Training School on
Acoustic & Elastic (Meta)-Materials

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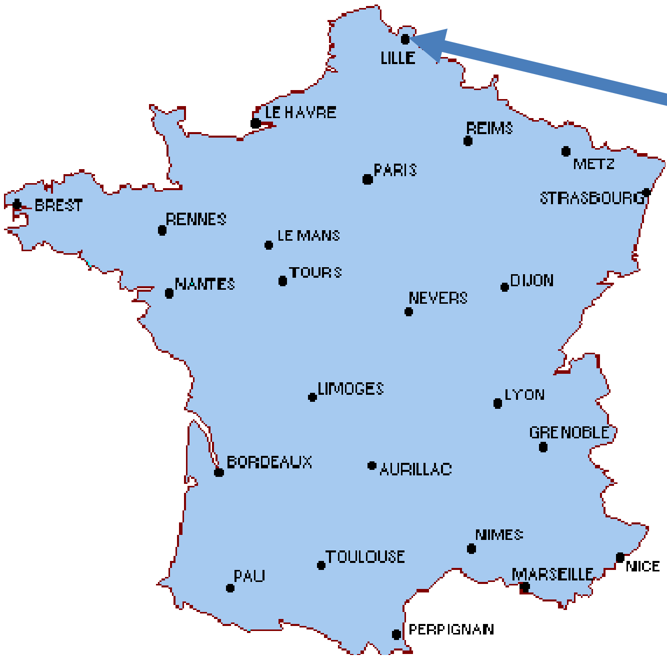
Basic theoretical tools for investigating periodic media



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Head : DR CNRS T. MELIN

ACOUSTICS GROUP

« PHONONIC CRYSTALS AND ACOUSTIC / ELASTIC METAMATERIALS »

- Tunable phononic crystals (piezoelectric / piezomagnetic constituents)
- Time-dependant phononic crystals
- Topological metamaterials
- Metamaterials for underwater acoustics

Basic theoretical tools for investigating periodic media

- *Direct Lattice / Reciprocal Lattice*
- *Brillouin zone / Irreducible Brillouin zone*
- *Dispersion relations (band structures)*
- *Plane Wave Expansion (PWE) method*

OUTLINE

Introduction : Infinite one-dimensional linear chains of atoms (mass-spring model)

I) Periodic structures and their properties (fundamental notions from the theory of crystalline solids) :

A) Bravais lattices, primitive vectors, Wigner-Seitz cells, examples

B) Reciprocal lattices, irreducible Brillouin zones, examples

II) **Periodic structures and band structures :**

A) Equations of propagation of elastic waves, Bloch theorem, Fourier series, Plane Wave Expansion (PWE) method for phononic crystals of infinite extent ("*bulk phononic crystals*"), band structures, advantages and drawbacks of the PWE method

B) Modified PWE method for complex band structures, complex wave vectors, evanescent waves, applications

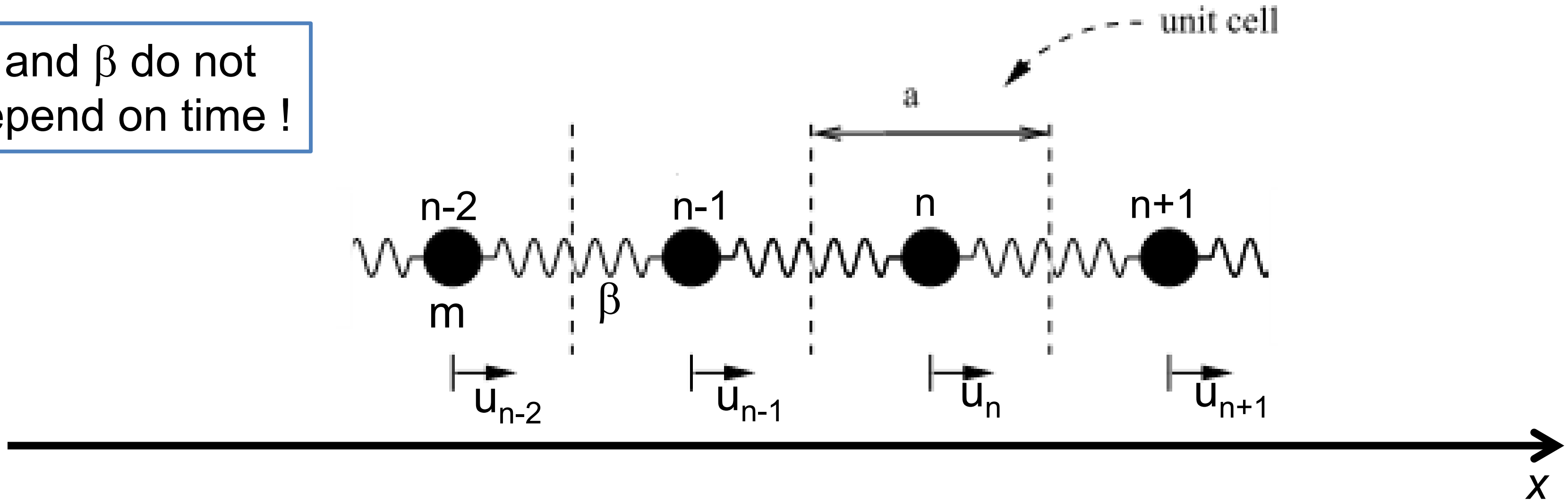
C) PWE method for *"phononic crystal plates"*

D) Comments

INTRODUCTION

A very simple periodic structure : an infinite one-dimensional linear chain of atoms of identical masses m, connected by springs with the same spring constant β

m and β do not depend on time !



Equilibrium position of atom n is $x_{n,eq}=na$ where a is the distance between two atoms in their equilibrium position.

Atoms are free to move slightly around their respective equilibrium position.

Position, at any date t, of moving atoms is given as $x_n(t)=na+u_n(t)$ with $|u_n(t)| << |x_n(t)|$ and $u_n = x_n - x_{n,eq} \equiv$ displacement of the n^{th} atom from the equilibrium position

a ≡ lattice spacing ≡ periodicity !!!

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Newton's second law applied to atom n (interaction between first neighbours)

$$\Rightarrow m\frac{d^2u_n}{dt^2} = -\beta(u_n - u_{n-1}) + \beta(u_{n+1} - u_n) = \beta(u_{n+1} + u_{n-1} - 2u_n)$$

Solutions ≡ propagating sinusoidal waves of the form $u_n(n,t) = U_0 e^{i(kna-\omega t)}$

$$\Rightarrow -m\omega^2 = \beta(e^{ika} + e^{-ika} - 2) = 2\beta(\cos(ka) - 1) = -4\beta\sin^2\left(\frac{ka}{2}\right) \Rightarrow \boxed{\omega(k) = \sqrt{\frac{4\beta}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|}$$

m ≡ mass (kg)

β ≡ spring constant ($N.m^{-1}$)

ω ≡ circular frequency ($rad.s^{-1}$)

a ≡ periodicity of the « direct lattice » (m)

k ≡ wave number (m^{-1}) = $\frac{2\pi}{\lambda}$ (λ ≡ wavelength (m))

↳ « reciprocal lattice »

⇒ *ω(k)* ≡ dispersion relation

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Note : If $ka \ll 1 \Leftrightarrow a \ll \lambda,\ \ \omega(k) \approx \sqrt{\frac{4\beta}{m}}.\frac{ka}{2} = a\sqrt{\frac{\beta}{m}}.k = C.k$

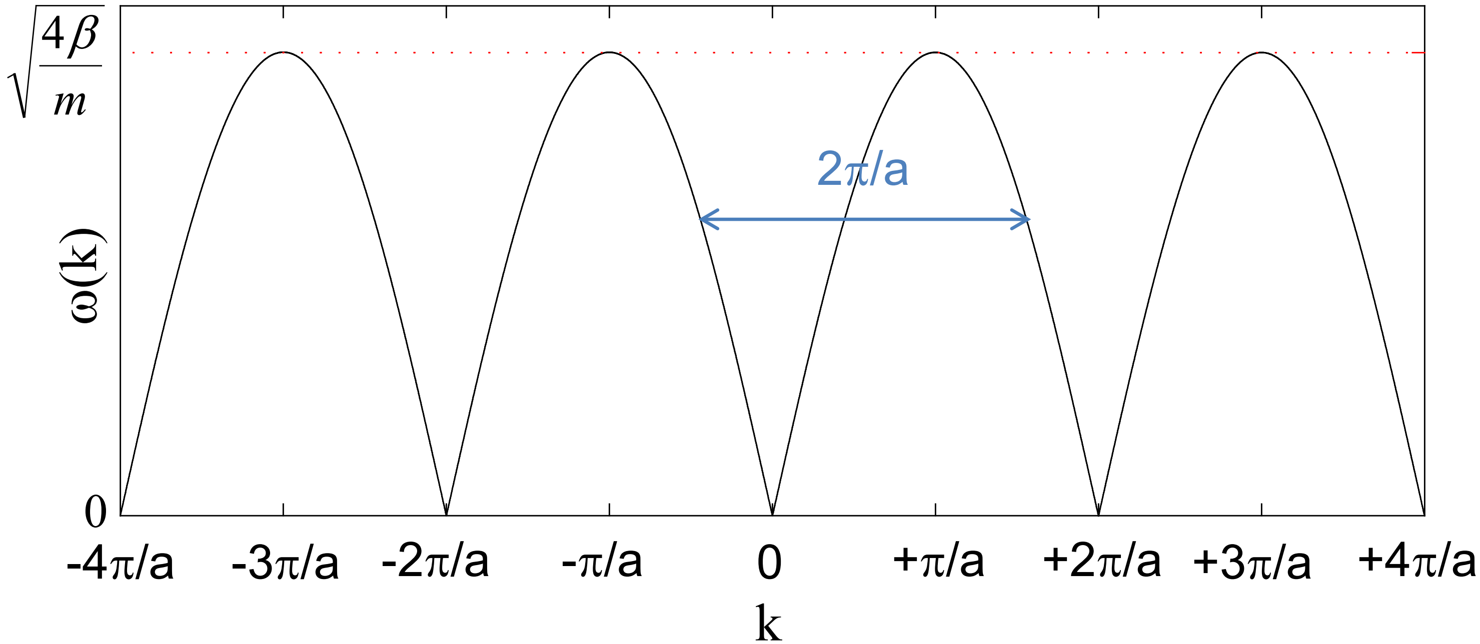
$\Rightarrow$ Linear dispersion relation where $[C] = m.\left(\frac{N.m^{-1}}{kg}\right)^{1/2} = m.\left(\frac{kg.m.s^{-2}m^{-1}}{kg}\right)^{1/2} = m.s^{-1}$

$\Rightarrow$ *C* has the same dimensions than a speed

$\Rightarrow$ Large wavelength limit $\Leftrightarrow$ Continuum limit

$\Rightarrow$ Phonons (periodic array of atoms)

$\leftrightarrow$ Elastic waves (homogeneous continuous medium)



$$|\sin x| \text{ is } \pi\text{-periodic} \Rightarrow \left|\sin\left(\frac{ka}{2}\right)\right| = \left|\sin\left(\frac{ka}{2}+\pi\right)\right| = \left|\sin\left(\frac{a}{2}\left(k+\frac{2\pi}{a}\right)\right)\right|$$

⇒ ω(k) is a periodic function of k with periodicity G=2π/a

⇒ ω(k+nG)=ω(k), n integer

⇒ A propagation mode of wave number k and a mode with wave number (k+G) are the same mode !!!

→ G is associated with the «reciprocal lattice» (periodicity 2π/a) of the chain («direct lattice» of periodicity a)

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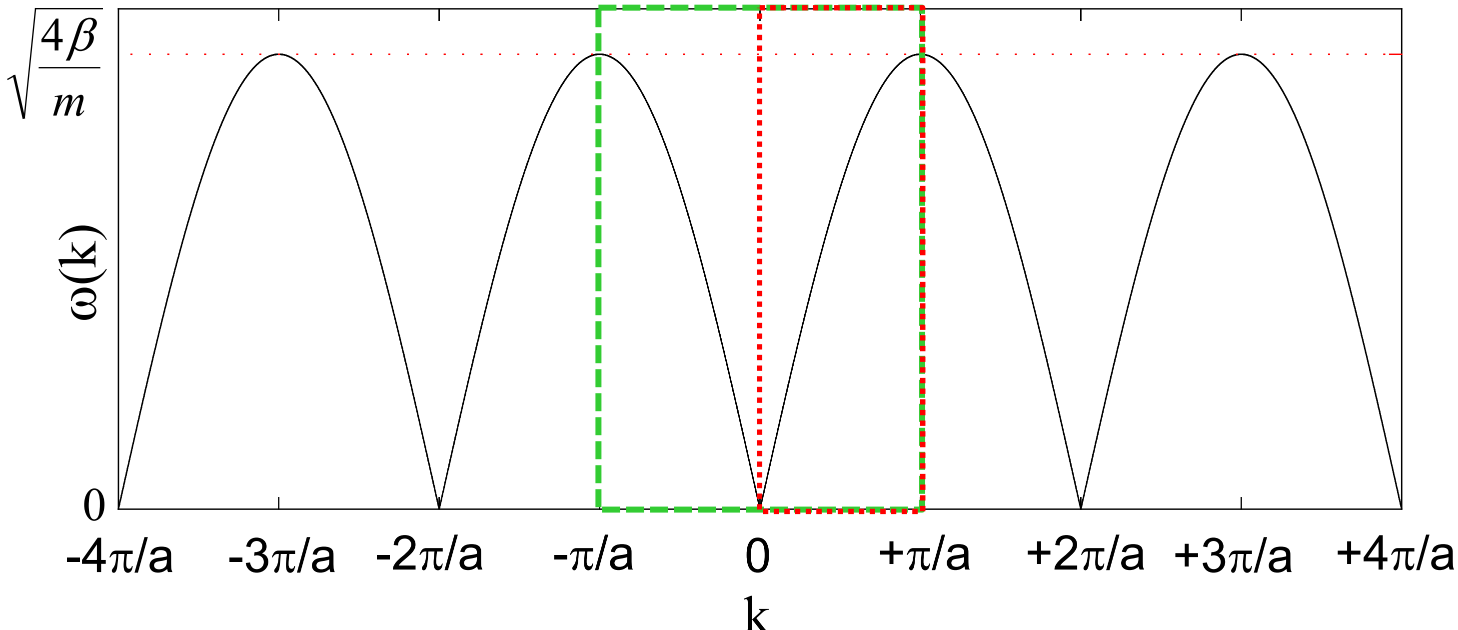
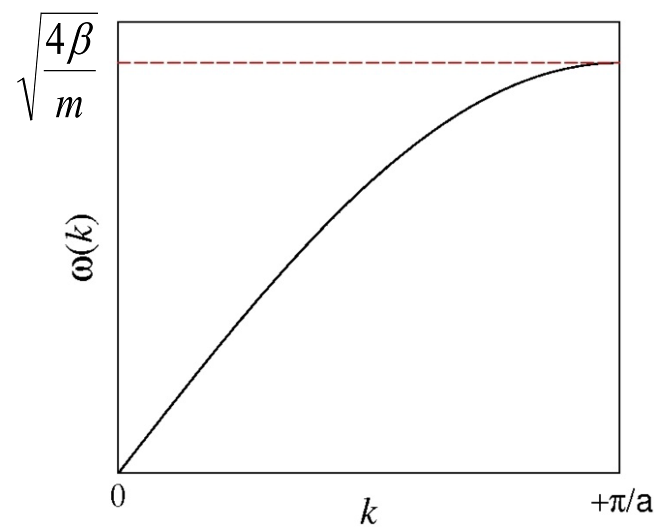


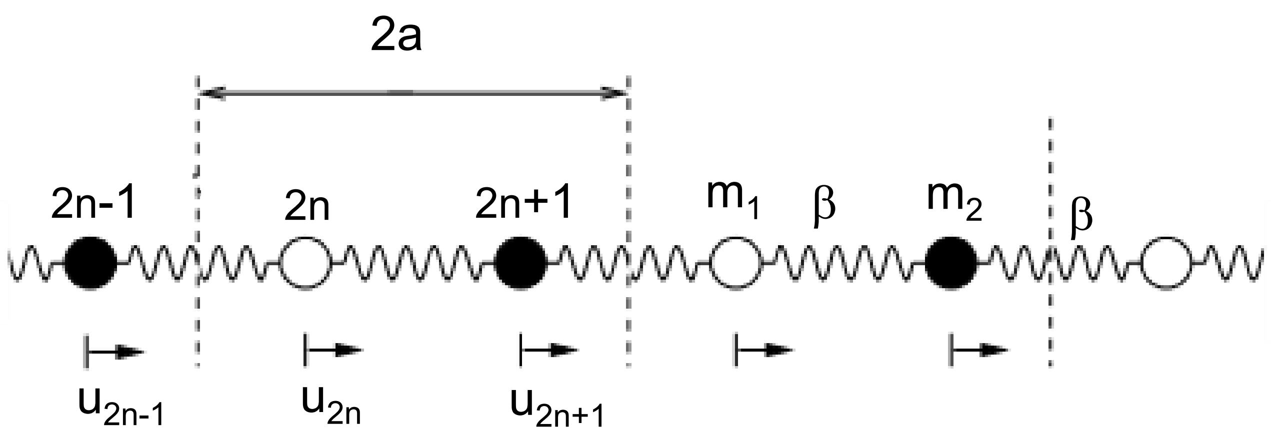
Due to the periodicity of the dispersion relation in the wave number space (reciprocal space), the useful information is contained in the waves with wave numbers lying between the limits –π/a and +π/a

⇔ 1D first Brillouin zone (centred on k=0)

Dispersion relation is also symmetric with respect of the plane k=0 (« reciprocity principle »), and one may focus the study on wave numbers ranging from 0 to +π/a ⇒ 1D Irreducible Brillouin zone



A bit more complicated periodic structure : an infinite one-dimensional linear chain with two atoms of different masses in the unit cell



Assumptions : - All the springs have the same constant β
- m_1, m_2 and β independent of time

The equations of motion of two adjacent odd (2n+1) and even (2n) atoms are

$$\begin{cases} m_1 \dfrac{d^2 u_{2n}}{dt^2} = -\beta(u_{2n} - u_{2n-1}) + \beta(u_{2n+1} - u_{2n}) = \beta(u_{2n+1} + u_{2n-1} - 2u_{2n}) \\ m_2 \dfrac{d^2 u_{2n+1}}{dt^2} = -\beta(u_{2n+1} - u_{2n}) + \beta(u_{2n+2} - u_{2n+1}) = \beta(u_{2n+2} + u_{2n} - 2u_{2n+1}) \end{cases}$$

Solutions ≡ propagating sinusoidal waves of the form $\begin{cases} u_{2n}(n,t) = Ae^{i(k2na-\omega t)} \\ u_{2n+1}(n,t) = Be^{i(k(2n+1)a-\omega t)} \end{cases}$

One obtains a set of two equations with 2 unknowns A and B

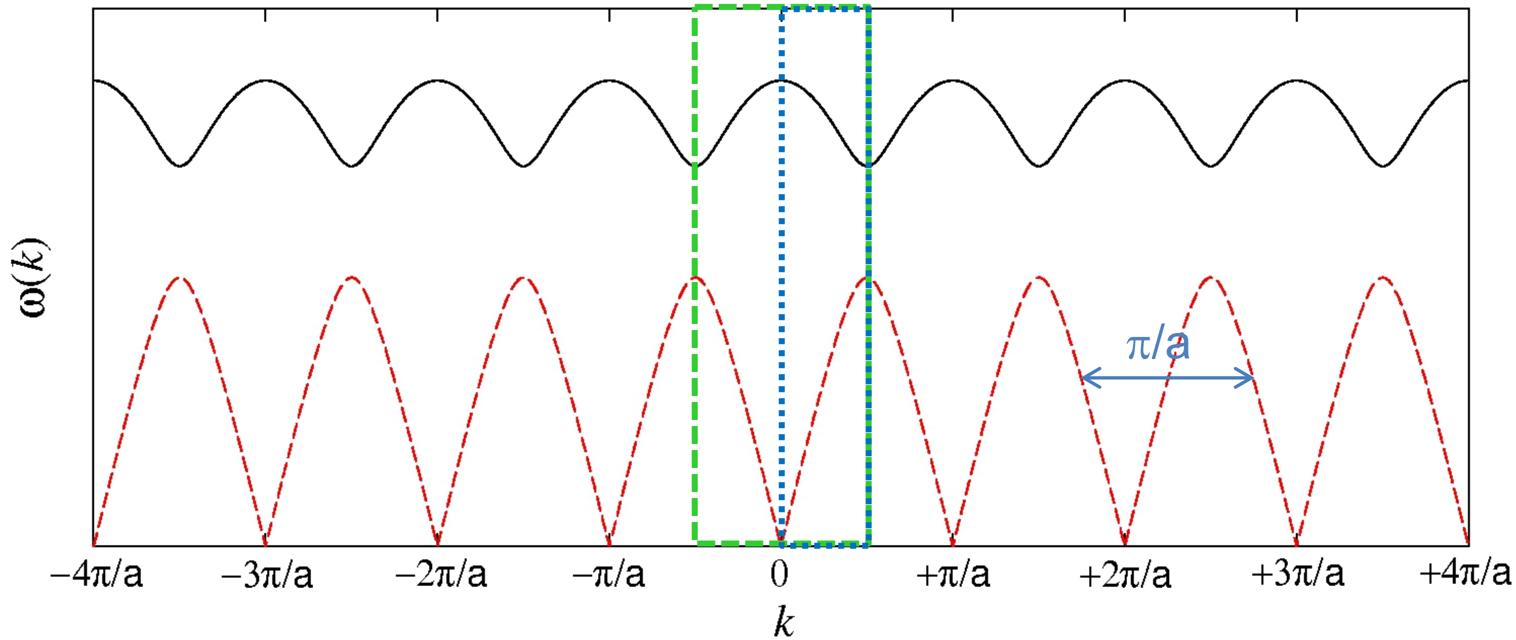
$$\begin{cases} -m_1\omega^2 A = \beta\left(Be^{ika} + Be^{-ika} - 2A\right) \\ -m_2\omega^2 B = \beta\left(Ae^{ika} + Ae^{-ika} - 2B\right) \end{cases} \Leftrightarrow \begin{cases} \left(2\beta - m_1\omega^2\right)A - 2\beta\cos(ka)B = 0 \\ 2\beta\cos(ka)A - \left(2\beta - m_2\omega^2\right)B = 0 \end{cases}$$

Non-trivial (A=B=0!!!) solutions of this set of equations are obtained if

$$\begin{vmatrix} 2\beta - m_1\omega^2 & -2\beta\cos(ka) \\ 2\beta\cos(ka) & -\left(2\beta - m_2\omega^2\right) \end{vmatrix} = 0 \quad \text{then} \quad \omega^4 - 2\beta\left(\frac{m_1+m_2}{m_1m_2}\right)\omega^2 + \frac{4\beta^2}{m_1m_2}\sin^2(ka) = 0$$

and $$\omega(k) = \sqrt{\beta\left(\frac{m_1+m_2}{m_1m_2}\right) \pm \sqrt{\beta^2\left(\frac{m_1+m_2}{m_1m_2}\right)^2 - \frac{4\beta^2}{m_1m_2}\sin^2(ka)}}$$

⇒ Two solutions, $\omega_-(k)$ and $\omega_+(k)$, that are periodic in wave number, k, with a period of π/a (due to the dependence with $\sin^2(ka)$ rather than $\sin^2(ka/2)$)



Periodicity of the «direct lattice» = 2a

⇒ Periodicity of the «reciprocal lattice» =2π/2a=π/a !

