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Hosting University Supervisor: prof. Katia Bertoldi

Obtaining tunable phononic crystals from shape memory polymers

Research activity carried out at

Bertoldi Group

SEAS – Harvard University – Boston, MA

February 27th, 2015

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Outline

- Shape memory polymers description
- Goal of the project
- Material modeling
- Experiments
- Wave propagation analysis

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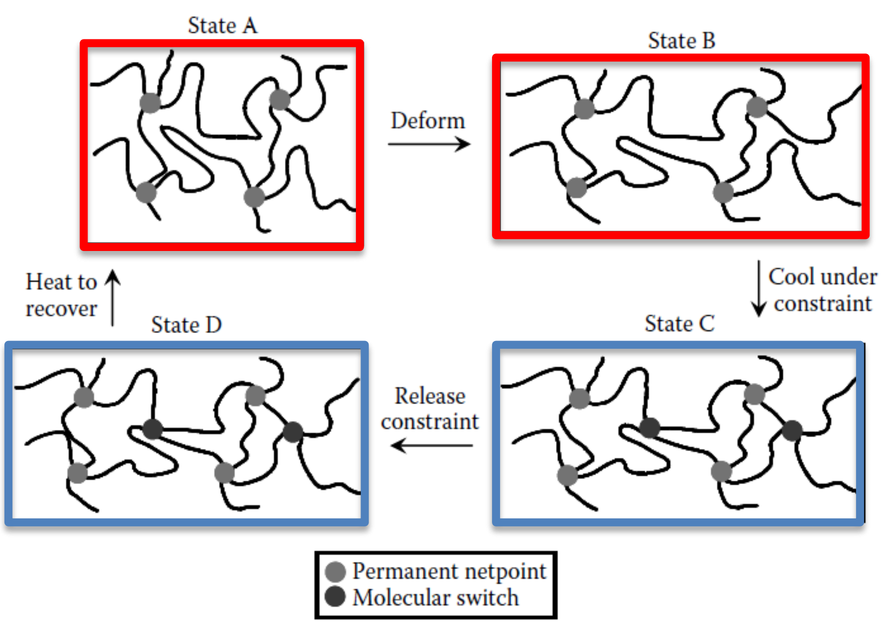
Shape memory polymers (SMPs)

- Ability to store a **temporary** shape and recover the **original** (processed) shape
- **Netpoints** provide the permanent shape, **switching domains** provide the temporary shape
- Chemical (covalent bonds) or physical (intermolecular interactions) crosslinking



- **Temperature** activated shape memory polymers are the most common: the driving force is the micro-Brownian motion, i.e. the variation of the chain mobility with temperature

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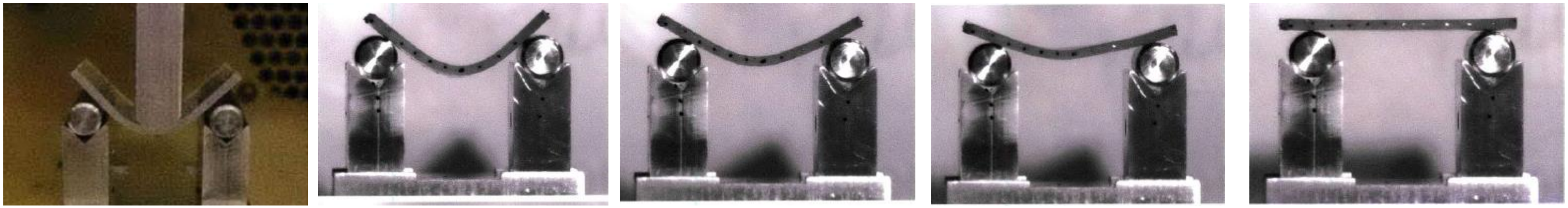
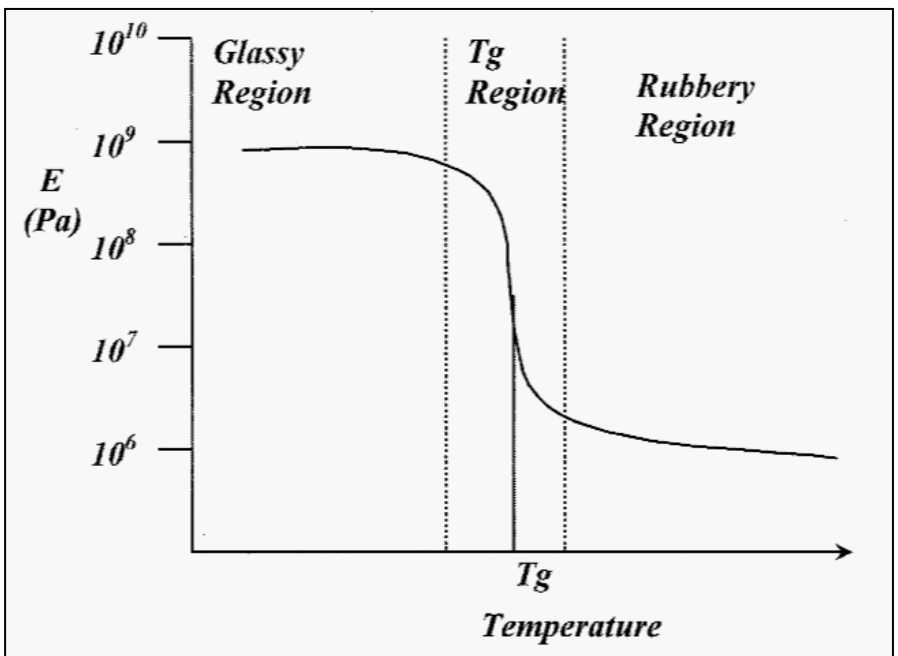
Shape memory polymers (SMPs)



Deformation at
$T > T_t$
and cooling

Heating



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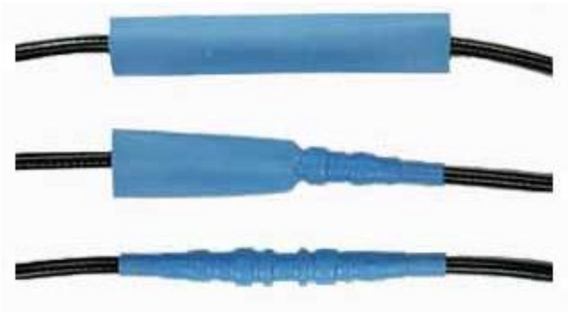
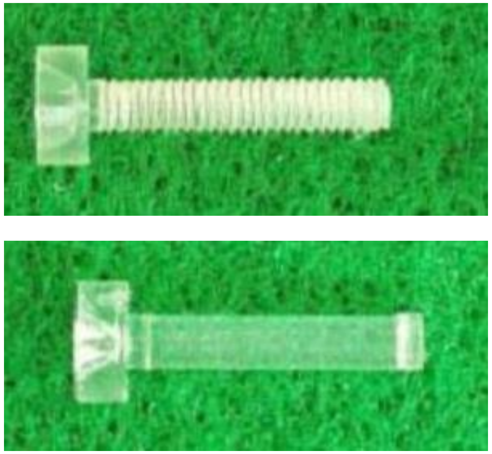
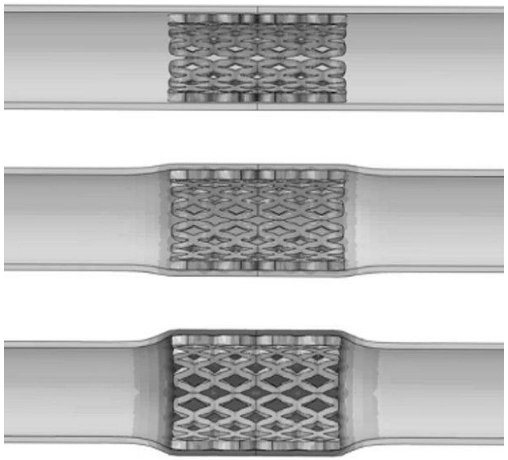
Shape memory polymers (SMPs)

- Application examples:
  - Heat shrinkable tubes
  - Toys and items
  - Soft grippers
  - Smart fabrics
  - Cardiovascular stents
  - Wound closure stitches
  - Drug delivery systems
  - Damping systems
  - Deployable structures
  - Food packaging
  - Fasteners
  - …



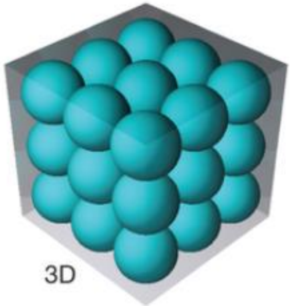
Intravenous syringe cannula

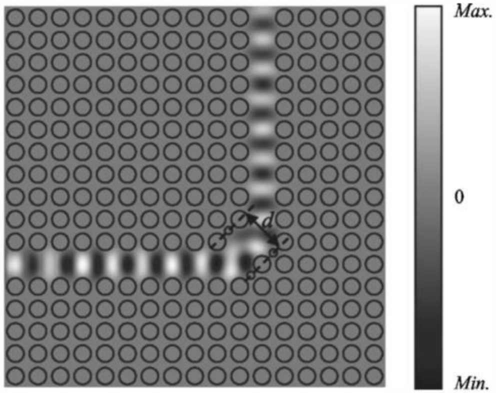




Phononic crystal

- Phononic crystals are periodic structures which display a wave band gap
- The explanation for the band gap can be found in the multiple interference of sound waves scattered
- Example applications:
  - Noise Cancelling
  - Vibration Insulation
  - Wave Filter
  - Wave Guide / Mirror
  - Acoustic Imaging





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Phononic crystal

- Example of phononic crystal: sculpture by Eusebio Sempere (1923-1985) in Madrid → two-dimensional periodical arrangement of steel tubes.

- In 1995, measurements performed by Francisco Meseguer and colleagues showed that attenuation occurs at certain frequencies, a phenomenon that can not be explained by absorption, since the steels tubes are extremely stiff and behave as very efficient scatterers for sound waves.

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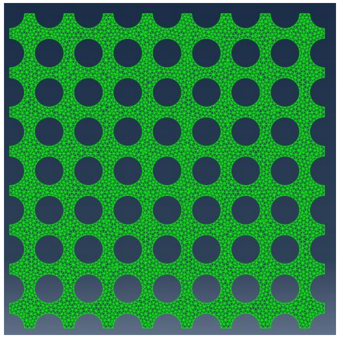
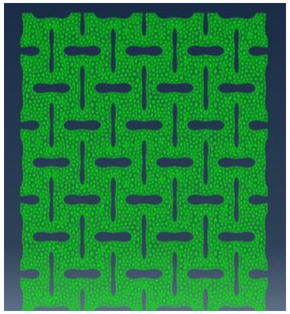
Phononic crystal

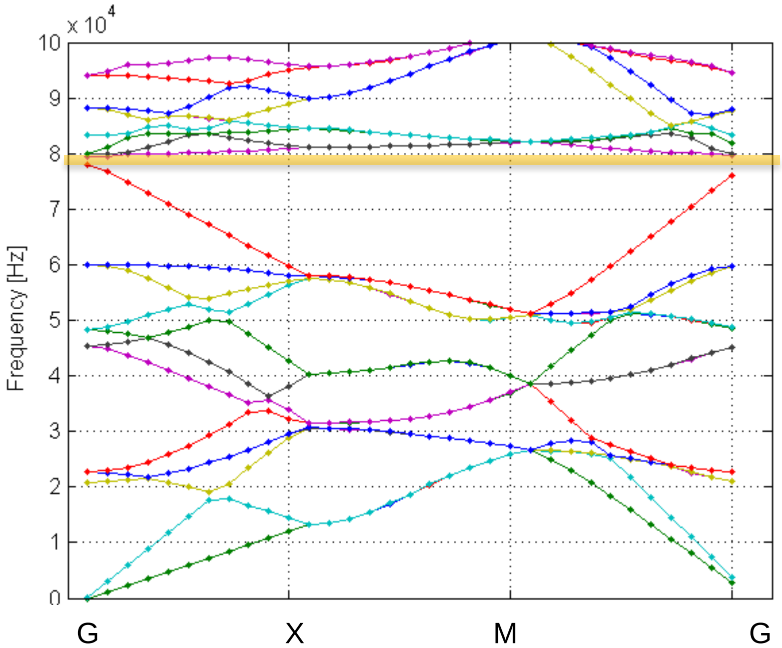
- To identify the band gap, i.e., the range(s) of frequencies which are barred by the crystal, we need to perform a wave propagation analysis.
- I considered 2 simulation types: the **Bloch wave analysis** and the **steady-state dynamics analysis**.
- Analyses performed on Abaqus software.

