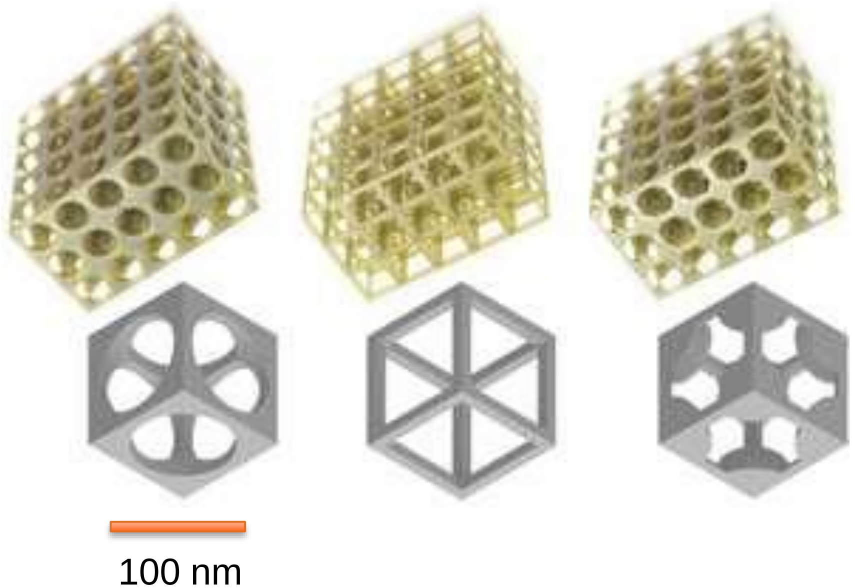
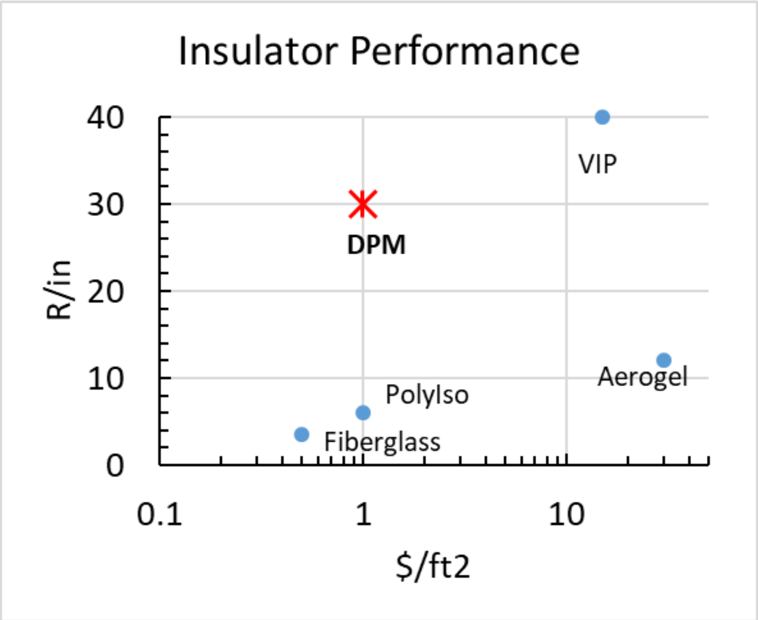
Dynamic Phononic Metamaterial (DPM) for Building Envelopes





Argonne National Laboratory
Ralph T. Muehleisen, Principal Building Scientist
630-252-2547, rmuehleisen@anl.gov

Project Summary

Timeline:

Start date: 10/01/2019

Planned end date: 9/30/2019

Key Milestones

1. Simulate k<0.005 (W/mK) with FEM (Q3)
2. Simulate k<0.01 (W/mK) with LAMMPS (Q3)
3. Fabricate with 80% reduction in k (Q4)

Budget:

Total Project $ to Date:

- DOE: $500,000
- Cost Share: $0

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- DOE: $500,000
- Cost Share: $0

Key Partners:

Alcorix Co., Plainfield, IL

Project Outcome:

- Show feasibility of generating a superinsulator through nanoscale structural design with a process potentially amenable to low cost
  - Design, in simulation, a material capable of R >28/in
  - Fabricate a material structure that reduces bulk conductivity > 5x

Ultimate Goal:

- Design a low cost, highly durable, high strength superinsulator with R/in > 30 and cost premium of under $0.50/sqft)
- Design the material to have dynamic properties to provide “free cooling” under appropriate conditions

Team

Dr. Ralph T. Muehleisen, PI, Principal Building Scientist
Expert in building science, thermodynamics, and metamaterials for acoustics and vibration. Will provide program management and primary material design as well as knowledge of building construction, performance requirements and cost targets.

