Photonic and phononic crystal research at Sandia

Sandia National Laboratories and University of New Mexico

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Quantum, Molecular and High Performance Modeling and Simulation for Devices and Systems (QMHP)

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
Outline

- Sandia missions, capabilities and interests.
- Recent work in photonic and phononic crystals
Sandia’s Institutional Resources

**MESA**
Microsystems and Engineering Sciences Applications

**CCIM**
National Leadership in High Performance Computing

**Information Systems Analysis Center**
Information Assurance & Survivability Assessment Analysis

**Center for Integrated Nanotechnologies**
One Scientific Community Focused on Nanoscience Integration
A U.S. DOE Nanoscale Science Research Center

**Microsystems**
Science, Technology & Components

Providing the foundation for tomorrow’s technologies
The Physical, Chemical & Nano Sciences Center is recognized for its world-class focused research, having significant impact on important national security issues while contributing to Sandia’s missions. Our unique expertise is essential in supporting enduring DOE needs.
Supports Sandia's role as a "Science-Based Engineering" Laboratory

**NNSA Science and Technology Thrust**
- Physical and chemical understanding of NW component operation, aging, failure mechanisms, and response to radiation exposure.

**Collective Hierarchical Systems Thrust**
- The study and simulation of dynamic self-assembly processes and cooperative behaviors in living systems.

**Compound Semiconductor Science and Technology Thrust**
- Advancing semiconductor research in areas such as quantum phenomena, defect physics, materials and device modeling, and heteroepitaxy.

**Nanosciences**
- Explore phenomena that are new and unique at the nanometer length scale, and develop bridges from the nanometer length scale to longer scales.

**Optical Sciences**
- We emphasize innovative work in laser development, nonlinear optics, spectroscopy, remote sensing, and photon - material interactions.
• 96,000-square-foot CINT Core Facility will be a distribution point for researchers best served at smaller “gateways” at LANL and Sandia
• $75.8 million Center — one of five funded nationwide by the Office of Science

Nano-bio-micro Interfaces: Import biological principles and functions into artificial bio-mimetic nano- and microsystems.

Nanophotonics and Nanelectronics: Precise control of electronic and photonic wavefunctions to invoke novel and unique properties.

Complex Functional Nanomaterials: Promote complex and collective interactions between individual components in materials to yield emergent properties and functions.

Nanomechanics: Understanding the underlying mechanisms of mechanical behavior of nanoscale materials and structures is the objective of the nanomechanics theme.
Distinguishing Enabler: Tungsten 3-D Fabrication Process

The process is low temperature (CMOS compatible), and can be used to fabricate highly complex structures from dielectrics and tungsten.
Linear ion trap chip micro-fabricated with a metal MEMS process at Sandia National Laboratories. Planar metallic trap electrodes (W overcoated with Au) and a hole through the Si substrate define the trapping region and allow 3D optical access for lasers to ions trapped between RF leads stretched lengthwise over the hole. Control electrodes at the hole edges define seven trapping segments. Air bridge metal leads reduce capacitance and RF dissipation to the substrate.
Photonic crystal research

The Why: insurmountable problems in electronic circuits

- Bandwidth (few GHz) – high inductances from small wire features.
- Thermal issues (fast degradation in performance at elevated temperatures).
- Slow interchip communication and signal synchronization issues limits high speed interchip communications.

An optical solution is needed

Photonic crystal offers a new perspective to these problems:

- Guide and bend light in a unique way.
- Photonic crystal light source such as selective emitter and threshold-less lasers.
- Large density of states at the bandedge can be used to control radiative processes of quantum dot systems.
- Fabrication technologies are compatible to microelectronic tool sets.
**Si 3-D Photonic Lattice Revolutionizing Photonics**

1) Photonic lattices - the optical analogues of semiconductors.

2) Sandia is developing novel Photonic Lattice designs.

3) This enables a high level of control over optical properties.

4) Si processing enables the development of well defined structures.

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**Graphs and Images:**
- Energy vs. Angle (degree) graph showing Photonic Band Gap.
- Transmission vs. Wavelength graph with > 98% attenuation.
- SEM images of photonic lattice structures.
Physics questions:
- Emissivity is a thermodynamical quantity describing equilibrium property of electrons, photons and phonons interacting in a common space.
- In metallic photonic crystal, photons and other entities do not occupy the same space except on the surface.
- It is interesting to study what are the conditions to drive a photonic crystal system out of equilibrium.

