DOE Award # 118660 / DE-SC0004624 and DE-FG02 - 10ER46720

Date of Report: November 27, 2013 (Final Submission July 9, 2015)

Period Covered by Report: October 18, 2010 – June 30, 2013

Title of Project: Manipulation of Phonons with Phononic Crystals

Approved Budget: 585,253 USD

Principal Investigator:

Zayd Chad Leseman

Associate Professor of Mechanical Engineering

National Laboratory Collaborator:

Ihab El-Kady

Principal Member of Technical Staff – Sandia National Laboratories

Project Goals

There were three research goals associated with this project. First, was to experimentally demonstrate phonon spectrum control at THz frequencies using Phononic Crystals (PnCs), i.e. demonstrate coherent phonon scattering with PnCs. Second, was to experimentally demonstrate analog PnC circuitry components at GHz frequencies. The final research goal was to gain a fundamental understanding of phonon interaction using computational methods. As a result of this work, 7 journal papers have been published, 1 patent awarded, 14 conference presentations given, 4 conference publications, and 2 poster presentations given. Note that this report was submitted more than 2 years after the project's end date due to Sandia National Laboratories holding the report form 'unlimited' submission until the final publication was published – Ref. 7, the Nature Communications article.

Papers Generated as a Result of this Work

Published

1. D. F. Goettler, M. F. Su, C. M. Reinke, S. Alaie, P. E. Hopkins, R. H. Olsson III, I. El-Kady, and Z. C. Leseman, *Realization of a 33 GHz Phononic Crystal Fabricated in a Freestanding Membrane*, *AIP Advances.* **1**, 042001 (2011).
2. C. M. Reinke, M. F. Su, B. L. Davis, B. Kim, M. I. Hussein, Z. C. Leseman, R. H. Olsson, I. and El-Kady, "Thermal conductivity prediction of nanoscale phononic crystal slabs using a hybrid lattice dynamics-continuum mechanics technique," *AIP Advances* 1, 042001, 2011.
3. S. Alaie, M. F. Su, D. F. Goettler, I. El-Kady, and Z. C. Leseman, "Effects of flexural and extensional excitation modes on the transmission spectrum of phononic crystals operating at gigahertz frequencies," *J. Appl. Phys.*, vol. 113, no. 10, p. 103513, 2013.
4. Alaie, S., Goettler, D. F., Abbas, K., Su, M. F., Reinke, C. M. El-Kady, I., & Leseman, Z. C. (2013). Microfabricated Suspended Island Platform for the Measurement of In-Plane Thermal Conductivity of Thin Films and Nanostructured Materials with Consideration of Contact Resistance. *Review of Scientific Instruments, 84, 105003, 2013.*
5. Abbas, K., Mousavi, A. K., Elahi, M. M., Lima, E., Moya, S., Butner, J. D., Pinon, D., Benga, A., Mousavi, B. K., and Leseman, Z. C., Vacuum, revision submitted (2014).
6. S. Alaie, D. F. Goettler, Y.-B. Jiang, K. Abbas, M. G. Baboly, D. H. Anjum, S. Chaieb, and Z. C. Leseman, "Thermal conductivity and nanocrystalline structure of platinum deposited by focused ion beam," *Nanotechnology*, vol. 26, no. 8, p. 085704, 2015.
7. S. Alaie, D. F. Goettler, M. F. Su, Z. C. Leseman, C. M. Reinke, and I. F. El-Kady, "Thermal Transport in Phononic Crystals and the Observation of Coherent Phonon Scattering at Room Temperature," *Nat. Commun.*, 6:7228 doi: 10.1038/ncomms8228, 2015.

Example Excerpt from Acknowledgments Sections:

"This work was supported by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering Experimental Program to Stimulate Competitive Research (EPRSCoR) under Contract No. DE - FG02 - 10ER46720."

Demonstrate Phonon Spectrum Control at THz Frequencies Using Phononic Crystals

In order to demonstrate phonon control at THz frequencies we chose to use Phononic Crystals, which have a periodic spacing of air holes in Si. This is the first experimental evidence (reinforced by major theoretical development) proving that phonons can indeed undergo substantial coherent scattering at room temperature! The platform for our study is based on PnCs. By undertaking this effort we delved into the controversy surrounding the ability of PnCs with relatively large (>100 nm) features to influence the propagation of the high frequency phonons dominant in room-temperature thermal transport. The ability of a PnC to coherently influence a phonon population depends on whether or not that population remains coherent as it traverses the lattice. With minimum features sizes ≥100nm, the claim of coherent phonon scattering in PnCs at room temperature has generated widespread controversy. Since the major portion of phonon thermal conductivity is carried by phonons with wavelengths as small as tens of nanometers, it is questionable whether such phonons can traverse the comparatively widely spaced PnC lattice while maintaining coherence to be influenced by the topology of the arrangement.

To delaminate incoherent from coherent scattering, we proposed a first-of-its-kind experiment that holds the contribution of incoherent boundary scattering constant and varies only the coherent component. Our results are supported by extensive modeling, and yield conclusive evidence that significant coherent phonon scattering does indeed take place in these PnC structures at room temperature.

This effort occurred in three main stages: (1) creating the PnCs, (2) measuring the PnCs, and (3) validating results with a computational model. In order to create the PnCs a novel method was developed that utilized a focused ion beam (FIB) in order to pattern air holes in Si. In this method a protective metal coats the PnC substrate to protect it from incoming Ga ions from the FIB. The protective layer is later removed in a vapor etch in order to avoid stiction failure of the samples, see Fig. 1.