Dr. Mathew Cherukara, CO-I, Assistant Physicist
He is an expert in detailed computer simulation of materials and chemical processes.. Leading high fidelity molecular simulation work.

Dr. Michael Pellin, CO-I, Argonne Distinguished Fellow
Expert in material science and chemistry. Leading 3-D nanoprinting fabrication.

- Will produce at least one nanofabrication sample for testing by end of project.

Dr. S. Hales Swift. Postdoctoral Staff
Expert in acoustics and vibration. Developing continuum mechanics simulations using Comsol Multiphysics and contributing to design.

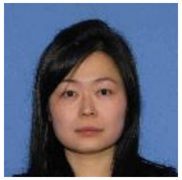
- Will show simulations and optimization of of 3 potential designs in Q3 and 5 by end of project.

Dr. Raghuveer Chimata, Postdoctoral Staff
Expert in material . Developing detailed molecular dynamics simulations on HPC using LAMMPS molecular dynamics software.

- Will show high fidelity simulations of at least one design in Q3 and for actual fabrication sample by end of project.

Team

Dr. Nwike Iloeje, Postdoctoral Staff
Expert in thermodynamics, chemical processes, and design.
- Will work Dr. Swift to develop nanostructure design.



Dr. Clarisse Kim, Energy Scientist
Expert condensed matter physics.
- Will work with Dr. Cheruka and Dr. Chimata on self-assembling molecules and solid-gas interface physics

Cathy Milostan, Market & Technology Development Analyst
Expert in techno-economic analysis, market assessment, and business development.
- Will work with team on TEA and with Dr. Muehleisen on finding investment and industry partners

Dr. Jonathan Logan, Alcorix Co.
Expert in nanomaterial fabrication
- Will work Dr. Pellin on sample fabrication and with C. Milostan on TEA

Current Team Gaps:
- Molecular Engineering, Manufacturing Engineering

We plan to fill these gaps by consulting with researchers at the Materials Engineering Research Facility (MERF) in the Advanced Materials Division at Argonne and a Technical Advisory Group

Challenge

Problem: Heating and cooling energy lost through walls, roofs, and foundations accounts for 51% (5.7 Quad) of all building HVAC energy and 17% of all the building energy use in the US, at a cost of over $100B per year.

Current insulators: Limited heat blocking capability and long term stability problems; difficulty in using in retrofits

Current superinsulators (VIP and Aerogels) : Limited by cost and durability

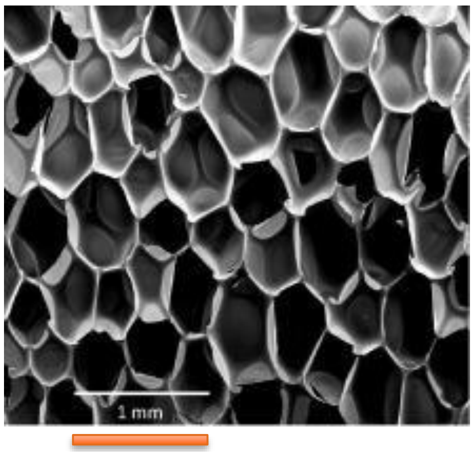
All current insulator: Static performance

Need: A dynamic superinsulator that has much better cost, weight, durability and retrofit integration than currently available

