Numerical Simulation of Phonon Dispersion Relations for 2D Phononic Crystals

Gaohua Zhu, Eric Dede

Toyota Research Institute of North America

10/03/2012

Excerpt from the Proceedings of the 2012 COMSOL Conference in Boston

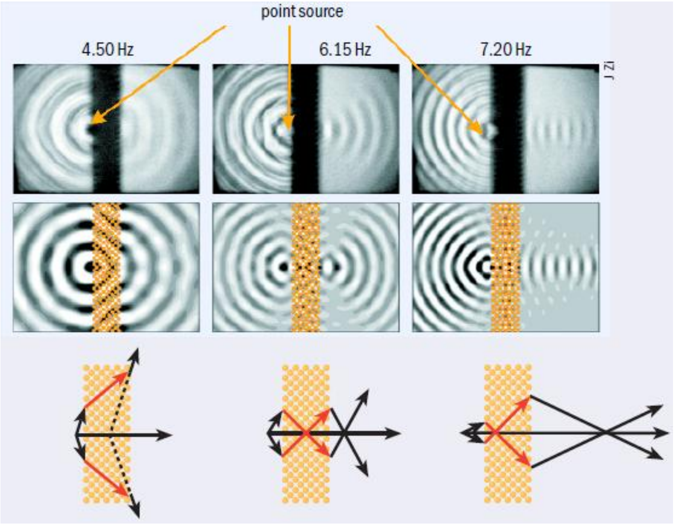
Outline

- Introduction to Phononic Crystals
- Theoretical Background
- COMSOL Multiphysics Model
- Simulation Results and Experiments
- Conclusions

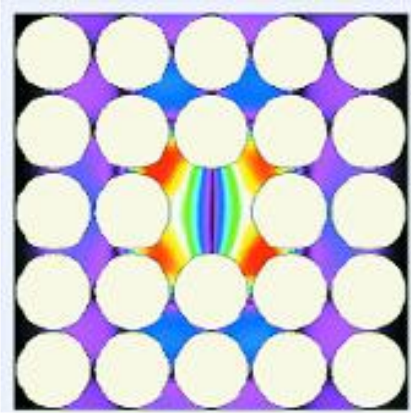
Phononic Crystals

- Phononic crystal are materials that have periodic variations in their mechanical properties
- Phononic structures provide a route to control the propagation of mechanical wave by engineering the structure of the materials
- The concept has been extended to the high frequency phonon domain

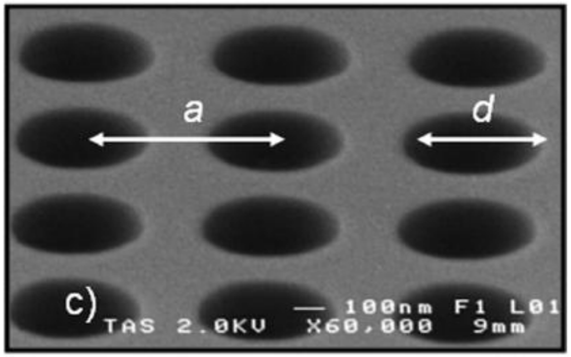
Negative Refraction



Acoustic waveguide



Heat manipulation



Phys Rev E 69, 030201(2004)
Physica World 12,2 (2005)
Nano Letters 11, 107 (2011)

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Phonon Dispersion Relation Simulation

- Plane Wave Expansion (PWE)
  - Easy to implement
  - Convergence problem for structures with large elastic mismatch
- Finite Difference Time Domain (FDTD)
  - Real time and transmission simulation
  - Band folding problem for super cell
- Multiple Scattering Theory (MST)
  - Accurate
  - Long computation time and limitation overlap scatters
- Finite Element Method (FEM)
  - Good for complicated structure design
  - Shows displacement fields
  - Requires lots of memory
- Molecular Dynamics (MD)
  - For nano-scale structures(< 100 nm, THz phonons)
  - Large computation amount when scales up

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Governing Equation for Wave Propagation