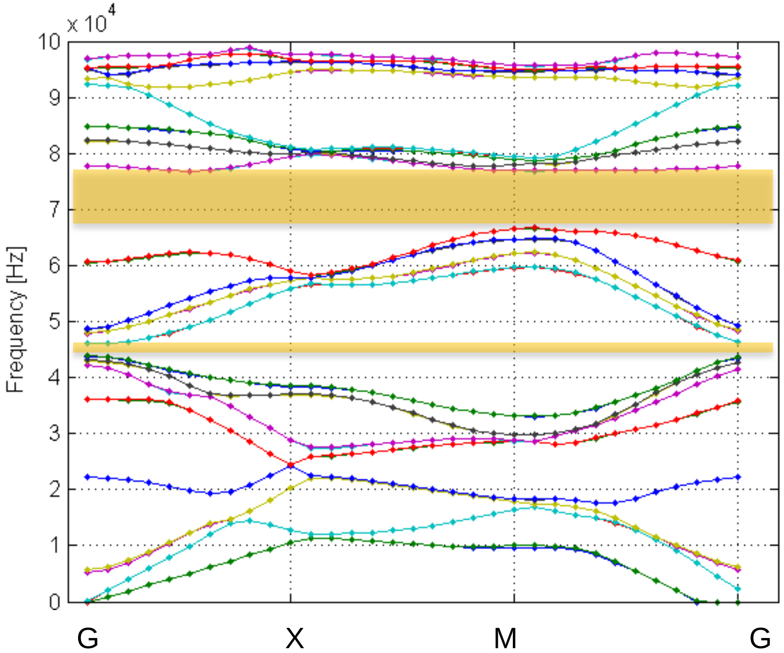
Goal

- Obtaining a phononic structure which displays a tunable band-gap, along with good wave propagation properties









Goal

- SMP vs rubbery material: pros and cons

SMP

- Can be deformed until buckling (when hot)
- **Stiffer (when cold): better wave propagation**
- Partial shape memory recovery; need for reshaping (when hot) in order to completely recover original shape
- While cold, it does not need continuous load to keep the buckled shape
- Buckling at high temperature, wave propagation at room temperature

Rubbery material
(*Shan 2013 paper*)

- Can be deformed until buckling
- Sloppy and dissipative: waves are damped
- Elastic recovery of original shape when unloaded
- Need to maintain the loading constraint to keep the buckled shape
- All happens at room temperature

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SMP model

- Two main constitutive modeling approaches:

Phase-change

- Change of the material state according to temperature variation (“frozen” and “active” phases)
- Variable indicating fraction of “frozen” phase
- Rule of mixtures is usually used
- Examples:
  - Liu et al. (2006)
  - Chen and Lagoudas (2008)
  - Reese et al. (2010)

Viscoelastic

- Based on standard linear viscoelastic models commonly used to simulate polymers behavior
- More close to the real mechanisms but usually more complex
- Huge number of material parameters
- Examples:
  - Diani et al. (2006)
  - Nguyen et al. (2008)
  - Srivastava et al. (2010)

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SMP model

- 3D phenomenological finite-strain model for amorphous SMPs, based on Reese 2010 paper
- Based on distinction between **rubbery** (subscript "r") and **glassy** (subscript "g") phase, and on **frozen deformation** storage
- Assume the glass volume fraction (z) as a variable dependent only on temperature

$$z = \frac{1}{1 + Exp(2\, w\, (\theta - \theta_t))}$$

θ = current temperature

θ_t = transformation temperature

w = material parameter determining the slope of the transformation curve

- Consider Neo-Hookean model for both rubbery and glassy phases, with proper material parameters
- Use rule of mixtures to derive the global Helmoltz potential

$$\Psi = (1 - z)\ \Psi_r + z\ \Psi_g$$

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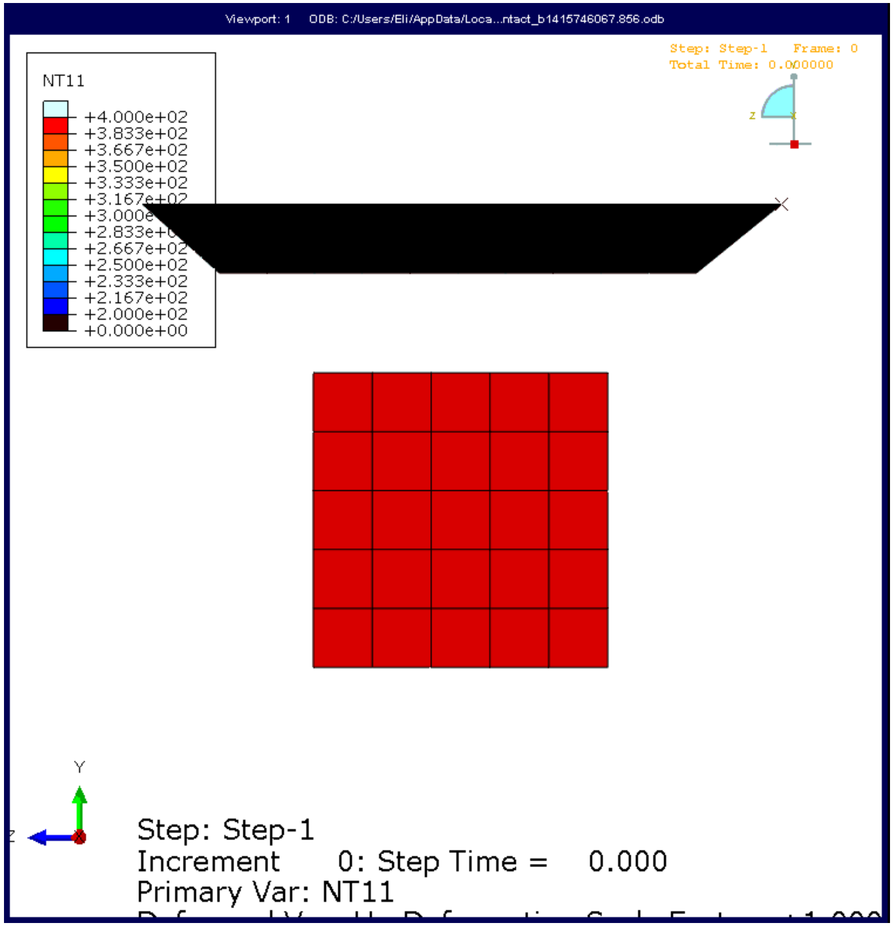
SMP model

- Model implemented in an Abaqus UMAT



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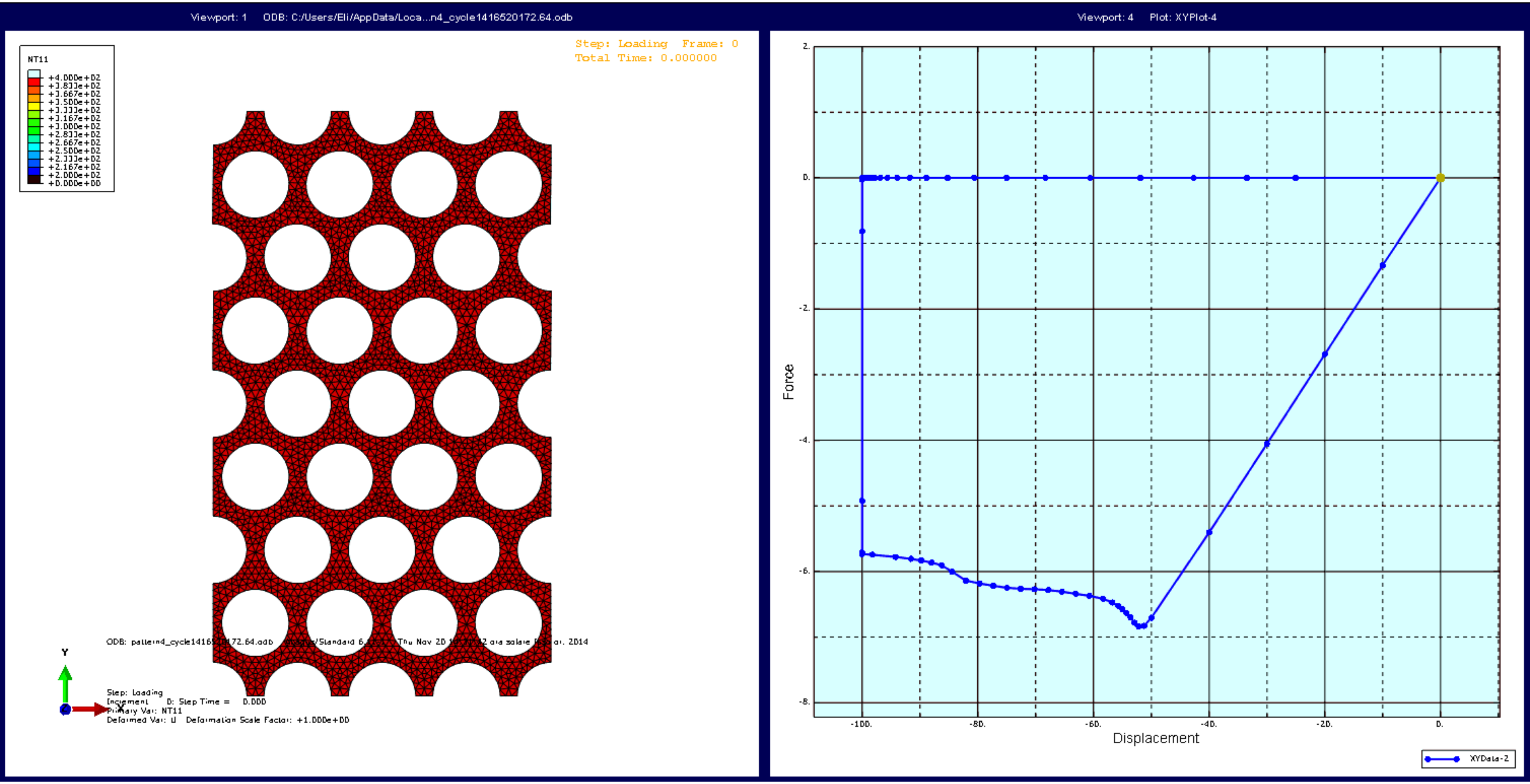
SMP model