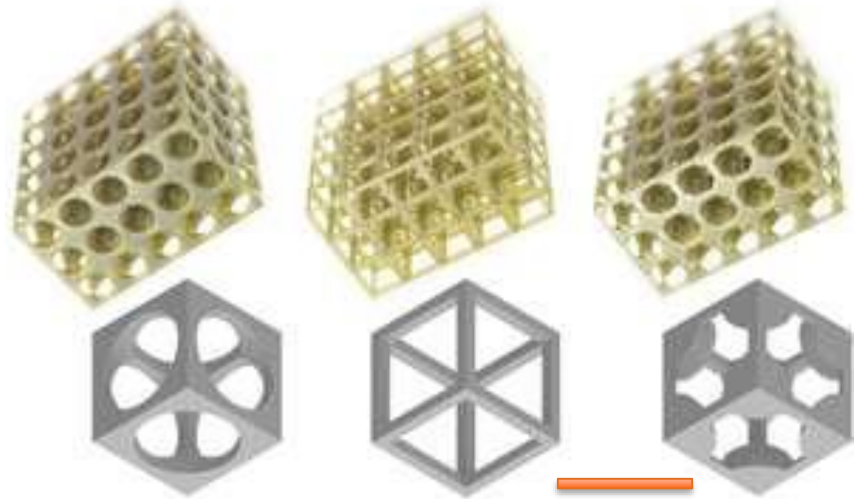
Our Solution: DPM. 2.5x better price/performance than current foams with better durability and long term stability and dynamic capabilities

Approach: Dynamic Phononic Metamaterial (DPM)

- Create a nanostructured porous polymer with metamaterial properties to dramatically decrease heat transfer, increase strength, and possibly allow dynamic operation. High R/in allows for better retrofit integration.
- Develop a low cost, high yield manufacturing process



1mm



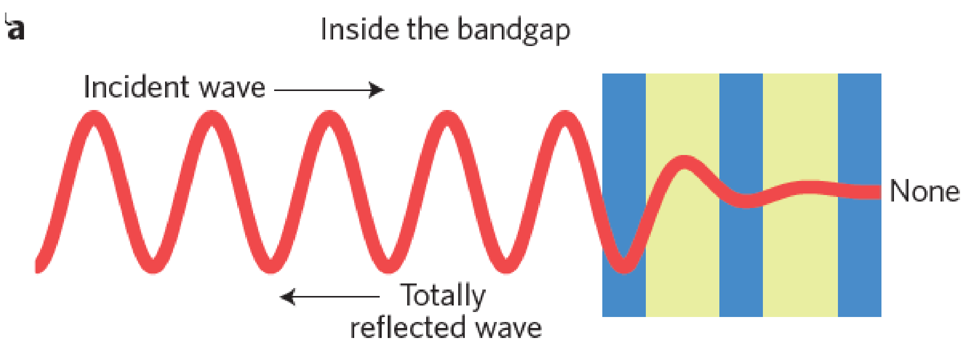
100 nm

Typical polyiso foam insulator – 100’s of μm sized pores.

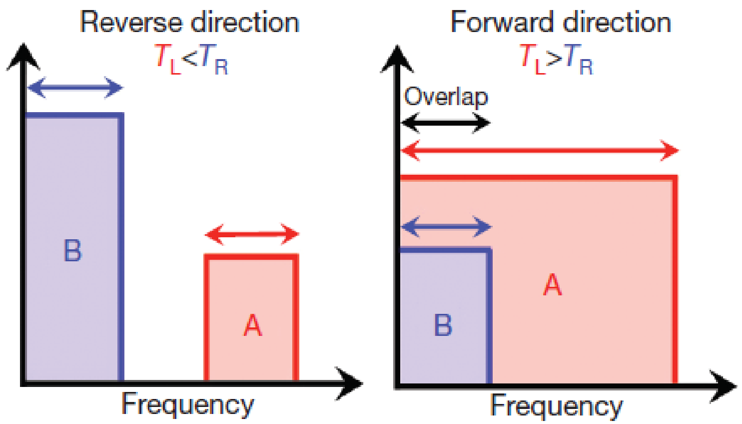
Nanostructure has <100 nm sized pores and periodic structure to reduce heat transfer further through phonon interference. Dynamic properties arise through careful design of temperature sensitive phononic spectra

Approach – How Does This Work?