⇒ first Brillouin zone : $k \in [-\pi/2a, +\pi/2a]$

⇒ Irreducible Brillouin zone : $k \in [0, +\pi/2a]$

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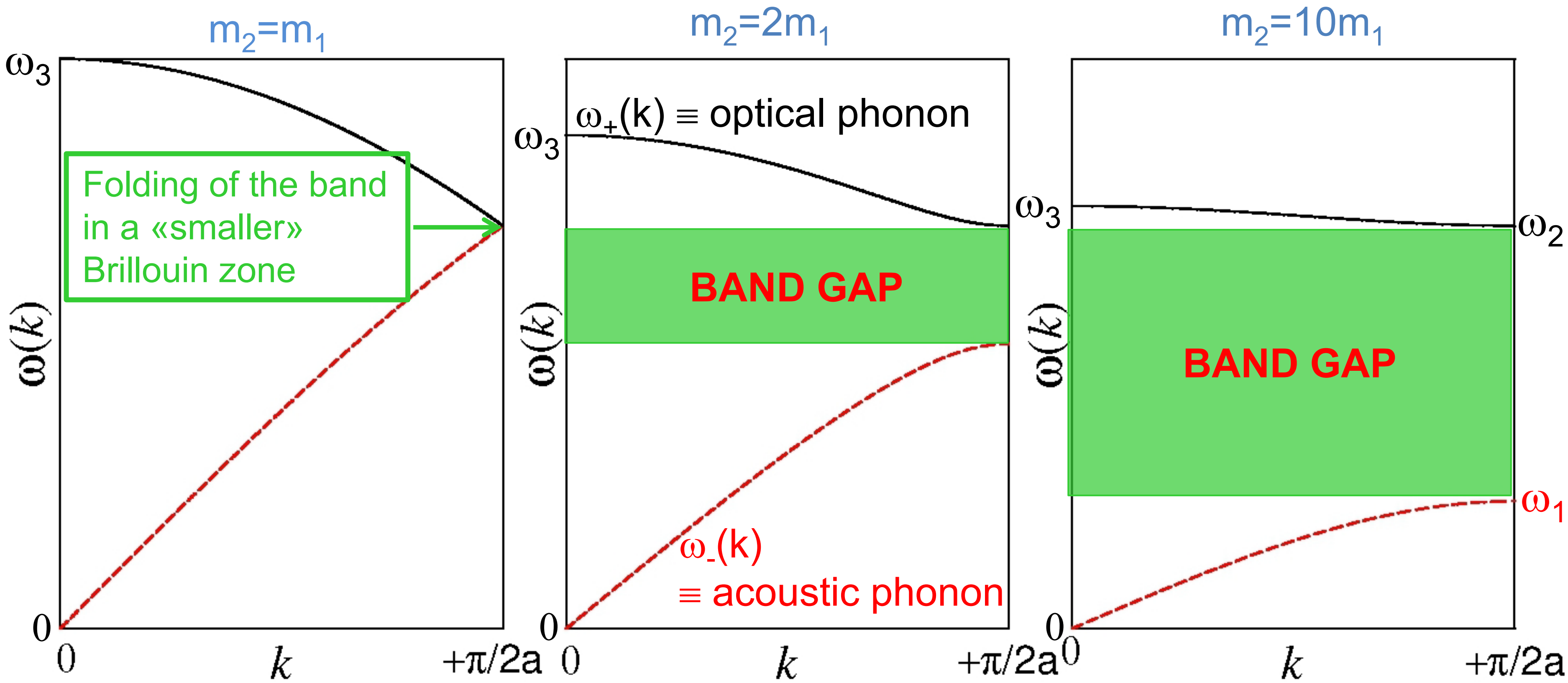


Band structure plotted in the irreducible Brillouin zone : $k \in [0, +\pi/2a]$

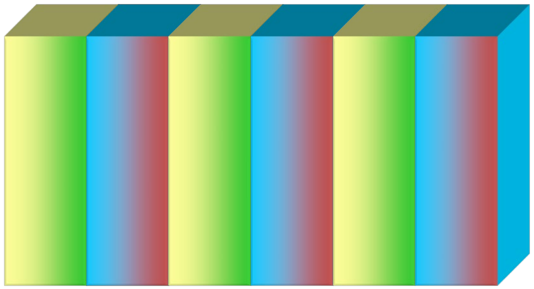
With two different atoms in the unit cell, the band structure exhibits a band gap (or stop band) for $\omega_1 < \omega < \omega_2$. Larger is m_2/m_1, larger is the gap!!!

$$\omega_1 = \sqrt{\frac{2\beta}{m_2}}, \omega_2 = \sqrt{\frac{2\beta}{m_1}}, \omega_3 = \sqrt{\frac{2\beta(m_1+m_2)}{m_1.m_2}}$$

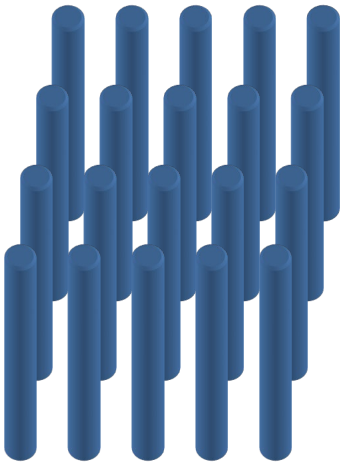
…. much more complicated periodic structures : the **phononic crystals**

Artificial crystals whose physical characteristics (elastic constants and density) are periodic functions of the position (1D, 2D, 3D)

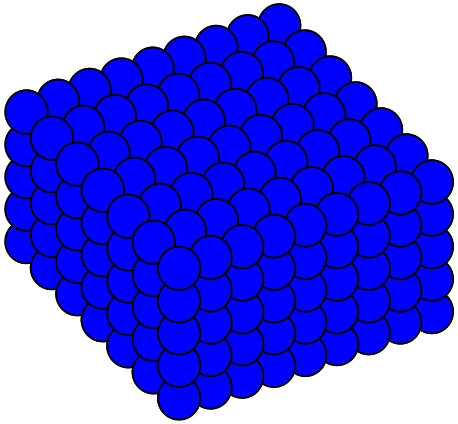
1D: Multilayers materials



2D: Array of cylinders of circular, square, … cross section embedded in a matrix



3D: Array of spheres, cubes, … embedded in a matrix



⇒ Study of such «artificial» crystals can be done using the same «tools» as those developed for «natural crystals» (direct and reciprocal lattices, Brillouin zones, band structures ….)

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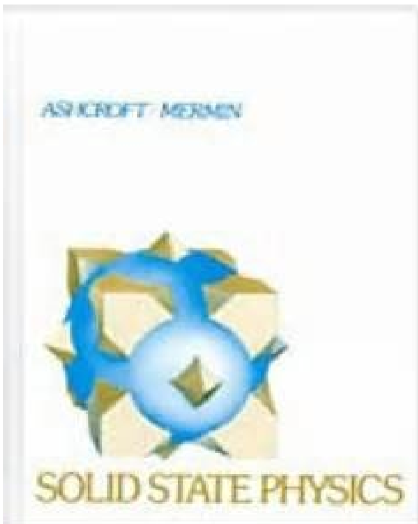
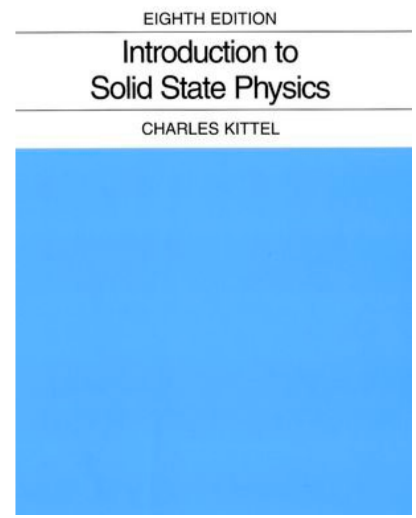
I - PERIODIC STRUCTURES AND THEIR PROPERTIES

A few elements of solid state physics …. necessary for the study of periodic structures properties ….

For more details, see ….



«*Solid State Physics*»,
N.W. Ashcroft and N.D. Mermin,
Saunders College,
Philadelphia, 1976



«*Introduction to Solid State Physics, 8th Edition*”, C. Kittel, Wiley, 2004

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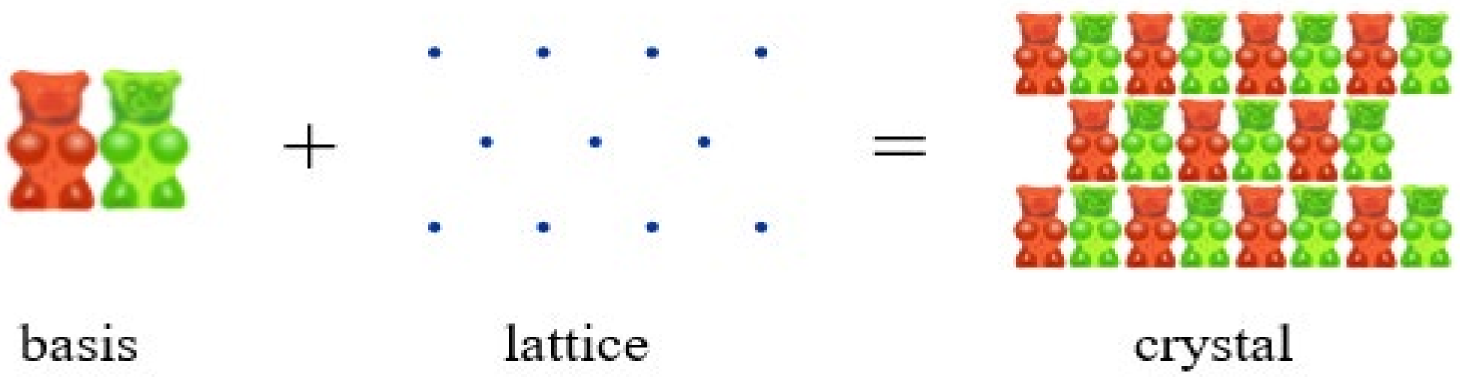
A) Bravais lattices, primitive vectors, Wigner-Seitz cells, examples

« Crystals are periodic arrays of atoms »

Crystal ≡ Bravais lattice+basis

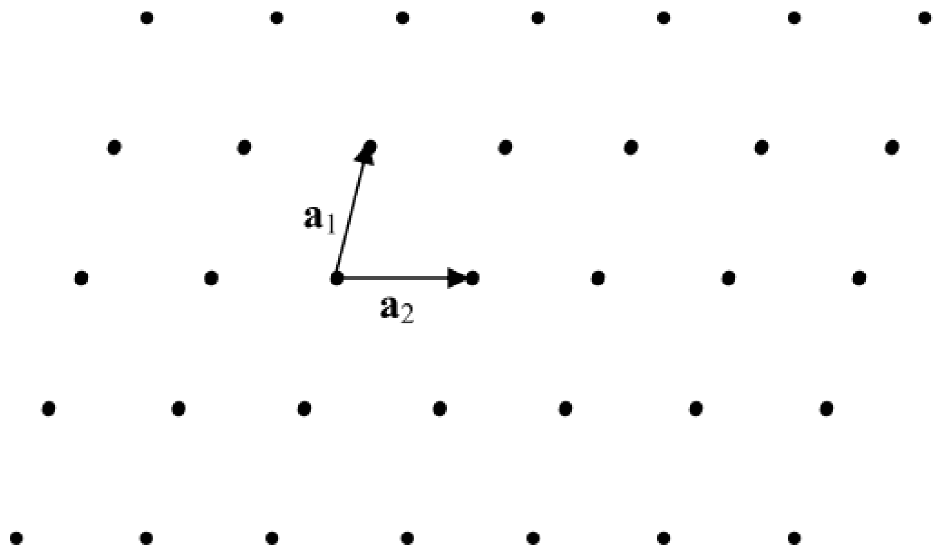


Basis is attached to each point of the Bravais lattice
Basis may contain several atoms

Bravais lattice ≡ An infinite array of discrete points (or atoms) with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed (all the points have the same environment).

In 3D, from the mathematical point of view, a **Bravais lattice** is a collection of points with position vectors $\vec{R}$ of the form $\vec{R} = n\vec{a}_1 + m\vec{a}_2 + l\vec{a}_3$ where $\vec{a}_1, \vec{a}_2, \text{and } \vec{a}_3$ are three vectors (the primitive vectors of the Bravais lattice) not in the same plane and *n, m* and *l* are three integers

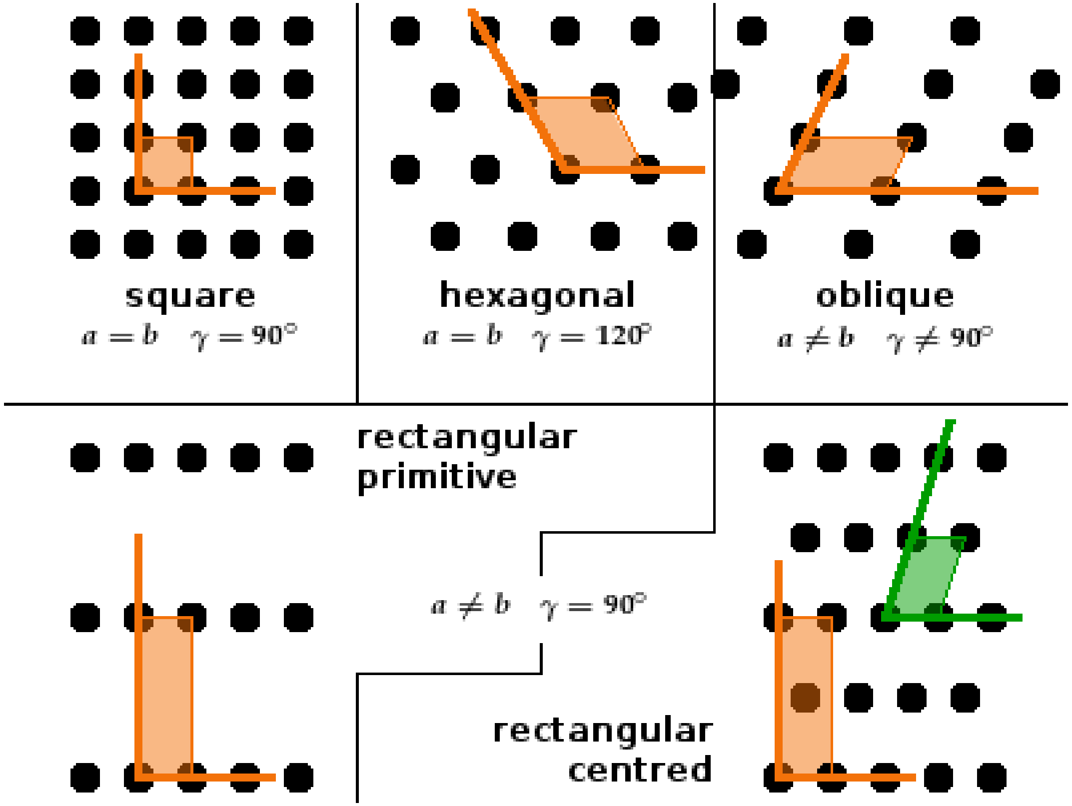
An example in 2D



The choice of primitive vectors is not unique!!!!

1 Bravais lattice in 1D !!

5 Bravais lattices in 2D



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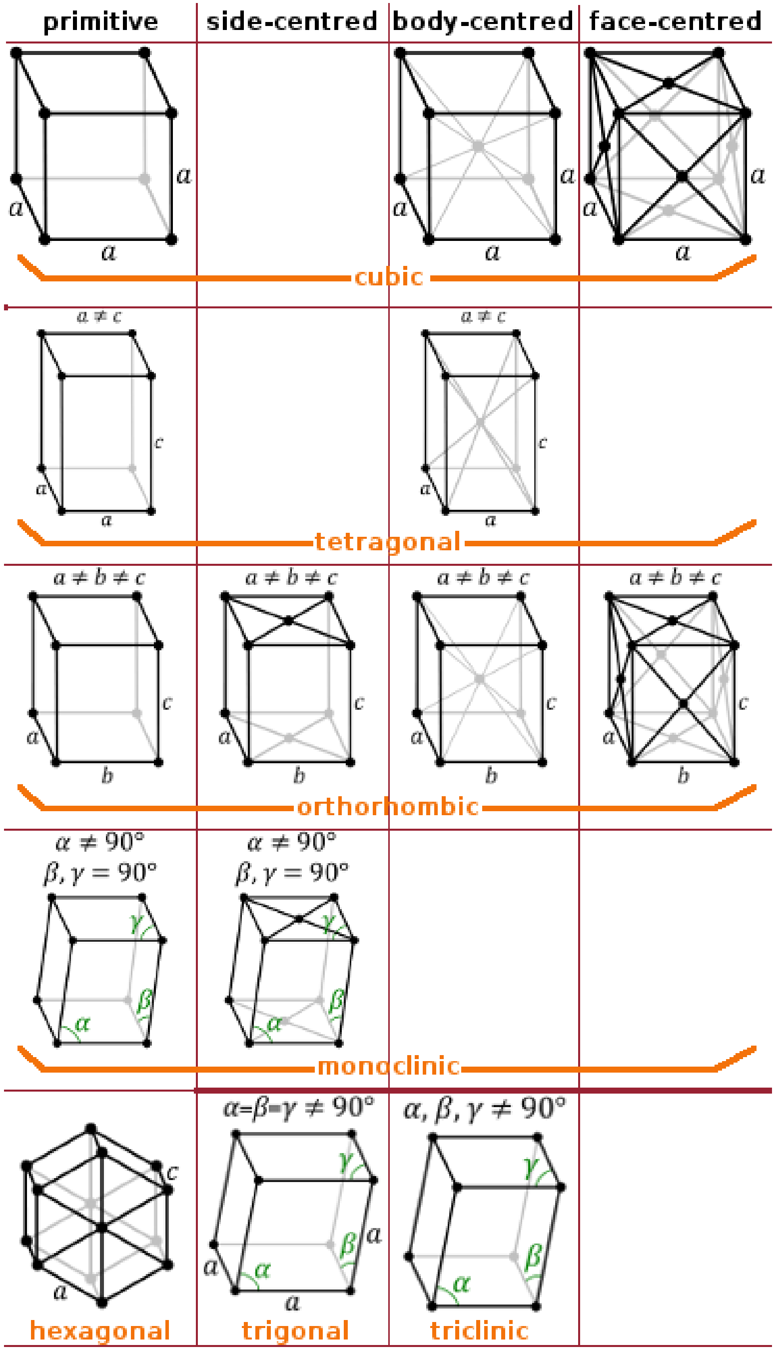
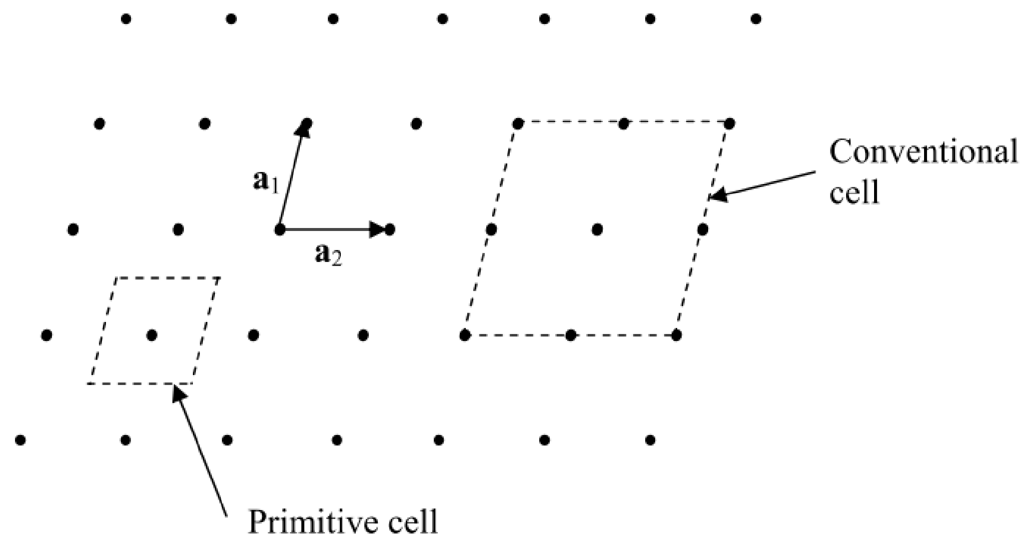
14 Bravais lattices in 3D



Primitive cell : Volume of space that contains precisely one lattice point and can be translated through all the vectors of a Bravais lattice to fill all the space without overlapping itself or leaving voids



There is no unique way of choosing a primitive cell …..

« Conventional cell » does not contain one lattice point

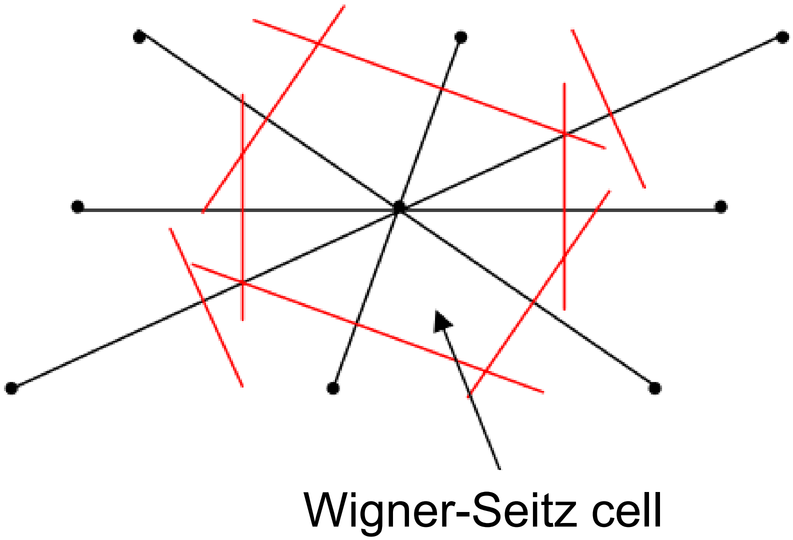
<u>One particular primitive cell</u>: The Wigner-Seitz cell

A Wigner-Seitz cell is a primitive cell constructed by the following method:

(i) draw lines to connect a given lattice point to all nearby lattice points;

(ii) at the mid point and normal to these lines, draw new lines or planes;

(iii) the smallest volume enclosed by these new lines or planes is the Wigner-Seitz cell.



The Wigner-Seitz cell has the full symmetry of the underlying Bravais lattice

Bravais lattice ≡ Direct lattice (defined in the real space)

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B) Reciprocal lattices, irreducible Brillouin zones, examples

For any function $f(\vec{r})$ periodic in the direct lattice, there exists a set of vectors $\vec{G}$

such as $f(\vec{r}) = \sum_{\vec{G}} f(\vec{G}) e^{i\vec{G}\cdot\vec{r}}$ (Fourier series)

In the Bravais lattice, a periodic function satisfies

$$f(\vec{r}) = f(\vec{r}+\vec{R}) \text{ where } \vec{R} = n\vec{a}_1 + m\vec{a}_2 + l\vec{a}_3$$

$$\Rightarrow f(\vec{r}+\vec{R}) = \sum_{\vec{G}} f(\vec{G}) e^{i\vec{G}\cdot(\vec{r}+\vec{R})} = f(\vec{r}) = \sum_{\vec{G}} f(\vec{G}) e^{i\vec{G}\cdot\vec{r}}$$

$$\Rightarrow e^{i\vec{G}\cdot\vec{R}} = 1$$

$$\Rightarrow \vec{G}\cdot\vec{R} = 2\pi.N \quad \text{where } N \equiv \text{integer}$$

Reciprocal lattice : It is a set of points whose positions are given by a set of vectors $\vec{G}$ (the reciprocal lattice vectors) satisfying the condition $\vec{G}\cdot\vec{R} = 2\pi.N$ where $N \equiv$ integer, for all $\vec{R}$ in the Bravais lattice

EXERCISE : How to define the reciprocal lattice vectors $\vec{G}$?

- Assumption : Because $\vec{R}$ is a linear combination of the primitive vectors $\{\vec{a_i}\}$, $\vec{G}$ may be written also as a linear combination of some basis vectors $\{\vec{b_j}\}$ as $\vec{G} = n'\vec{b_1} + m'\vec{b_2} + \ell'\vec{b_3}$ where n', m', ℓ' and the $\{\vec{b_j}\}$ are initially undefined

* Constraint : One imposes that $\vec{a_i}.\vec{b_j} = 2\pi\delta_{i,j}, \ldots (i,j) \in (1,2,3)$

$\Longrightarrow \vec{G}.\vec{R} = nn' + mm' + \ell\ell' = N$ integer

$\Longrightarrow n',\ m'$ and ℓ' are integers ! $\Rightarrow$ A reciprocal lattice of a direct lattice is also a Bravais lattice !!

- Define $\{\vec{b_j}\}$ as an orthonormal basis?