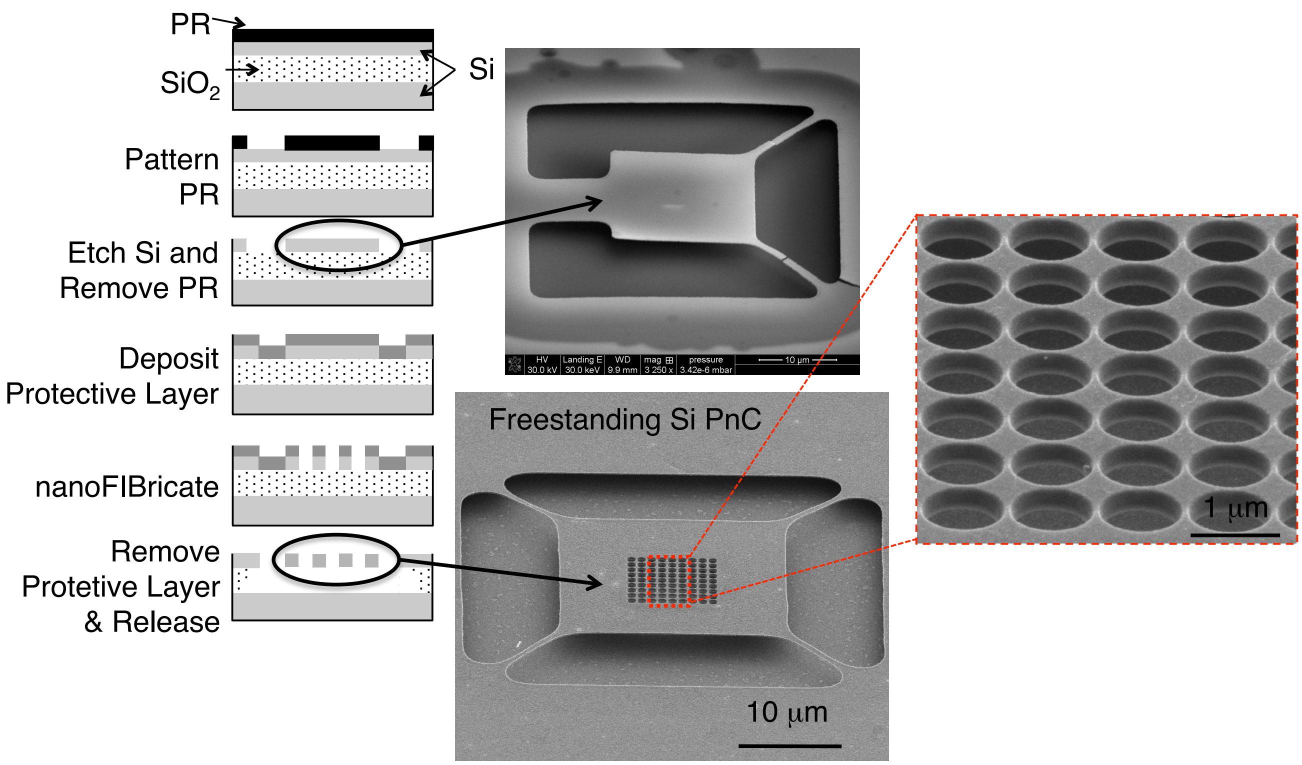

Fig. 1: Process flow for the creation of PnCs for this work.

Measuring the thermal conductivity of the PnCs was the next challenge. In order to undertake this effort a new method for measurement of nanostructured materials was developed. In order to reach this stage two enabling technologies were also developed and they are contained in the submitted publications marked 5 and 6 in the above list. The core idea is place a PnC sample between a hot and cold island and measure the thermal transport across the PnC, see Fig. 2. The difficulty in making this type of measurement, however, comes when one takes into account the thermal resistance introduced by 'placing' the sample using a FIB. This error needs to be quantified.