- Heat Xfer in non-metallic solids is through molecular vibration (phonons)
- With careful design, periodic variations in structure can create destructive interference of phonons and shape changes can block phonon transfer
- With even more careful design, the blocking can be made temperature dependent and allow heat transfer at the right temperatures creating a thermal diode that lets heat flow at some conditions



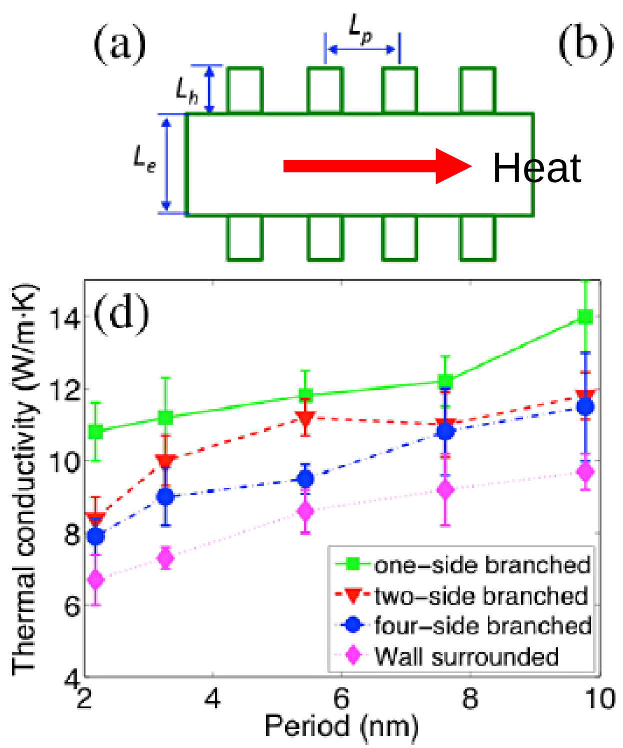
Maldovan. *Nature Materials* **14**, 667–674 (2015).



Maldovan, M. *Nature* **503**, 209–217 (2013).

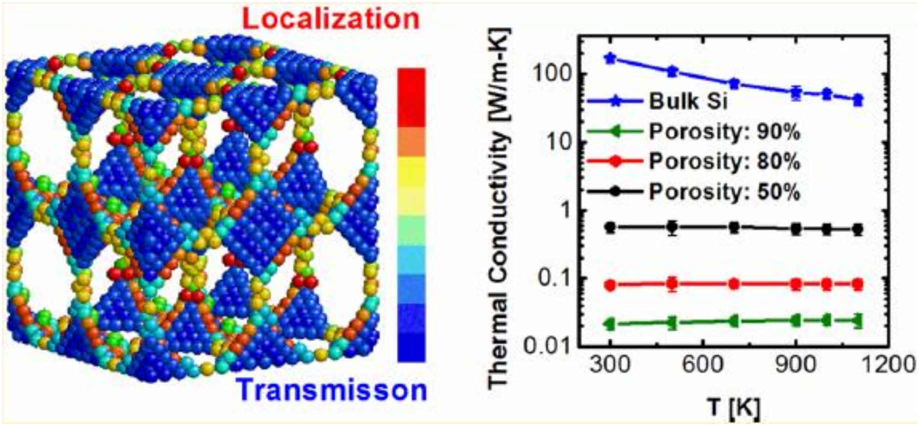
Approach – How Does This Work?

- 1D/2D geometry that reduces heat xfer purely through phononic interference

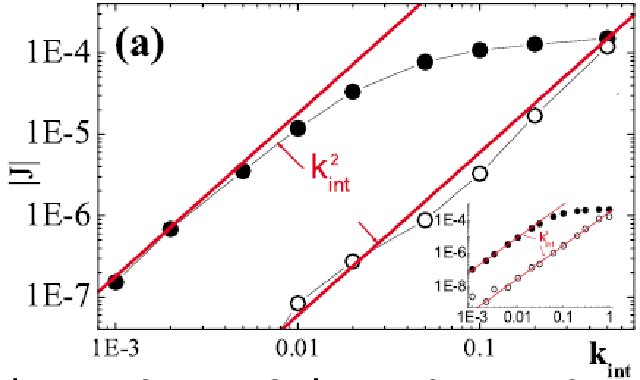


Xiong, S. *et al. Phys. Rev. Lett.* **117**, 025503 (2016).