Complete cycle

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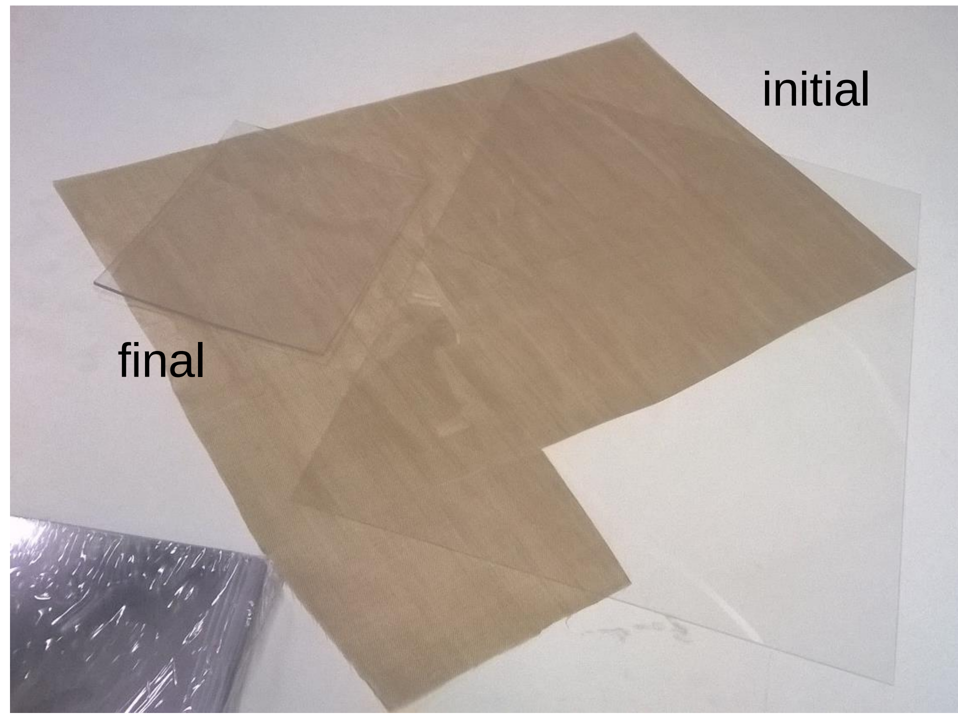
Material



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Material

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Material

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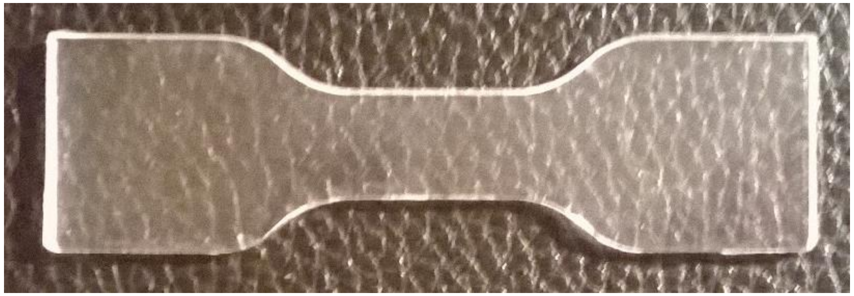
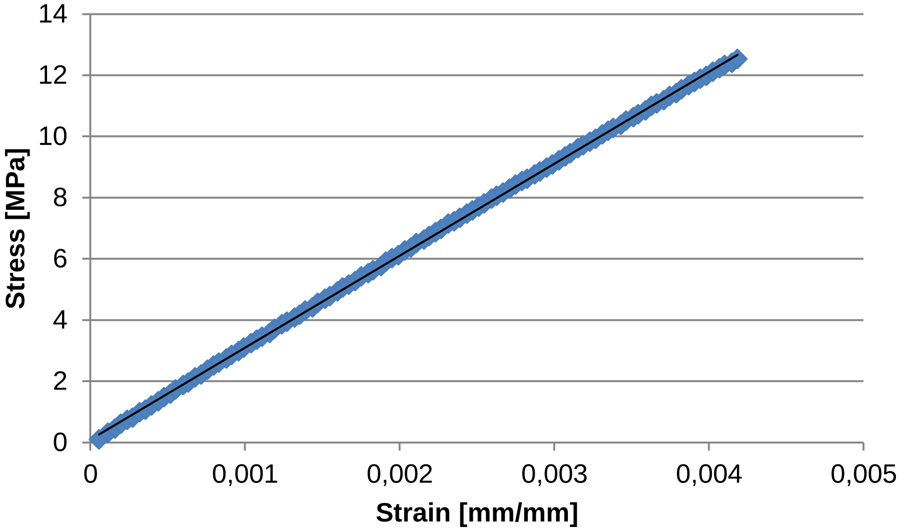
Traction test





Young's modulus = 3000 MPa

User material parameters:

Young's modulus glassy phase = 3000 MPa
Poisson's coefficient glassy phase = 0.35
Young's modulus glassy phase = 10 MPa
Poisson's coefficient glassy phase = 0.49

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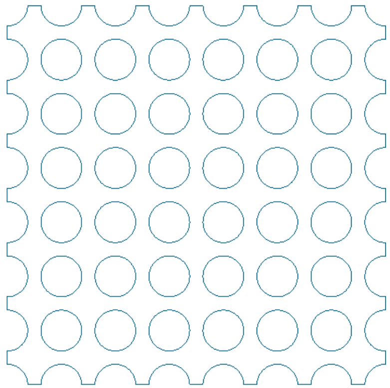
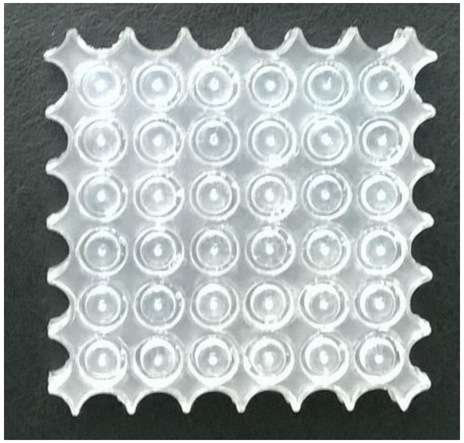
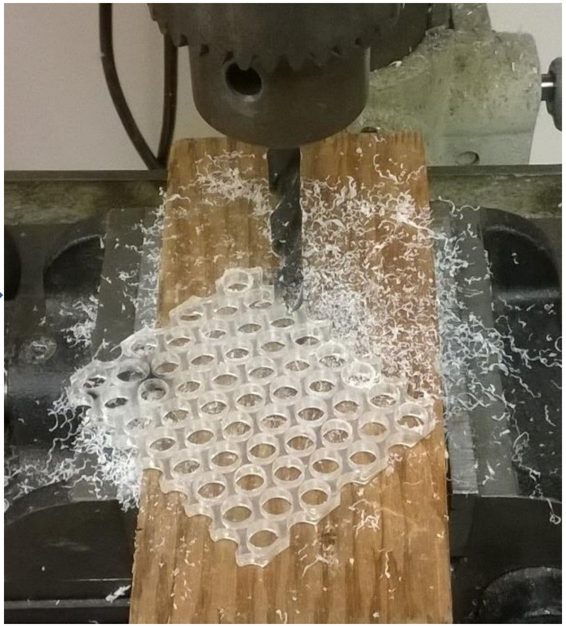
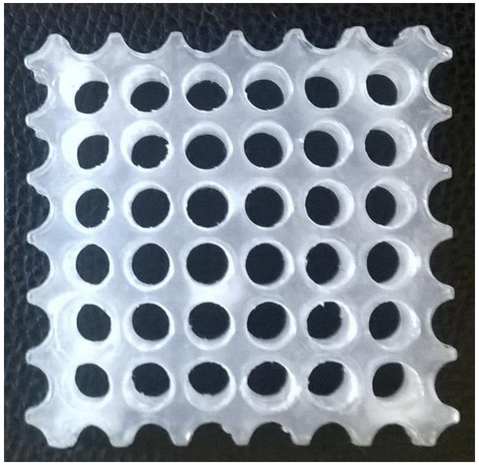
Manufacturing

- After MANY (!) trials …found the ideal way to manufacture the samples, using both the laser-cutter and the drilling machine









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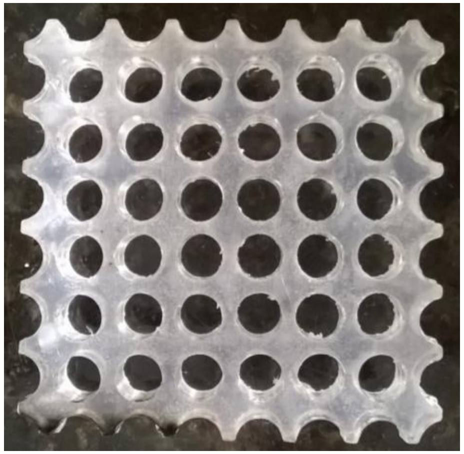
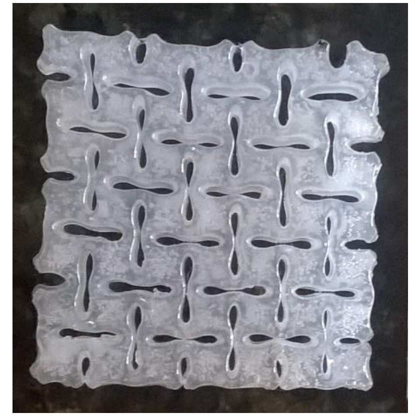
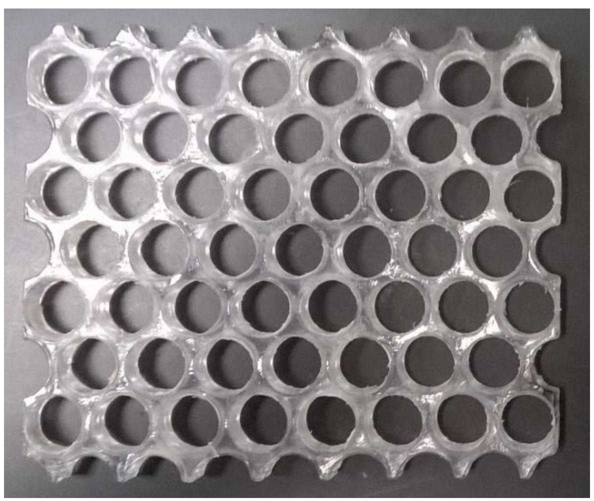
Heating → buckling → cooling

