- Measured record κ reduction for lattice constant/porosity parameters and at elevated T
- Self-consistent continuum mechanics/lattice dynamics model of κ
- 2 invited talks at international conferences
- Contributed talk at an international conference
- 2 journal papers

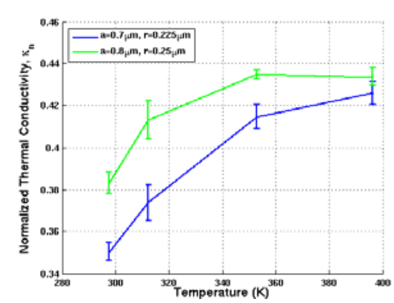


Significance of Results

- Enable a new class of thermal materials and devices
  - Efficient thermoelectric cooling
  - Competitive waste heat scavenging
- Examine a low-cost solution for creating high-ZT materials
- Explore the continuum/quantum regime boundary
- Uncover new physical phenomena
  - High-temperature thermodynamic properties
  - Electronic band-bending at nano-scale metal-semiconductor interfaces
  - Simultaneously engineering the electrical and thermal conductivities and the Seebeck coefficient

R&D Goals and Milestones

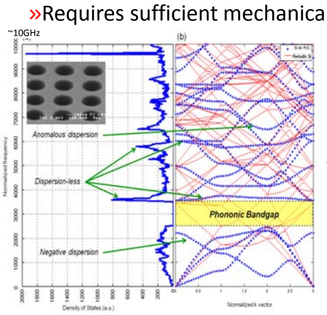
- Demonstrate κ reduction in Si-air PnCs at elevated temperatures
  - CM/LD hybrid model - *90%*
  - Full TE characterization - *70%*
- Demonstrate σ enhancement with Si-W PnC
  - Fabrication - *100%*
  - Measurements - *70%*
- Demonstrate Seebeck enhancement with metallic nano-shells
  - Fabrication - *50% (using previous samples)*
  - Measurements - *10% (test-bed currently ready)*

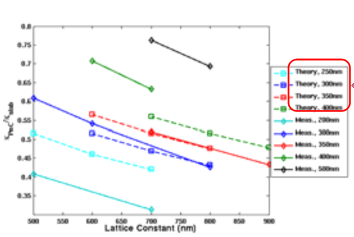


What is a Phononic Crystal?

» Periodic arrangement of elastic scattering centers in a matrix material that exhibits both incoherent and Mie and Bragg resonant scattering

» Requires sufficient mechanical impedance mismatch





How does a Phononic Crystal effect κ?

» Modification of phonon dispersion "$\omega(k)$", which is related to the and influences the phonon scattering lifetime

» Incoherent scattering due to the interface at each inclusion

» Redistribution of the phonon density of states as compared with bulk

- Thermal conductivity is given by the Callaway-Holland model as:

$$\kappa = \frac{1}{6\pi^2}\sum_j \int_k \frac{\hbar^2\omega_j^2(k)}{k_B T^2} \frac{\exp\left[\frac{\hbar\omega_j(k)}{k_B T}\right]}{\left(\exp\left[\frac{\hbar\omega_j(k)}{k_B T}\right]-1\right)^2} \upsilon_j^2(k)\tau_j(k)k^2 dk$$

$\omega(k)$ is the phonon dispersion
$\upsilon(k) = \partial\omega(k)/\partial k$ is the phonon group velocity
$\tau(k)$ is the scattering lifetime of the phonons
k is the wavenumber
j = 1,2,3 (1longitudinal and 2 transverse modes)
L is the minimum feature size

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

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

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

$$\frac{1}{\tau_{boundary,j}} = \frac{L}{\upsilon_j(k)}$$

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

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