- 3D geometry that reduces heat xfer through phononic interference and porosity

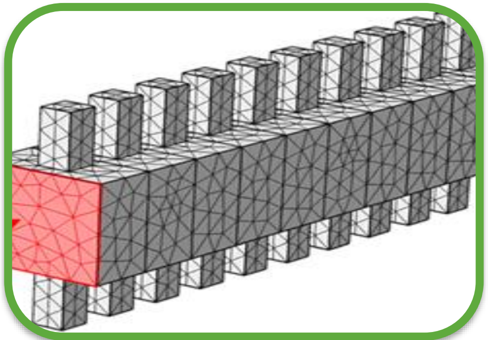


Yang, L. *et al. Nano Letters* **14**, 1734–1738 (2014).

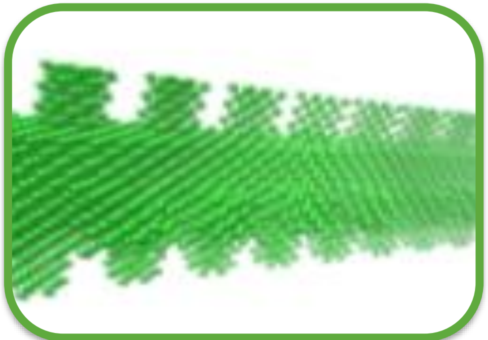


Chang, C. W., *Science* **314**, 1121–1124 (2006).

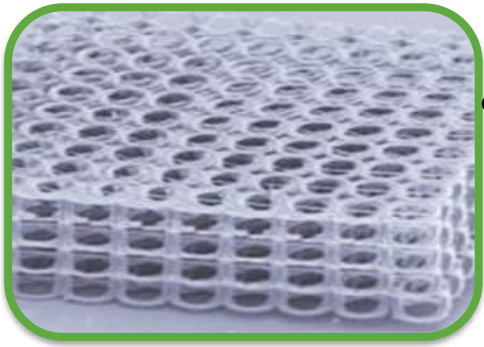
Approach – How Will We Do It?