The general elastic wave equation

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \nabla \cdot (\rho c_t^2 \nabla u_i) + \nabla \cdot \left[\rho c_t^2 \frac{\partial u}{\partial x_i}\right] + \frac{\partial}{\partial x_i}\left[\left(\rho c_l^2 - 2\rho c_t^2\right)\nabla \cdot u\right]$$

$$c_l = \sqrt{C_{11}/\rho} \qquad c_t = \sqrt{C_{44}/\rho}$$

The solutions satisfying the Block theorem due to the periodic nature of phononic crystals

$$u_i(\vec{r},t) = e^{i\vec{G}\cdot\vec{r}} U_i(\vec{r},t)$$

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Plane Strain and Mindlin Plate Models

Plane Strain and Mindlin Plate modules were applied to solve for the in-plane and out-of-plane phonon eigen-frequencies respectively

$$\sigma = D\varepsilon$$

In-plane:

$$D = \frac{E}{(1+\nu)(1-2\nu)}\begin{pmatrix} 1-\nu & \nu & \nu & 0 \\ \nu & 1-\nu & \nu & 0 \\ \nu & \nu & 1-\nu & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} \end{pmatrix}$$

Out-of-plane:

$$D_p = \frac{E}{1-\nu^2}\begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{pmatrix}$$

$$D_s = \begin{pmatrix} \frac{E}{2(1+\nu)S_f} & 0 \\ 0 & \frac{E}{2(1+\nu)S_f} \end{pmatrix}$$

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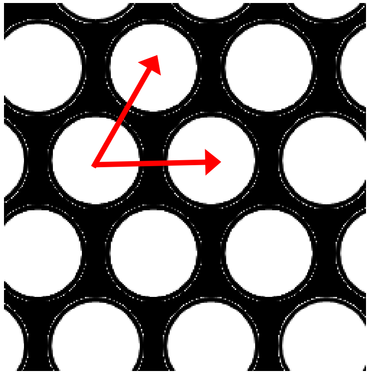
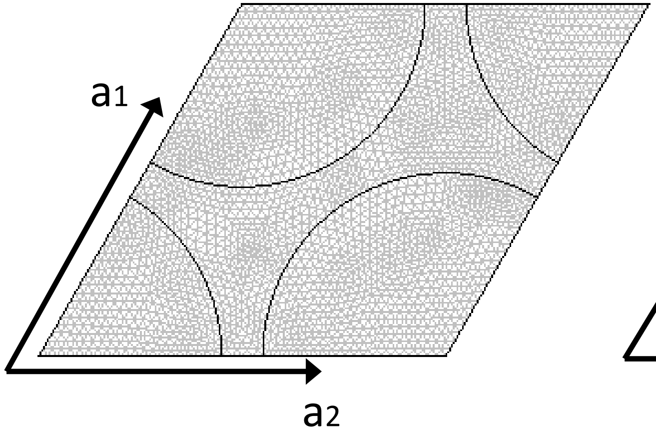
COMSOL Multiphysics Model

- Unit cell was built in COMSOL Multiphysics with the periodic boundary conditions
- Plane strain and Mindlin modules were applied to solve the eigen-frequencies for in-plane and out-of-plane vibrations
- Phonon dispersion relations along symmetric directions in the reciprocal space are plotted using a Matlab code