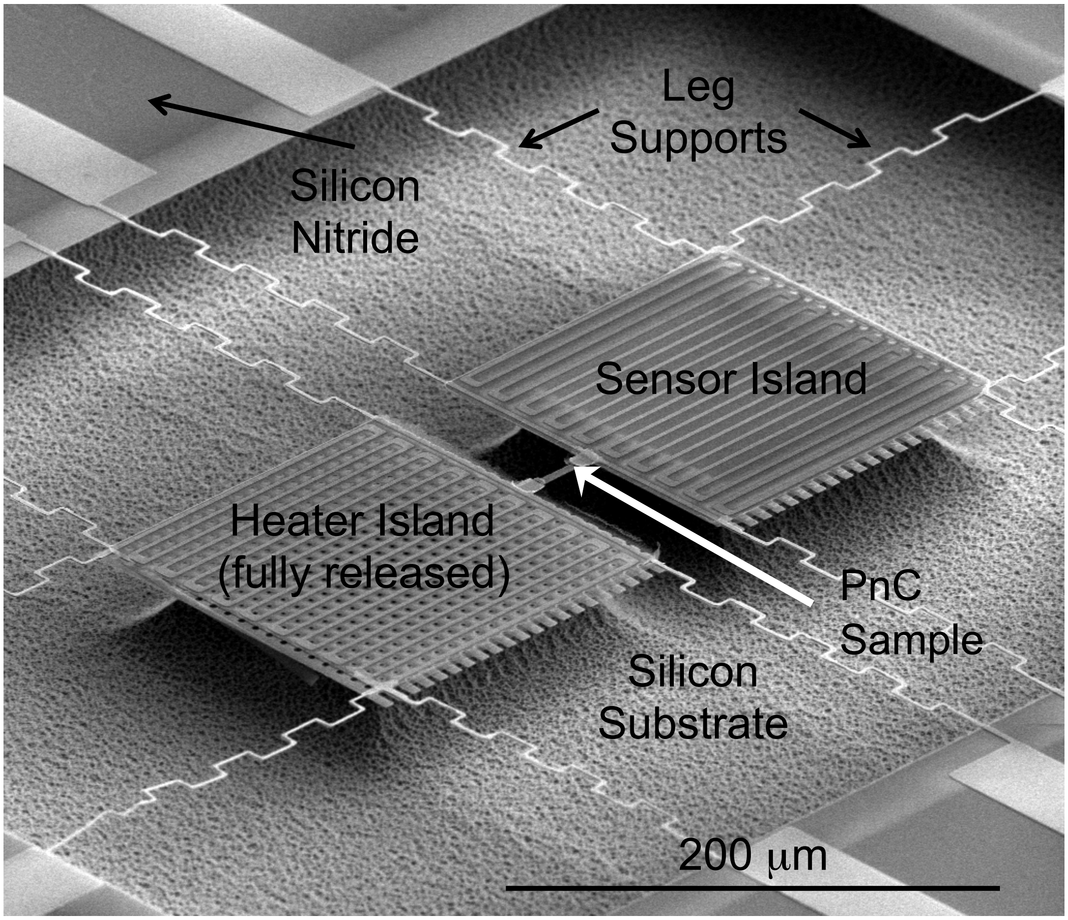

Fig. 2: SEM image of the measurement platforms used in this work.

In order to quantify this error a systematic technique was developed. Using systematic steps for measurements, the characterization of the thermal resistances of a sample and its contacts are studied, see Fig. 3. The calibration of the contacts in this method is independent of the geometry, size, materials and uniformity of contacts. To verify the technique, two different Si samples with different thicknesses and two samples of the same SiN_x wafer are characterized on a single device. One of the Si samples is also characterized by another technique, which verifies the current results.

Characterization of the two SiN_x samples taken from the same wafer showed less than 1% difference in the measured thermal conductivities, indicating the precision of the method. Additionally, one of the SiN_x samples is characterized and then demounted, remounted, and characterized for a second time. The comparison showed the change in the thermal resistance of the contact in multiple measurements could be as small as 0.2 K/μW, if a similar sample is used. Using this technique all error can be taken into account in order to measure the thermal conductivity of the PnCs.