Emissivity measurements:
- Temperature of the emitter.
- Detector gain response.
- Detector spectral response.
Spectral intensity response

- Detector response is non-linear.
- Cubic fit the detector response for each wavelength (1490 points).
- The actual intensity for each wavelength (1490 of them) is determined by solving the cubic equation.

\[ y = 0.2257x^3 - 0.8533x^2 + 1.8869x + 0.0133 \]

\[ R^2 = 0.9998 \]
Thermal analysis

Silicon thickness = 653 um

- Heat loss from the silicon is by radiation with emissivity in accordance to its temperature.
- Use room temperature thermal conductivity.

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<tr>
<th>Heater block temp [K]</th>
<th>Emissivity</th>
<th>Top center temp [K]</th>
<th>Top center temp averaged over 2mm [K]</th>
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Emissivity measurements of photonic crystal

Uncoupled model

Without temperature correction
Harvesting multi-exciton energies with photonic crystal

Solar source to excite multi-exciton states

Multi-excitons in quantum dots

Solar cell tuned to single exciton energy

Use photonic crystal to enhance emission

Multiple-exciton energy conversion

One photon yields three e^- - h^+ pairs

1st e^- energy level

1st h^+ energy level

Quantum Dot (QD)

QD Energy Levels

Use photonic crystal to enhance emission

Photocell

1S_s

1S_h

0.8 eV for PbSe QD

Quadexciton Triexciton Biexciton

Single exciton
Quantum information processing requires non-classical light (single photon source).

**Coupling parameter** $g = (\text{Rabi Frequency})(\text{interaction time})$

**Critical atom number** $n_0 = \frac{4}{3}(\text{radiative lifetime})(\text{dephasing time})/(\text{Rabi Frequency})^2$

**Critical photon number** $N_0 = 2(\text{radiative lifetime})(\text{cavity lifetime})/(\text{Rabi Frequency})^2$

**Requirements**
- $g \sim \text{dipole moment} > 1$
- $n_0 \sim V << 1$
- $N_0 \sim V/Q << 1$

- Quantum dot acts like an atom.
- Photonic crystals provide high Q and small mode volume.
- Ideal system to study radiative control and dephasing processes.

**Single photon source and photonic crystal**
What about phonon control?
Acoustic Bandgap Crystals: Why, What, and How?

Motivation: Telecom (the why):

- Radio/Cellular Operation:
  - Half Duplex
  - Full Duplex: Requires high resolution steep filtering
  - Figure of merit $Q \approx 1000$–$2000$

ASP: Electro-Acoustic Coupling Losses:

Coupling Loss

Signal Power

Analogue Signal Processing:

Cascaded insertion losses imply that once we are in the acoustic domain we would like to remain in...

Why not Digital Signal Processing:

Requires high power at high frequencies.

Low resolution ADC

Acoustic Signal Processing

⇒ ABG’s
**Acoustic Bandgap Crystals:**

**The What**

- **What does this have to do with PBG’s?**
  - Direct analogy between 2D Acoustic (phononic) and photonic crystals.
  - Wealth of Literature on 2D PC that can be used as a first iteration for the design and study of ABG crystal applications.

<table>
<thead>
<tr>
<th><strong>PBG Photons</strong></th>
<th><strong>ABG Phonons</strong></th>
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</thead>
<tbody>
<tr>
<td>2nd order coupled vector equations with 2 polarizations</td>
<td>2nd order coupled Tensor Equations with 3 polarizations</td>
</tr>
<tr>
<td>Light line constraints and ability to couple to free space modes mandates that full control of waves can only be achieved in 3D devices</td>
<td>Mechanical wave nature and low coupling to air modes along with the possibility of vacuum packaging allow for full control using only 2D devices</td>
</tr>
<tr>
<td>No inherent structural resonances. Finite size leads only to evanescent mode issues.</td>
<td>Inherent physical size dependent structural resonances.</td>
</tr>
<tr>
<td>THZ applications require sub-micron length scales</td>
<td>GHZ applications require sub-micron length scales</td>
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<tr>
<td>Inherently linear</td>
<td>Inherently non-linear</td>
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</table>
Acoustic Bandgap Crystals:

Contrast to Photonic Bandgap Crystals

- **ABG = Superposition of Bragg and Mie Scattering:**
  - A cermet topology (disconnected) of high density inclusions in a low density background matrix.
  - Acoustic impedance mismatch between the inclusions and the matrix.
  - A maximization of the gaps is achieved by requiring the ratio of the longitudinal velocity $c_l$ to the shear velocity $c_s$ values in both the matrix and inclusion to be as close to the fundamental limit of a hard scatterer $\sqrt{2}$.