Square





Diagonal



- Optimized using FEA simulations → 60% porosity

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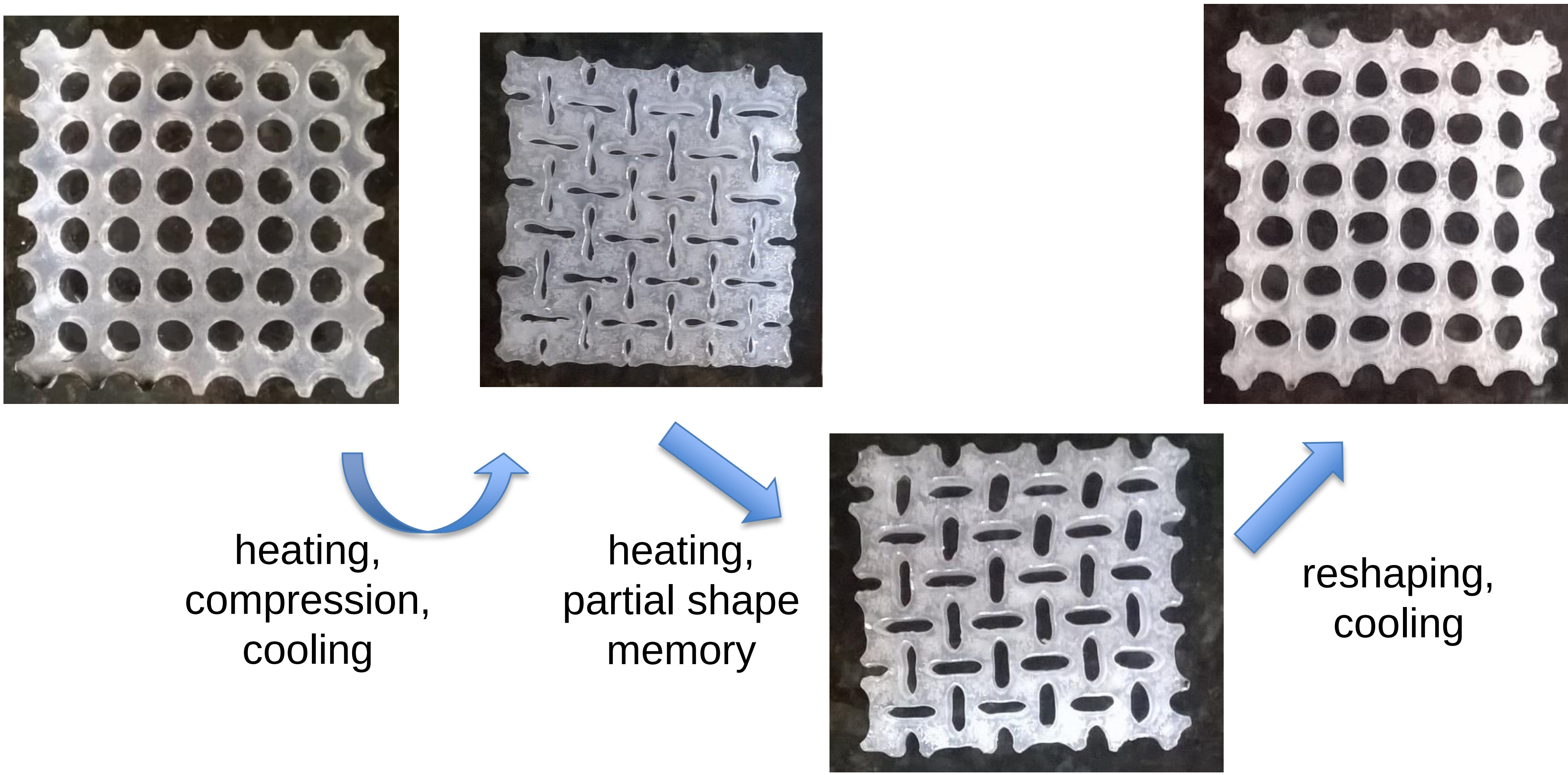
Re-heating and …recovery?



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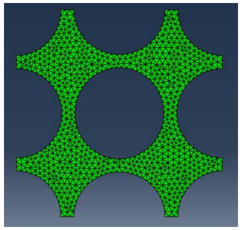
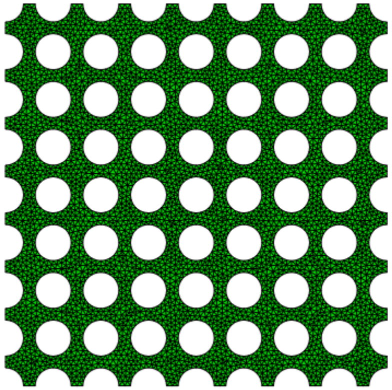
Simulations



infinite structure
+
periodic boundary conditions



finite-size structure

- Buckling
- Post-buckling

both on **infinite** and **finite-size**

- Wave propagation analysis

Bloch wave analysis for **infinite**

Dynamics steady-state for **finite-size**

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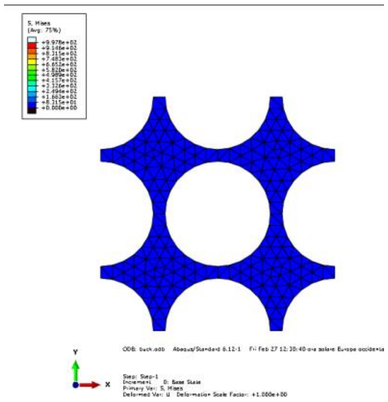
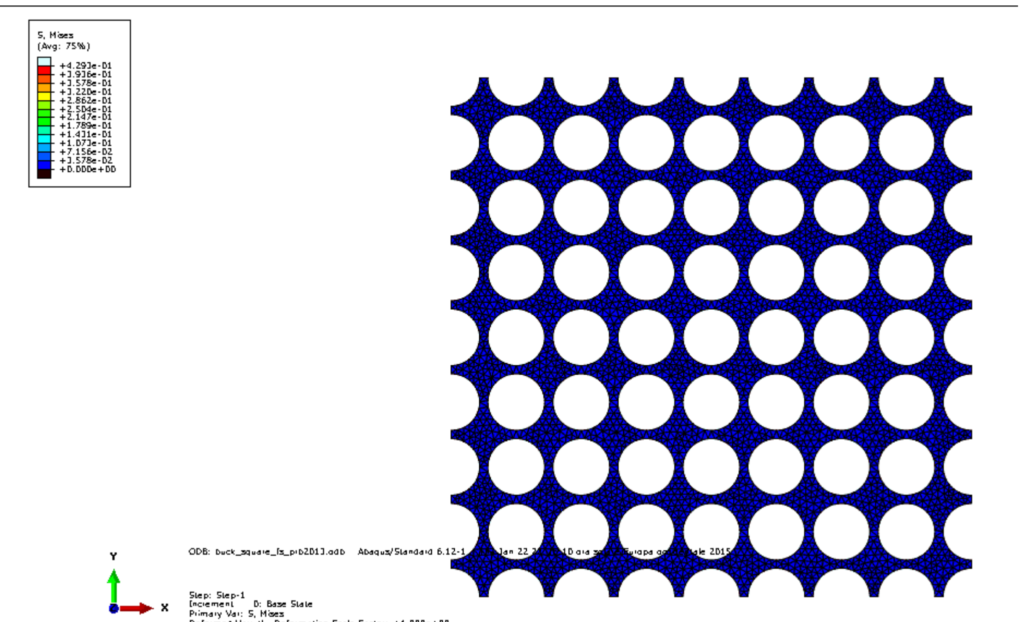
Buckling



Buckling modes



ABAQUS PROCEDURE:

- Linear perturbation → buckle
- Load (0, 1)
- Additional line in input file:

  *NODE FILE
  U

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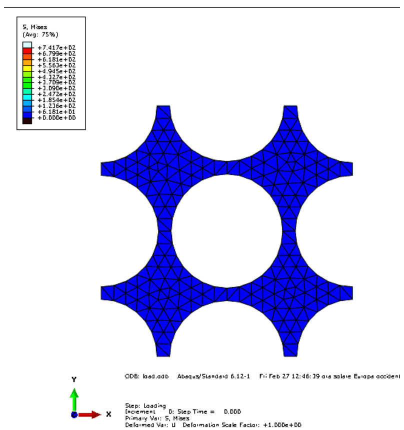
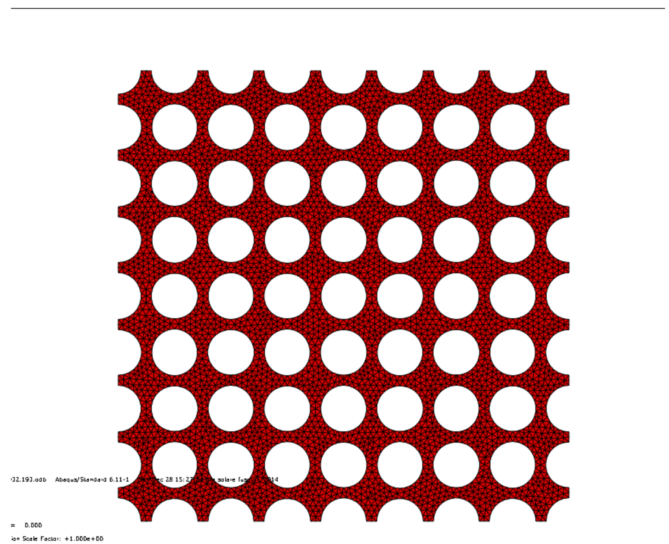
Post-buckling





ABAQUS PROCEDURE:

- Static general step
- Apply required load
- Additional line in input file:

  *IMPERFECTION, …

  related to the buckling analysis file

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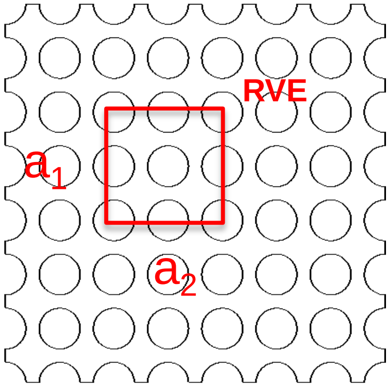
Bloch wave analysis

- The Bloch wave analysis considers an infinite periodic structure and is based on a RVE, which is the smaller unit-cell of the structure:



- The *reciprocal lattice* can be defined as the set of wave vectors **k** that creates plane waves that satisfy the spatial periodicity of the point lattice:

$$e^{i\mathbf{k}\cdot\mathbf{r}} = e^{i\mathbf{k}\cdot(\mathbf{r}+\mathbf{R})}$$

$$\mathbf{u}_T(\mathbf{r}, t) = \mathrm{Re}(\mathbf{u}_{T0}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)})$$

$$\mathbf{u}_L(\mathbf{r}, t) = \mathrm{Re}(\mathbf{u}_{L0}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)})$$

Elastic plane waves propagation

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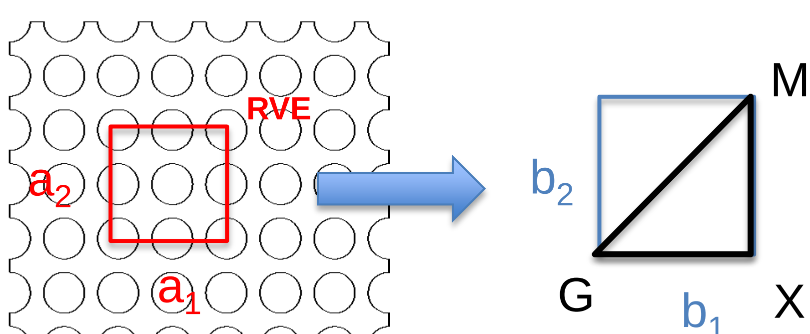
Bloch wave analysis

- The subset of wave vectors **k** that contains all the information about the propagation of plane waves in the structure is called the *Brillouin zone*.
- The phononic band gaps are identified by checking all eigenfrequencies ω(**k**) for all **k** vectors in the irreducible Brillouin zone: the band gaps are the frequency ranges within which no ω(**k**) exists.



$$b_1 = 2\pi \frac{a_2 \times z}{\|z\|^2}$$

$$b_2 = 2\pi \frac{z \times a_1}{\|z\|^2}$$

$$z = a_1 \times a_2$$

(In this case, a_1=a_2=a)

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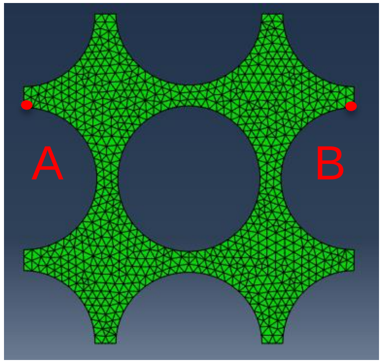
Bloch wave analysis

- Bloch-Floquet conditions are applied to the boundaries:

$$\mathrm{Real}(\mathbf{u}_i^B) = \mathrm{Real}(\mathbf{u}_i^A)\cos[\mathbf{k}\cdot\mathbf{r}_{A_iB_i}] - \mathrm{Imag}(\mathbf{u}_i^A)\sin[\mathbf{k}\cdot\mathbf{r}_{A_iB_i}]$$
$$\mathrm{Imag}(\mathbf{u}_i^B) = \mathrm{Real}(\mathbf{u}_i^A)\sin[\mathbf{k}\cdot\mathbf{r}_{A_iB_i}] + \mathrm{Imag}(\mathbf{u}_i^A)\cos[\mathbf{k}\cdot\mathbf{r}_{A_iB_i}]$$

$$\mathbf{r}_{A_iB_i} = \mathbf{x}_i^B - \mathbf{x}_i^A$$

$\mathbf{k}$ is the wave propagation direction



- Coupling of real and imaginary parts.