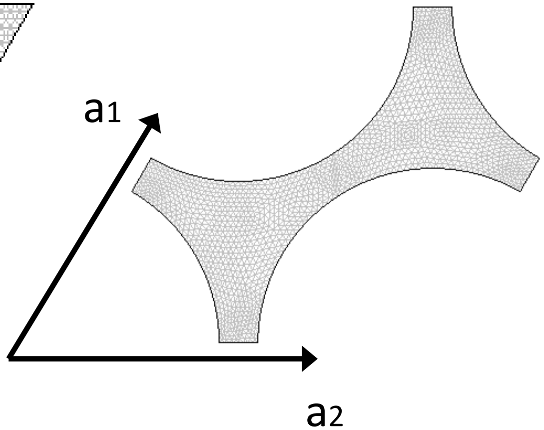
Triangular cylinder array



Air cylinder in epoxy matrix

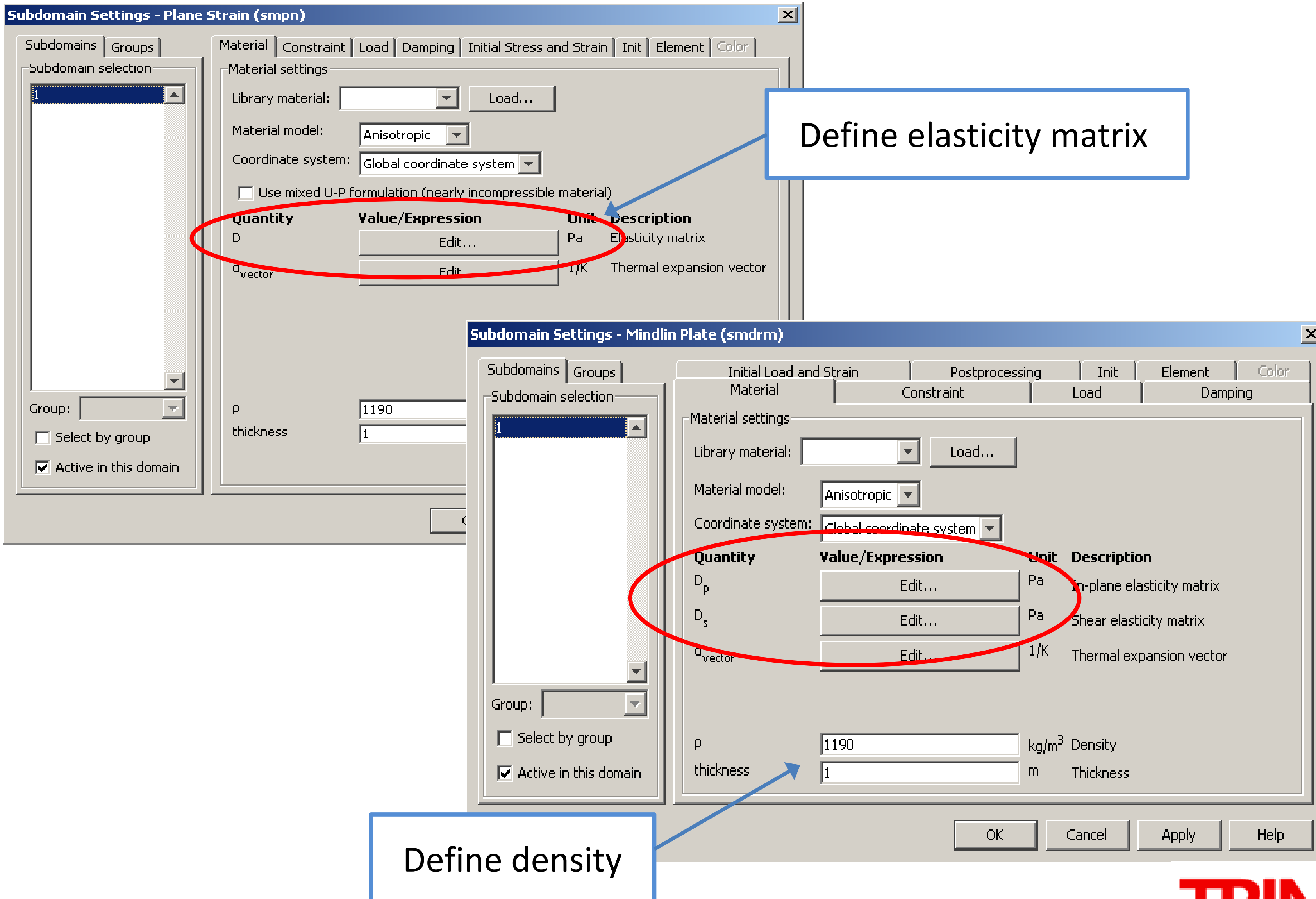


Vacuum cylinder in epoxy matrix