**Challenges:**
- Finding high Q pair systems.
- Compatibility with AlN and Si-processing techniques for integration
- Scaling to um size designs.
Acoustic Bandgap Crystals:

Advantages of ABG Circuitry

**Added Benefits of the Acoustic Domain:**

- High-Q distributed ABG filters at GHz frequencies at significant improvement over current FBAR technologies resulting in new low power radio architectures.
- Integration of multiple components on one chip with little or no losses at a size that is $10^4$-times smaller than current optical or micro-strip technology.
- Allows for distributed circuit techniques that are commonly used in microwave circuit design to be applied to lower frequency systems (such as cell phones and WLAN) using acoustic rather than EM waves.

- Speed of Light = $3 \times 10^8$ m/s
- Speed of Sound in SiO$_2$ = $5.8 \times 10^3$ m/s
- Optical Delay Line of 1 µs = 300 m
- ABG Delay Line of 1 µs = 5.8 mm
- **ABG delay line is 52,000 times smaller than an optical one!**

**Miniature**

- Filters
- Delay Lines
- Phase Shifters
- Acoustic Signal Processing
- Power Combiners/Dividers
**Acoustic Bandgap Crystals:**

**The Path to GHz ABG’s**

**Proposed System:**

- Suspended membrane topology of 2D rod arrays of W ($\rho = 19,300 \text{ kg/m}^3$, $Z = 89 \text{ M} \Omega$) in SiO$_2$ ($\rho = 2,200 \text{ kg/m}^3$, $Z = 13 \text{ M} \Omega$) matrix (both are high Q materials).

- AlN Piezoelectric transducers (allows us to leverage FBAR low insertion loss technologies).

- 1$^{st}$ generation: MHz devices using a 7 Levels Post-CMOS Compatible process.

**Modeling:**

- FDTD algorithm for the temporal integration of the full elastic wave equation that incorporates both Lame coefficients.

- Periodic boundary conditions are used at the edges of the cell along the x and y directions and space is terminated along the z axis (direction of propagation) by Mur’s first order absorbing boundary.

- The time series results collected at the detection point are converted into the frequency domain using the fast Fourier transform.
Acoustic Bandgap Crystals: Theory Versus Experiment

- **Excellent Qualitative Agreement.**

- **Differences due to:**
  - Use of bulk properties in the simulation versus actual measured values of the deposited materials.
  - Theoretical gap appears to be wider, (low frequency end is red-shifted and high frequency end is blue shifted), can be attributed to:
    - Use of lossless materials in model.
    - Infinite size extent in the lateral dimensions.
Acoustic Bandgap Crystals:

Line Defects: Theory v.s. Experiment

![Graphs showing transmission vs. frequency for different guides and modes.](Image)
Proof of Concept and Lessons Learned

- **Phononic Bandgap Recipe.**
- **Possibility of introduction of multiple rejection bands per crystal**
- **Because of low coupling to air modes 2D periodicity is sufficient and we do not need to go for the more complicated 3D structures.**

That’s not all!
**Phonon Taming by Elastic Bandgaps**

- **Idea:**
  - Mold and shape the phonon distribution by artificially changing the density of states.

- **Path:**
  - Create the phonon equivalent of the band theory of solids: Allowed states separated by a phonon gap (forbidden phonon states).

- **Approach:**
  - Superpose Mie resonant scattering by individual scattering centers and Bragg scattering due to their periodic arrangement in a lattice.
  - Requires Mie resonances scattering centers and background matrix to be sufficiently separated by an acoustic impedance mismatch.

[Diagram showing phonon distribution with allowed and forbidden states, and Mie resonances superposition.]
Energy Harvesting Scheme:

1. Engineer Elastic band gap to possess single/multiple rejection bands whose boundaries lie at the desired harvesting frequency.