- AI Assisted Design Space Exploration with COMSOL FEM



- Detail Optimization using LAMMPS Molecular Dynamics Simulation on HPC

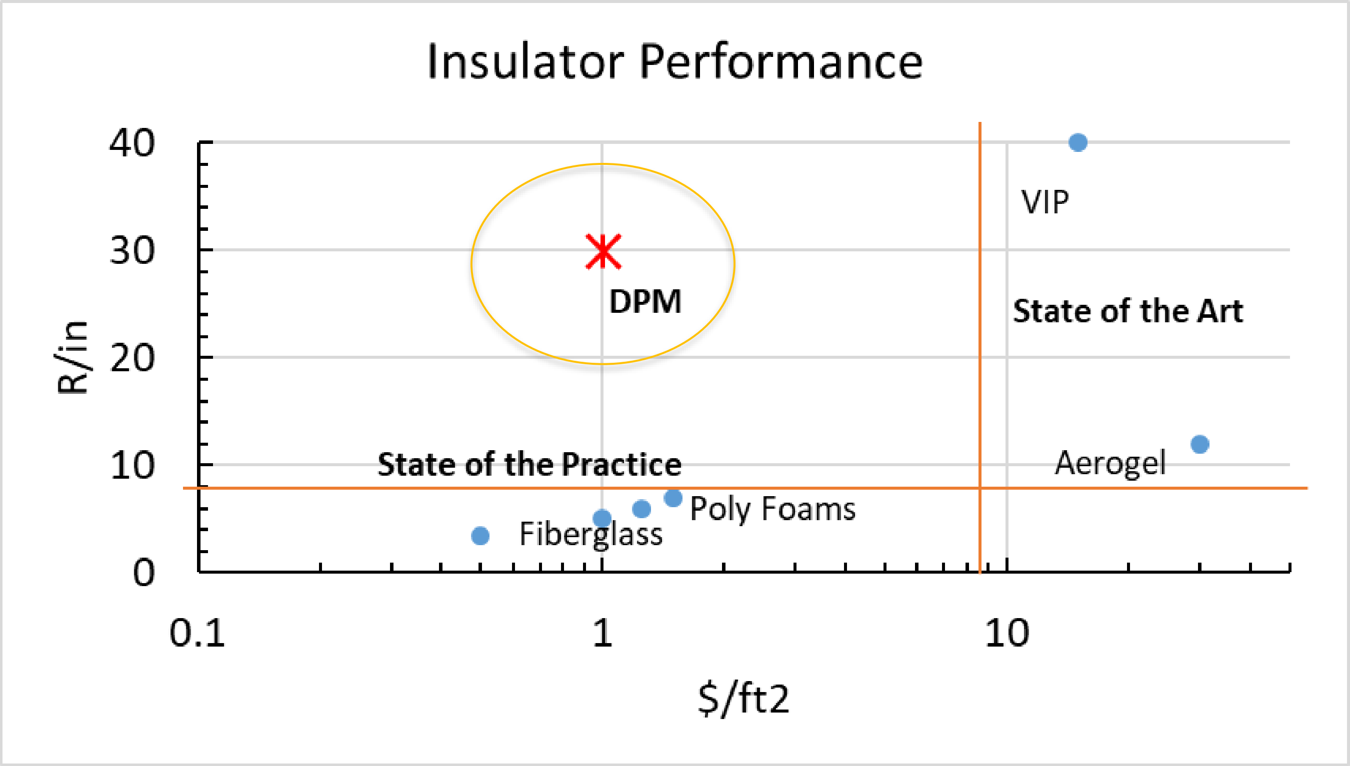


- Fabricate & Measure Candidate

Impact

BTO Goals are for increased performance including:

- High R, strength, durability, and easier integration into retrofits (highly insulating sheathing and siding)



Progress: Computer Aided Literature Review

Project is Very Early Stage, High Risk, Fundamental Research in a new area for Buildings

- **Scanned 500+ papers, collected over 150+ papers in shared database**

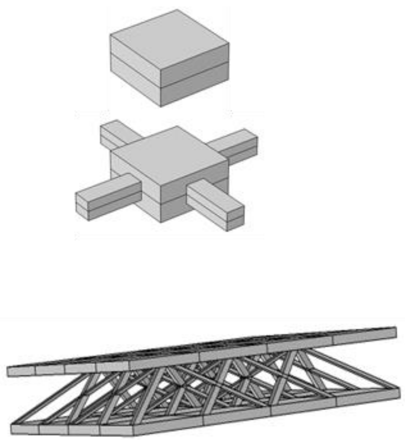
First Goal: Identifying Key Nanoscale Research	Second Goal: Defining material design space
• Phonon Propagation Modeling • Heat Transfer at Solid-Gas interface • Self-Assembly	• Selecting Target Materials • Selecting Target Structures

Key takeaways

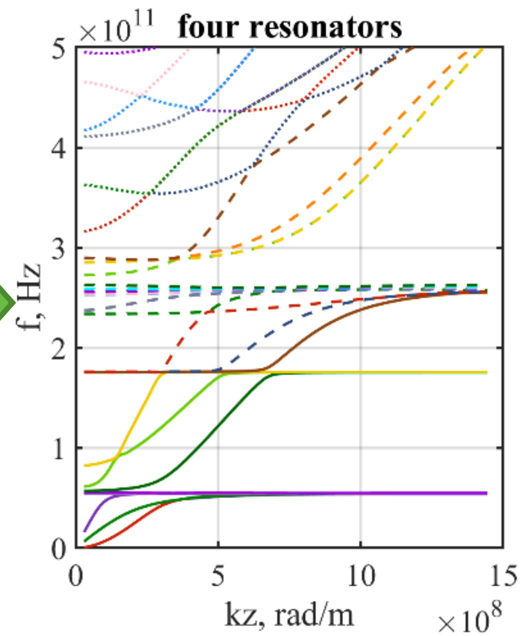
- **PMMA, PEG, SiO_2 are good target materials**
- **Periodic Slabs (2-D Structures)**
  - Self-Assembly Easier but low porosity & High Material Costs
- **3D Structures**
  - Self Assembly Harder but high porosity & lower material costs