  $\rightarrow$ Consider $\vec{b_1}$:

$\vec{b_1} \perp \vec{a_2}$ and $\vec{b_1} \perp \vec{a_3} \Longrightarrow \vec{b_1}$ is colinear to $\vec{a_2} \times \vec{a_3}$ $(\times \equiv \text{cross product})$ and

$$\vec{b_1} = \gamma\vec{a_2} \times \vec{a_3} \text{ where } \gamma \text{ is a constant to be determined}$$

$$\rightarrow \vec{a_1}.\vec{b_1} = 2\pi = \vec{a_1}.(\gamma\vec{a_2} \times \vec{a_3}) \Longrightarrow \gamma = \frac{2\pi}{\vec{a_1}.(\vec{a_2} \times \vec{a_3})}$$

$$\Rightarrow \vec{b_1} = 2\pi \frac{\vec{a_2} \times \vec{a_3}}{\vec{a_1}.(\vec{a_2} \times \vec{a_3})}$$

$\rightarrow \vec{b_2}$ and $\vec{b_3}$ can be derived in the same way …

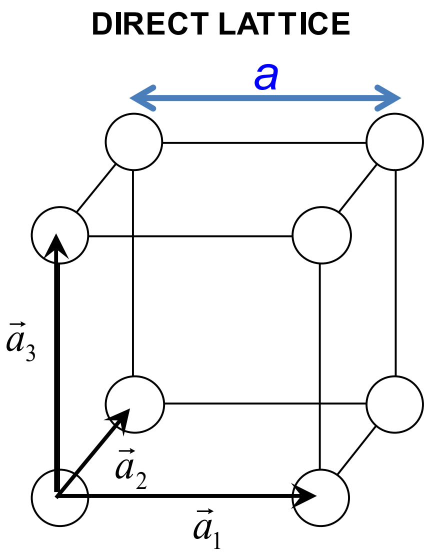
⇒ We have shown that :

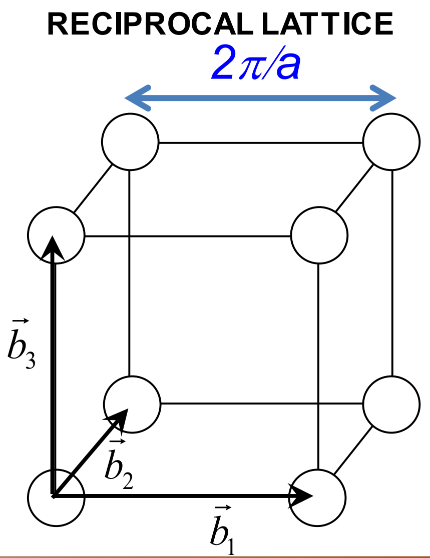
If $\vec{a}_1, \vec{a}_2$ and $\vec{a}_3$ are the primitive vectors of the direct lattice, then the primitive vectors $\vec{b}_1, \vec{b}_2$ and $\vec{b}_3$ of the reciprocal lattice are given in 3D as

$$\begin{cases} \vec{b}_1 = 2\pi \dfrac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1.(\vec{a}_2 \times \vec{a}_3)} \\ \vec{b}_2 = 2\pi \dfrac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_2.(\vec{a}_3 \times \vec{a}_1)} \\ \vec{b}_3 = 2\pi \dfrac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_3.(\vec{a}_1 \times \vec{a}_2)} \end{cases}$$

and $\vec{G} = n'\vec{b}_1 + m'\vec{b}_2 + l'\vec{b}_3$ where n', m', l' integers

An example in 3D : Simple-cubic direct lattice (of lattice parameter a) and its reciprocal lattice (of lattice parameter $2\pi/a$). The reciprocal lattice is also a Bravais lattice….





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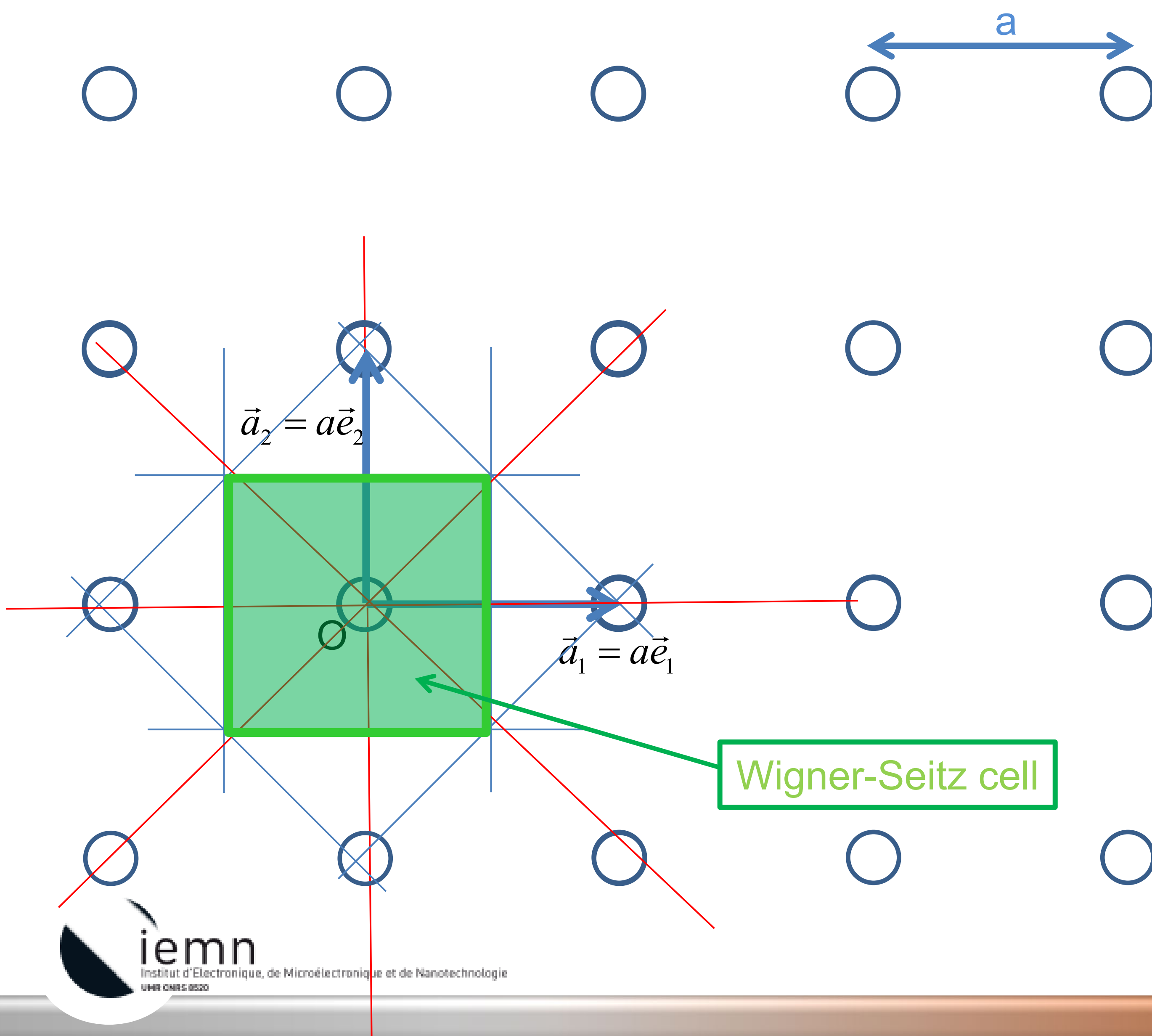
Brillouin zone :

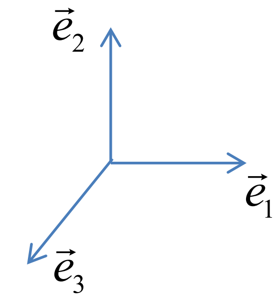
The reciprocal lattice is a Bravais lattice

$\Rightarrow$ One may define a Wigner-Seitz cell for the reciprocal lattice

$\Leftrightarrow$ The first Brillouin zone

An example in 2D : the square lattice of lattice parameter a





$(\overrightarrow{e_1}, \overrightarrow{e_2}, \overrightarrow{e_3})$ ≡ orthonormal basis in the 3D space

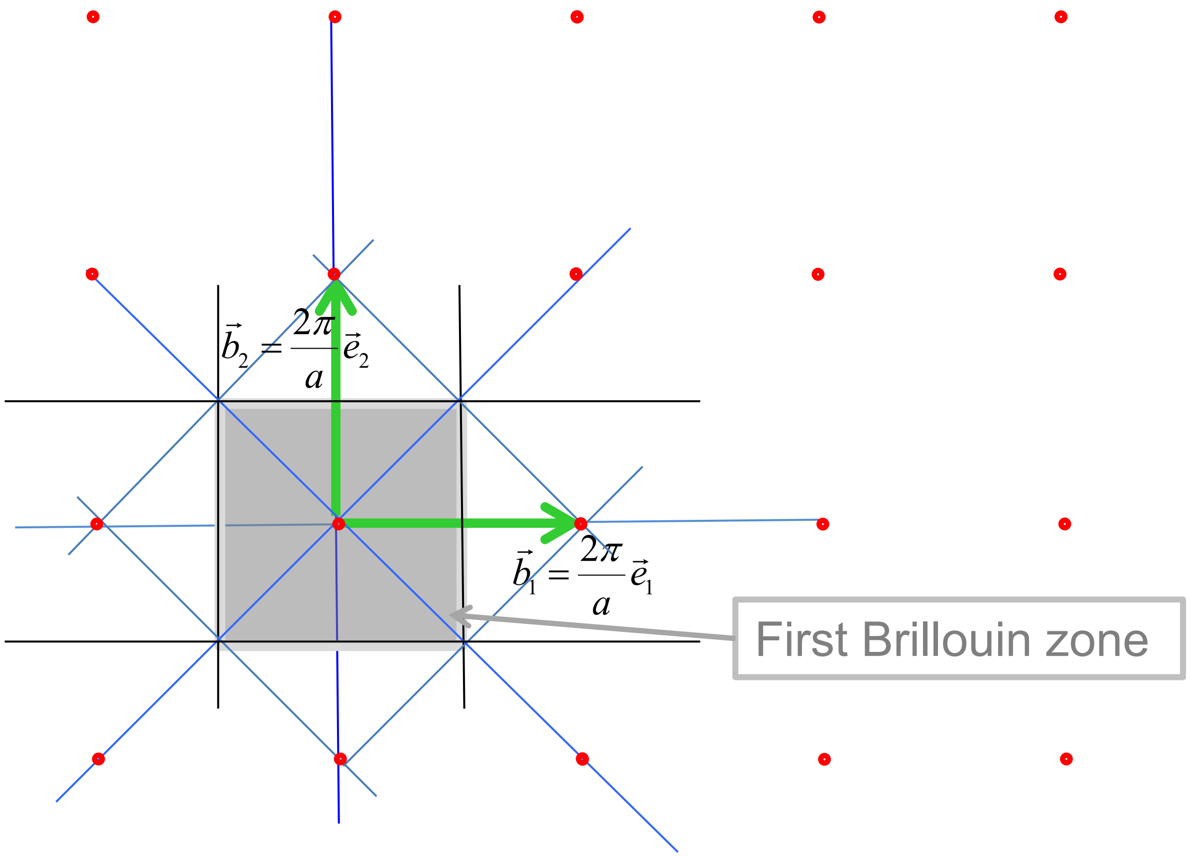
2D Direct lattice of primitive vectors

$$\begin{cases} \overrightarrow{a_1} = a\ \overrightarrow{e_1} \\ \overrightarrow{a_2} = a\ \overrightarrow{e_2} \end{cases}$$

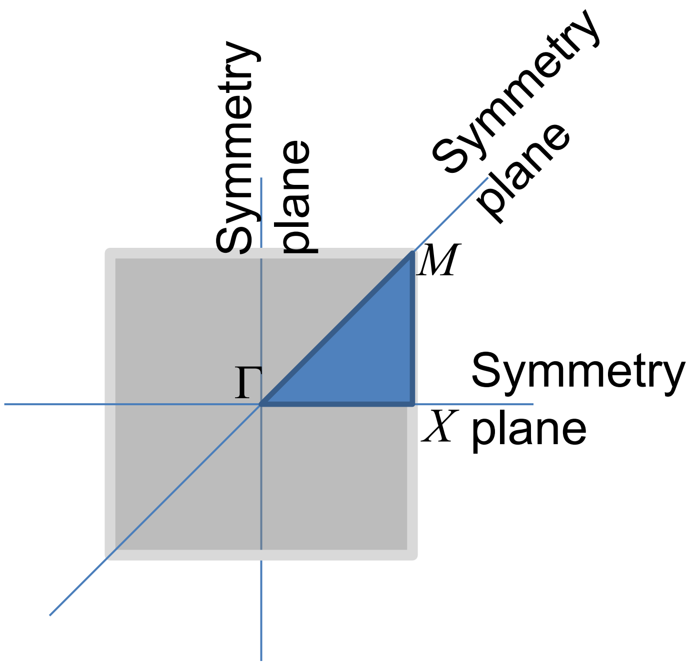
2D Reciprocal lattice of primitive vectors …

$$\begin{cases} \vec{b}_1 = 2\pi \dfrac{\vec{a}_2 \times \vec{e}_3}{\vec{a}_1.(\vec{a}_2 \times \vec{e}_3)} = 2\pi \dfrac{a\vec{e}_2 \times \vec{e}_3}{a\vec{e}_1.(a\vec{e}_2 \times \vec{e}_3)} = 2\pi \dfrac{a\vec{e}_1}{a\vec{e}_1.(a\vec{e}_1)} = \dfrac{2\pi}{a}\vec{e}_1 \\ \vec{b}_2 = 2\pi \dfrac{\vec{e}_3 \times \vec{a}_1}{\vec{a}_2.(\vec{e}_3 \times \vec{a}_1)} = \dfrac{2\pi}{a}\vec{e}_2 \end{cases}$$

$$\vec{G} = m'\overrightarrow{b_1} + n'\overrightarrow{b_2}$$



Due to the symmetries of the first Brillouin zone, study can be limited to the triangle ΓXM



Irreducible Brillouin zone *ΓXM*

$$\Gamma : \overrightarrow{\Gamma\Gamma} = \vec{0} \Rightarrow \Gamma : \frac{2\pi}{a}(0,0),$$

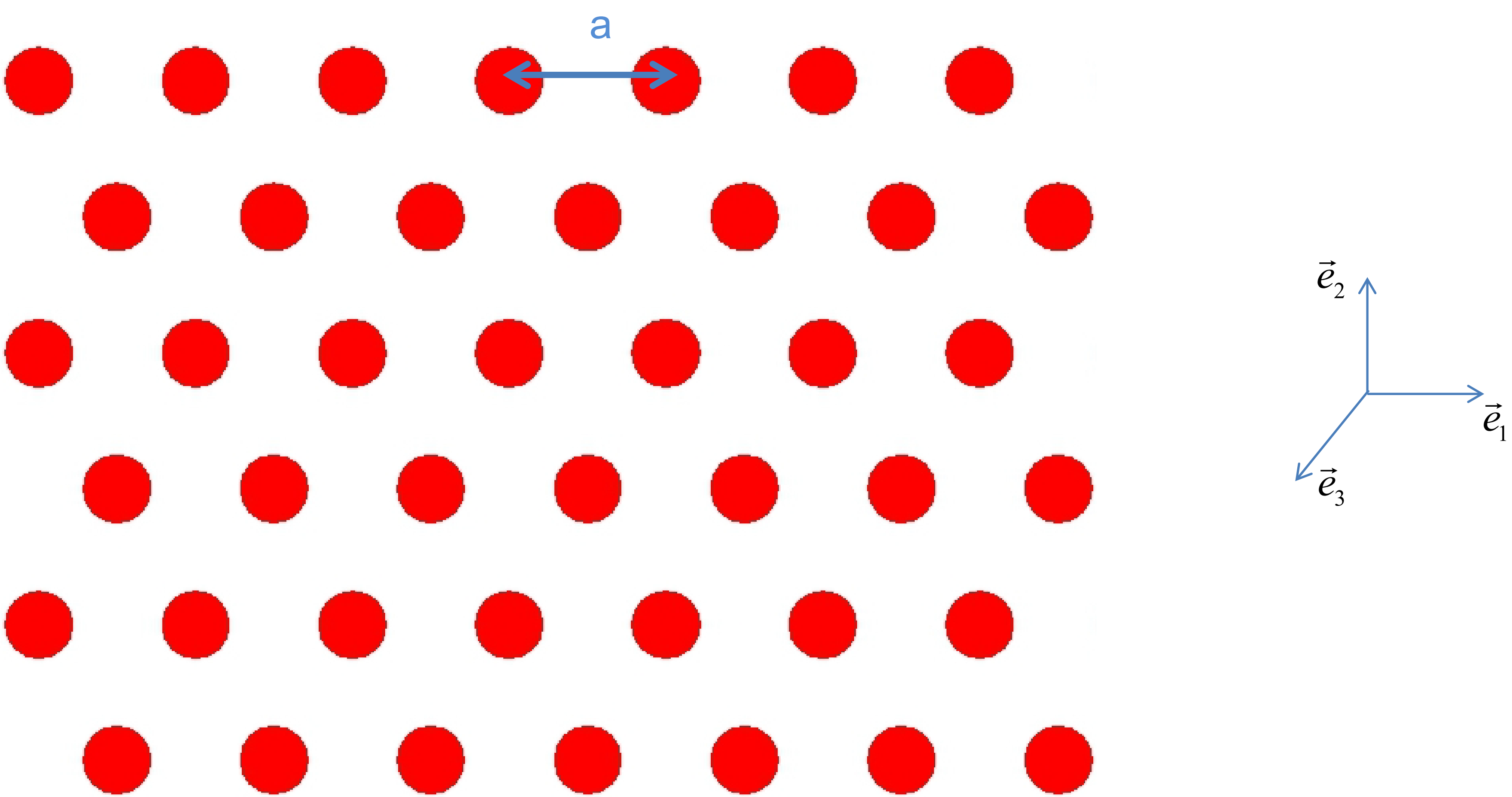
$$X : \overrightarrow{\Gamma X} = \frac{\vec{b}_1}{2} \Rightarrow X : \frac{2\pi}{a}\left(\frac{1}{2},0\right),$$

$$M : \overrightarrow{\Gamma M} = \frac{\vec{b}_1 + \vec{b}_2}{2} \Rightarrow M : \frac{2\pi}{a}\left(\frac{1}{2},\frac{1}{2}\right).$$

Γ, X, M : points of high symmetry

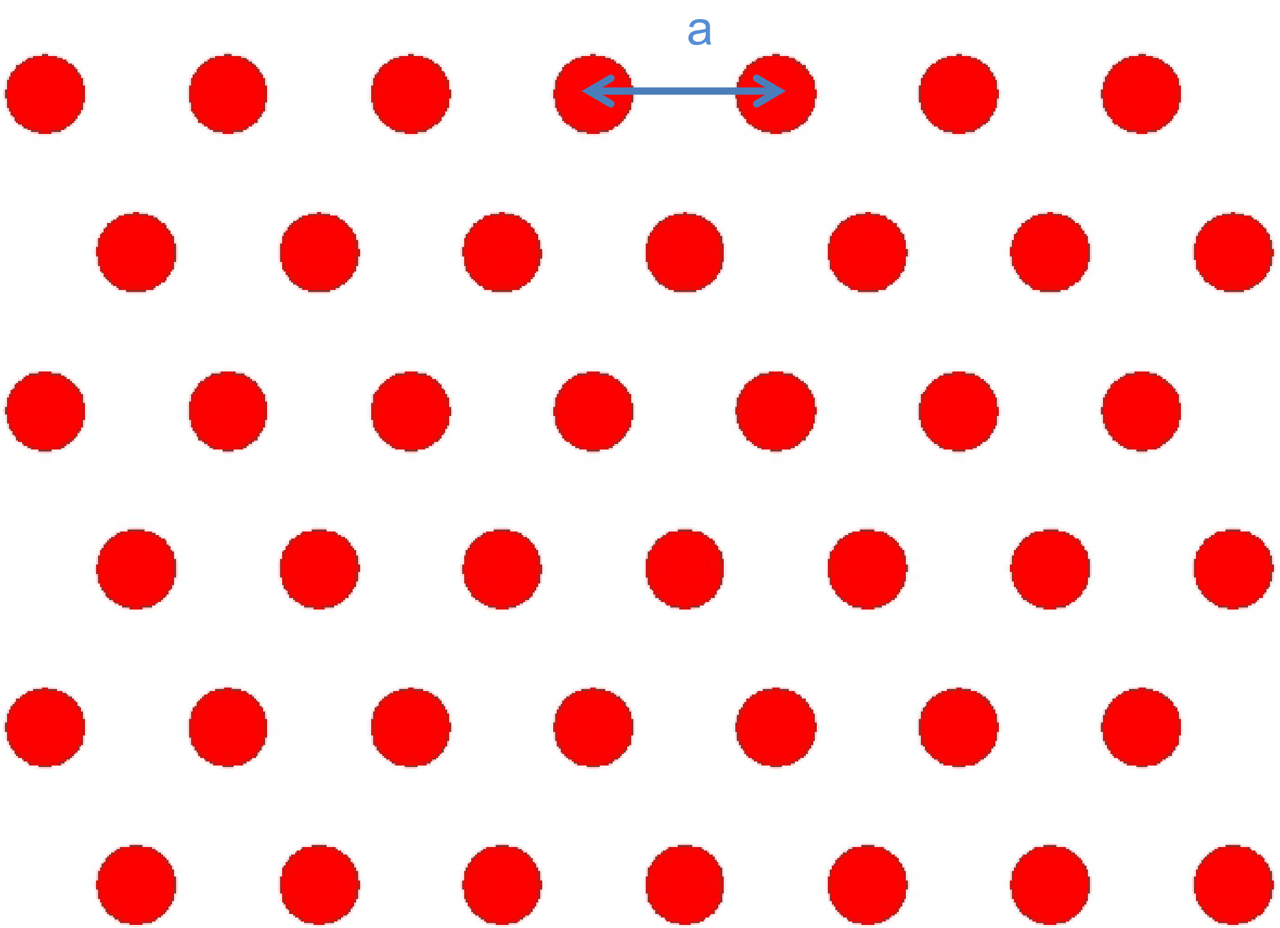
⇒ *Calculation of the band structure for a wave vector describing the periphery of the irreducible Brillouin zone*

EXERCISE : 2D hexagonal (or triangular) array of lattice parameter a



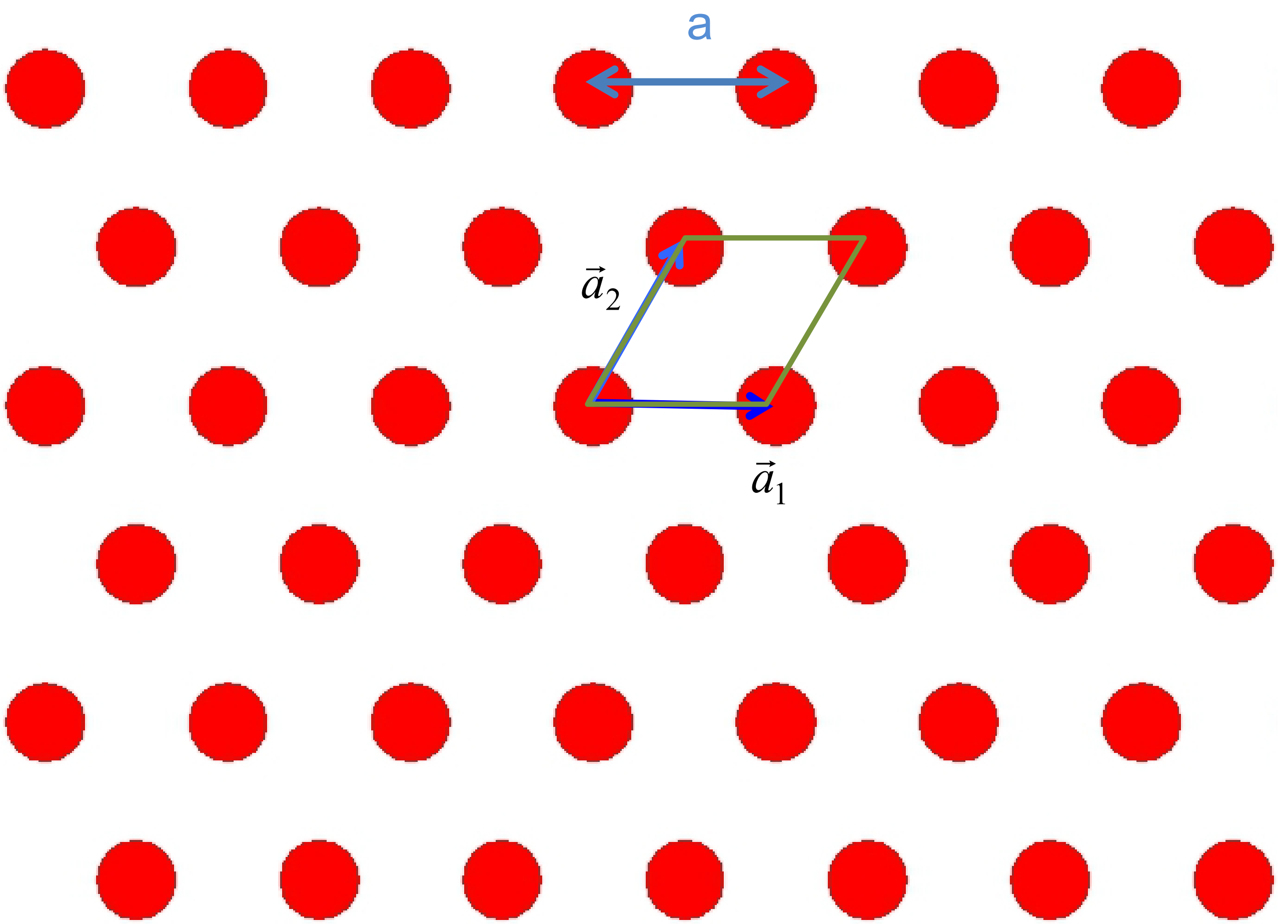
EXERCISE : 2D hexagonal (or triangular) array of lattice parameter a