2. Depleted density of phonon states in the rejection band will force multi-phonon processes to perform up/down frequency conversion allowing phonons to escape in the allowed bands. $\text{Eph}_1 + \text{Eph}_2 \leftrightarrow \text{Eph}_3$

3. Couple lattice to a Piezoelectric material to generate EM radio signal.

4. Cascade crystals of different periods and/or design a single crystal with multiple higher order bands (overtones) to generate discrete multiple communication channels.

Thermal To RF: Energy Harvesting and Passive Tagging

Thermal phonon spectrum

+  

Phononic Crystal rejection bands

up Conversion

$\text{Piezoelectric Crystal}$

Down Conversion

Frequency Bar Code!

RF Emission Spectrum
Thermal Energy Harvesting Via Elastic Bandgap Phonon Engineering

- **Power Economy:**
  - Room temperature produces 40mW/cm² of power
  - RF detection limit is in the microwatts (μW)
  - Must insure that the phononic rejection band spans at least a μW.
  - Conversion efficiency of piezoelectric materials is well within $10^{-3}$.

- **Impacts**
  - **Passive Tagging:** Converting exhaust body heat to a discrete set of frequency lines *(Radio transmitted frequency bar code!)*
  - **Inter-chip wireless communications:** multiple bands allow for an overall wider communication bandwidth at zero additional cost.

- **Challenges**
  - Impedance matching the piezoelectric material to the lattice if used in a separate stage configuration
  - Micromachining the piezoelectric material as the background matrix when using a single stage configuration

- **Sandia and UNM Capabilities:**
  - World class **System Integration, Microfabrication and AlN** capability *(MEMS, NEMS, Sandia-MDL, Roy H. Olsson)*
  - Leading **Photonic/Phononic experimental R&D** teams *(Photonic Microsystems Technologies, T.S. Luk)*
  - Unique **3D E&M modeling capabilities:** FDTD, TMM, PW, Far and Near Field Fourier Analysis, and Inverse and forward problem solutions *(PMT, and UNM-EECE, I. El-Kady)*
Accelerated Cooling and Modification of the Global Heat Capacity

- **Rapid Accelerated Cooling (ballistic phonon) Scheme:**
  - **Conventional:**
    - Random Phonon Scattering
    - Overall Drift velocity $v_d$
  - **EBG Solution:**
    - Directive Phonon Guides
    - Guide Group velocity $v_g$

- **Concerns:**
  - Can we engineer the bands so that:
    - $V_g > V_d$?
  - Match guide impedance

- **Modification of the Global Heat Capacity:**
  - $Q$ vs. $T$
    - Bulk
    - $c_p$
  - $E_{ph}(kT)$ vs. $T$
    - $c_p$
**Phonon Shielding** = Johnson Noise Reduction:

- **Conventional:**
  - White Noise
  - Cap on Sensitivity

- **EBG Solution:**
  - 1D Phonon Shield
  - 2D Phonon Mirrors on the interconnects

**Negative Refraction and Acoustic Focusing:**

- Pononic band gap
- Negative Sloping Bands
- Negative Refraction

Negative group-velocity or negative curvature (“eff. mass”):

Negative refraction, Super-Lensing

- super-lens
- Veselago (1968)
Elastic Bandgap Phonon Engineering

- **Challenges:**
  - **Scaling**
    - Most relevant applications lie in the GHz-to-THz range; these require sub-μm to nm length scales.
    - Unclear how the elastic wave equations scale as we go from the continuum length scales (KHz) to the quantum length scales (THz).
  - Back fill thermalization?
    - Unclear how a modification of the phonon distribution affects the heat capacity.
    - Unclear how a phonon insulation scheme for Johnson noise reduction can be setup in a frame work that prevents re-thermalization of the phonon states.
  - Drift Versus Group Velocities and impedance matching.
    - Unclear whether or not we can create a preferred direction for phonon propagation where the group velocity is higher than the drift velocity and hence allow for accelerated cooling.
  - Efficiency of multiphonon processes for up/down frequency conversion?

- **Problem Statement:**
  - Phononic crystals offer a unique vehicle for full phonon control and as such open the door to a vast group of novel applications, however there is a great deal of ambiguity in the efficiency of this control and whether or not recipes borrowed from conventional photonic can be immediately applied or not.