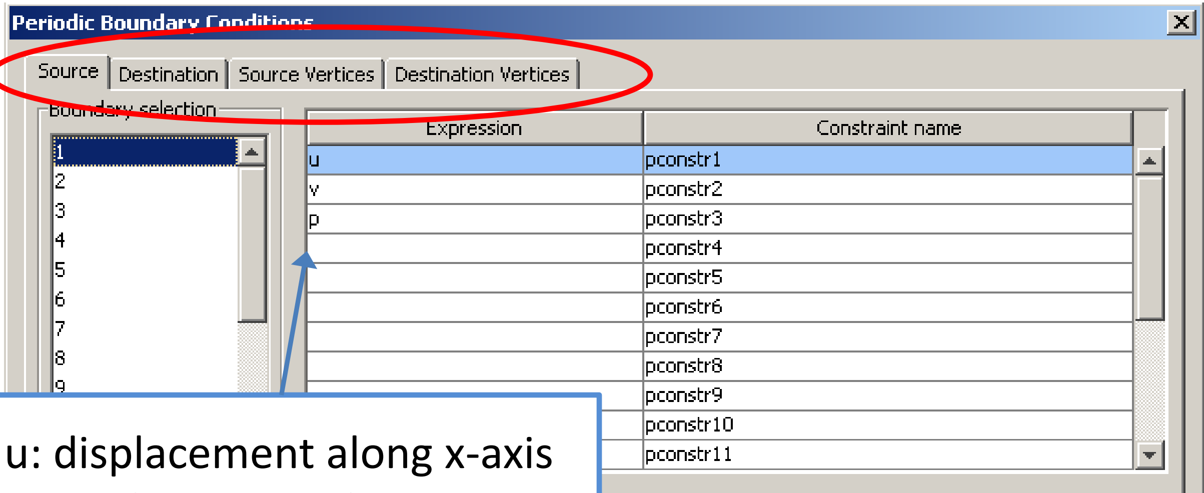


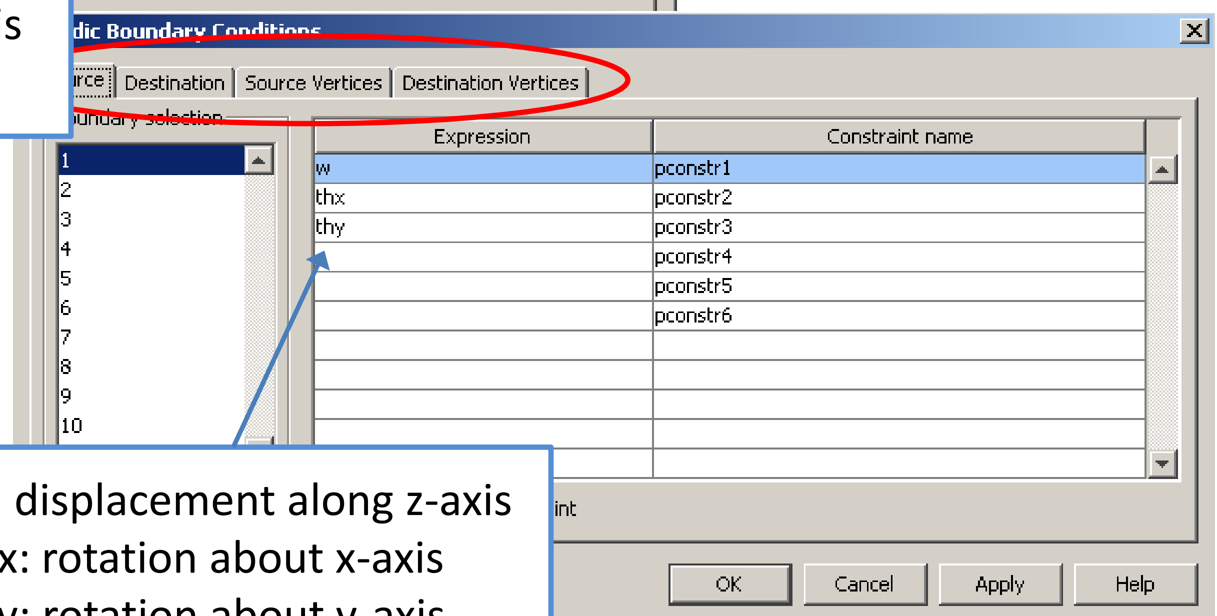
$$u_i(\vec{r}+\vec{a}) = e^{i\vec{G}\cdot\vec{a}}u_i(\vec{r}) = e^{i(G_x a_x + G_y a_y)}u_i(\vec{r})$$