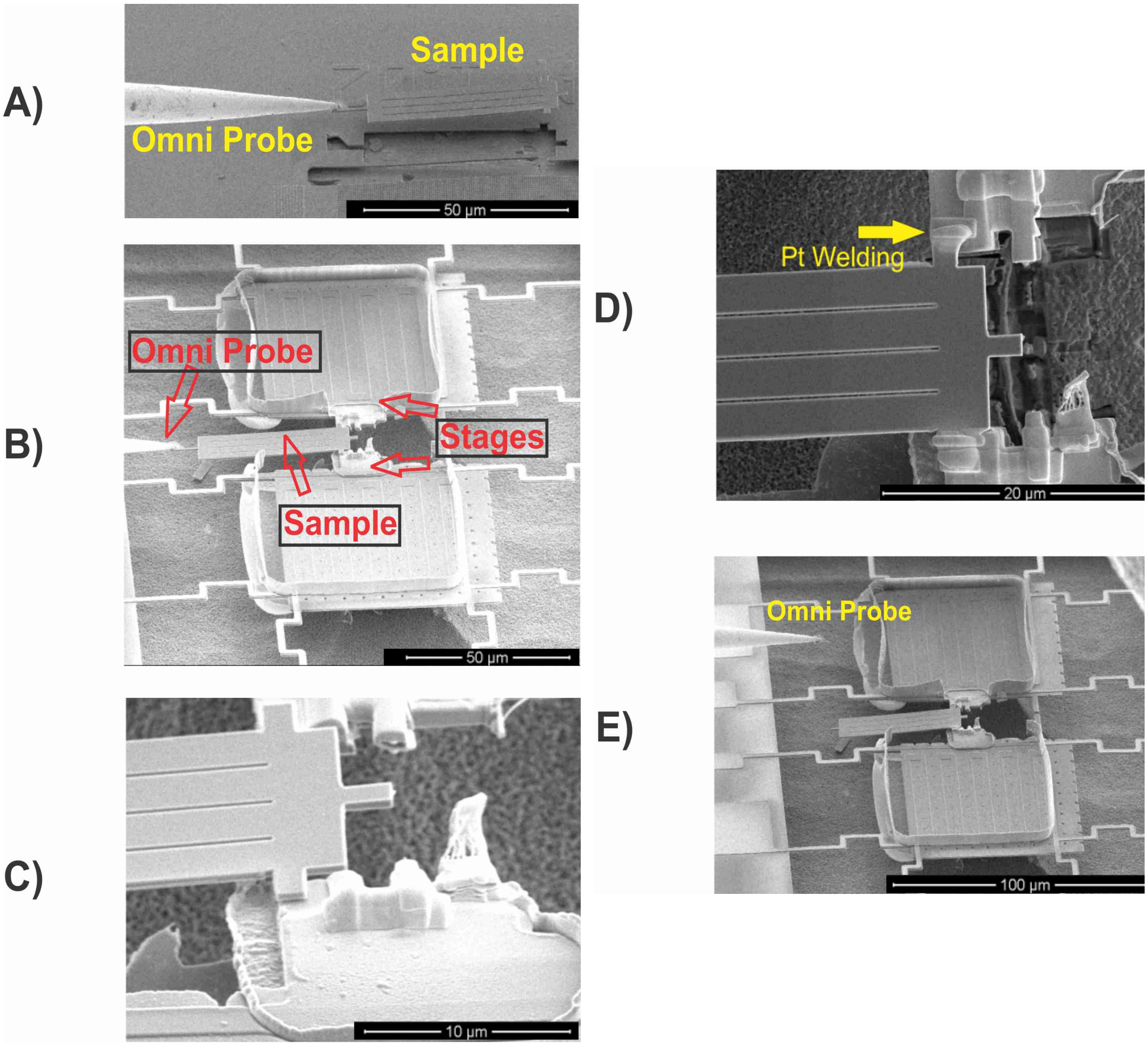

Fig. 3: SEM images of the subsequent steps for characterization of nanomaterials.

In order to study the effect of coherent scattering PnCs a design was developed for the PnC's unit cells that fixed the incoherent scattering strength yet allows for varying of the coherent scattering component. By introducing a small hole into a square lattice of circular holes one can create a set of supercells for which there is a constant critical length, Lc, see Fig. 4. In this way, the coherent scattering will vary due to Brillouin Zone Folding.

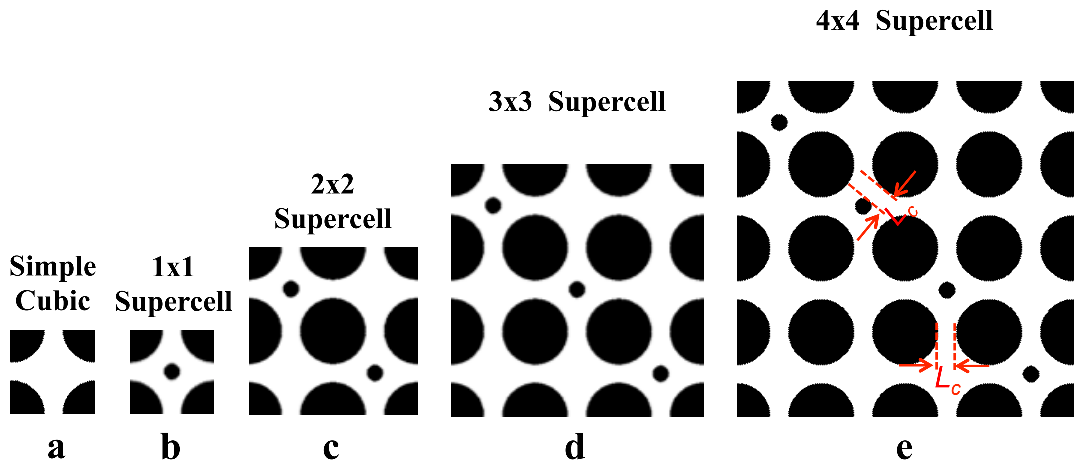

Fig. 4: Schematic of the unit cells used in this work. L_c is fixed at 250 nm.

Figure 5 shows the measurements made on all five samples made in this work. The thermal conductivities of the supercells are normalized to the thermal conductivity of the simple cubic (SC) lattice. There is only a small variation, a few percent, in the amount of porosity of the samples. Due to this porosity change there should be a small change in the thermal conductivity of the samples according to continuum models that take into account porosity. However we found that there is an additional reduction of ~10% to the thermal conductivity of the 1x1 supercell at room temperature. This difference is attributed to coherent scattering of phonons and is the subject of an article published in Nature Communications.