Progress: COMSOL FEM

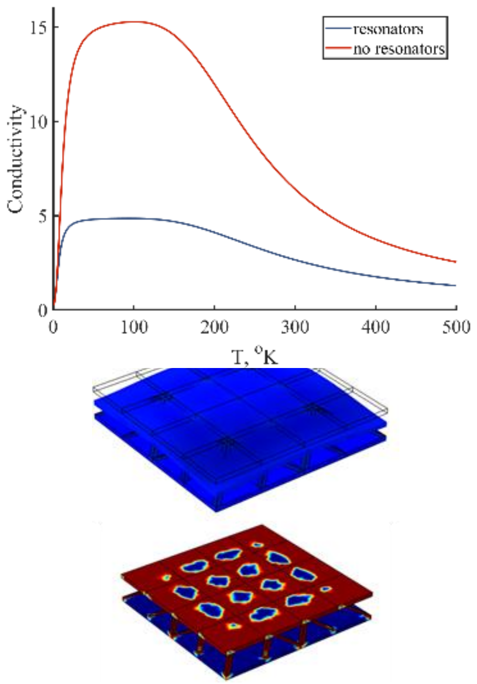
- Developing FEM Models to Compute Phonon Spectra and Scripts/Tools for Converting Spectra to Conductivity



Geometry



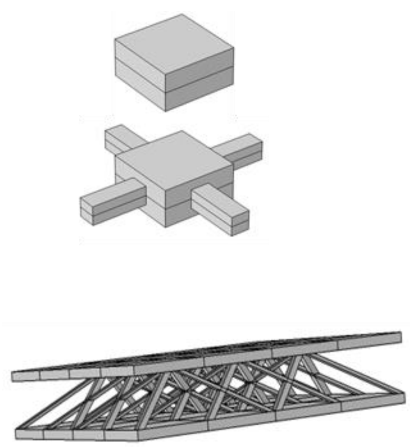
Spectra

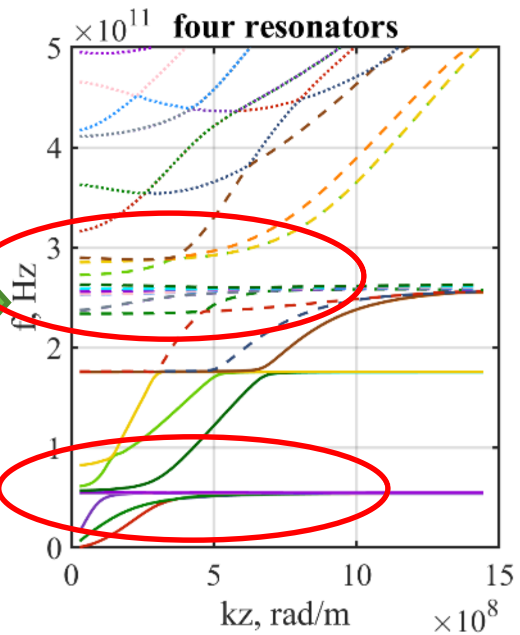


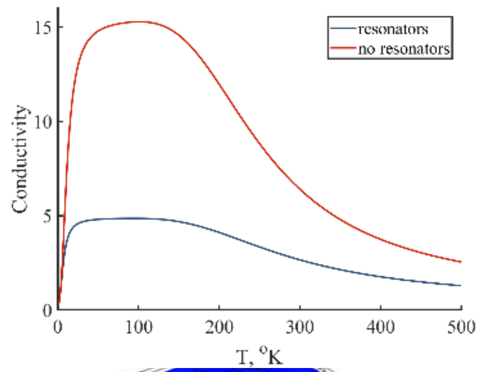
Therm. Cond. and Strength

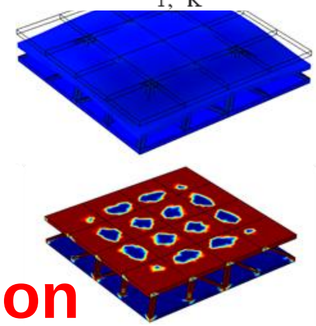
Progress: COMSOL FEM

- Developing FEM Models to Compute Phonon Spectra and Scripts/Tools for Converting Spectra to Conductivity