1) Define a primitive unit cell and primitive lattice vectors

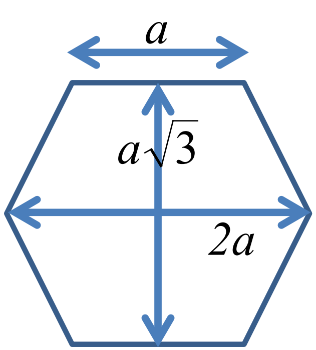


EXERCISE : 2D hexagonal (or triangular) array of lattice parameter a

1) Define a primitive unit cell and primitive lattice vectors



$$\begin{cases} \vec{a}_1 = a\vec{e}_1 \\ \vec{a}_2 = \frac{a}{2}\vec{e}_1 + \frac{a\sqrt{3}}{2}\vec{e}_2 \end{cases}$$



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EXERCISE : 2D hexagonal (or triangular) array of lattice parameter a

2) Define the reciprocal lattice vectors

$$\begin{cases} \vec{a}_1 = a\vec{e}_1 \\ \vec{a}_2 = \frac{a}{2}\vec{e}_1 + \frac{a\sqrt{3}}{2}\overrightarrow{e_2} \end{cases}$$

$$\begin{cases} \vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{e}_3}{\vec{a}_1 . (\vec{a}_2 \times \vec{e}_3)} = 2\pi \frac{1}{a^2 \frac{\sqrt{3}}{2}} \left(a \frac{\sqrt{3}}{2} \vec{e}_1 - \frac{a}{2} \vec{e}_2 \right) = \frac{2\pi}{a} \left(\vec{e}_1 - \frac{1}{\sqrt{3}} \vec{e}_2 \right) \\ \vec{b}_2 = 2\pi \frac{\vec{e}_3 \times \vec{a}_1}{\vec{a}_2 . (\vec{e}_3 \times \vec{a}_1)} = 2\pi \frac{1}{a^2 \frac{\sqrt{3}}{2}} (a\vec{e}_2) = \frac{2\pi}{a} \left(\frac{2}{\sqrt{3}} \right) \vec{e}_2 \end{cases}$$

$$\vec{G} = m'\vec{b}_1 + n'\vec{b}_2 = \frac{2\pi}{a}\left(m'\vec{e}_1 + \frac{1}{\sqrt{3}}(-m' + 2n')\vec{e}_2 \right) \quad \text{in 2D}$$

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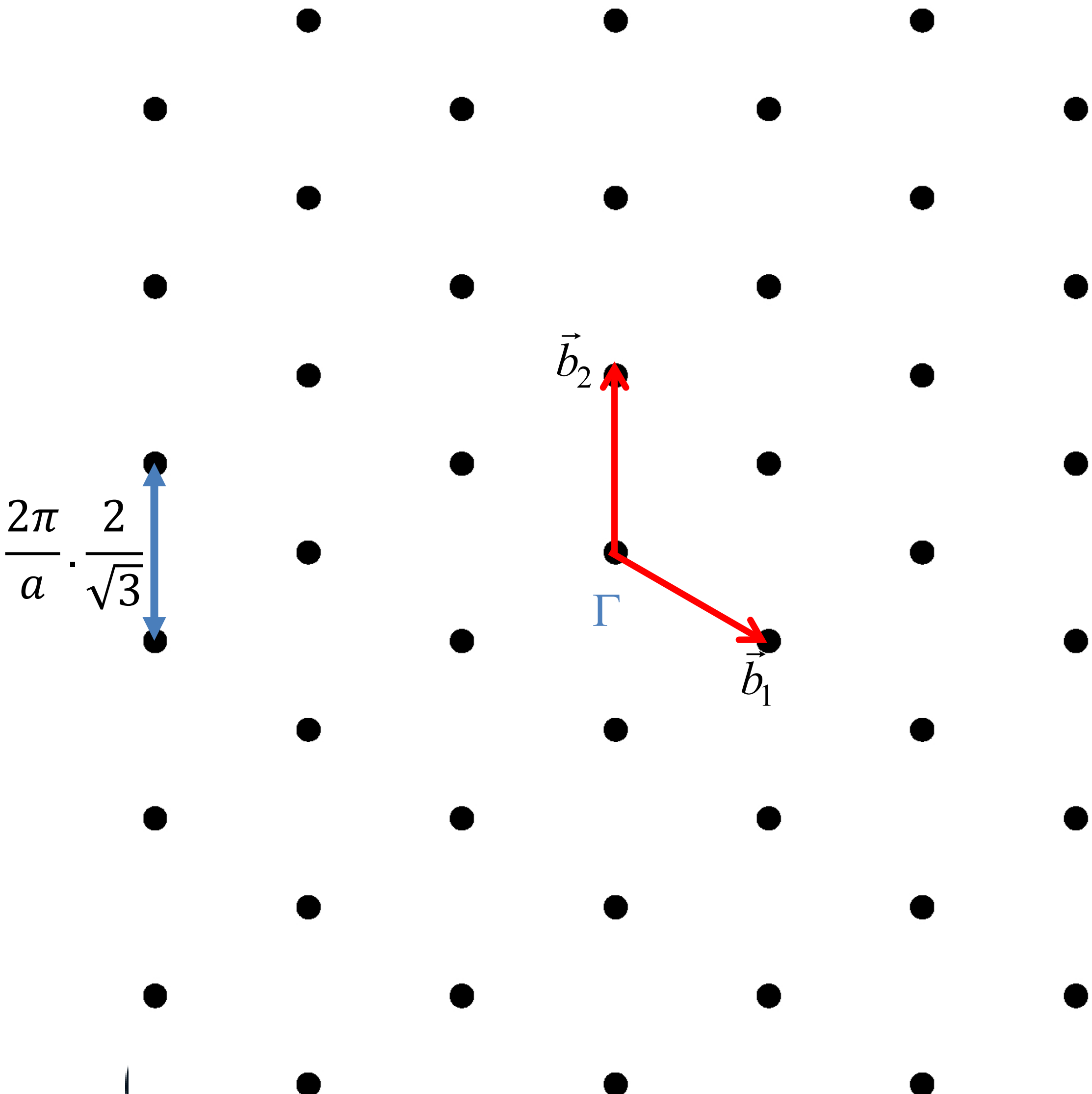
EXERCISE : 2D hexagonal (or triangular) array of lattice parameter a

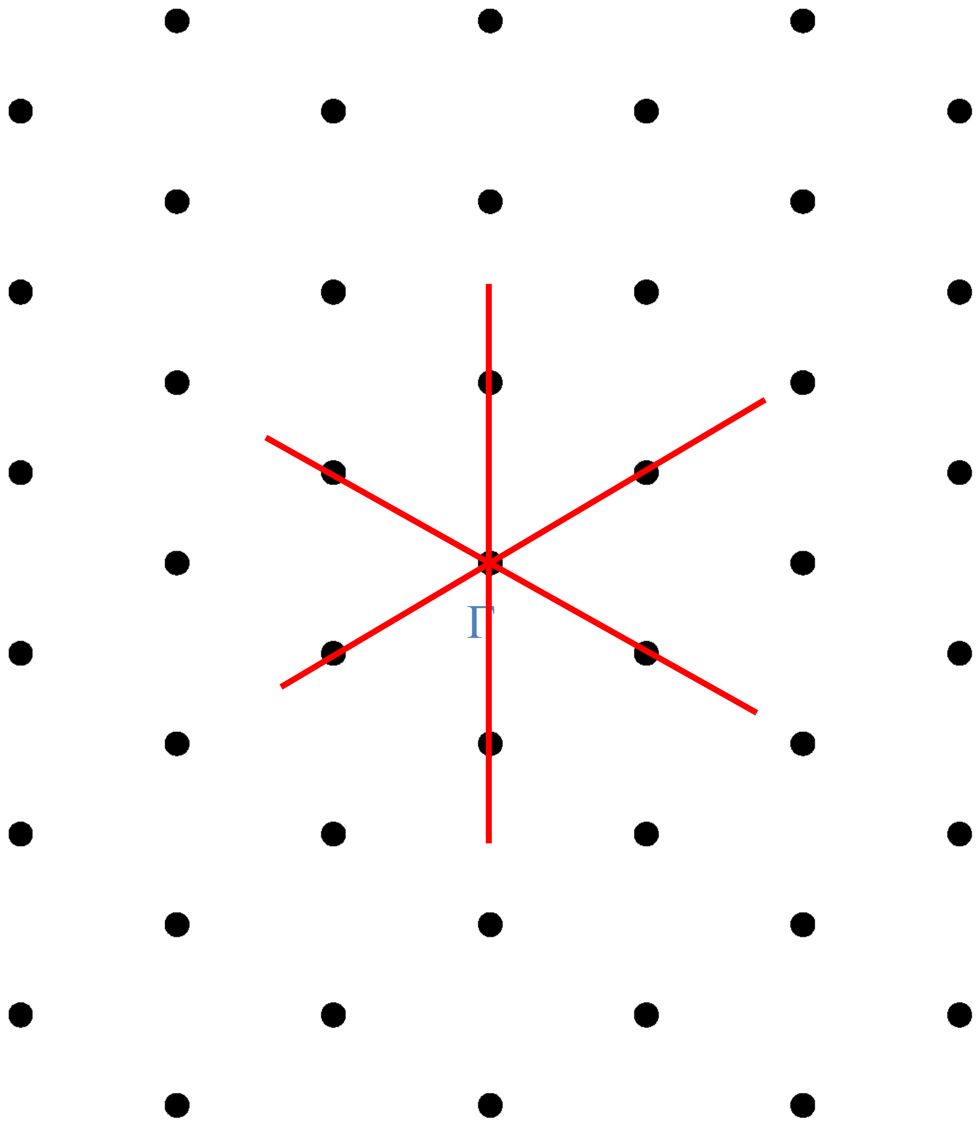
3) Draw the first Brillouin zone



1) Choose an origin Γ

EXERCISE : 2D hexagonal (or triangular) array of lattice parameter a

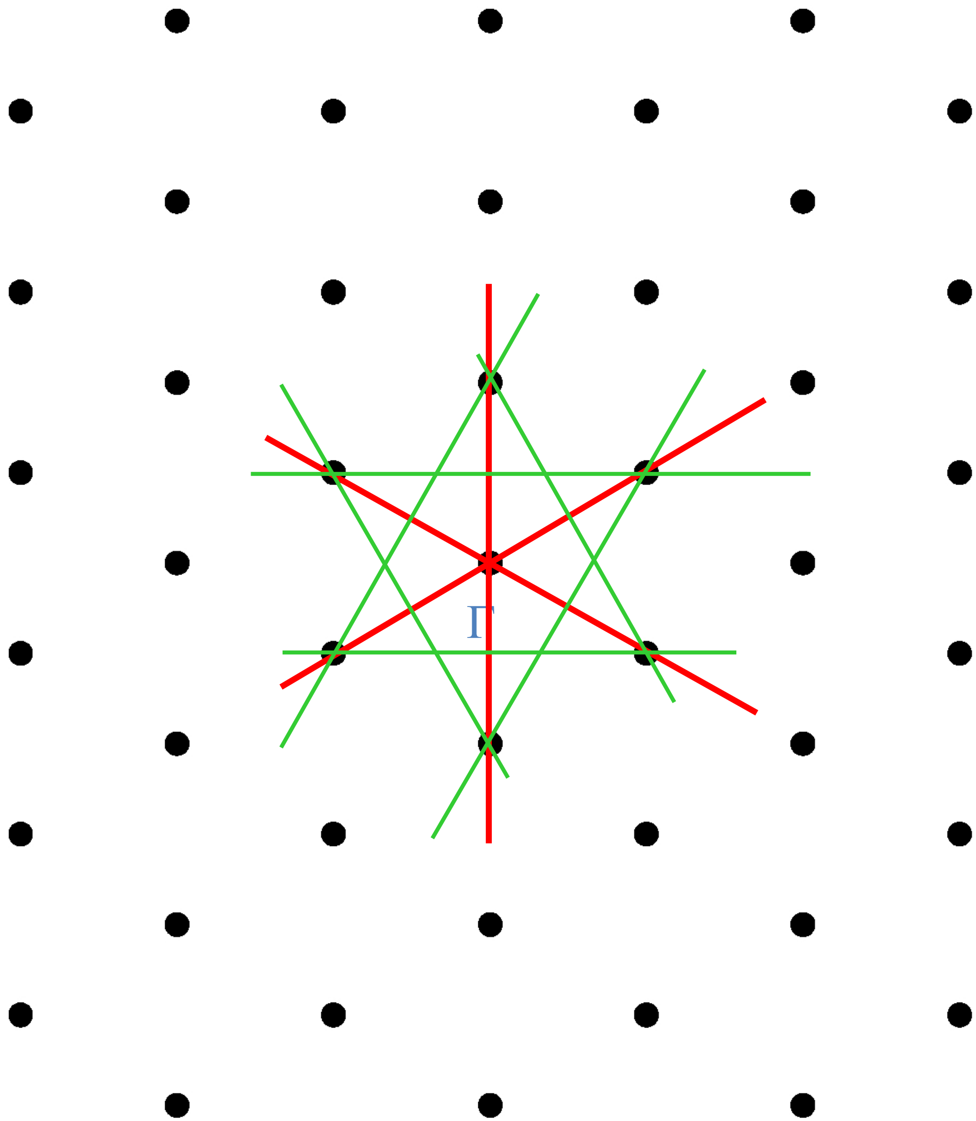
3) Draw the first Brillouin zone



2) Draw lines (red) connecting Γ to its first neighbours

EXERCISE : 2D hexagonal (or triangular) array of lattice parameter a

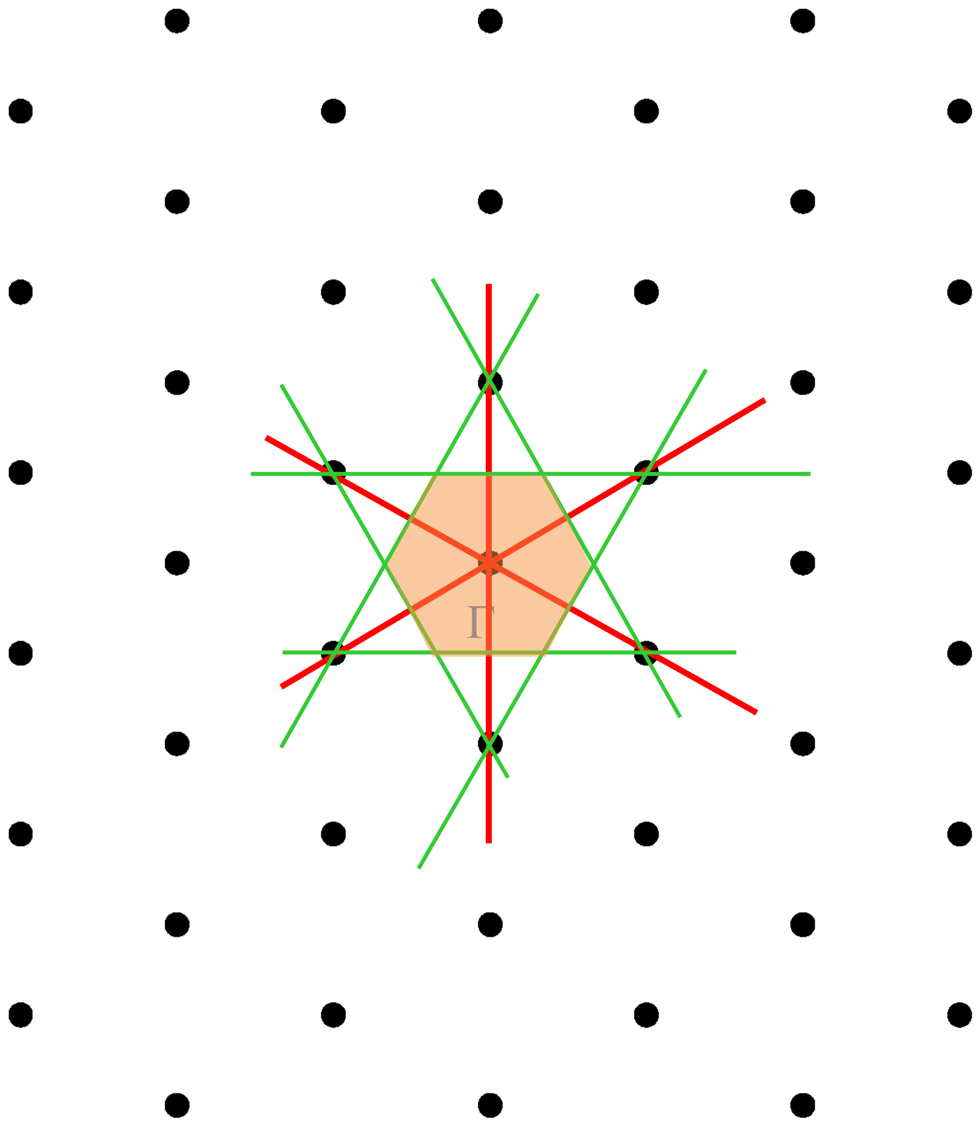
3) Draw the first Brillouin zone



3) At the mid point and normal to red lines draw new lines (green)

EXERCISE : 2D hexagonal (or triangular) array of lattice parameter a

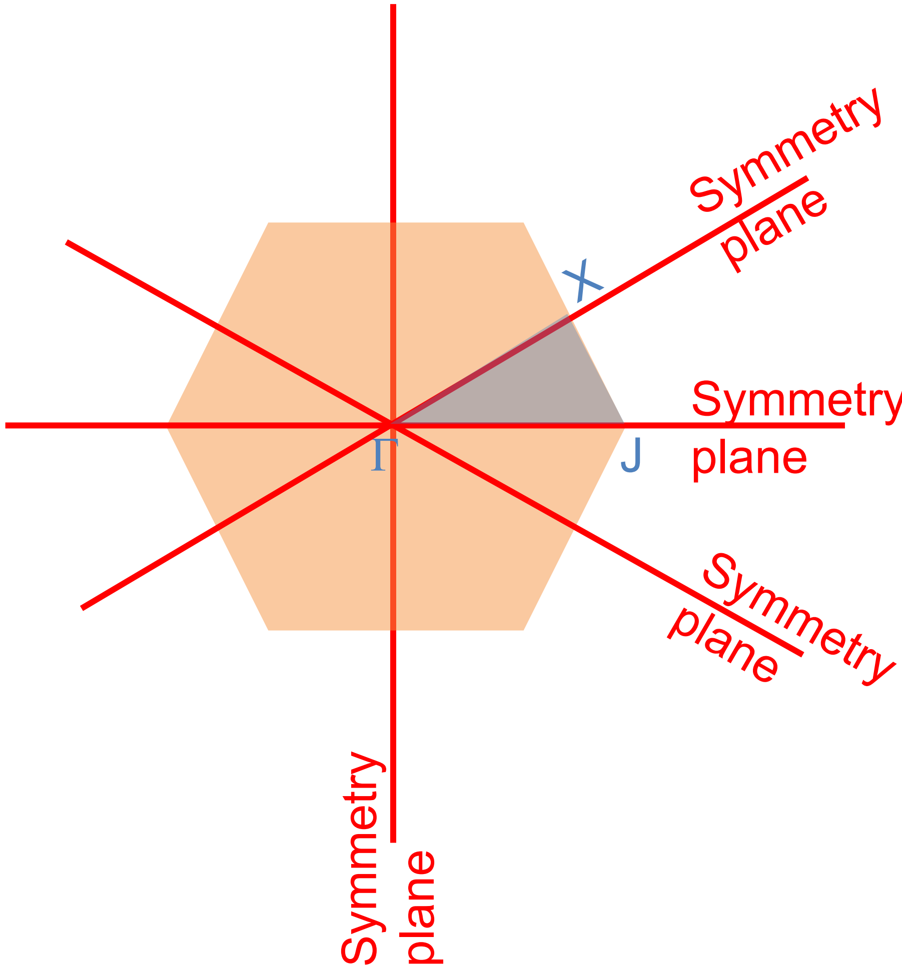
3) Draw the first Brillouin zone



4) The smallest volume (surface in 2D) enclosed by the green lines is the first Brillouin zone

<u>EXERCISE</u> : 2D hexagonal (or triangular) array of lattice parameter a

4) Determine the irreducible Brillouin zone and the coordinates of the points of highest symmetry



Due to the symmetries of the first Brillouin zone, study can be limited to the triangle ΓJX

$$\Gamma : \overrightarrow{\Gamma\Gamma} = \vec{0} \Rightarrow \Gamma : \frac{2\pi}{a}(0,0),$$

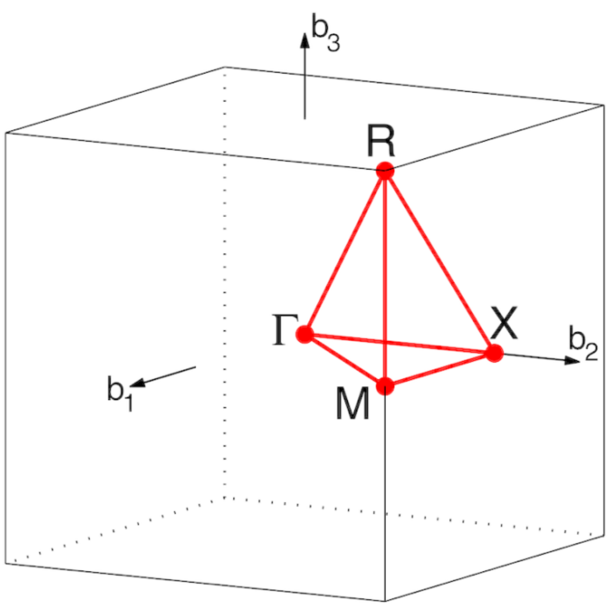
$$X : \overrightarrow{\Gamma X} = \frac{\vec{b}_1 + \vec{b}_2}{2} \Rightarrow X : \frac{2\pi}{a}\left(\frac{1}{2}, \frac{1}{2\sqrt{3}}\right),$$

$$J : \Gamma X^2 + XJ^2 = \Gamma J^2 \Rightarrow x_{1,J} = \frac{2}{3} \Rightarrow J : \frac{2\pi}{a}\left(\frac{2}{3}, 0\right).$$

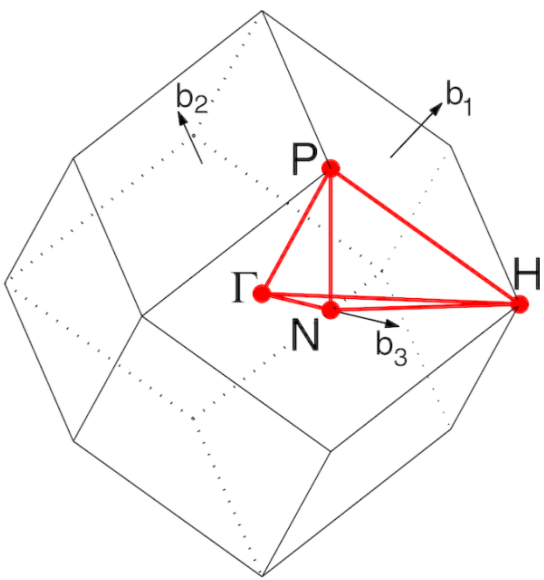
ΓJX ≡ Irreducible Brillouin zone

BRILLOUIN ZONES FOR SOME 3D LATTICES ….

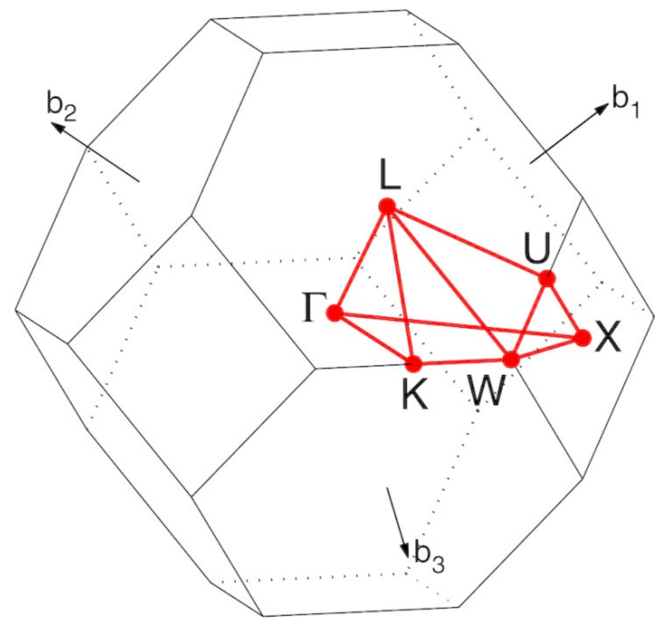
Cubic | Body Centred Cubic | Face Centred Cubic



CUB path: Γ-X-M-Γ-R-X|M-R



BCC path: Γ-H-N-Γ-P-H|P-N



FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

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II - PERIODIC STRUCTURES AND BAND STRUCTURES

A) Equations of propagation of elastic waves and the plane wave expansion method.