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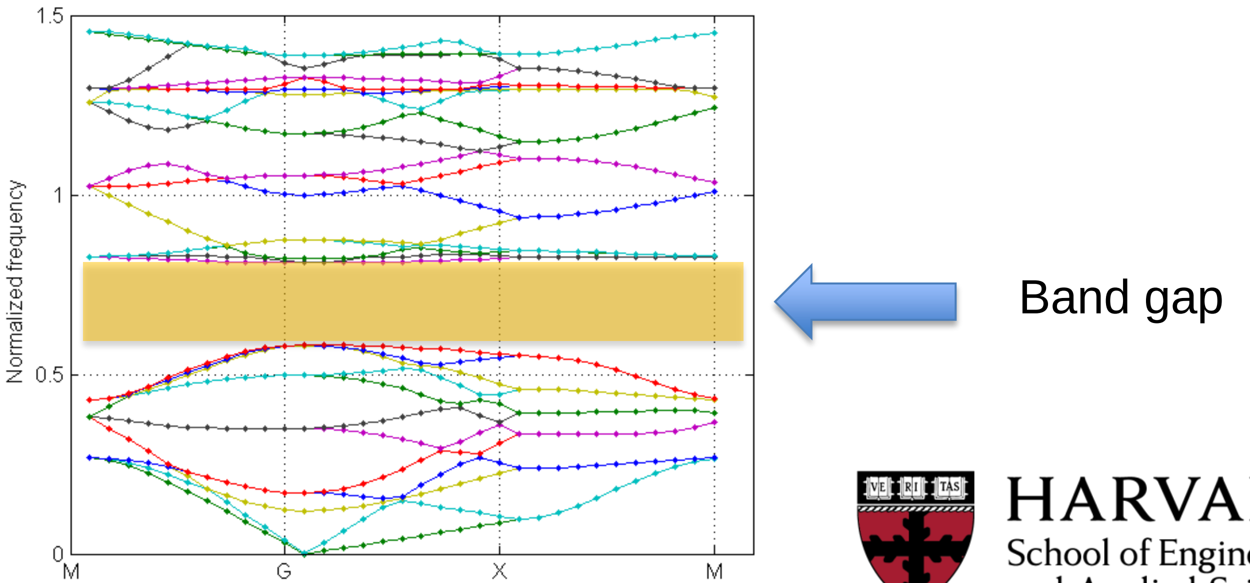
Bloch wave analysis

- These eigenvalues ω(**k**) are continuous functions of the vectors **k** (which individuate the wave direction), but they are discretized when computed through numerical methods such as FEA.
- Once checked all the eigenvalues in the Brillouin zone, the eigenvalues ω(**k**) can be plotted vs **k**.
- The ω(**k**) vs **k** plot is called dispersion diagram.

Normalized frequency:

$$\omega a / 2 \pi c_T$$

where c_T is the wave propagation speed in the considered material.



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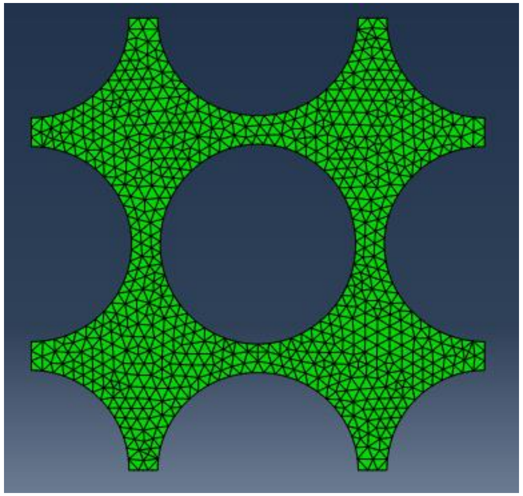
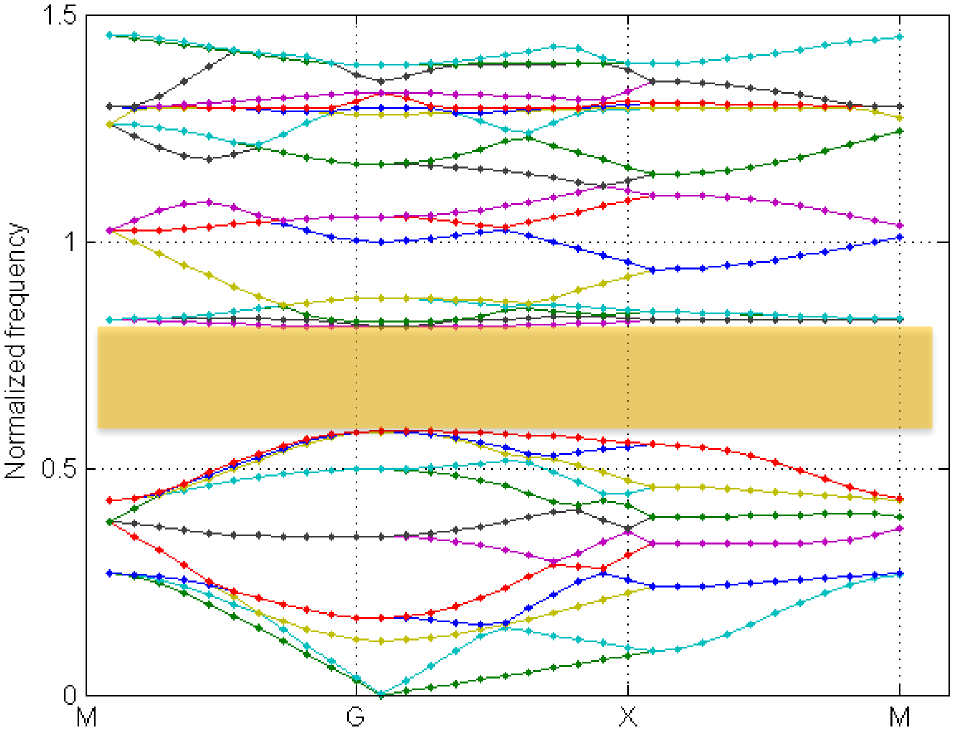
Bloch wave analysis example

Radius ≈ 4.37 mm **porosity = 60%**



Compression = 0%

<u>Biaxial</u>



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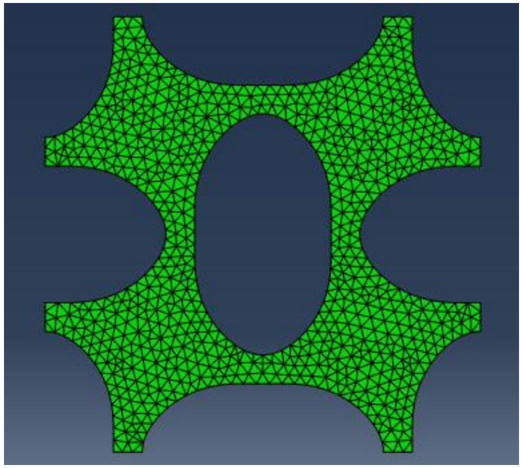
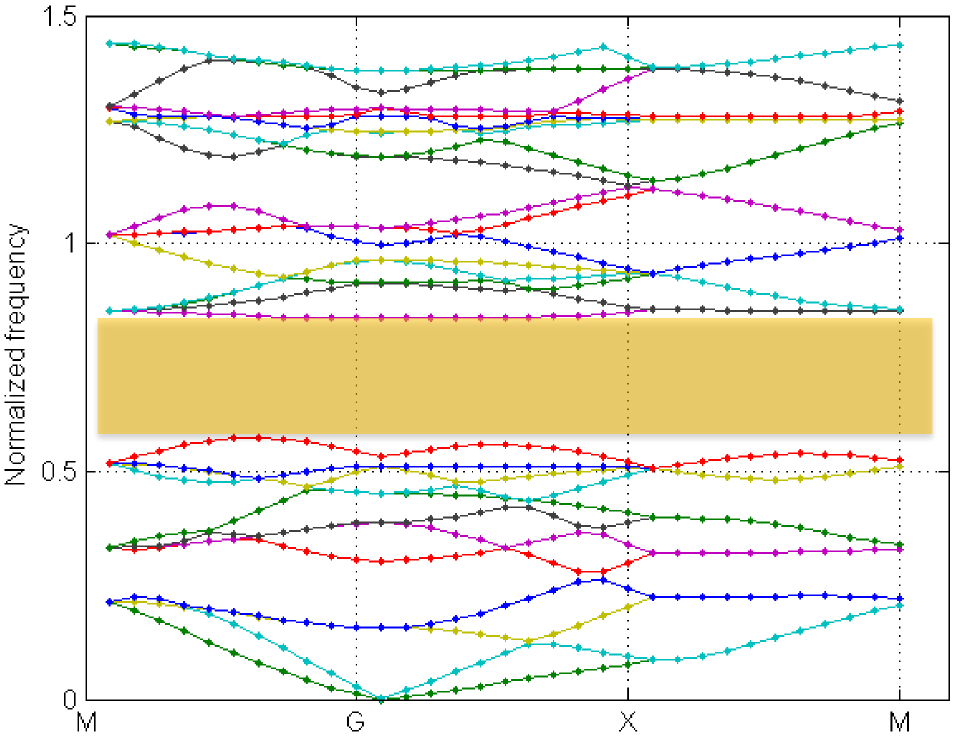
Bloch wave analysis example

Radius ≈ 4.37 mm **porosity = 60%**



Compression = 25%



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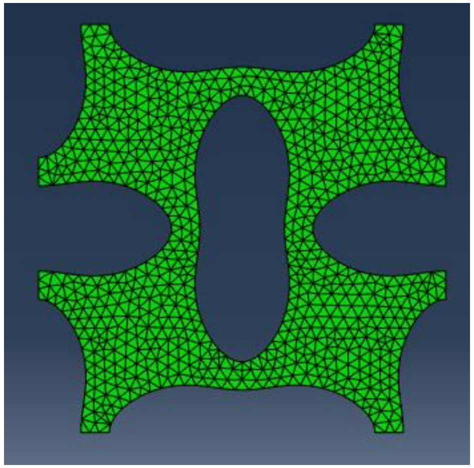
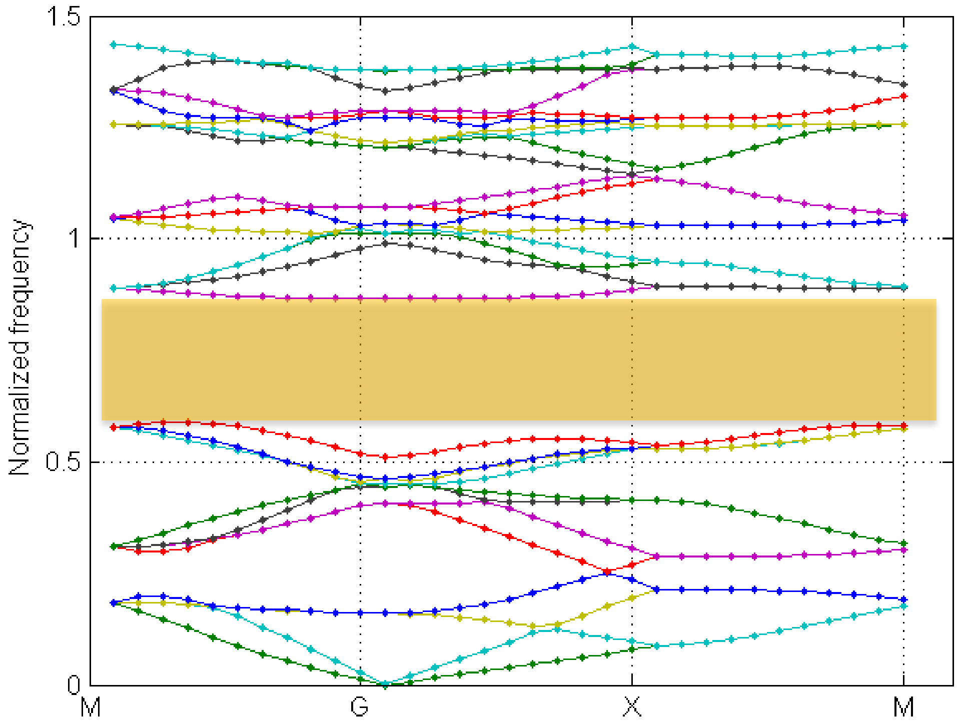
Bloch wave analysis example