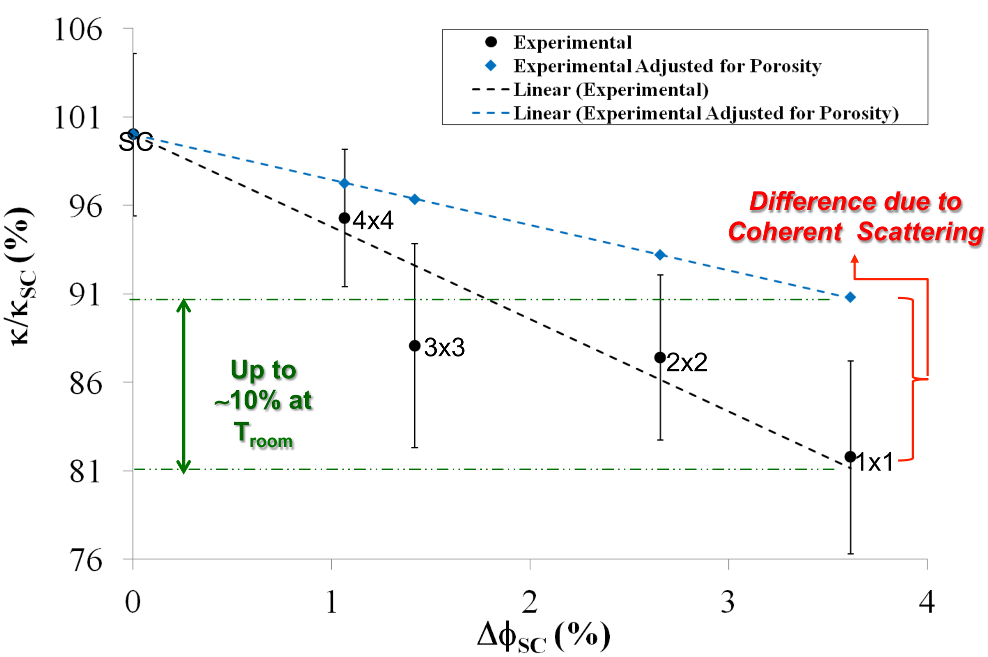

Fig. 5: Data taken for the PnC supercells in Figure 4.

Demonstrate Analog PnC Circuitry Components at GHz Frequencies

During the grant we have managed to model, design, fabricate and test several PnC circuitry components that operate at GHz frequencies. Firstly, the models were developed in finite difference time domain codes and finite element codes (more detail are available in next section on modeling). Then all designs were transferred into computer aided drafting packages and then fabricated at Sandia National Laboratories, the partner lab for this project. All PnC logic structures were modeled and fabricated as mentioned in the proposal, see Fig. 6.

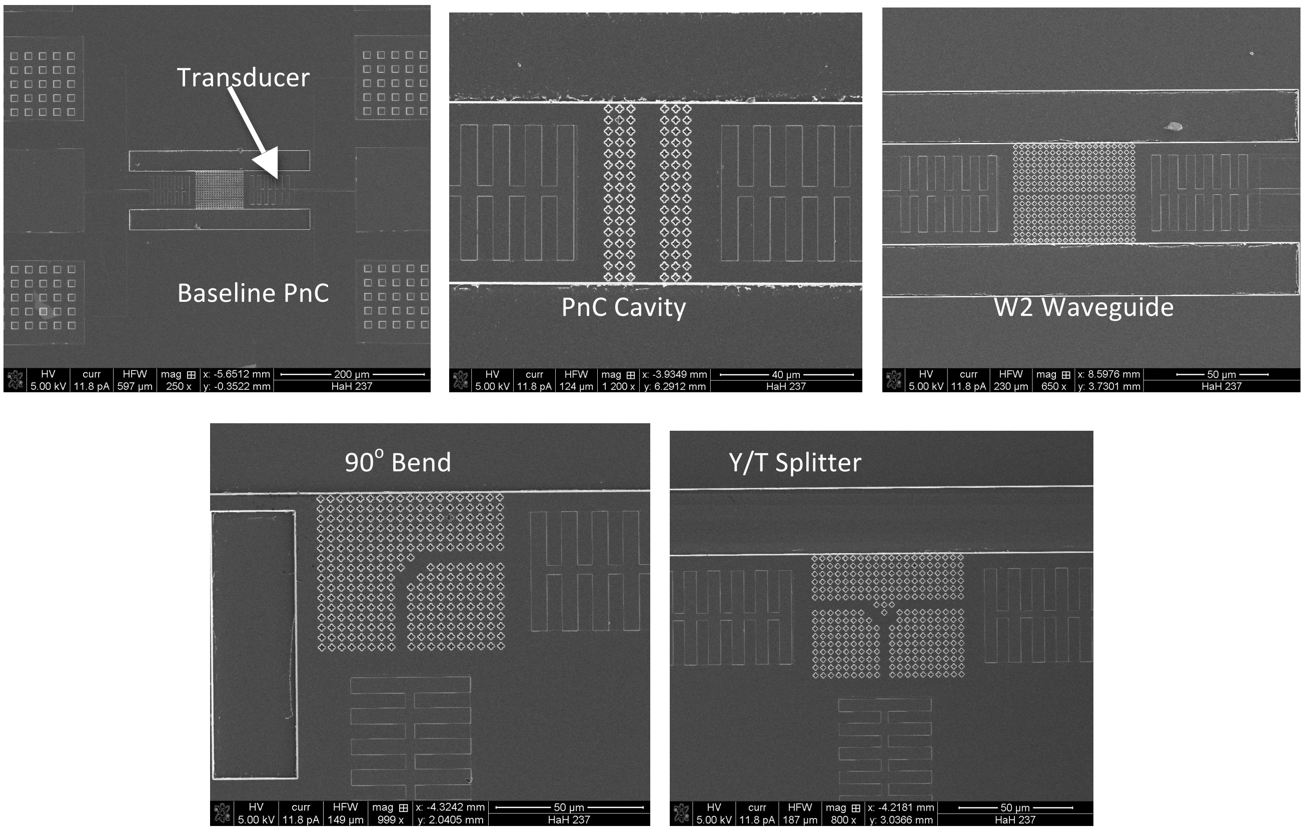

Fig. 6: SEM images of GHz Pnc structures fabricated in this work: Top from left to right – baseline PnC, PnC Cavity, PnC W2 Waveguide; Bottom from left to right – 90^o bend and a T/Y Splitter

Fabricated structures were received from Sandia in the summer of 2013. Unfortunately, there were many unforeseen delays in the fabrication run which allowed us to only have one iteration of devices. Geometries of the small feature sizes (750 nm) did not transfer correctly during fabrication. However, the baseline PnC and slab devices did work and produced a bandgap at 1.15 GHz as seen in Fig. 7. However, due to the altered geometry during fabrication the other devices are not working as predicted. Though this project is over, through further collaboration with Sandia, another fabrication run will be undertaken to correct these issues and have all PnC logic components work properly.