Equations of propagation of elastic waves in an «inhomogeneous solid» ?

- Inhomogeneous elastic medium of infinite extent along the 3 spatial directions (x_1,x_2,x_3), made of constituent materials of specific crystallographic symmetry (isotropic, cubic, …).

- At every point, $\vec{r}$, the medium is characterized by the material parameters : mass density $\rho(\vec{r})$ and elastic moduli $C_{ijkl}(\vec{r})$

- $C_{ijkl}(\vec{r})$ depend on the crystallographic symmetry of the constituent materials and

$C_{ijkl} = C_{jikl}$ and $C_{ijkl} = C_{ijlk}$ (due to energetic and thermodynamic considerations)

-The elements of the stress tensors (T_{ij}) and those of the strain tensors (S_{kl}) are

related through the Hooke's law $T_{ij}(\vec{r}) = \sum_{kl} C_{ijkl}(\vec{r}) S_{kl}(\vec{r})$

- Constituent materials are assumed to be linear materials (small strains) and the

elements of the strain tensor are expressed as $S_{kl}(\vec{r}) = \frac{1}{2}\left(\frac{\partial u_k(\vec{r})}{\partial x_l} + \frac{\partial u_l(\vec{r})}{\partial x_k}\right)$

where $u_i \left(i = 1,2,3\right)$ refers to the components of the displacement vector $\vec{u}\left(\vec{r},t\right)$

$$T_{ij} = \sum_{kl} C_{ijkl} S_{kl} = \sum_{kl} C_{ijkl} \left[\frac{1}{2} \left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \right] = \frac{1}{2} \sum_{kl} C_{ijkl} \frac{\partial u_k}{\partial x_l} + \frac{1}{2} \sum_{kl} C_{ijkl} \frac{\partial u_l}{\partial x_k}$$

$$= \frac{1}{2} \sum_{kl} C_{ijkl} \frac{\partial u_k}{\partial x_l} + \frac{1}{2} \sum_{kl} C_{ijlk} \frac{\partial u_l}{\partial x_k} = \sum_{kl} C_{ijkl} \frac{\partial u_k}{\partial x_l}$$

-For the sake of simplicity, constituent materials are supposed to be of cubic symmetry. In that case, the «matrix » of elastic moduli writes,

$$\overline{\overline{C}} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

3 independent elastic moduli : C_{11}, C_{12}, C_{44}

For isotropic materials,

$$\begin{cases} C_{12} = C_{11} - 2C_{44} \\ C_{11} = \rho V_L^2 \quad \text{and} \quad C_{44} = \rho V_T^2 \end{cases}$$

using the Voigt notation: *pair of indices kl becomes «index» m such as*

ij	11	22	33	23 or 32	31 or 13	12 or 21
m	1	2	3	4	5	6

• EXERCISE : Writes T_{ij} as functions of C_{mn} and u_i ?

$$T_{11} = \sum_{kl} C_{11kl} \frac{\partial u_k}{\partial x_l} = C_{1111}\frac{\partial u_1}{\partial x_1} + C_{1112}\frac{\partial u_1}{\partial x_2} + C_{1113}\frac{\partial u_1}{\partial x_3}$$

$$+ C_{1121}\frac{\partial u_2}{\partial x_1} + C_{1122}\frac{\partial u_2}{\partial x_2} + C_{1123}\frac{\partial u_2}{\partial x_3}$$

$$+ C_{1131}\frac{\partial u_3}{\partial x_1} + C_{1132}\frac{\partial u_3}{\partial x_2} + C_{1133}\frac{\partial u_3}{\partial x_3}$$

$$= C_{11}\frac{\partial u_1}{\partial x_1} + \underbrace{C_{16}}_{0}\frac{\partial u_1}{\partial x_2} + \underbrace{C_{15}}_{0}\frac{\partial u_1}{\partial x_3}$$

$$+ \underbrace{C_{16}}_{0}\frac{\partial u_2}{\partial x_1} + C_{12}\frac{\partial u_2}{\partial x_2} + \underbrace{C_{14}}_{0}\frac{\partial u_2}{\partial x_3}$$

$$+ \underbrace{C_{15}}_{0}\frac{\partial u_3}{\partial x_1} + \underbrace{C_{14}}_{0}\frac{\partial u_3}{\partial x_2} + C_{13}\frac{\partial u_3}{\partial x_3}$$

$$\Rightarrow T_{11} = C_{11}\frac{\partial u_1}{\partial x_1} + C_{12}\left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right)$$

In the same way, one obtains

$$T_{12} = \sum_{kl} C_{12kl} \frac{\partial u_k}{\partial x_l} = C_{44}\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) = T_{21}$$

$$T_{13} = \sum_{kl} C_{13kl} \frac{\partial u_k}{\partial x_l} = C_{44}\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right) = T_{31}$$

$$T_{22} = \sum_{kl} C_{22kl} \frac{\partial u_k}{\partial x_l} = C_{11}\frac{\partial u_2}{\partial x_2} + C_{12}\left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_3}{\partial x_3}\right)$$

$$T_{23} = \sum_{kl} C_{23kl} \frac{\partial u_k}{\partial x_l} = C_{44}\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right) = T_{32}$$

$$T_{33} = \sum_{kl} C_{33kl} \frac{\partial u_k}{\partial x_l} = C_{11}\frac{\partial u_3}{\partial x_3} + C_{12}\left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2}\right)$$

- In absence of external forces, Newton's second law leads to the equations of motion

$$\rho(\vec{r})\frac{\partial^2 u_i(\vec{r},t)}{\partial t^2} = \sum_j \frac{\partial T_{ij}(\vec{r})}{\partial x_j} = \sum_j \frac{\partial}{\partial x_j}\left[\sum_{kl} C_{ijkl}(\vec{r})\frac{\partial u_k(\vec{r})}{\partial x_l}\right]$$

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$$\rho(\vec{r})\frac{\partial^2 u_1(\vec{r},t)}{\partial t^2} = \frac{\partial T_{11}(\vec{r})}{\partial x_1} + \frac{\partial T_{12}(\vec{r})}{\partial x_2} + \frac{\partial T_{13}(\vec{r})}{\partial x_3}$$

$$= \frac{\partial}{\partial x_1}\left(C_{11}(\vec{r})\frac{\partial u_1}{\partial x_1} + C_{12}(\vec{r})\left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right)\right) + \frac{\partial}{\partial x_2}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\right) + \frac{\partial}{\partial x_3}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right)\right)$$

$$\rho(\vec{r})\frac{\partial^2 u_2(\vec{r},t)}{\partial t^2} = \frac{\partial T_{21}(\vec{r})}{\partial x_1} + \frac{\partial T_{22}(\vec{r})}{\partial x_2} + \frac{\partial T_{23}(\vec{r})}{\partial x_3}$$

$$= \frac{\partial}{\partial x_1}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\right) + \frac{\partial}{\partial x_2}\left(C_{11}(\vec{r})\frac{\partial u_2}{\partial x_2} + C_{12}(\vec{r})\left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_3}{\partial x_3}\right)\right) + \frac{\partial}{\partial x_3}\left(C_{44}(\vec{r})\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right)\right)$$

$$\rho(\vec{r})\frac{\partial^2 u_3(\vec{r},t)}{\partial t^2} = \frac{\partial T_{31}(\vec{r})}{\partial x_1} + \frac{\partial T_{32}(\vec{r})}{\partial x_2} + \frac{\partial T_{33}(\vec{r})}{\partial x_3}$$

$$= \frac{\partial}{\partial x_1}\left(C_{44}(\vec{r})\left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3}\right)\right) + \frac{\partial}{\partial x_2}\left(C_{44}(\vec{r})\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right)\right) + \frac{\partial}{\partial x_3}\left(C_{11}(\vec{r})\frac{\partial u_3}{\partial x_3} + C_{12}(\vec{r})\left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_1}{\partial x_1}\right)\right)$$

Equations of propagation of elastic waves in an heterogeneous elastic material of infinite extent are three coupled differential equations of order 2

For «periodic» distributions of inhomogeneities, these equations can be solved using the Plane Wave Expansion (PWE) method

Basic principles of the PWE method for infinite phononic crystals

- Method derived from the electronic theory of solids (electronic band structure)

- Direct lattice (DL), of specific geometry, characterized by its unit cell (UC)

- Reciprocal lattice (RL) of 3D vectors $\left(\overrightarrow{G_1}, \overrightarrow{G_2}, \overrightarrow{G_3}\right)$ with respect to the orthonormal basis $(O, \overrightarrow{e_1}, \overrightarrow{e_2}, \overrightarrow{e_3})$

- One search sinusoidally time varying solutions of the equations of propagation in the form $\vec{u}(\vec{r}, t) = \vec{u}(\vec{r}).e^{-i\omega t}$ where ω is the circular frequency

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- Due to the periodicity of the structure, the **Bloch-Floquet theorem** states that $\vec{u}(\vec{r})$ can be written in the form $\vec{u}(\vec{r}) = e^{i\vec{K}.\vec{r}}\vec{U}_{\vec{K}}(\vec{r})$ where $\vec{K}(K_1, K_2, K_3)$ is the 3D Bloch wave vector and $\vec{U}_{\vec{K}}(\vec{r})$ has the periodicity of the direct lattice

⇒ $\vec{U}_{\vec{K}}(\vec{r})$ can be developped in Fourier series as

$$\vec{U}_{\vec{K}}(\vec{r}) = \sum_{\vec{G}'} \vec{U}_{\vec{K}}(\vec{G}')e^{i\vec{G}'\cdot\vec{r}} \text{ where } \vec{G}' \in RL$$

⇒ $$\vec{u}(\vec{r},t) = e^{i(\vec{K}.\vec{r}-\omega t)} \sum_{\vec{G}'} \vec{U}_{\vec{K}}(\vec{G}')e^{i\vec{G}'\cdot\vec{r}}$$

-The material parameters, mass density $\rho(\vec{r})$ and elastic moduli $C_{ijkl}(\vec{r})$ are periodic functions of the position i.e. $\rho(\vec{r}) = \rho(\vec{r} + \vec{R})$ and $C_{ijkl}(\vec{r}) = C_{ijkl}(\vec{r} + \vec{R})$ where $\vec{R} \in (\mathrm{DL})$ and can be expanded in Fourier series such as

$$\begin{cases} C_{ijkl}(\vec{r}) = \sum_{\vec{G}''} C_{ijkl}(\vec{G}'') e^{i\vec{G}''\cdot\vec{r}} \\ \rho(\vec{r}) = \sum_{\vec{G}''} \rho(\vec{G}'') e^{i\vec{G}''\cdot\vec{r}} \end{cases} \quad \text{where } \vec{G}'' \in (RL)$$

- $\vec{u}(\vec{r},t)$, $\rho(\vec{r})$, $C_{ijkl}(\vec{r})$ in the equations of propagation are then replaced by these expressions …

Equation of propagation for u_1

$$\rho(\vec{r})\frac{\partial^2 u_1(\vec{r},t)}{\partial t^2} =$$

$$= \frac{\partial}{\partial x_1}\left(C_{11}(\vec{r})\frac{\partial u_1}{\partial x_1} + C_{12}(\vec{r})\left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right)\right) + \frac{\partial}{\partial x_2}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\right) + \frac{\partial}{\partial x_3}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right)\right)$$

<u>Left hand side</u> $\rho(\vec{r})\frac{\partial^2 u_1(\vec{r},t)}{\partial t^2}$ becomes $-\omega^2 e^{i(\vec{K}.\vec{r}-\omega t)} \sum_{\vec{G}',\vec{G}''} \rho(\vec{G}'') U_{1,\vec{K}}(\vec{G}') e^{i(\vec{G}'+\vec{G}'')\vec{r}}$ ….

Multiplication of this term by $e^{-i\vec{G}.\vec{r}}$ and integration over the unit cell

$$\rightarrow \frac{1}{V_{(UC)}} \int_{(UC)} e^{i(\vec{G}'+\vec{G}''-\vec{G}).\vec{r}} d\vec{r} = \delta_{\vec{G}'+\vec{G}''-\vec{G},\vec{0}} = \begin{cases} 1 \text{ if } (\vec{G}'+\vec{G}''-\vec{G}) = \vec{0} \\ 0 \text{ if } (\vec{G}'+\vec{G}''-\vec{G}) \neq \vec{0} \end{cases} \Rightarrow \vec{G}'' = \vec{G} - \vec{G}'$$

$V_{(UC)} \equiv$ Volume of the unit cell

… and $-\omega^2 e^{i((\vec{K}+\vec{G}).\vec{r}-\omega t)} \sum_{\vec{G}'} [\rho(\vec{G}-\vec{G}')] U_{1,\vec{K}}(\vec{G}')$

Right hand side

$$\frac{\partial}{\partial x_1}\left(C_{11}(\vec{r})\frac{\partial u_1}{\partial x_1}+C_{12}(\vec{r})\left(\frac{\partial u_2}{\partial x_2}+\frac{\partial u_3}{\partial x_3}\right)\right)+\frac{\partial}{\partial x_2}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)\right)+\frac{\partial}{\partial x_3}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_3}+\frac{\partial u_3}{\partial x_1}\right)\right)$$

becomes ?????

Method

$$u_1(\vec{r},t) = e^{i(\vec{K}.\vec{r}-\omega t)} \sum_{\vec{G}\prime} U_{1,\vec{K}}(\vec{G}')e^{i\vec{G}\prime\cdot\vec{r}} = e^{-i\omega t} \sum_{\vec{G}\prime} U_{1,\vec{K}}(\vec{G}')e^{i(\vec{K}+\vec{G}\prime)\cdot\vec{r}}$$

with $(\vec{K}+\vec{G}').\vec{r} = (K_1 + G'_1)x_1 + (K_2 + G'_2)x_2 + (K_3 + G'_3)x_3$

then $$\frac{\partial u_1(\vec{r},t)}{\partial x_1} = e^{i(\vec{K}.\vec{r}-\omega t)} \sum_{\vec{G}\prime} [i(K_1 + G'_1)]U_{1,\vec{K}}(\vec{G}')e^{i\vec{G}\prime\cdot\vec{r}}$$

$$C_{11}(\vec{r})\frac{\partial u_1(\vec{r},t)}{\partial x_1} = e^{-i\omega t} \sum_{\vec{G}\prime,\vec{G}\prime\prime} [i(K_1 + G'_1)]U_{1,\vec{K}}(\vec{G}')C_{11}(\vec{G}'')e^{i(\vec{K}+\vec{G}\prime+\vec{G}\prime\prime)\cdot\vec{r}}$$

$$\frac{\partial}{\partial x_1}\left[C_{11}(\vec{r})\frac{\partial u_1(\vec{r},t)}{\partial x_1}\right] = -e^{-i\omega t} \sum_{\vec{G}\prime,\vec{G}\prime\prime} [(K_1 + G'_1)(K_1 + G'_1 + G_1'')]U_{1,\vec{K}}(\vec{G}')C_{11}(\vec{G}'')e^{i(\vec{K}+\vec{G}\prime+\vec{G}\prime\prime)\cdot\vec{r}}$$

$$= -e^{i(\vec{K}.\vec{r}-\omega t)} \sum_{\vec{G}\prime,\vec{G}\prime\prime} [(K_1 + G'_1)(K_1 + G'_1 + G_1'')]U_{1,\vec{K}}(\vec{G}')C_{11}(\vec{G}'')e^{i(\vec{G}\prime+\vec{G}\prime\prime)\cdot\vec{r}}$$

Multiplication of all these terms by $e^{-i\vec{G}.\vec{r}}$ and integration of all these terms over the unit cell

→ $\frac{\partial}{\partial x_1}\left[C_{11}(\vec{r})\frac{\partial u_1(\vec{r},t)}{\partial x_1}\right]$ becomes

$$-e^{i((\vec{K}+\vec{G}).\vec{r}-\omega t)} \sum_{\vec{G}\prime} [(K_1 + G'_1)(K_1 + G_1)C_{11}(\vec{G}-\vec{G}')]U_{1,\vec{K}}(\vec{G}')$$

After lengthy algebra (!!!), one obtains

$$\begin{cases} \omega^2 \sum_{\vec{G}'} B^{(11)}_{\vec{G},\vec{G}'} U_{1,\vec{K}}\left(\vec{G}'\right) = \sum_{\vec{G}'} \left\{ U_{1,\vec{K}}\left(\vec{G}'\right) A^{(11)}_{\vec{G},\vec{G}'} + U_{2,\vec{K}}\left(\vec{G}'\right) A^{(12)}_{\vec{G},\vec{G}'} + U_{3,\vec{K}}\left(\vec{G}'\right) A^{(13)}_{\vec{G},\vec{G}'} \right\} \\ \omega^2 \sum_{\vec{G}'} B^{(22)}_{\vec{G},\vec{G}'} U_{2,\vec{K}}\left(\vec{G}'\right) = \sum_{\vec{G}'} \left\{ U_{1,\vec{K}}\left(\vec{G}'\right) A^{(21)}_{\vec{G},\vec{G}'} + U_{2,\vec{K}}\left(\vec{G}'\right) A^{(22)}_{\vec{G},\vec{G}'} + U_{3,\vec{K}}\left(\vec{G}'\right) A^{(23)}_{\vec{G},\vec{G}'} \right\} \\ \omega^2 \sum_{\vec{G}'} B^{(33)}_{\vec{G},\vec{G}'} U_{3,\vec{K}}\left(\vec{G}'\right) = \sum_{\vec{G}'} \left\{ U_{1,\vec{K}}\left(\vec{G}'\right) A^{(31)}_{\vec{G},\vec{G}'} + U_{2,\vec{K}}\left(\vec{G}'\right) A^{(32)}_{\vec{G},\vec{G}'} + U_{3,\vec{K}}\left(\vec{G}'\right) A^{(33)}_{\vec{G},\vec{G}'} \right\} \end{cases}$$

where

$$\begin{cases}
B^{(11)}_{\vec{G},\vec{G}'} = B^{(22)}_{\vec{G},\vec{G}'} = B^{(33)}_{\vec{G},\vec{G}'} = \rho\left(\vec{G}-\vec{G}'\right) \\
\\
A^{(11)}_{\vec{G},\vec{G}'} = C_{11}\left(\vec{G}-\vec{G}'\right)(G_1+K_1)(G'_1+K_1) + C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_2+K_2)(G'_2+K_2)+(G_3+K_3)(G'_3+K_3)\right] \\
A^{(12)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)(G_1+K_1)(G'_2+K_2) + C_{44}\left(\vec{G}-\vec{G}'\right)(G'_1+K_1)(G_2+K_2) \\
A^{(13)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)(G_1+K_1)(G'_3+K_3) + C_{44}\left(\vec{G}-\vec{G}'\right)(G'_1+K_1)(G_3+K_3) \\
\\
A^{(21)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)(G'_1+K_1)(G_2+K_2) + C_{44}\left(\vec{G}-\vec{G}'\right)(G'_2+K_2)(G_1+K_1) \\
A^{(22)}_{\vec{G},\vec{G}'} = C_{11}\left(\vec{G}-\vec{G}'\right)(G_2+K_2)(G'_2+K_2) + C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_1+K_1)(G'_1+K_1)+(G_3+K_3)(G'_3+K_3)\right] \\
A^{(23)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)(G'_3+K_3)(G_2+K_2) + C_{44}\left(\vec{G}-\vec{G}'\right)(G'_2+K_2)(G_3+K_3) \\
\\
A^{(31)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)(G'_1+K_1)(G_3+K_3) + C_{44}\left(\vec{G}-\vec{G}'\right)(G_1+K_1)(G'_3+K_3) \\
A^{(32)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)(G'_2+K_2)(G_3+K_3) + C_{44}\left(\vec{G}-\vec{G}'\right)(G_2+K_2)(G'_3+K_3) \\
A^{(33)}_{\vec{G},\vec{G}'} = C_{11}\left(\vec{G}-\vec{G}'\right)(G_3+K_3)(G'_3+K_3) + C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_1+K_1)(G'_1+K_1)+(G'_2+K_2)(G_2+K_2)\right]
\end{cases}$$

Conclusion : After Fourier transform, the equations of propagation can be rewritten as a standard generalized eigenvalues equation in the form

$$\omega^2 \begin{pmatrix} B^{(11)}_{\vec{G},\vec{G}'} & 0 & 0 \\ 0 & B^{(22)}_{\vec{G},\vec{G}'} & 0 \\ 0 & 0 & B^{(33)}_{\vec{G},\vec{G}'} \end{pmatrix} \begin{pmatrix} U_{1,\vec{K}}(\vec{G}') \\ U_{2,\vec{K}}(\vec{G}') \\ U_{3,\vec{K}}(\vec{G}') \end{pmatrix} = \begin{pmatrix} A^{(11)}_{\vec{G},\vec{G}'} & A^{(12)}_{\vec{G},\vec{G}'} & A^{(13)}_{\vec{G},\vec{G}'} \\ A^{(21)}_{\vec{G},\vec{G}'} & A^{(22)}_{\vec{G},\vec{G}'} & A^{(23)}_{\vec{G},\vec{G}'} \\ A^{(31)}_{\vec{G},\vec{G}'} & A^{(32)}_{\vec{G},\vec{G}'} & A^{(33)}_{\vec{G},\vec{G}'} \end{pmatrix} \begin{pmatrix} U_{1,\vec{K}}(\vec{G}') \\ U_{2,\vec{K}}(\vec{G}') \\ U_{3,\vec{K}}(\vec{G}') \end{pmatrix}$$

or $$\omega^2 \overleftrightarrow{B}.\vec{U}_{\vec{K}} = \overleftrightarrow{A}.\vec{U}_{\vec{K}}$$

where $\overleftrightarrow{A}$ and $\overleftrightarrow{B}$ are square matrices whose size depends on the number of reciprocal lattice vectors taken into account in the Fourier series.

The resolution of this eigenvalue equation is performed along the principal directions of propagation of the irreducible Brillouin zone of the array of inclusions :

→for a given $\vec{K}$, one obtains a set of ω values

Question : What is the meaning of terms of the form $\eta\left(\vec{G}-\vec{G}'\right)$ that appear in the Fourier transformed equations of propagation?

$$\eta(\vec{r}) = \sum_{\vec{G}} \eta(\vec{G}) e^{i\vec{G}\cdot\vec{r}} \quad \text{where } \vec{G} \in (RL)$$

Fourier coefficients of the Fourier series

$$\eta(\vec{G}) = \frac{1}{V_{(uc)}} \int_{(UC)} \eta(\vec{r}).e^{-i\vec{G}.\vec{r}}.d\vec{r}$$

Calculation of $\eta\left(\vec{G}\right)$?

In the particular case of two-dimensional phononic crystals !