Band Gaps = Reduced Conduction

Geometry

Spectra

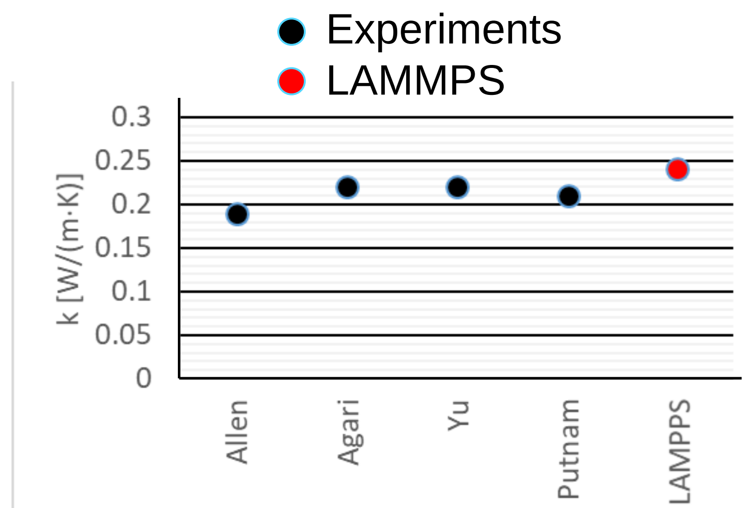
Conductivity and Strength

Progress: Molecular Dynamics Simulation

- **Using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) for high fidelity simulation**
- **Hired postdoc early in Q2, developing LAMMPS workflow**
  - Over 300,000 core hours of LAMMPS code on Bebop in Q2 alone
- **Accurately computed bulk conductivity for PMMA as a check to ensure we had valid potential functions and atom packing geometry**

Bebop: 1.5 PF HPC

K for PMMA @ 300K



Stakeholder Engagement

Early Stage Project: High Risk – Limited Scope

- Assembling a Technical Advisory Group (TAG)
  - Assess both high level process and specific design choices
  - Team includes researchers and industry that have developed phononic and photonic metamaterials for other applications
  - Advise and plan follow-on if this project is successful

- Already talking with several R&D Investment Firms and Industry
  - Investors focused on augmenting early stage R&D to create IP
    - IP Group, Osage Partners, Shultz Innovation Fund
  - Industry focused on scalability and ability to license IP or collaborate through CRADA (limited conversations for IP security reasons)
    - 3M, DOW, USG, Johns Manville, Alcorix (nanomaterial startup)

Remaining Project Work

<u>Q3 and Q4 (Project scheduled to end in Q4)</u>

- **At least 2 TAG Meetings**
- **Begin Securing IP (filing patents)**
- **Begin AI assisted design optimization using FEM**
  - Find at least 1 design capable of *k* < 0.005 W/(m·K) (R28/in)
- **Refining calculation and verifying FEM configuration using LAMMPS**
  - Confirm at least 1 design capable of *k* < 0.01 W/(m·K) (R14/in)
- **Fabricate potential designs using 3-D 2 photon printing or other method**
  - Fabricate at least 1 design with *k* reduction of 80% of bulk material k

<u>Follow On Work (With additional BTO funding and/or Industry Partners)</u>

- **Continue Design Optimization to reach R > 30/in with increased strength**
- **Develop variations that provide dynamic performance Develop self-assembly process using block copolymers**
- **Strength and Durability Testing**

Thank You

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Ralph T. Muehleisen
(630) 252-2547, rmuehleisen@anl.gov

REFERENCE SLIDES

Project Budget

Project Budget: $500K FY19 (New 1 year project)
Variances: No budget variances
Cost to Date:180K (spending rate picking up after recent hiring)
Additional Funding: None

Budget History					
FY 2018 (past)		FY 2019 (current)		FY 2020 – (planned)	
DOE	Cost-share	DOE	Cost-share	DOE	Cost-share
-	-	500K	-	-	-

Project Plan and Schedule

Project Schedule									
Project Start: 10-1-2018		Completed Work							
Projected End: 9-30-2019		Active Task (in progress work)							
		Milestone/Deliverable (Originally Planr							
		Milestone/Deliverable (Actual)							
	FY2013				FY2014				
Task	Q1 (Oct-Dec)	Q2 (Jan-Mar)	Q3 (Apr-Jun)	Q4 (Jul-Sep)	Q1 (Oct-Dec)	Q2 (Jan-Mar)	Q3 (Apr-Jun)	Q4 (Jul-Sep)	
Past Work									
Experimental Designs Reviewed by TAG									
Identify 3 materials & Structures with potential to meet thermal requirements and amenable to self assembly									
Current/Future Work									
Simulate at leat 1 material + structure meeting k=0.005 with FEM									
Simulate at least 1 material meeting K=0.01 using molecular dynamics									
Fabricate at least one material with a reduction in conductivity of at least 5x									