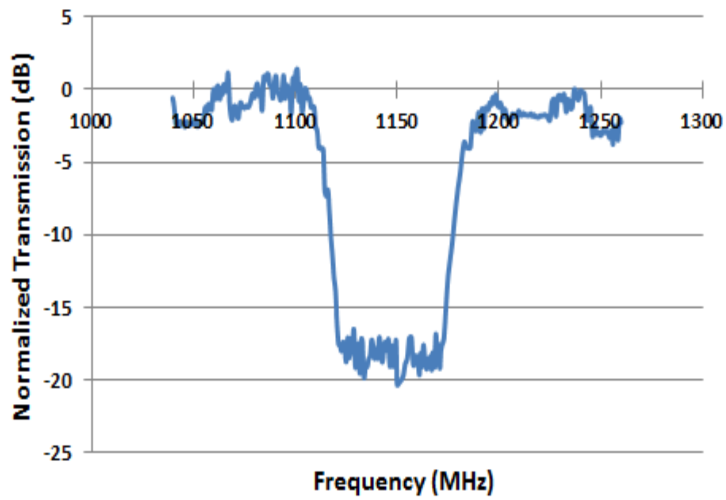

Fig. 7: Demonstration of a phononic bandgap for the device in the upper left hand corner of Fig. 6

Using Computational Methods to Determine Phonon Interactions

In order to model the thermal conductivity of the PnCs that show phonon spectrum control we formulated and implemented a hybrid method that augments the Callaway-Holland model for the analysis of the thermal conductivity of finite-thickness PnC devices. The technique involves an atomistic approach at the bulk material level combined with the application of Bloch theory at the continuum level. The lattice dynamics technique is used for the atomistic modeling and the 3-D plane-wave expansion (PWE) method is used to calculate PnC dispersion relations and density of states (DOS) at the continuum level. Finally, the Callaway-Holland model is employed for thermal conductivity prediction. The theoretical results thus obtained were compared with experimental results from samples fabricated in Si with cylindrical air inclusions.

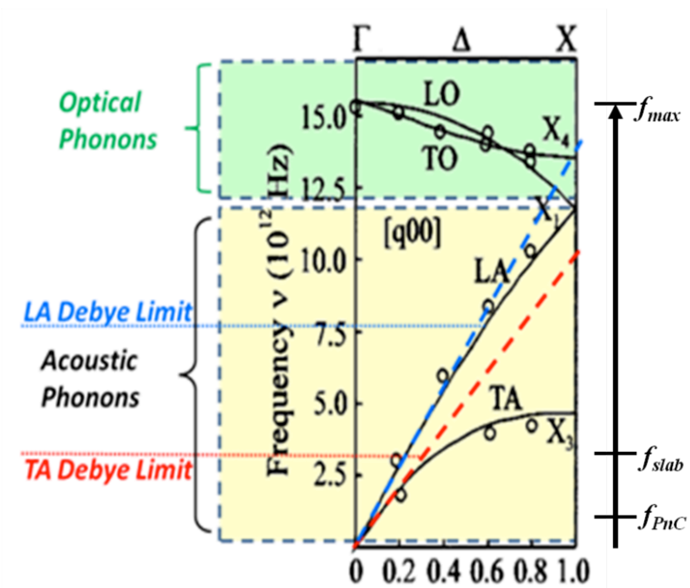

Fig. 8: Phonon dispersion of bulk Si for Γ–X (black curves), along with the corresponding dispersion from the Debye approximation for transverse (red dashed curve) and longitudinal (blue dashed curve) modes.

The Callaway-Holland method combines phonon group velocity, heat capacity, and phonon scattering rates to predict thermal conductivity, and is applicable for materials where the thermal conductivity is dominated by phonon, rather than electron, transport. While all these properties can be obtained from phonon dispersion relations, some approximations are made in practice. For example, the phonon group velocity is approximated as the average speed of sound and Debye approximation (Fig. 8) is used to make the dispersion of the acoustical branches linear and follow the slopes at low wave numbers. For higher wave numbers, the acoustical branches are considered to contribute less to the thermal conductivity due to the flattening of the bands and the resulting lower group velocities, and thus are not considered. For the same reasons, the optical branches are disregarded altogether. An additional result of using the Debye approximation is that the group and phase velocities become interchangeable due to the linearized form of dispersion. While these shortcomings are acceptable in traditional uses of the Callaway-

Holland method, PnC dispersion relations provide more than sufficient number of complications to make the aforementioned approximations inaccurate.

Results from the developed hybrid technique provide an improved understanding of coherent phonon scattering, as well as guidance in the planning of the experimental effort. An example calculation from the paper for a slab of Si and a PnC of similar thickness to the slab is shown in Fig. 9.