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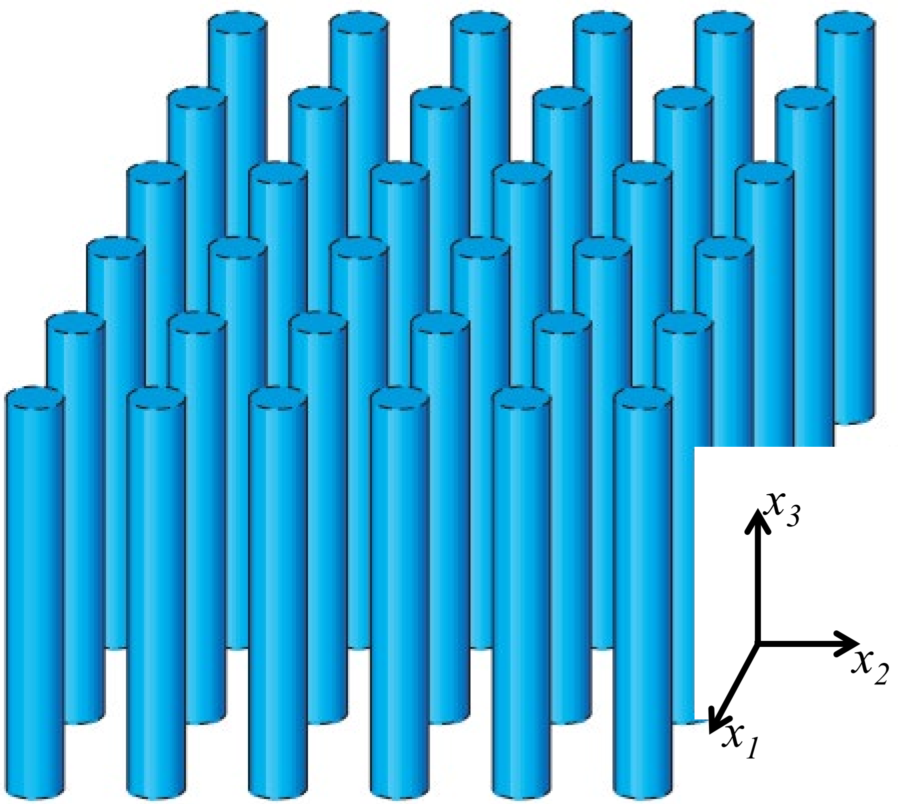
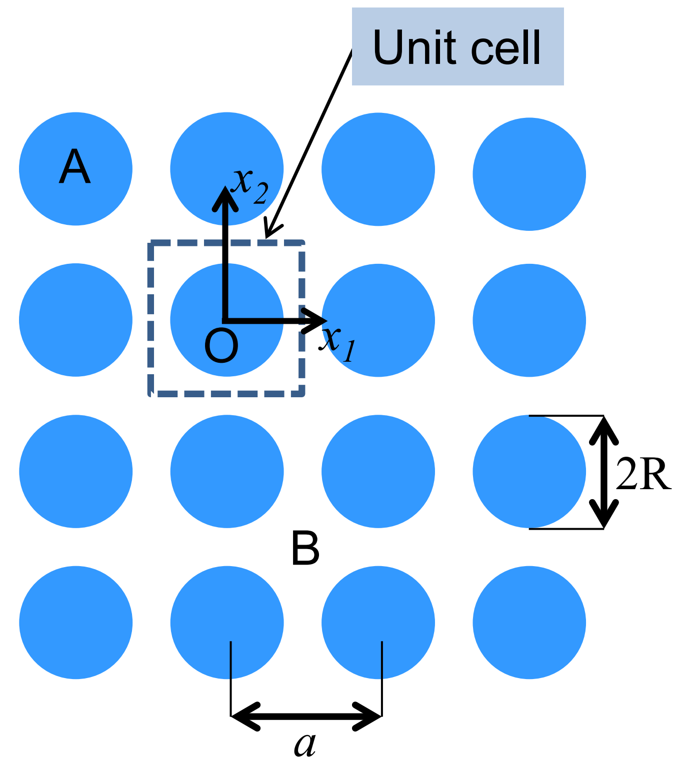
TWO-DIMENSIONAL PHONONIC CRYSTALS

Array of cylinders of circular, square, … cross section embedded in a matrix





A ≡ Constituent material of the inclusions
B ≡ Constituent material of the matrix

Hypothesis

-Infinite cylinders along the x_3 direction

⇒Translational symmetry along the x_3 direction

⇒ All quantities (materials parameters, displacement field) independent of x_3

⇒This is a «purely» 2D problem

⇒$G_3=G'_3=0$ and $K_3=0$

Then ……

$$
\begin{cases}
B^{(11)}_{\vec{G},\vec{G}'} = B^{(22)}_{\vec{G},\vec{G}'} = B^{(33)}_{\vec{G},\vec{G}'} = \rho\left(\vec{G}-\vec{G}'\right) \\
\\
A^{(11)}_{\vec{G},\vec{G}'} = C_{11}\left(\vec{G}-\vec{G}'\right)(G_1+K_1)(G'_1+K_1) + C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_2+K_2)(G'_2+K_2)\right] \\
A^{(12)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)(G_1+K_1)(G'_2+K_2) + C_{44}\left(\vec{G}-\vec{G}'\right)(G'_1+K_1)(G_2+K_2) \\
A^{(13)}_{\vec{G},\vec{G}'} = 0 \\
\\
A^{(21)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)(G'_1+K_1)(G_2+K_2) + C_{44}\left(\vec{G}-\vec{G}'\right)(G'_2+K_2)(G_1+K_1) \\
A^{(22)}_{\vec{G},\vec{G}'} = C_{11}\left(\vec{G}-\vec{G}'\right)(G_2+K_2)(G'_2+K_2) + C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_1+K_1)(G'_1+K_1)\right] \\
A^{(23)}_{\vec{G},\vec{G}'} = 0 \\
\\
A^{(31)}_{\vec{G},\vec{G}'} = 0 \\
A^{(32)}_{\vec{G},\vec{G}'} = 0 \\
A^{(33)}_{\vec{G},\vec{G}'} = C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_1+K_1)(G'_1+K_1) + (G'_2+K_2)(G_2+K_2)\right]
\end{cases}
$$

and

$$\omega^2\begin{pmatrix} B^{(11)}_{\vec{G},\vec{G}'} & 0 & 0 \\ 0 & B^{(22)}_{\vec{G},\vec{G}'} & 0 \\ 0 & 0 & B^{(33)}_{\vec{G},\vec{G}'} \end{pmatrix}\begin{pmatrix} U_{1,\vec{K}}\left(\vec{G}'\right) \\ U_{2,\vec{K}}\left(\vec{G}'\right) \\ U_{3,\vec{K}}\left(\vec{G}'\right) \end{pmatrix} = \begin{pmatrix} A^{(11)}_{\vec{G},\vec{G}'} & A^{(12)}_{\vec{G},\vec{G}'} & 0 \\ A^{(21)}_{\vec{G},\vec{G}'} & A^{(22)}_{\vec{G},\vec{G}'} & 0 \\ 0 & 0 & A^{(33)}_{\vec{G},\vec{G}'} \end{pmatrix}\begin{pmatrix} U_{1,\vec{K}}\left(\vec{G}'\right) \\ U_{2,\vec{K}}\left(\vec{G}'\right) \\ U_{3,\vec{K}}\left(\vec{G}'\right) \end{pmatrix}$$

These 2 matrices are “super-diagonal” and one can separate this matrix equation into two independent uncoupled eigen-values equations

$$\omega^2\begin{pmatrix} B^{(11)}_{\vec{G},\vec{G}'} & 0 \\ 0 & B^{(22)}_{\vec{G},\vec{G}'} \end{pmatrix}\begin{pmatrix} U_{1,\vec{K}}\left(\vec{G}'\right) \\ U_{2,\vec{K}}\left(\vec{G}'\right) \end{pmatrix} = \begin{pmatrix} A^{(11)}_{\vec{G},\vec{G}'} & A^{(12)}_{\vec{G},\vec{G}'} \\ A^{(21)}_{\vec{G},\vec{G}'} & A^{(22)}_{\vec{G},\vec{G}'} \end{pmatrix}\begin{pmatrix} U_{1,\vec{K}}\left(\vec{G}'\right) \\ U_{2,\vec{K}}\left(\vec{G}'\right) \end{pmatrix}$$

↔ x_1x_2 (or XY) vibration modes polarized in the transverse plane (x_1Ox_2)

$$\omega^2\sum_{\vec{G}'} B^{(33)}_{\vec{G},\vec{G}'} U_{3,\vec{K}}\left(\vec{G}'\right) = \sum_{\vec{G}'} A^{(33)}_{\vec{G},\vec{G}'} U_{3,\vec{K}}\left(\vec{G}'\right)$$

↔ x_3 or (Z) vibration modes with a displacement field along the x_3 direction

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Calculation of $$\eta(\vec{G}) = \frac{1}{V_{(uc)}} \int_{(UC)} \eta(\vec{r}).e^{-i\vec{G}.\vec{r}}.d\vec{r}$$

For two-dimensional phononic crystals, this equation becomes

$$\eta(\vec{G}) = \frac{1}{\Sigma_{(uc)}} \int_{(UC)} \eta(\vec{r}).e^{-i\vec{G}.\vec{r}}.d^2\vec{r}$$

where $\Sigma_{(UC)}$ is the area of the two-dimensional unit cell in the (x_1Ox_2) plane

$$\eta(\vec{G}) = \frac{1}{\Sigma_{(UC)}} \iint_{(UC)} \eta(\vec{r}) e^{-i\vec{G}\vec{r}}\, d^2\vec{r} \quad = \frac{1}{\Sigma_{(UC)}} \left\{ \iint_{(A_{(UC)})} \eta_A e^{-i\vec{G}\vec{r}} d^2\vec{r} \quad + \iint_{(B_{(UC)})} \eta_B e^{-i\vec{G}\vec{r}} d^2\vec{r} \right\}$$

$$= \frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} \eta_A e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} - \frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} \eta_B e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} + \frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} \eta_B e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} + \frac{1}{\Sigma_{(UC)}} \iint_{(B_{(UC)})} \eta_B e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r}$$

$$= \frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} \eta_A e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} - \frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} \eta_B e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} + \eta_B \left\{ \frac{1}{\Sigma_{(UC)}} \iint_{(UC)} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} \right\}$$

$$= \frac{1}{\Sigma_{(UC)}} (\eta_A - \eta_B) \iint_{(A_{(UC)})} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} + \eta_B \left\{ \frac{1}{\Sigma_{(UC)}} \iint_{(UC)} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} \right\}.$$

but $\frac{1}{\Sigma_{(UC)}} \iint_{(UC)} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} = \delta_{\vec{G},\vec{0}} = \begin{cases} 1 \text{ if } \vec{G} = \vec{0} \\ 0 \text{ if } \vec{G} \neq \vec{0} \end{cases}$

$$\Rightarrow \eta(\vec{G}) = (\eta_A - \eta_B) \frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} + \eta_B \delta_{\vec{G},\vec{0}}$$

$\Rightarrow \eta(\vec{G}) = (\eta_A - \eta_B) F(\vec{G}) + \eta_B \delta_{\vec{G},\vec{0}}$ where $F(\vec{G}) = \frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r}$ ≡ Structure Factor

depends on the geometry of the inclusions …

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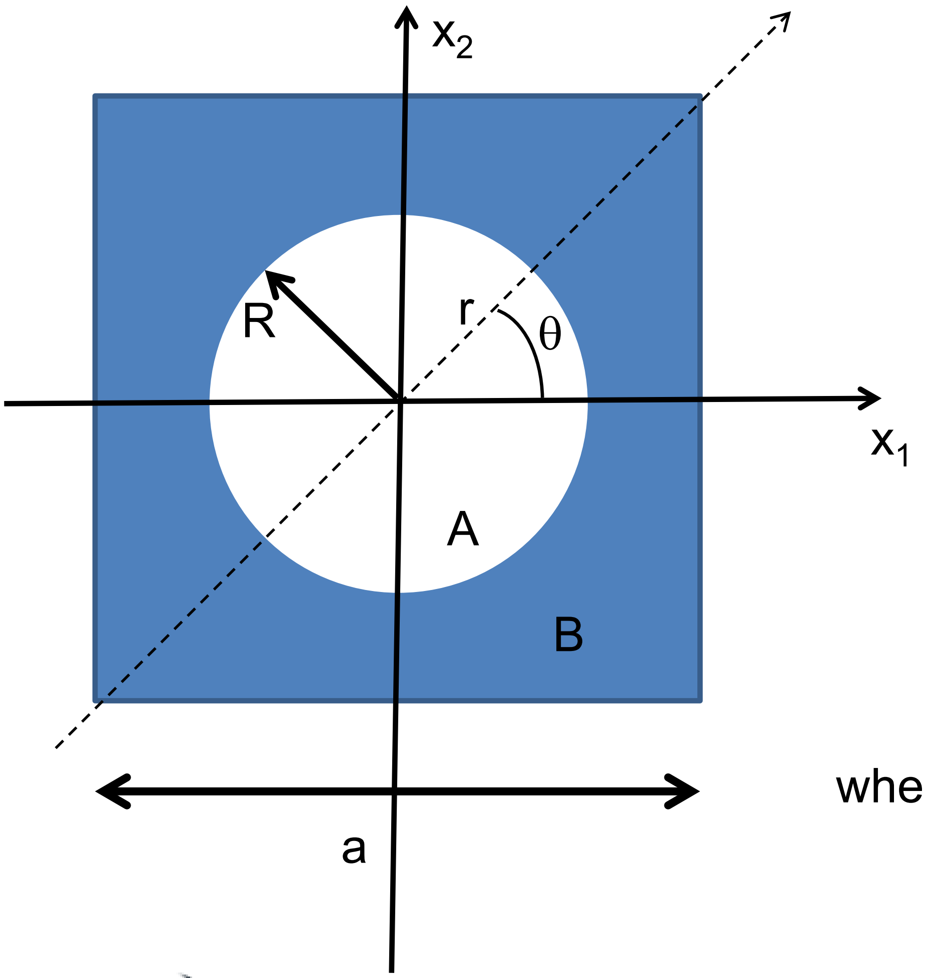
Example : Square array (lattice parameter a), of cylinders (circular cross section) of radius R made of material A

$\Rightarrow$ Unit cell = square of side length a



Using polar coordinates (r,θ)

$$F(\vec{G}) = \frac{1}{a^2}\int_0^R \int_0^{2\pi} e^{-iG\cdot r\cos\theta} r dr d\theta$$

$$= \frac{1}{a^2}\int_0^R 2\pi r dr J_0(Gr)$$

$$= \frac{2\pi}{a^2G^2}\int_0^{G_{//}R}(Gr)J_0(Gr)d(Gr)$$

$$= \frac{2\pi}{a^2G^2}GR.J_1(GR) = 2f\frac{J_1(GR)}{GR}$$

where $f = \pi\left(\frac{R}{a}\right)^2 \equiv \text{filling factor}; 0 \le f \le \frac{\pi}{4}$

$$G = \left\|\vec{G}\right\| = \sqrt{G_1^2 + G_2^2}$$

J_0 and J_1 are Bessel functions of the first kind of orders 0 and 1

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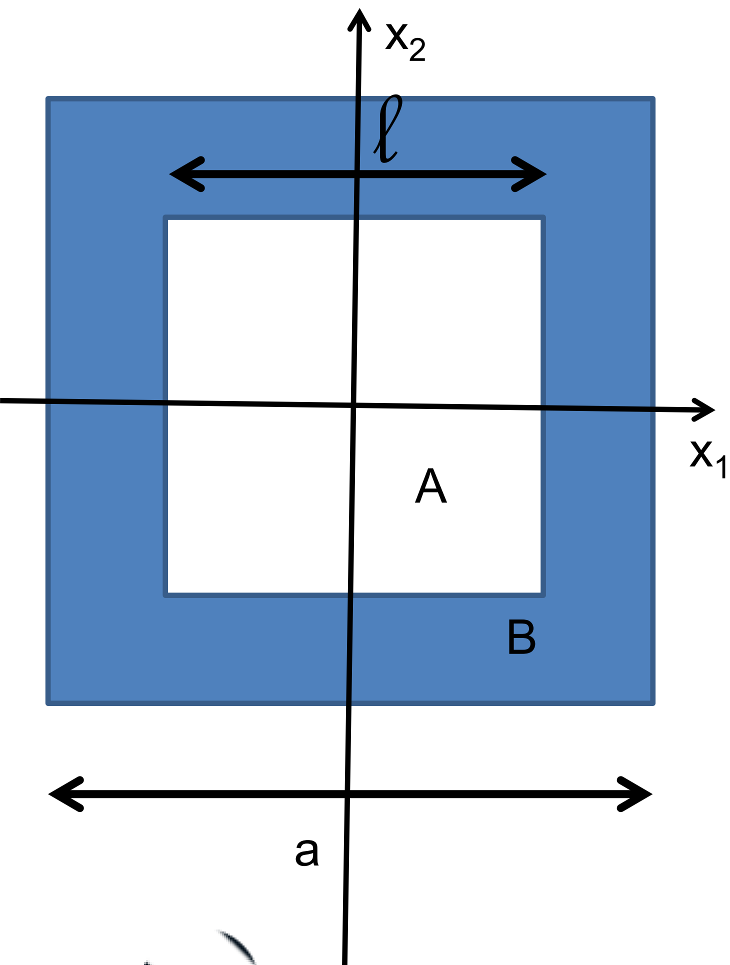
Exercises : Calculate the structure factor for cylinders of square cross section of side length ℓ



$$F(\vec{G}) = \frac{1}{a^2} \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} e^{-iG_1 \cdot x_1} dx_1 \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} e^{-iG_2 \cdot x_2} dx_2$$

$$= \frac{1}{a^2} \left[\frac{e^{-iG_1 \cdot \frac{\ell}{2}} - e^{+iG_1 \cdot \frac{\ell}{2}}}{-iG_1} \right] \left[\frac{e^{-iG_2 \cdot \frac{\ell}{2}} - e^{+iG_2 \cdot \frac{\ell}{2}}}{-iG_2} \right]$$

$$= \frac{1}{a^2} \left[\frac{2i \sin\left(G_1 \cdot \frac{\ell}{2} \right)}{iG_1} \right] \left[\frac{2i \sin\left(G_2 \cdot \frac{\ell}{2} \right)}{iG_2} \right]$$

$$= \frac{1}{a^2} \left[\ell \frac{\sin\left(G_1 \cdot \frac{\ell}{2} \right)}{G_1 \cdot \frac{\ell}{2}} \right] \left[\ell \frac{\sin\left(G_2 \cdot \frac{\ell}{2} \right)}{G_2 \cdot \frac{\ell}{2}} \right]$$

$$= f \left[\frac{\sin\left(G_1 \cdot \frac{\ell}{2} \right)}{G_1 \cdot \frac{\ell}{2}} \right] \left[\frac{\sin\left(G_2 \cdot \frac{\ell}{2} \right)}{G_2 \cdot \frac{\ell}{2}} \right] \quad \text{with } f = \left(\frac{\ell}{a} \right)^2 \text{ and } 0 \le f \le 1$$

… whatever the cross-section of the cylinder :

$$\eta(\vec{G}) = (\eta_A - \eta_B)F\left(\vec{G}\right) + \eta_B \delta_{\vec{G},\vec{0}} \quad \text{where } F\left(\vec{G}\right) = \frac{1}{\Sigma_{(UC)}} \iint_{\left(A_{(UC)}\right)} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r}$$

$$\text{If } \vec{G} = \vec{0}, \eta(\vec{G} = \vec{0}) = (\eta_A - \eta_B)F\left(\vec{G} = \vec{0}\right) + \eta_B$$

$$\text{and } F\left(\vec{G} = \vec{0}\right) = \frac{1}{\Sigma_{(UC)}} \iint_{\left(A_{(UC)}\right)} d^2\vec{r} = \frac{1}{\Sigma_{(UC)}} \cdot \left(\begin{array}{c} \text{inclusion} \\ \text{area } \left(\pi R^2 \text{ or } \ell^2\right) \end{array} \right) = f$$

$$\text{then } \eta(\vec{G} = \vec{0}) = (\eta_A - \eta_B)f + \eta_B = \eta_A f + (1 - \eta_B)f = \overline{\eta} \equiv \text{Average value of } \eta \text{ on the unit cell}$$

$$\text{If } \vec{G} \neq \vec{0}, \eta(\vec{G} \neq \vec{0}) = (\eta_A - \eta_B)F\left(\vec{G} \neq \vec{0}\right)$$

$$\eta(\vec{G}) = (\eta_A - \eta_B)F\left(\vec{G}\right) + \eta_B \delta_{\vec{G},\vec{0}} = \begin{cases} \overline{\eta} = f\eta_A + (1\text{-f})\eta_B \text{ if } \vec{G} = \vec{0} \\ (\eta_A - \eta_B)F\left(\vec{G} \neq \vec{0}\right) \text{if } \vec{G} \neq \vec{0} \end{cases}$$

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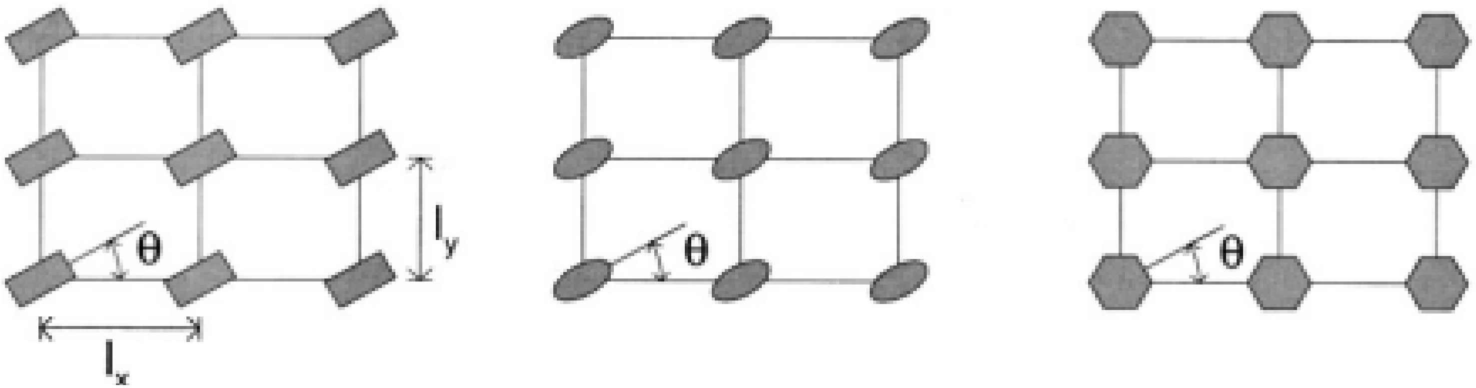
Other cross sections of inclusions can be considered :

rectangular, elliptical, hexagonal, …



Calculation of the structure factor can be made analytically or

numerically for more complicated geometries

Numerical implementation :

Particular case of the Z modes in a square array of circular cylinders

Vectors of the reciprocal lattice are $\vec{G} = \frac{2\pi}{a}\vec{g} = \frac{2\pi}{a}(m\vec{e}_1 + n\vec{e}_2),\ (m,n)\,\text{integers}$

Bloch wave vectors are $\vec{K} = \frac{2\pi}{a}\vec{k} = \frac{2\pi}{a}(k_1\vec{e}_1 + k_2\vec{e}_2)$ and $\vec{K}$ describes the periphery of the irreducible Brillouin zone (ΓXM) where

$$\Gamma \to \frac{2\pi}{a}(0,0),\ X \to \frac{2\pi}{a}\left(\frac{1}{2},0\right),\ M \to \frac{2\pi}{a}\left(\frac{1}{2},\frac{1}{2}\right)$$

$$\omega^2 \sum_{\vec{G}'} B^{(33)}_{\vec{G},\vec{G}'} U_{3,\vec{K}}\left(\vec{G}'\right) = \sum_{\vec{G}'} A^{(33)}_{\vec{G},\vec{G}'} U_{3,\vec{K}}\left(\vec{G}'\right)$$

$$\omega^2 \sum_{\vec{G}'} \rho\left(\vec{G}-\vec{G}'\right) U_{3,\vec{K}}\left(\vec{G}'\right) = \sum_{\vec{G}'} C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_1+K_1)(G'_1+K_1)+(G'_2+K_2)(G_2+K_2)\right] U_{3,\vec{K}}\left(\vec{G}'\right)$$

In the summations, one can separate the term $\vec{G} = \vec{G}'$ and one obtains

$$\omega^2 \left\{ \left[\rho(\vec{0}) U_{3,\vec{K}}(\vec{G}) \right] + \sum_{\vec{G}' \neq \vec{G}} \rho(\vec{G} - \vec{G}') U_{3,\vec{K}}(\vec{G}') \right\} =$$

$$= C_{44}(\vec{0}) \left[(G_1 + K_1)(G_1 + K_1) + (G_2 + K_2)(G_2 + K_2) \right] U_{3,\vec{K}}(\vec{G})$$

$$+ \sum_{\vec{G}' \neq \vec{G}'} C_{44}(\vec{G} - \vec{G}') \left[(G_1 + K_1)(G'_1 + K_1) + (G'_2 + K_2)(G_2 + K_2) \right] U_{3,\vec{K}}(\vec{G}')$$

$$\Leftrightarrow \omega^2 \left\{ \left[\overline{\rho}\, U_{3,\vec{K}}(\vec{G}) \right] + (\rho_A - \rho_B) . \sum_{\vec{G}' \neq \vec{G}} F(\vec{G} - \vec{G}') U_{3,\vec{K}}(\vec{G}') \right\} =$$

$$= \overline{C_{44}} (\vec{G} + \vec{K})^2 U_{3,\vec{K}}(\vec{G}) + (C_{44,A} - C_{44,B}) \sum_{\vec{G}' \neq \vec{G}} F(\vec{G} - \vec{G}') \left[(\vec{G} + \vec{K})(\vec{G}' + \vec{K}) \right] U_{3,\vec{K}}(\vec{G}')$$

$$\Leftrightarrow \omega^2 \overline{\rho} \left\{ U_{3,\vec{k}}(\vec{g}) + \frac{(\rho_A - \rho_B)}{\overline{\rho}} . \sum_{\vec{g}' \neq \vec{g}} F(\vec{g} - \vec{g}') U_{3,\vec{k}}(\vec{g}') \right\} =$$

$$= \overline{C_{44}} \left(\frac{2\pi}{a} \right)^2 \left\{ (\vec{g} + \vec{k})^2 U_{3,\vec{k}}(\vec{g}) + \left(\frac{C_{44,A} - C_{44,B}}{\overline{C_{44}}} \right) \sum_{\vec{g}' \neq \vec{g}} F(\vec{g} - \vec{g}') \left[(\vec{g} + \vec{k})(\vec{g}' + \vec{k}) \right] U_{3,\vec{k}}(\vec{g}') \right\}$$

$$\Leftrightarrow \Omega^2 \left\{ U_{3,\vec{k}}(\vec{g}) + (AP).\sum_{\vec{g}' \neq \vec{g}} F(\vec{g}-\vec{g}')\ U_{3,\vec{k}}(\vec{g}') \right\} =$$

$$= \left\{ (\vec{g}+\vec{k})^2 U_{3,\vec{k}}(\vec{g}) + (BP).\sum_{\vec{g}' \neq \vec{g}} F(\vec{g}-\vec{g}')[(\vec{g}+\vec{k})(\vec{g}'+\vec{k})]\ U_{3,\vec{k}}(\vec{g}') \right\}$$

where $\Omega = \left(\dfrac{\omega}{\left(\dfrac{2\pi}{a}\right)\sqrt{\dfrac{\overline{C_{44}}}{\overline{\rho}}}} \right)$ $\qquad AP = \dfrac{(\rho_A - \rho_B)}{\bar{\rho}}$ $\qquad BP = \left(\dfrac{C_{44,A} - C_{44,B}}{\overline{C_{44}}} \right)$

In the course of the numerical resolution of this equation, we consider

integers m and n (components of the reduced reciprocal lattice vectors $\vec{g}$)

such as $-MT \leq m \leq +MT$ and $-MT \leq n \leq +MT$.