Subdomain Settings



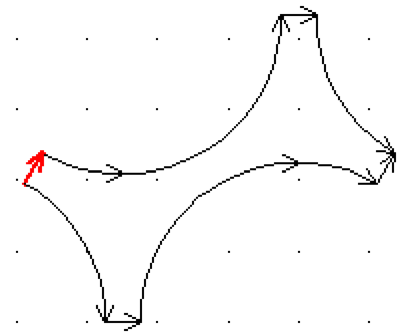
Boundary Condition Settings





u: displacement along x-axis
v: displacement along y-axis
p: pressure

w: displacement along z-axis
thx: rotation about x-axis
thy: rotation about y-axis



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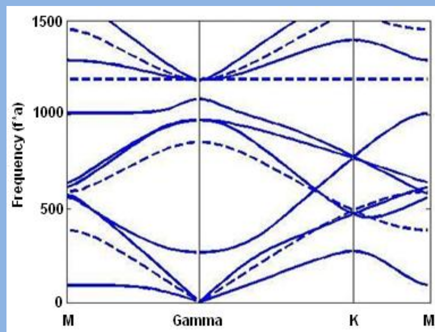
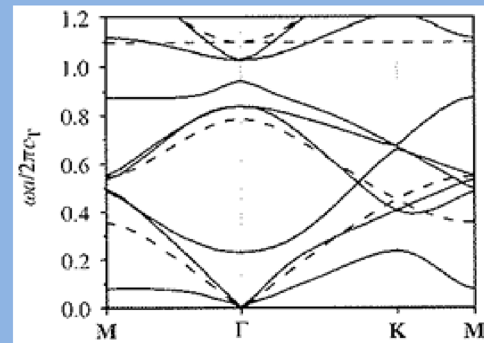
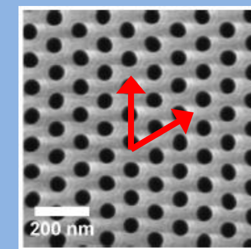
Compare Simulation Results

Epoxy - air hole triangular structure:



(COMSOL)

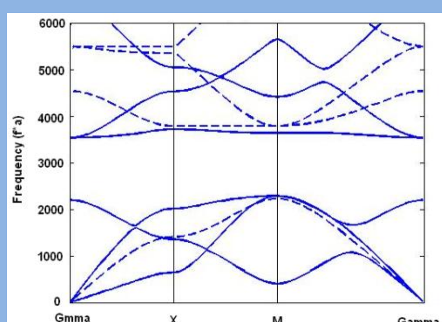




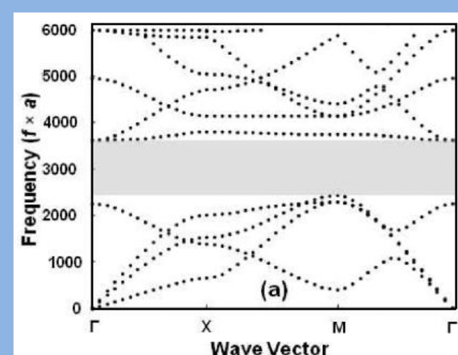
Maldovan *et al*, (2008)