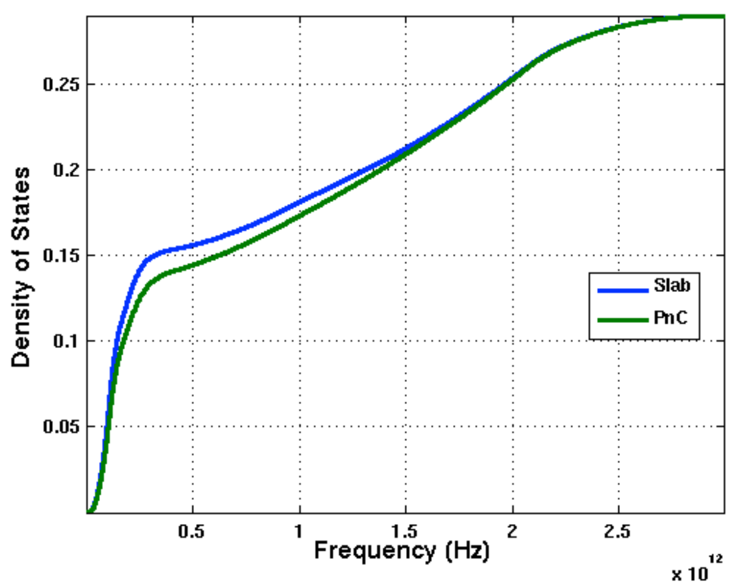

Fig. 9: Integrated density of states for a Si slab of 500 nm thickness and a PnC of the same thickness and with 150 nm radius air holes in a 600 nm lattice.

In order to model GHz frequency responses of PnC and PnC logic-circuitry components Finite Element Models (FEM) and Harmonic Finite Element (HFEM) methods were developed and employed. The former provides phonon dispersion relations, indicating the frequency, polarization and shape of the energy carrying modes sustained by the PnC waveguides and bends, while the latter yields transmittance, reflectance and wave guiding efficiencies. Simulations are performed using COMSOL Multiphysics and ANSYS commercial simulation software bought for this project.

Figure 10 shows a phonon band structure diagram for an AlN/Air design, obtained using COMSOL Multiphysics FEM analysis. The researchers have performed several hundred analyses during the course of this project. This PnC has a periodicity of a = 3 µm, hole radius-to-periodicity ratio of r/a = 0.46 and thickness-to-periodicity ratio of t/a = 0.5. The red-colored curves indicate the propagating modes with evenly symmetric profiles in the out-of-plane transverse direction, while the cyan-colored curves indicate propagating modes with odd symmetry. This distinction allows one to identify which modes are longitudinal, as only the longitudinal modes have even symmetry in the out-of-plane transverse direction. The band gap is visible (marked as a gray rectangle) as a frequency region devoid of propagating modes between 1.06-1.32 GHz. Waveguides and bends operate in the band gap where confinement in PnC occurs due to lack of propagating modes. The material system and designs were eventually implemented into the devices shown in Fig. 6.

A HFEM model for a W2 waveguide based on the previously discussed AlN/Air PnC is shown in Figure 11. This model has the PnC with a waveguide in the center, shown in detail in the figure inset, surrounded by auxiliary structures. The regions marked as D_1 and D_2 are buffer regions used for separation and wave energy measurement. The regions marked as PML have Perfectly Matched Layer absorbers to remove wave energy from the system. Energy is injected from the PML connected to the D_1 region and transmitted to the D_2 region. The profile of a propagating mode is depicted in Figure 5. As seen in the figure, the mode is confined into the waveguide section and propagates within it.

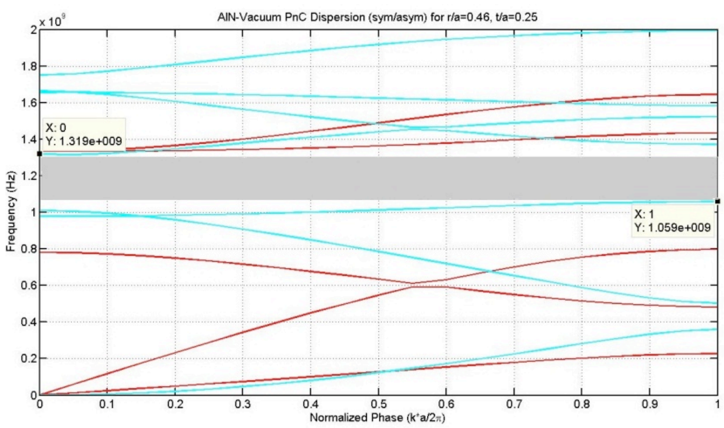

Fig. 10: Band structure diagram for AlN/Air PnC. Gap region is marked as a gray rectangle.

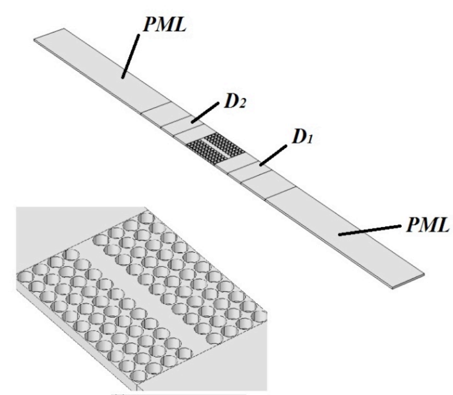

Fig. 11: HFEM model for a W2 PnC waveguide. Inset - the PnC and waveguide in detail.

During the considerable number of simulations run on the GHz PnC circuit components new observations and improvements to existing FEM and HFEM models for PnCs were developed. A summary of these conclusions is contained in Ref. 3. An example of an important observation is that multiple different mode shapes exist and dramatically affect the response of PnCs as is shown in Fig. 12.