$\Rightarrow$ $(2MT+1)^2$ two-dimensional $\vec{g}$ vectors are taken into account.

$\Rightarrow$This gives $(2MT+1)^2$ eigenfrequencies for a given wave vector describing

the principal directions of propagation in the irreducible Brillouin zone.

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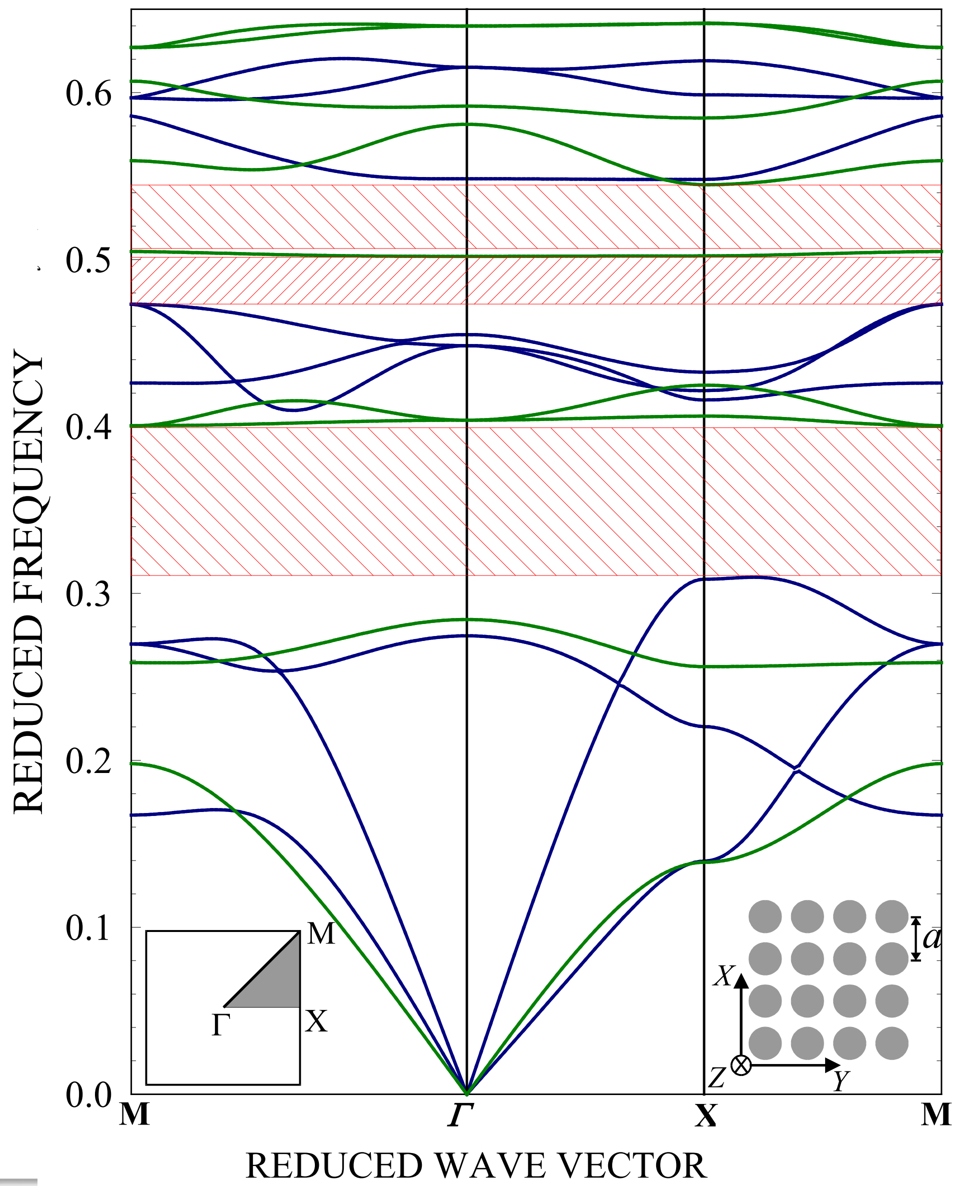
Example of FORTRAN code

Z_SquareArray_Circ_Lapack.txt

Numerical implementation for the XY modes can be done in the same way but matrices are twice larger than those for the Z modes …

Example of band structure



Square array of Carbon cylinders

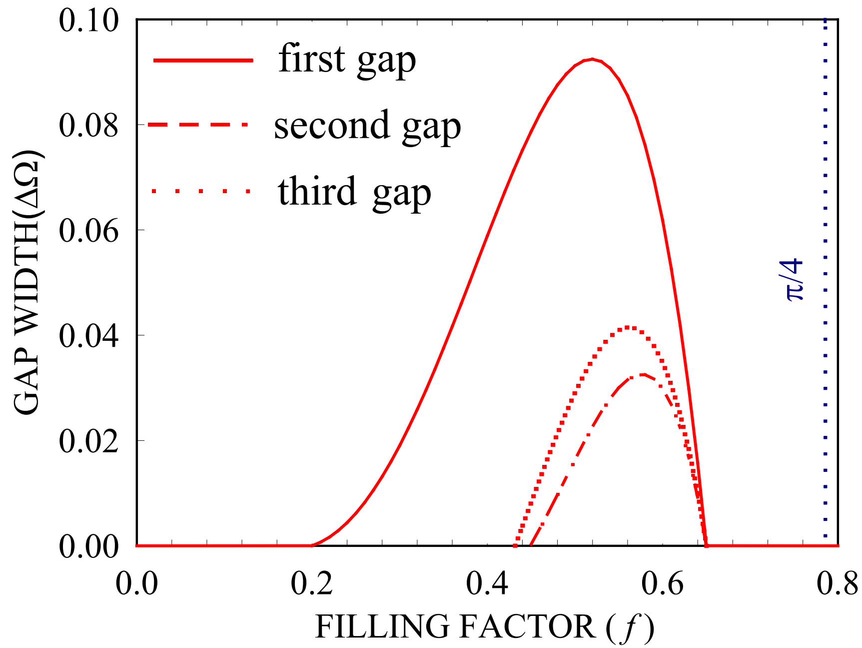
(circular cross section)

embedded in an epoxy resin matrix

***f* = 55 %**

Z modes

XY modes



Advantages and drawbacks of the PWE method

Advantages :

- Very easy to implement
- General (suitable *in theory* for 1D, 2D, 3D periodic structures)

Drawbacks :

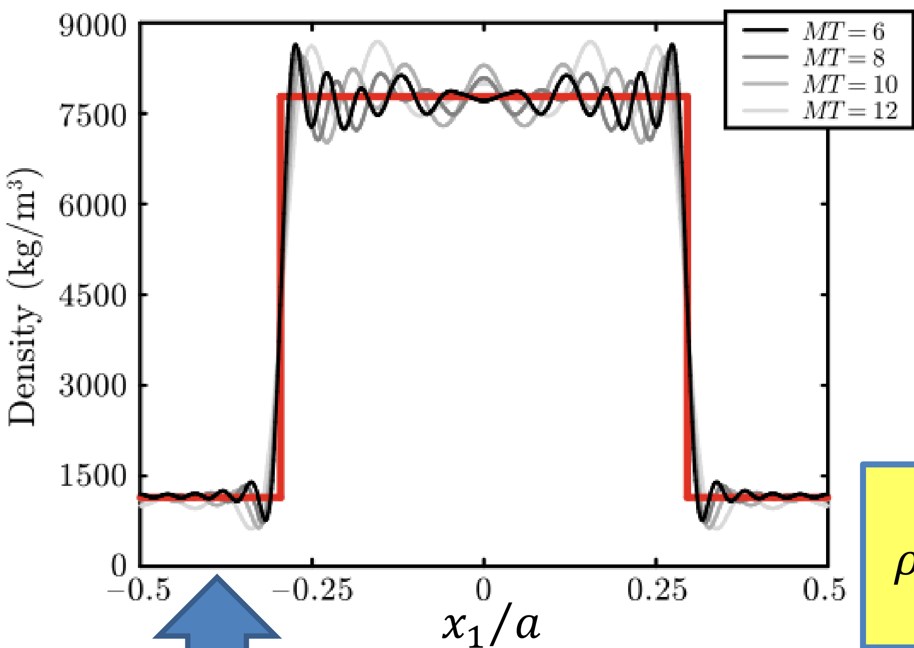
- Convergence of the (truncated) Fourier series is slow especially for constituent materials with very different densities and moduli
- Not reliable for mixed solid/fluid structures except for
  - Rigid solid inclusions in air
  - Holes in a solid matrix

LOW CONVERGENCE OF THE FOURIER SERIES ?

Problem intensively studied for PWE method applied to photonic crystals at the begining of the 1990's

See H.S. Sozuer *et al.*, Phys. Rev. B **45**, 13962 (1992))

$$\rho(\vec{r}) = \sum_{\vec{G}} \rho(\vec{G}) e^{i\vec{G}.\vec{r}}$$



Square array of steel cylinders ($f = 0.55$) embedded in an epoxy matrix
Red line : Density $\rho(\vec{r})$
Gray scale lines : "Truncated" densities along the path $x_1 = x_2$ in the unit cell for different MT values

$$\rho_{Trun}(x_1) = \sum_{m=-MT}^{m=+MT} \sum_{n=-MT}^{n=+MT} \rho(m,n)\, e^{i\frac{2\pi}{a}(m+n)x_1}$$

In the Fourier transform, one replaces a strongly discontinuous function (density or elastic moduli) by a summation of continous sinusoïdal functions ….

Gibbs phenomenon

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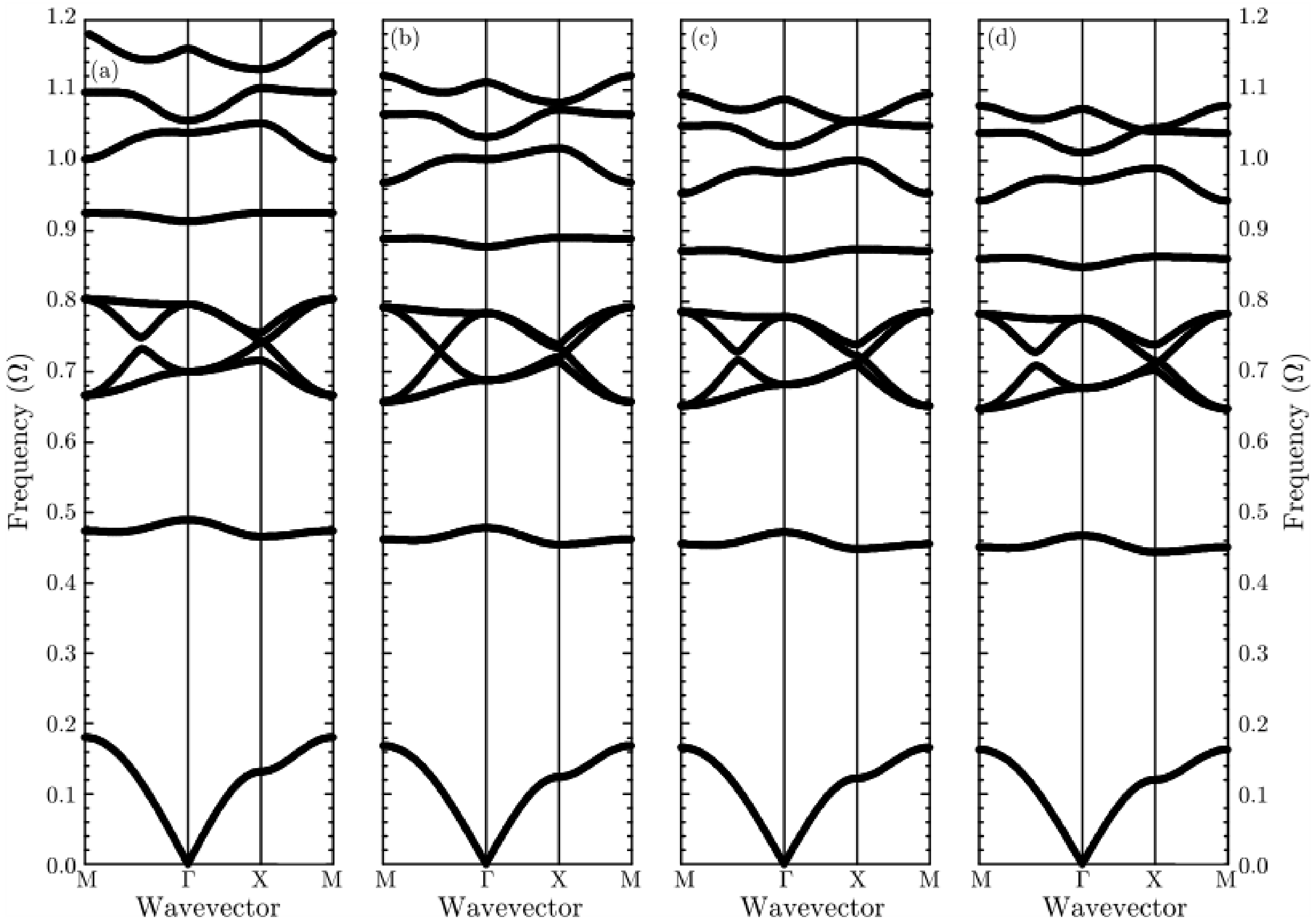
LOW CONVERGENCE OF THE FOURIER SERIES ?



Z modes band structure for a square array of steel cylinders embedded in an epoxy matrix for $MT = 6$ (**a**), $MT = 8$ (**b**), $MT = 10$ (**c**), $MT = 12$ (**d**). $\rho_A = 7780\ kg.m^{-3}$, $C_{44}^A = 8.1.10^{10}\ N.m^{-2}$, $\rho_B = 1142\ kg.m^{-3}$, $C_{44}^B = 0.148.10^{10}\ N.m^{-2}$ and $f = 0.55$

⇒ Location in frequency of some bands (for Ω around 0.2, 0.45 and 1.0 for examples) is strongly influenced by the value of MT, this effect being stronger for larger Ω

PWE METHOD FOR MIXED SOLID/FLUID PHONONIC CRYSTALS ?

First case

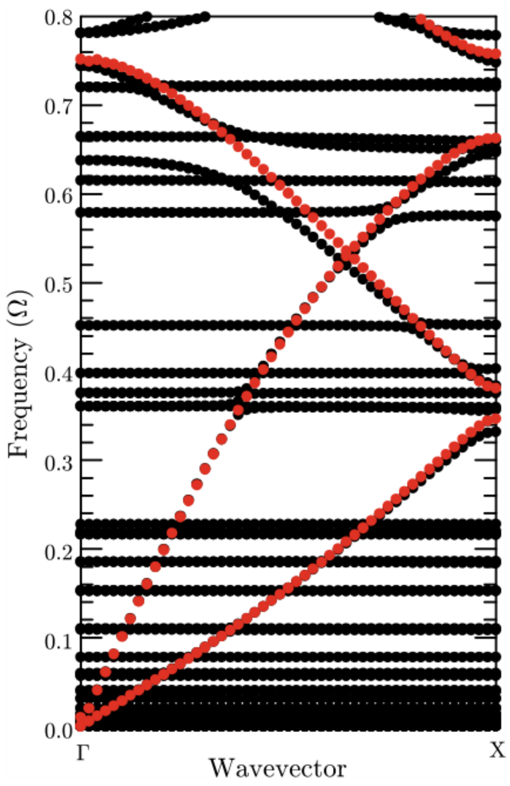
Square array of hollow cylinders in a solid matrix, filled with a non-viscous fluid

One may *intuitively* modelized the fluid as an isotropic *«solid»* material with C_{44}=0 because a transverse vibration does not exist inside a liquid …

… but the conventional PWE method still assumes a finite displacement amplitude for this transverse mode in the cylinders

$\Rightarrow$ numerical instabilities in the PWE code

Example:



XY modes in a two-dimensional square lattice of mercury circular cylinders in an Al substrate with filling fraction *f*=0.4.

Red dots : Finite element (Hg considered as a real fluid)

Black dots : PWE method (with C_{44} for Hg ≡ 0)

⇒Fictitious flat bands

(number of these bands increases when number of $\vec{G}$ vectors taken into account in the Fourier series increases !!!)

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Second case

Square array of hollow cylinders (holes) in a solid matrix

Air inside the holes can not be treated as a solid medium with $C_{44}=0$!!!!

For the same reason (fictitious flat branches), air inside the holes can not be replaced by vacuum with $\rho=0$ and $C_{11}=C_{44}=0$!!!!

Low Impedance Medium (LIM) rather than vacuum

Low density $\cong 10^{-4}$ kg.m^{-3} (<< 10^{3} kg.m^{-3} for usual solids)

Low elastic moduli $\cong 10^{5}$ N.m^{-2} (<< 10^{10} N.m^{-2} for usual solids)

$\Rightarrow$ Low impedance $\cong 10$ kg.m^{-2}.s^{-1} !!!

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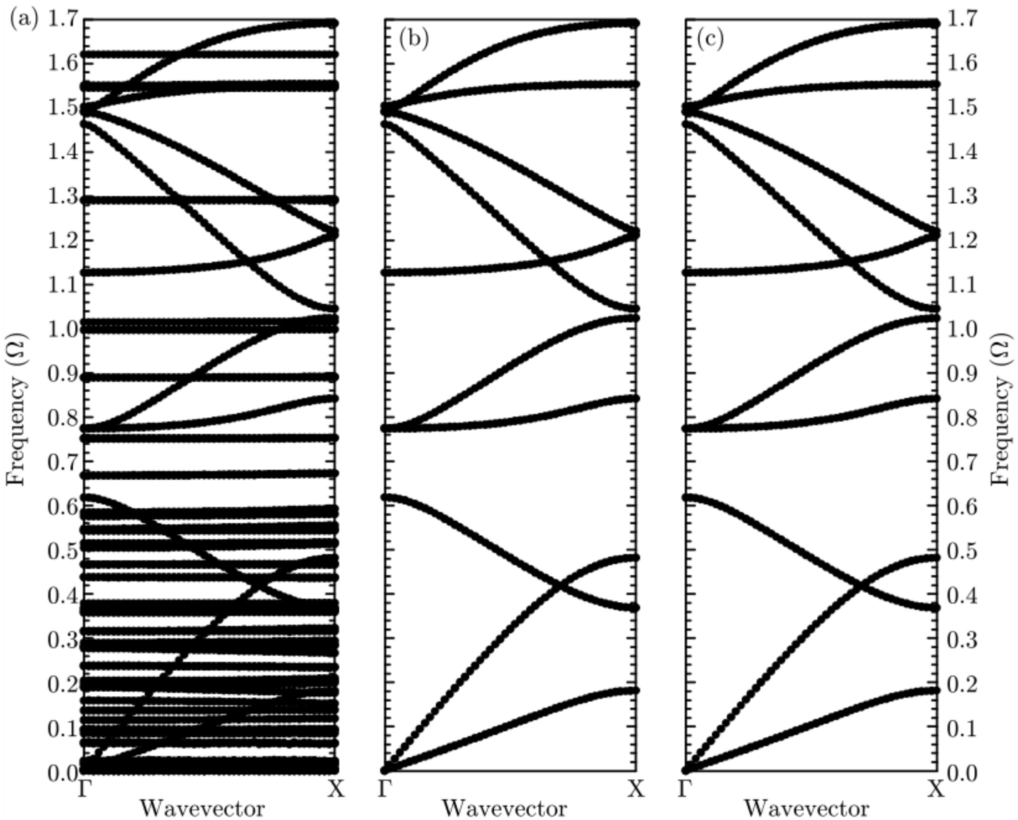

XY modes in a two-dimensional square lattice of hollow cylinders in an Al matrix with filling fraction *f*=0.55.

Left panel : PWE method with $C_{44}^{air} = 0$

Middle panel : PWE method (with material inside the cylinders is the LIM)

Right panel : Finite element method

⇒ Perfect agreement between FE and PWE with LIM

⇔ Spurious flat branches expected to appear in the PWE calculation with "real" air inside the holes are pushed out to the very high-frequency region.

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Third case

Square array of solid cylinders in air

* Due to the huge contrast between the physical characteristics of the solid and those of air, the solid cylinders are assumed infinitely hard (high density and high elastic moduli)

* It implies that the sound does not penetrate such inclusions, and hence the propagation of acoustic waves is predominant in air.

- Air is a fluid where only longitudinal waves can propagate

⇒ Equation of propagation of longitudinal acoustic waves in an inhomogeneous fluid medium

$$-\frac{\omega^2}{C_{11}(\vec{r})} p(\vec{r},t) = \vec{\nabla}.\left(\frac{1}{\rho(\vec{r})}\vec{\nabla} p(\vec{r},t)\right)$$

where $p(\vec{r},t) \equiv$ Acoustic pressure field

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In a « periodic » fluid medium, the equation of propagation of acoustic waves can be Fourier transformed in the form

$$\omega^2 \sum_{\vec{G}'} C_{11}^{-1}\left(\vec{G}-\vec{G}'\right) p_{\vec{K}}\left(\vec{G}'\right) = \sum_{\vec{G}'} \rho^{-1}\left(\vec{G}-\vec{G}'\right)\left[(G_1+K_1)(G'_1+K_1)+(G'_2+K_2)(G_2+K_2)\right] p_{\vec{K}}\left(\vec{G}'\right)$$

Equation similar to that of Z modes in an infinite 2D solid/solid phononic crystal

$$\omega^2 \sum_{\vec{G}'} \rho\left(\vec{G}-\vec{G}'\right) U_{3,\vec{K}}\left(\vec{G}'\right) = \sum_{\vec{G}'} C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_1+K_1)(G'_1+K_1)+(G'_2+K_2)(G_2+K_2)\right] U_{3,\vec{K}}\left(\vec{G}'\right)$$

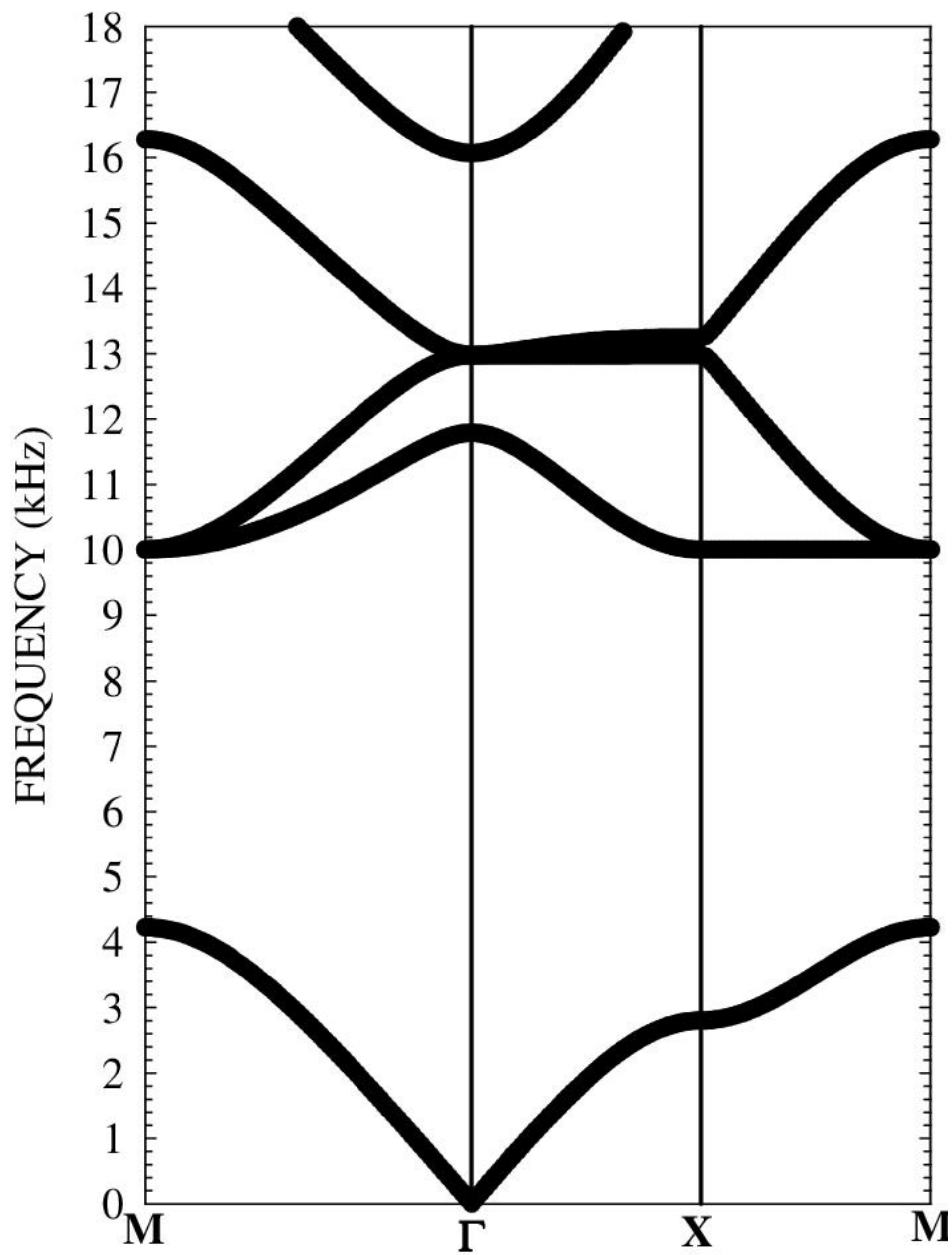
By analogy

$$\begin{cases} \text{Z modes} \leftrightarrow \text{Fluid} \\ \rho \leftrightarrow C_{11}^{-1} \\ C_{44} \leftrightarrow \rho^{-1} \end{cases}$$

$$C_{11} = \rho V_L^2$$

Example:

Square array of steel cylinders in air
a = 2.7 cm
R= 1.29 cm



Stop band in the audible frequency range

Sonic crystal

B) Modified PWE method for complex band structures, complex wave vectors, evanescent waves, examples.