Radius ≈ 4.37 mm **porosity = 60%**



Compression = 50%



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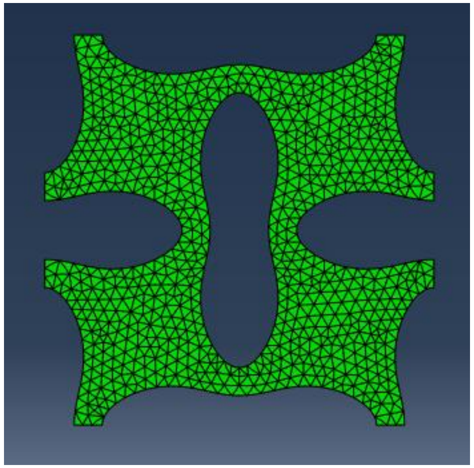
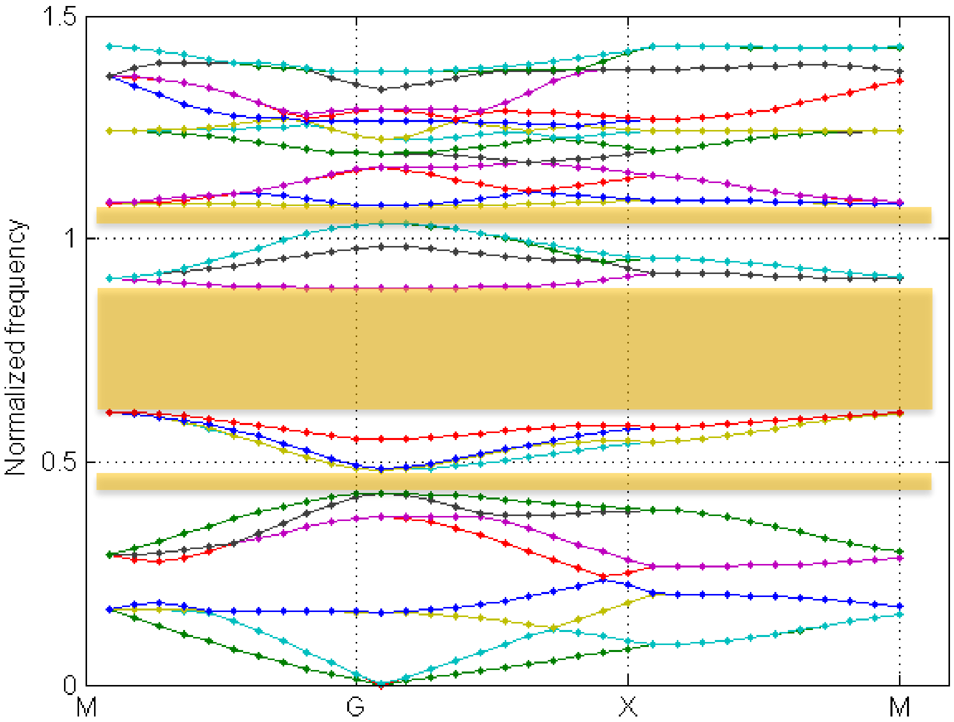
Bloch wave analysis example

Radius ≈ 4.37 mm **porosity = 60%**

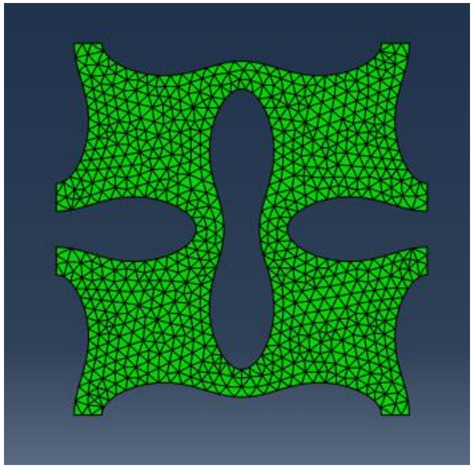


Compression = 75%

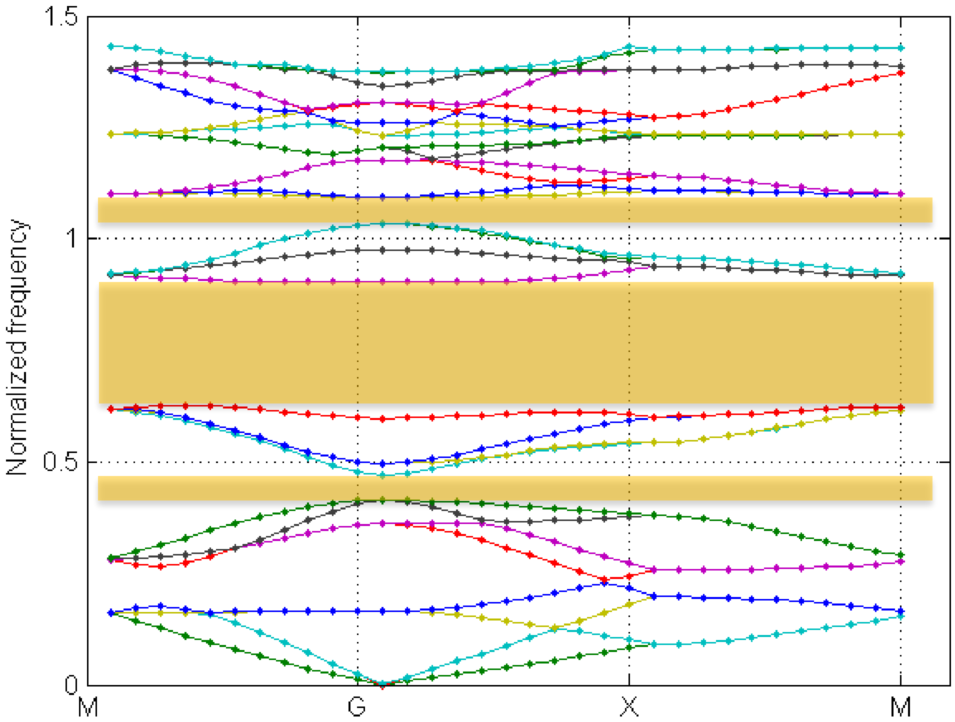


Bloch wave analysis example

Radius ≈ 4.37 mm **porosity = 60%**

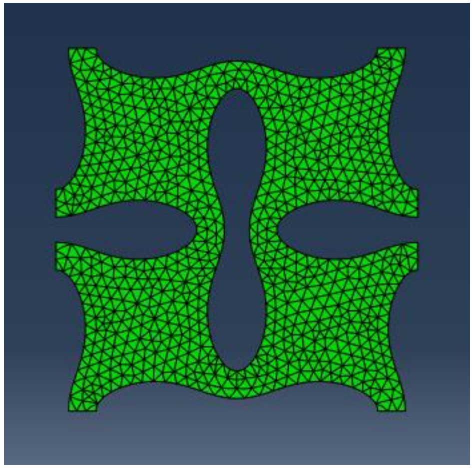


Compression = 90%



Bloch wave analysis example

Radius ≈ 4.37 mm **porosity = 60%**



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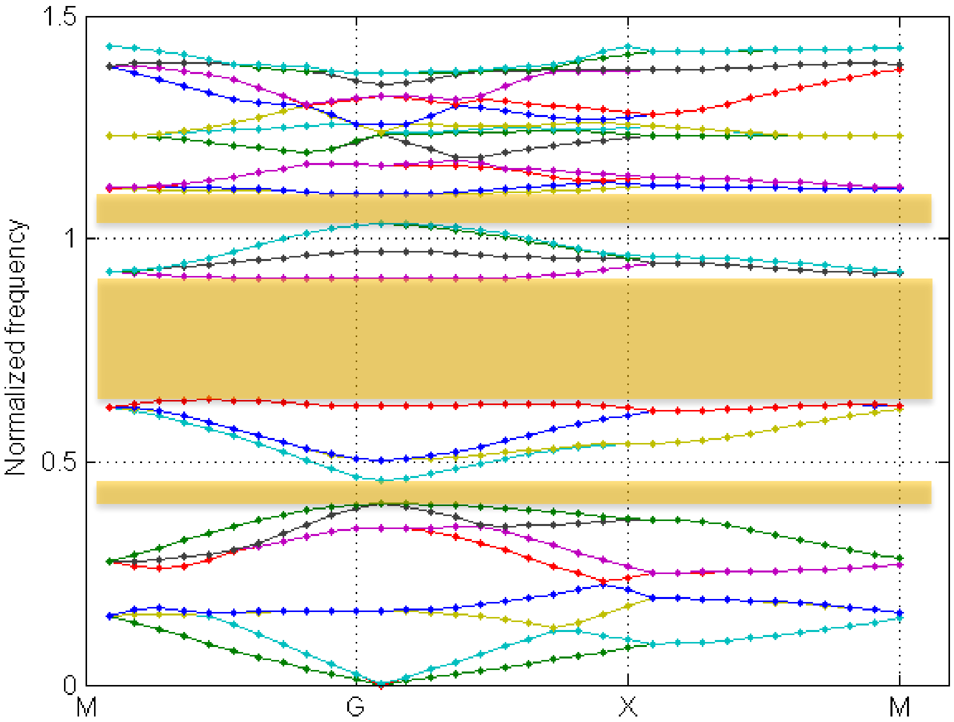

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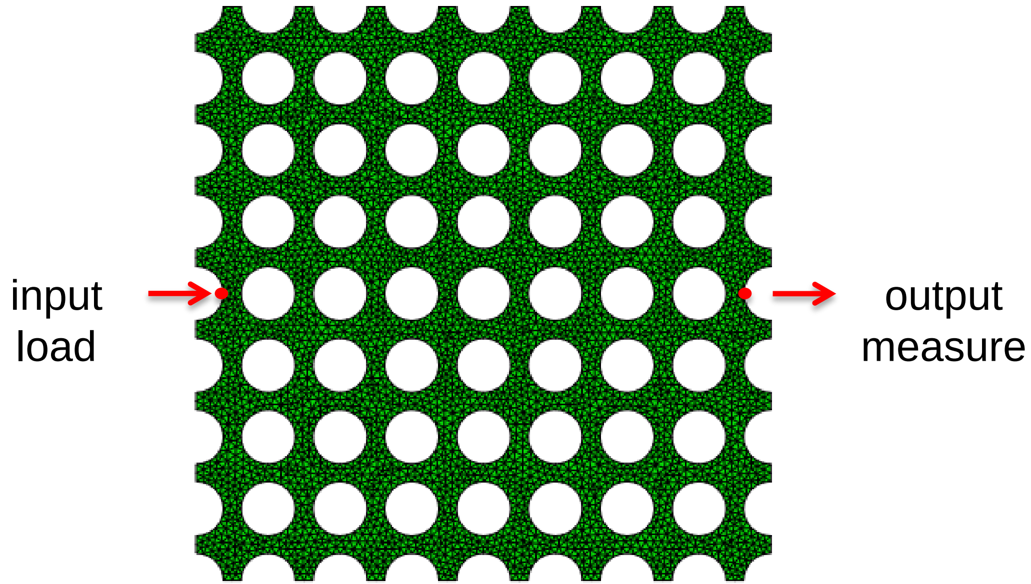
Steady-state dynamics analysis