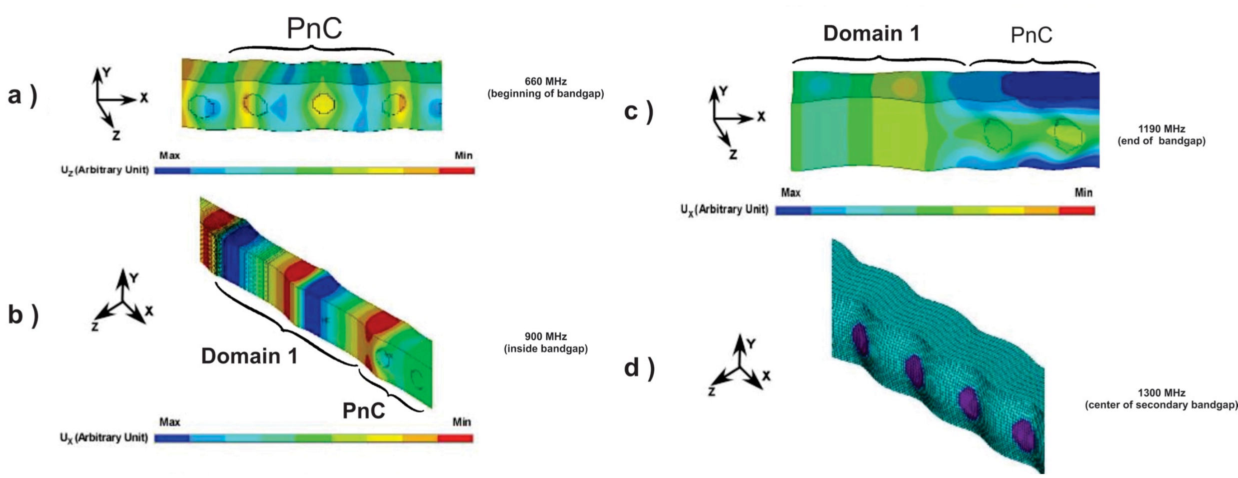

Fig. 12: Vibrational behavior of phononic crystals showing the different mode shapes that occur in a PnC over the frequencies spanning their bandgap.

List of Participants on Project

Person	Position	Approximate Level of Support
Zayd Leseman (PI)	UNM Prof. – Student/Postdoc Advisor	1 summer month per year
Ihab El-Kady	Primary Member of Technical Staff Sandia National Laboratory Partner	0%
Mehmet Su	Postdoc (now Assistant Research Prof.)	40% over 3 years
Hamid Alaie	Ph.D. Student	2.5 years
Khawar Abbas	Ph.D. Student	0.5 year
Drew Goettler	Ph.D. Student	0% (Sandia supported)
Juanita Trevino	Ph.D. Student	0% (Fellowship supported her)
Charles Reinke	Member of Technical Staff (Sandia)	0%

Current and Pending Support

1) Awarded – Agency: Sandia National Labs / Title: Nanotechnology Research / Award: $1,500,000 / ZL's subaward $25k per year for 3 years / Duration: 9/1/2013 – 8/30/2016
    a. Overlap with this DOE Proposal: YES - This collaboration was made possible due to the techniques and equipment developed and purchased with funding from this DOE proposal.
2) Agency: NSF / CAREER: Phononic Crystals: Theory and Practical Implementation / Award: $410,000 / Duration: 8/1/2011 – 6/30/2016
    a. Overlap with this DOE Proposal: YES – This proposal will also seek to make measurements on PnCs. However, the PnCs created in this proposal are much larger and can ben machined with end mills and as such operate in a much lower frequency range. In particular, this award would develop a heterodyne interferometer that would spatially map the vibrational pattern of GHz PnCs. The NSF effort complements the prior DOE work in that one can see vibrational patterns experimentally rather than infer them from transmission plots like Fig. 7.

Cost Status:

The costs for this project are shown in the subsequent spreadsheet. Total expenditures for this project were on target. Modeling, design, fabrication, and characterization for this project were more expensive than predicted. Reducing the amount of salaries that were paid, in order to make the project come in on budget, offset these increased costs. Approximately 3k USD of over expenditure was absorbed by the PIs discretionary funds.

	Proposed	Actual
	FULL BUDGET	**FULL BUDGET**
Faculty (summer salaries)		
Zayd Leseman	25,003	20,591
Post-Doc / Assistant Research Professor		
Mehmet F. Su	61,818	59,496
Total Post-Doc and Faculty Salaries	86,821	80,087
Graduate Students (stipends)		
Research Assistant (RA)	83,182	54,281
Total Fringe Benefits	26,838	28,176
Total Salaries & Fringe Benefits	196,841	162,543
Other direct costs		
Travel to DOE & Conferences	18,000	15,436
Materials and supplies	17,153	35,789
Workstations and Software	8,000	11,888
Other Res Costs Gen - User Facility Costs and Rental	52,200	69,184
RA Tuition	14,848	9,075
Overexpenditure that was Covered by the PI	0	-3,142
Total Other Direct Costs		
Equipment	129,673	141,168
Total Direct Costs	436,715	441,942
Modified Total Direct Costs	291,250	286,620
Facilities & Administrative Costs	148,537	143,310
Total Requested / Spent	585,252	585,252