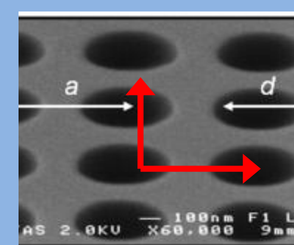
- Phonic band structures simulated using COMSOL show good agreement with published results

Silicon - air hole square structure:



(COMSOL)



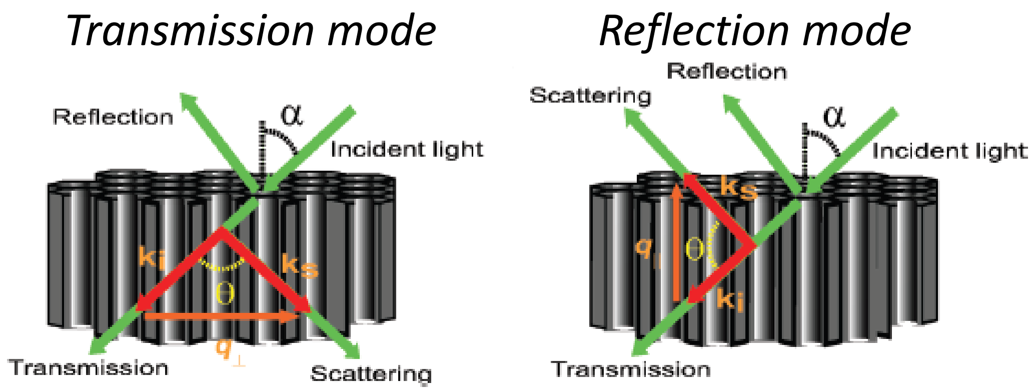


Mohammadi *et al*, *Optics Express* **18**(9), 9164 (2010)

- It can be used to simulation different materials combination and structural designs

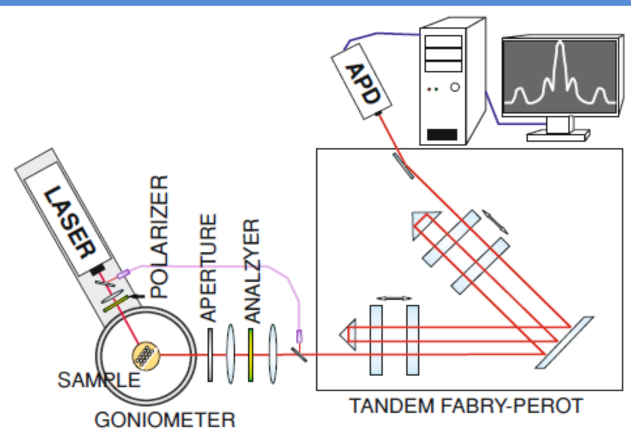
Characterize the Phononic Band Structure

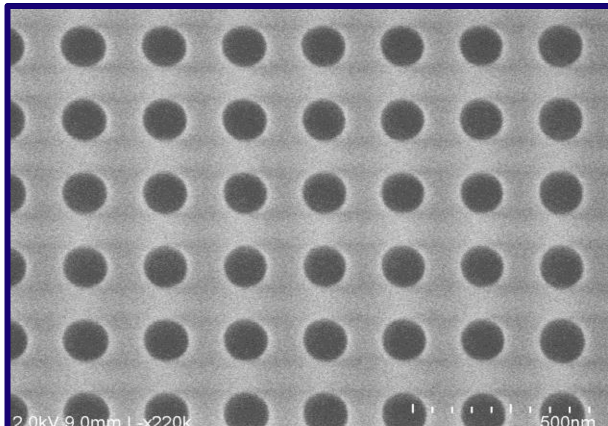
Phononic band structures in the low GHz range can be characterize by the Brillouin light scattering (BLS)



Sato *et al*, *ACS Nano* 4(6), 3473

Schematic of angle-resolved BLS





Phononic pattern with high aspect ratio made by ebeam lithography and DRIE

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Conclusions

- COMSOL models are created to calculate the phonon dispersion relations
- The simulation results show good agreement with existing numerical simulation results
- Inelastic scattering experiment will be perform to compare with the simulation results