- The steady-state dynamics analysis is performed on the finite-size sample.



input displacement: U = 1. cos(ω t)

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Steady-state dynamics analysis

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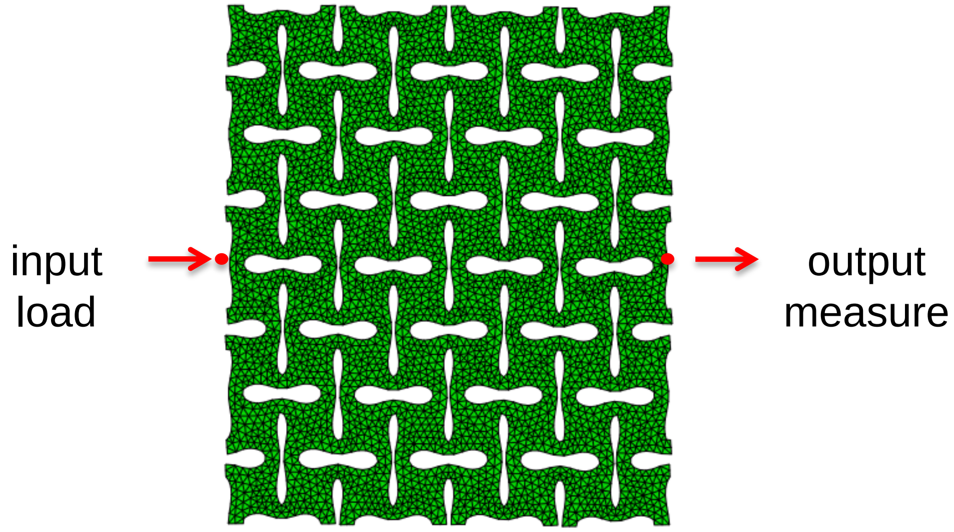
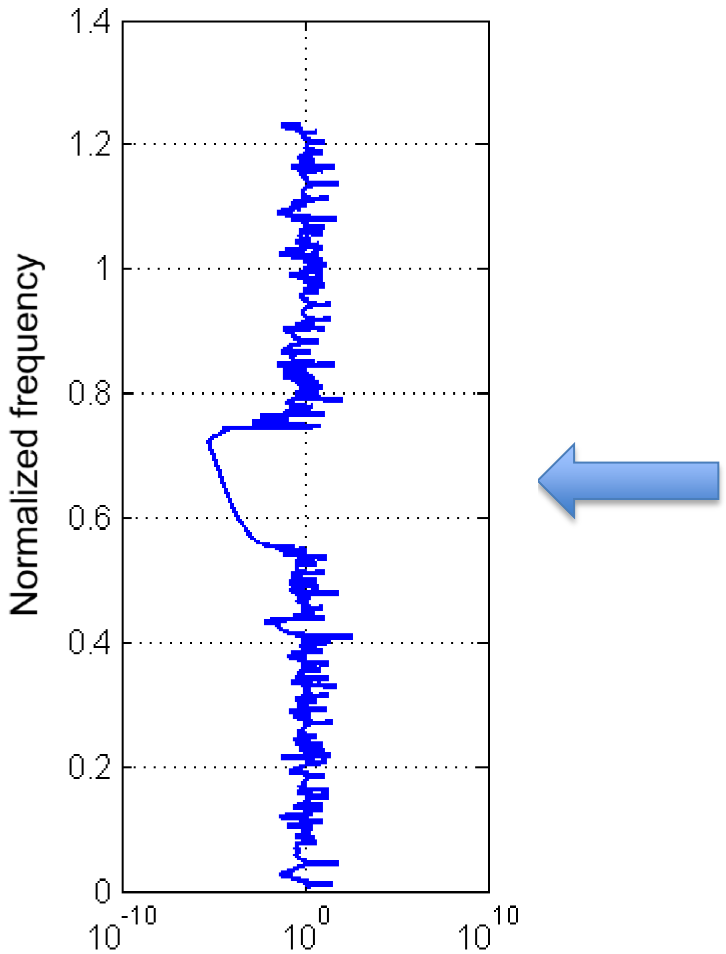


input displacement: U = 1. cos(ω t)

Steady-state dynamics analysis



Band gap

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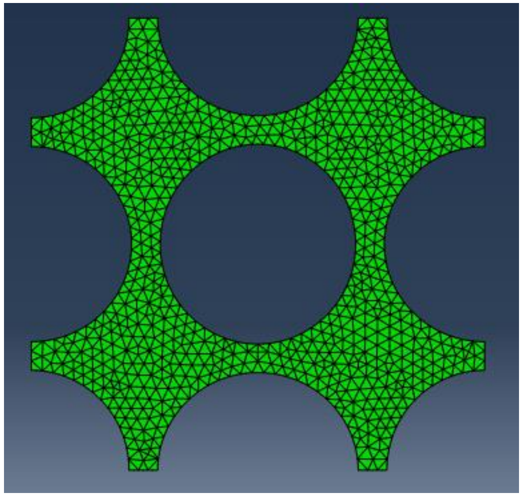
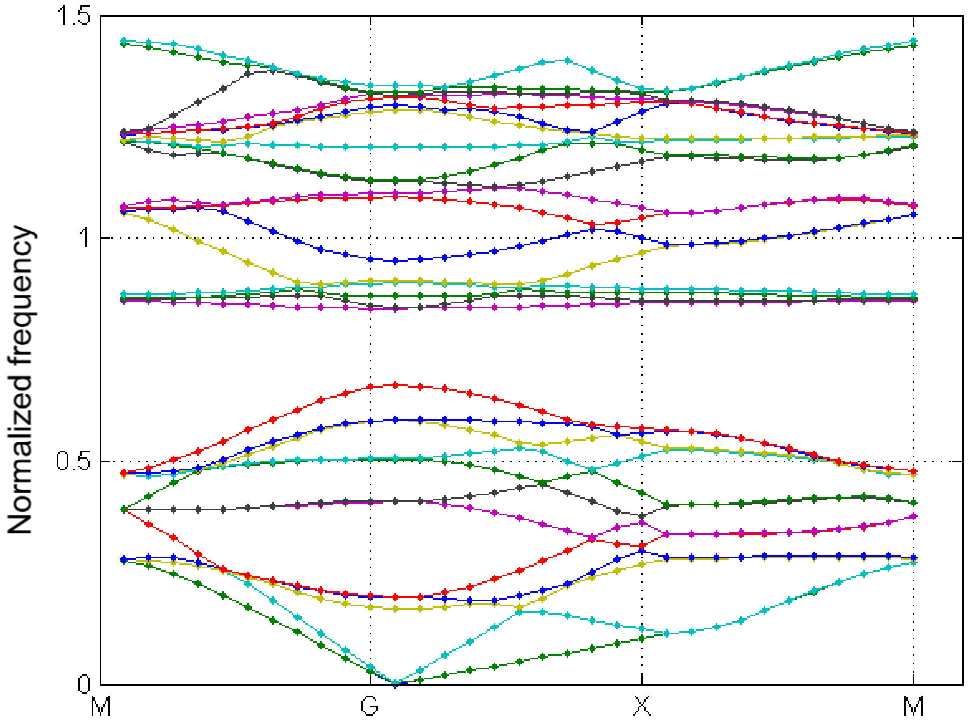
Wave propagation analysis

porosity = 60%





- Bloch wave analysis on SMP phononic crystal

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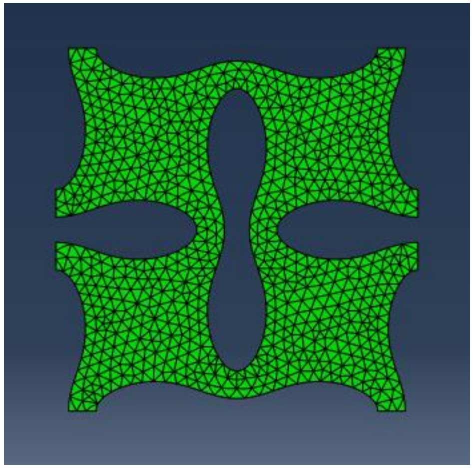
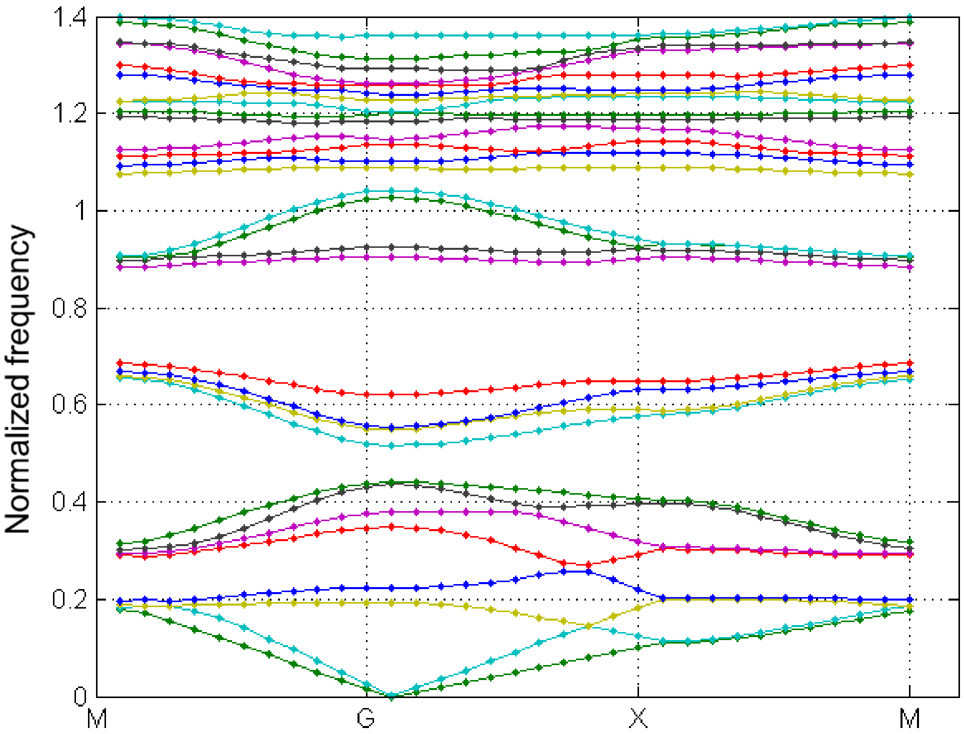
Wave propagation analysis

porosity = 60%





- Bloch wave analysis on SMP phononic crystal (compressed configuration)

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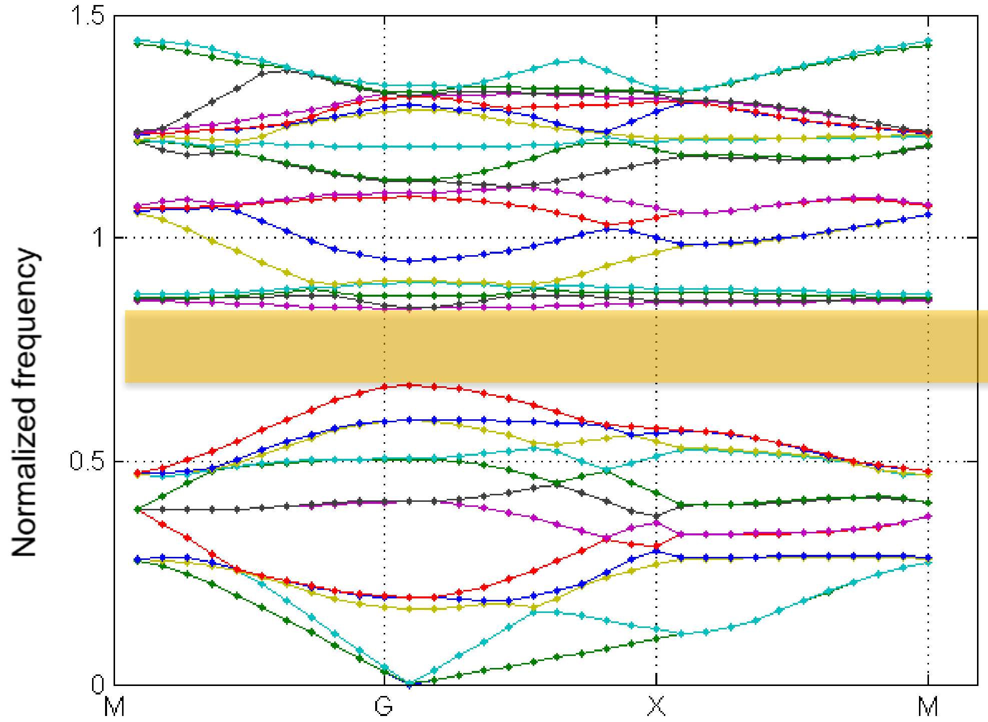
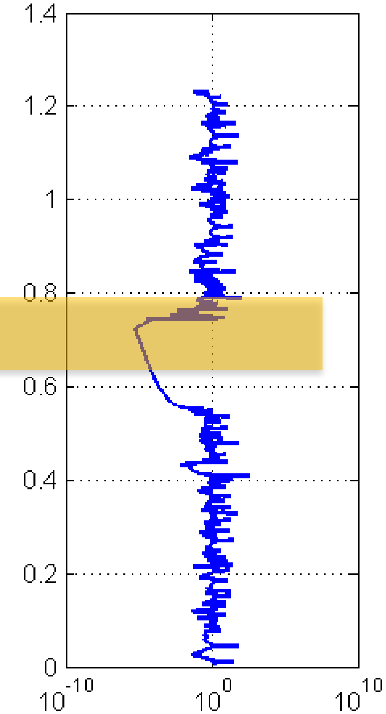
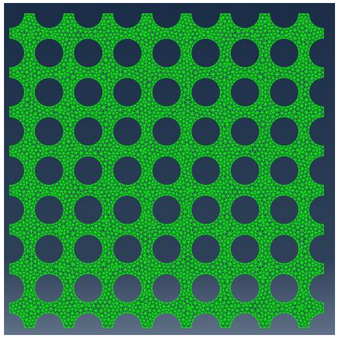
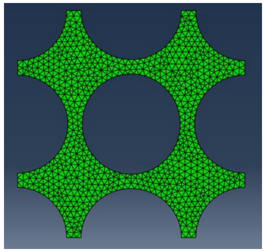
Wave propagation analysis

porosity = 60%









Bloch wave analysis + finite size analysis

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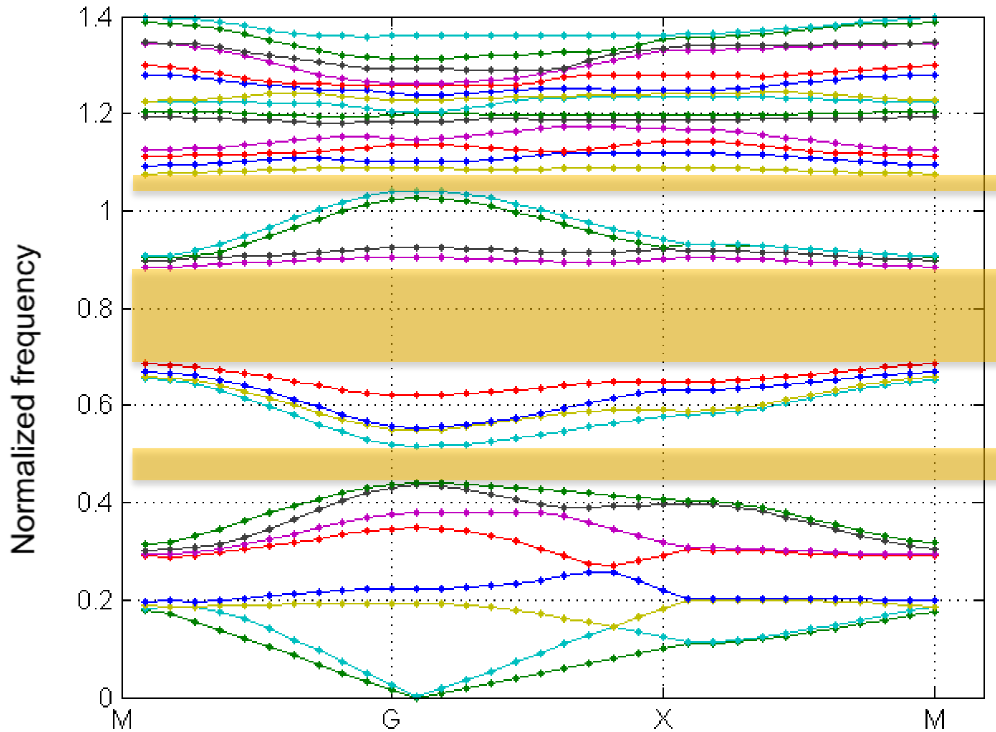
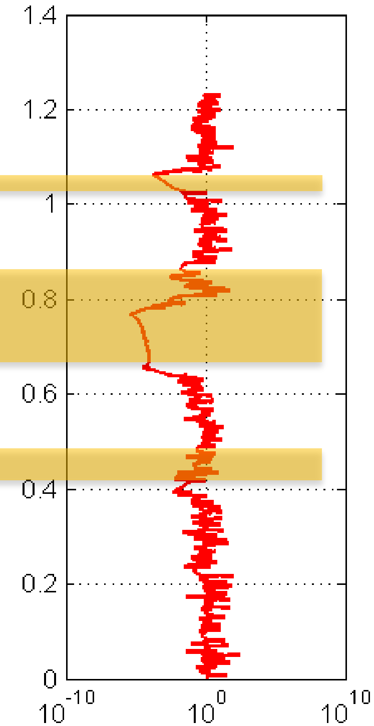
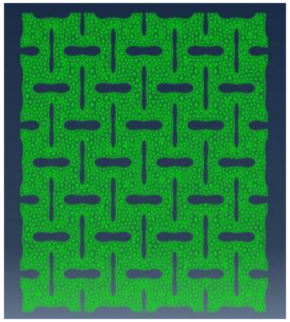
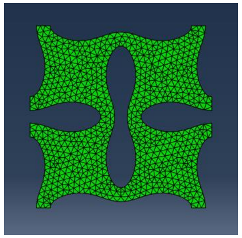
Wave propagation analysis

porosity = 60%









Bloch wave analysis + finite size analysis

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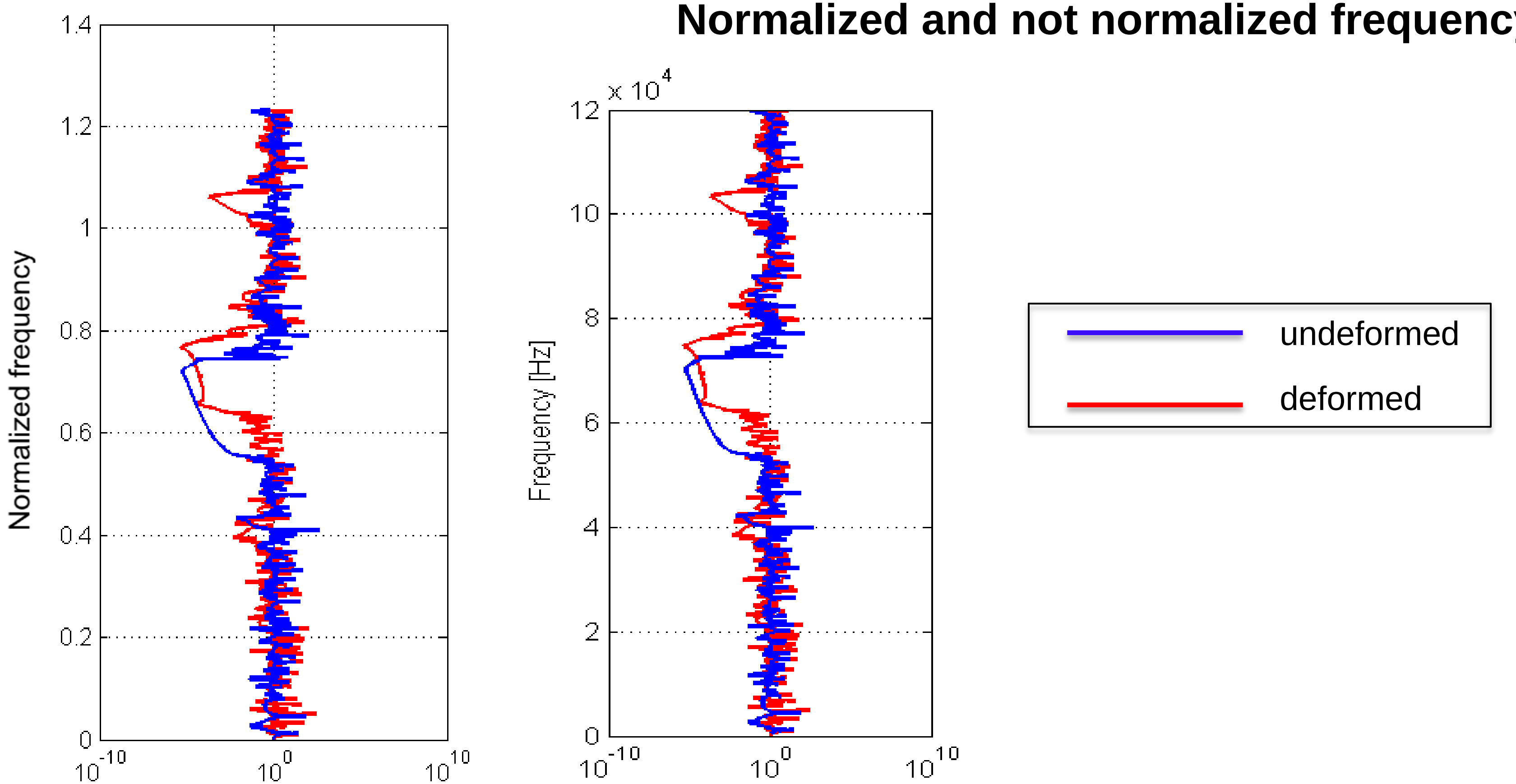
Wave propagation analysis

Finite-size:
Normalized and not normalized frequency



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Future work

- Experimental tests on waves propagation
- Find a SMP material with higher shape memory
- Further trials on diagonal structure

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Thank you

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