"Classical" PWE expansion method $\Rightarrow$ For a fixed wave vector $\vec{K}$ (with real components), one calculates a set of real eigenfrequencies $\Omega_n(\vec{K})$

"Modified" PWE expansion method $\Rightarrow$ For a fixed value of the frequency, one calculates the components of the wave vectors associated with this frequency

Principle

In the classical PWE method, the Fourier transform of the equation of propagation of elastic waves in a phononic crystal leads to the resolution of a generalized eigenvalue equation in the form $\omega^2 \overleftrightarrow{B}.\vec{U} = \overleftrightarrow{A}.\vec{U}$.

The matrix elements of $\overleftrightarrow{A}$ involve terms depending on the components of the wave vector $\vec{K}$.

$\Rightarrow$ One may rewrite matrix $\overleftrightarrow{A}$ as $\overleftrightarrow{A} = K_\alpha^2 \overleftrightarrow{A}_1 + K_\alpha \overleftrightarrow{A}_2 + \overleftrightarrow{A}_3$ where K_α is one of the components of the wave vector and $\overleftrightarrow{A}_1$, $\overleftrightarrow{A}_2$ and $\overleftrightarrow{A}_3$ are matrices of the same size as $\overleftrightarrow{A}$. The generalized eigenvalue equation $\omega^2 \overleftrightarrow{B}.\vec{U} = \overleftrightarrow{A}.\vec{U}$ may be recast as $K_\alpha^2 \overleftrightarrow{A}_1.\vec{U} = \omega^2 \overleftrightarrow{B}.\vec{U} - \overleftrightarrow{A}_3.\vec{U} - K_\alpha \overleftrightarrow{A}_2.\vec{U}$ and can be rewritten as

$$K_\alpha \begin{pmatrix} \overleftrightarrow{I} & \overleftrightarrow{0} \\ \overleftrightarrow{0} & \overleftrightarrow{A}_1 \end{pmatrix} \begin{pmatrix} \vec{U} \\ K_\alpha \vec{U} \end{pmatrix} = \begin{pmatrix} \overleftrightarrow{0} & \overleftrightarrow{I} \\ \omega^2 \overleftrightarrow{B} - \overleftrightarrow{A}_3 & -\overleftrightarrow{A}_2 \end{pmatrix} \begin{pmatrix} \vec{U} \\ K_\alpha \vec{U} \end{pmatrix} \text{ where } \overleftrightarrow{I} \text{ is the identity matrix}$$

⇔ Eigen-value problem where the eigen-values are the component of the wave vector

<u>Example</u> : Z elastic modes of a square array of cylinders embedded in a matrix

$$\omega^2 \sum_{\vec{G}'} \rho\left(\vec{G}-\vec{G}'\right) U_{3,\vec{K}}\left(\vec{G}'\right) = \sum_{\vec{G}'} C_{44}\left(\vec{G}-\vec{G}'\right)\left[\left(G_1+K_1\right)\left(G'_1+K_1\right)+\left(G'_2+K_2\right)\left(G_2+K_2\right)\right] U_{3,\vec{K}}\left(\vec{G}'\right)$$

Consider the direction of propagation ΓX ⇒ K_2=0

$$K_1{}^2 \sum_{\vec{G}'} C_{44}\left(\vec{G}-\vec{G}'\right) U_{3,\vec{K}}\left(\vec{G}'\right)$$
$$= \sum_{\vec{G}'} \left\{\omega^2 \rho\left(\vec{G}-\vec{G}'\right) - \left(G_1 G'_1 + G_2 G'_2\right) C_{44}\left(\vec{G}-\vec{G}'\right)\right\} U_{3,\vec{K}}\left(\vec{G}'\right) - K_1 \sum_{\vec{G}'} \left(G_1 + G'_1\right) C_{44}\left(\vec{G}-\vec{G}'\right) U_{3,\vec{K}}\left(\vec{G}'\right)$$

and

$$K_1\begin{pmatrix}\overleftrightarrow{I} & \overleftrightarrow{0}\\ \overleftrightarrow{0} & \overleftrightarrow{A}_1\end{pmatrix}\begin{pmatrix}\vec{U}\\ K_1\vec{U}\end{pmatrix}=\begin{pmatrix}\overleftrightarrow{0} & \overleftrightarrow{I}\\ \omega^2\overleftrightarrow{B}-\overleftrightarrow{A}_3 & -\overleftrightarrow{A}_2\end{pmatrix}\begin{pmatrix}\vec{U}\\ K_1\vec{U}\end{pmatrix}$$

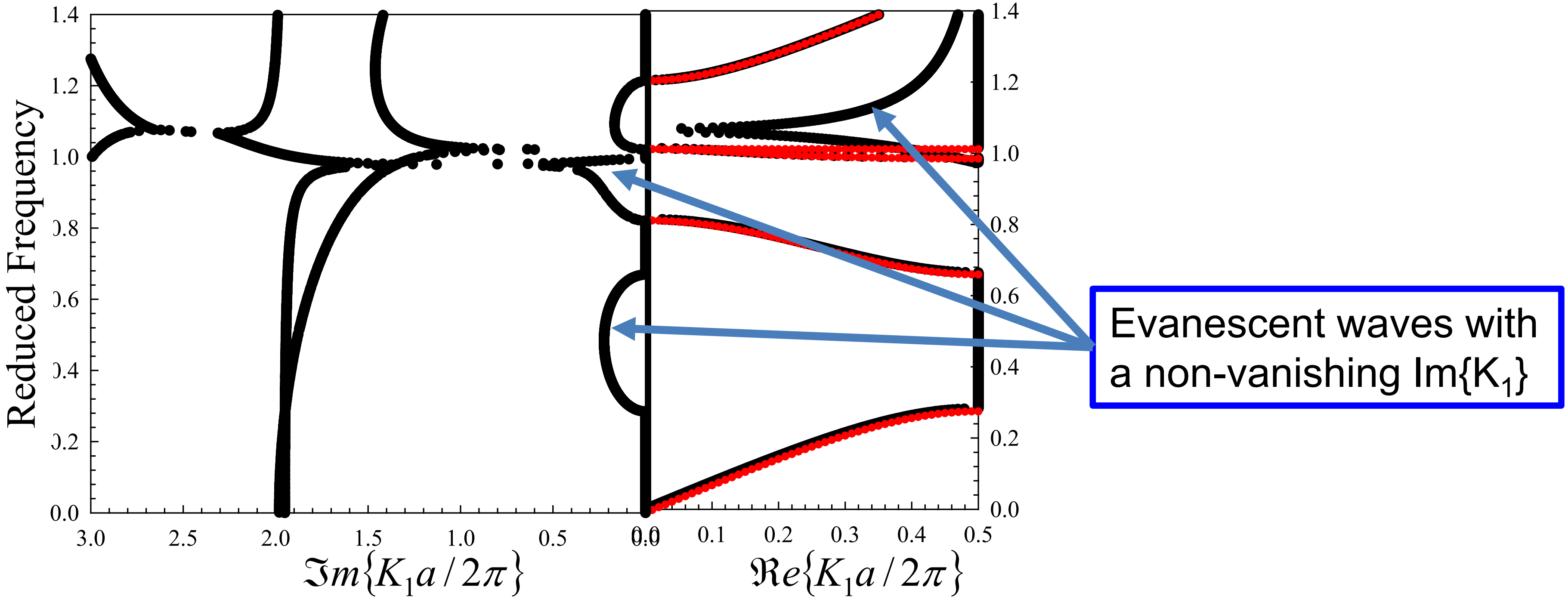
where

$$\begin{cases} B_{\vec{G},\vec{G}'} = \rho(\vec{G}-\vec{G}') \\ A^{(1)}_{\vec{G},\vec{G}'} = C_{44}(\vec{G}-\vec{G}') \\ A^{(2)}_{\vec{G},\vec{G}'} = C_{44}(\vec{G}-\vec{G}')(G_1+G'_1) \\ A^{(3)}_{\vec{G},\vec{G}'} = C_{44}(\vec{G}-\vec{G}')(G_1G'_1+G_2G'_2) \end{cases}$$

→ Eigen-value problem where, for a fixed value of the real frequency ω,

the complex eigen-values are $K_1 = \Re e\{K_1\} - i\Im m\{K_1\}$

An example of complex band structure



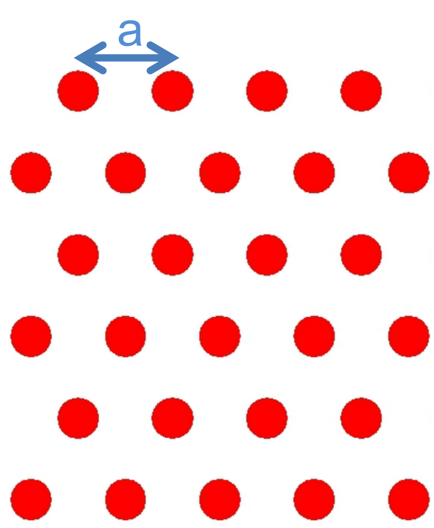
Band structure along the ΓX direction of the irreducible Brillouin zone for a square array of holes drilled in a Silicon matrix :

Red dots: Classical PWE method;
Black dots: Modified PWE method.

An application : Calculation of the Equifrequency contour at some specific frequency

Steel-Epoxy phononic crystal

Triangular array of steel cylindrical inclusions embedded in an epoxy matrix
Inclusion radius : R=1mm
Lattice parameter : a=2.84 mm
$\Rightarrow$ Filling factor = 45%



Band structure

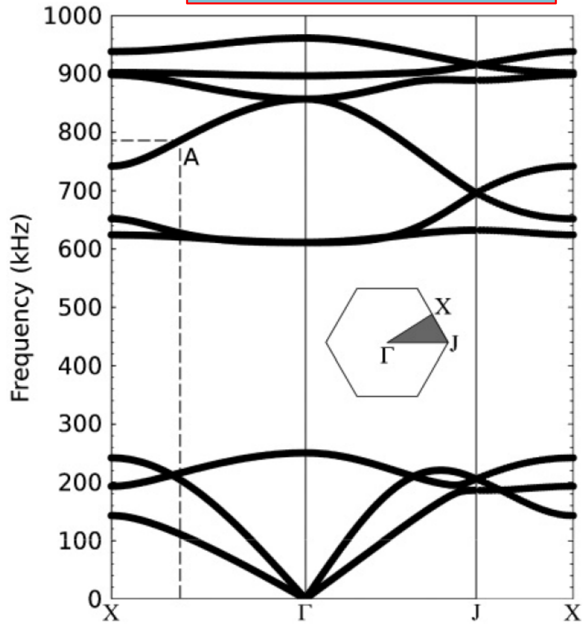


FIG. 1. Elastic band structure for the 2D PC made of a triangular array of steel rods in an epoxy matrix.

Equi-frequency contours
($f = f(k_x,k_y)$)

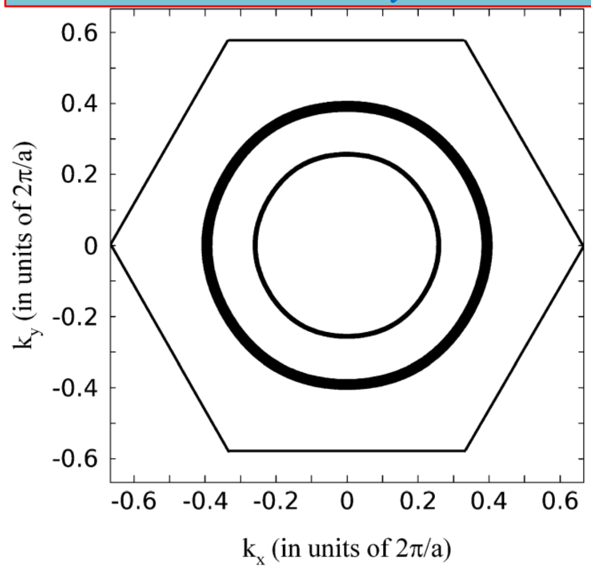


FIG. 3. EFCs of the PC at 780 kHz (thick line) and 820 kHz (thin line).

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Steel-Epoxy phononic crystal

Square array of steel cylindrical inclusions embedded in an epoxy matrix
Inclusion radius : R=1mm
Lattice parameter : a=3.23 mm and Filling factor = 30%

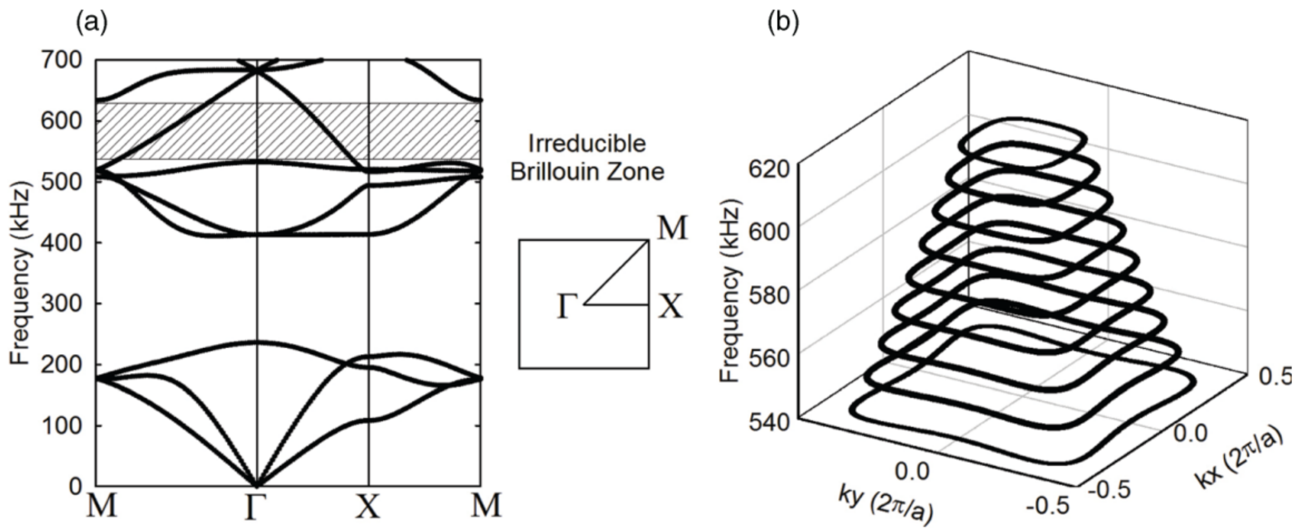

FIG. 1. (a) Band structure calculated with the plane wave expansion method (Refs. 2 and 3) of the infinite, periodic steel/epoxy PC (square array, lattice parameter $a = 3.23$ mm, filling factor $f = 30\%$) along high symmetry directions in the irreducible Brillouin zone. This band structure is limited to vibrational modes in the plane perpendicular to the inclusions. A large band gap is observed between 238 and 410 kHz. From 540 to 620 kHz (shaded region), a passing band with negative slope stands alone. (b) EFCs over frequency range 540–620 kHz [shaded region in (a)]. The squarelike shape of these contours allows for zero-angle refraction phenomena for a wide range of incidence angles of acoustic beams (after Ref. 25).

EFC's are usefull when investigating refraction phenomena in phononic crystals (negative refraction, zero-angle refraction)

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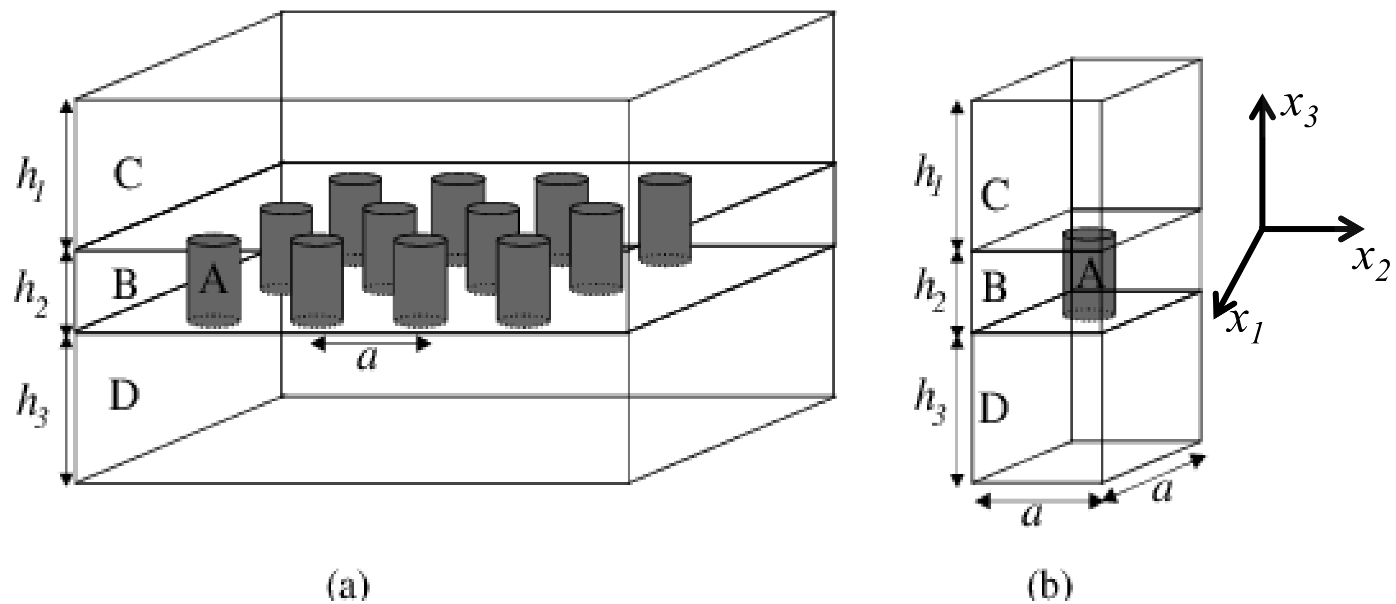
C) PWE method for phononic crystal plates

One considers a 2D phononic crystal of finite thickness h_2 along the x_3 direction sandwiched between two homogeneous plates made of materials C and D

Phononic crystal plate and the super-cell PWE method



(a) 2D phononic crystal plate sandwiched between two slabs of homogeneous materials, and (b) three-dimensional supercell considered in the course of the supercell-PWE computation

The super cell is a parallelepiped of side length a (the lattice parameter of the 2D array) and of height $\ell = h_1 + h_2 + h_3$ and is repeated periodically in the three spatial directions

Full 3D problem !!! (see FT equations of propagation in page 53)

but

$$\eta(\vec{G}) = \frac{1}{V_u} \iiint_{(super\ cell)} \eta(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r} \quad \text{where} \quad V_u = a^2\ell$$

$\equiv$ Volume of the supercell

For a square array of inclusions, the Fourier coefficients become :

$$\Rightarrow \eta(\vec{G}) = \begin{cases} f\eta_A\left(\frac{h_2}{\ell}\right) + (1-f)\eta_B\left(\frac{h_2}{\ell}\right) + \eta_C\left(\frac{h_1}{\ell}\right) + \eta_D\left(\frac{h_3}{\ell}\right), if\ \vec{G} = \vec{0} \\ (\eta_A - \eta_B)F^s{}_I(\vec{G}) + (\eta_C - \eta_B)F^s{}_{II}(\vec{G}) + (\eta_D - \eta_B)F^s{}_{III}(\vec{G}), if\ \vec{G} \neq \vec{0} \end{cases}$$

$$F^s{}_I(\vec{G}) = \frac{1}{V_u}\iiint\limits_{(A)} e^{-i\vec{G}\cdot\vec{r}}\, d^3\vec{r} = 2f\,\frac{J_1(G_{//}R)}{G_{//}R}\left(\frac{sin\left(G_3\dfrac{h_2}{2}\right)}{\left(G_3\dfrac{h_2}{2}\right)}\right).\left(\frac{h_2}{\ell}\right)$$

$$F^s{}_{II}(\vec{G}) = \frac{1}{V_u}\iiint\limits_{(C)} e^{-i\vec{G}\cdot\vec{r}}\, d^3\vec{r} = \left(\frac{sin\left(G_1\dfrac{a}{2}\right)}{\left(G_1\dfrac{a}{2}\right)}\right).\left(\frac{sin\left(G_2\dfrac{a}{2}\right)}{\left(G_2\dfrac{a}{2}\right)}\right).\left(\frac{sin\left(G_3\dfrac{h_1}{2}\right)}{\left(G_3\dfrac{h_1}{2}\right)}\right).\left(\frac{h_1}{\ell}\right).e^{-iG_3\left(\frac{h_1+h_2}{2}\right)}$$

$$F^s{}_{III}(\vec{G}) = \frac{1}{V_u}\iiint\limits_{(D)} e^{-i\vec{G}\cdot\vec{r}}\, d^3\vec{r} = \left(\frac{sin(G_1\dfrac{a}{2})}{(G_1\dfrac{a}{2})}\right).\left(\frac{sin(G_2\dfrac{a}{2})}{(G_2\dfrac{a}{2})}\right).\left(\frac{sin(G_3\dfrac{h_3}{2})}{(G_3\dfrac{h_3}{2})}\right).\left(\frac{h_3}{\ell}\right).e^{-iG_3\left(\frac{h_2+h_3}{2}\right)}$$

where $\vec{G} = (G_1, G_2, G_3) = (\vec{G}_{//}, G_3)$ and $G_3 = \dfrac{2\pi}{\ell} n_3,\ \ n_3$ integer

$\vec{K} = (K_1, K_2, K_3) = (\vec{K}_{//}, K_3)$ where $\vec{K}_{//} \in (2D$ Reduced BZ) and $0 < \mathrm{K}_3 < \dfrac{\pi}{\ell}$

What must be media C and D for isolating the vibrational modes of the plate with those of plates in the adjacent unit cells???

Rigorously : C and D must be vacuum with ρ and C_{ij} equal to 0

But numerical instabilities in the PWE code

Low Impedance Medium (LIM) rather than vacuum
Low density $\cong 10^{-4}$ kg.m^{-3}
Low elastic moduli $\cong 10^{5}$ N.m^{-2} (<< 10^{10} N.m^{-2} for usual solids)

$\Rightarrow$ Low impedance $\cong 10$ kg.m^{-2}.s^{-1} !!!

BUT

Due to the full 3D nature of the problem, the convergence of the Fourier series is very slow

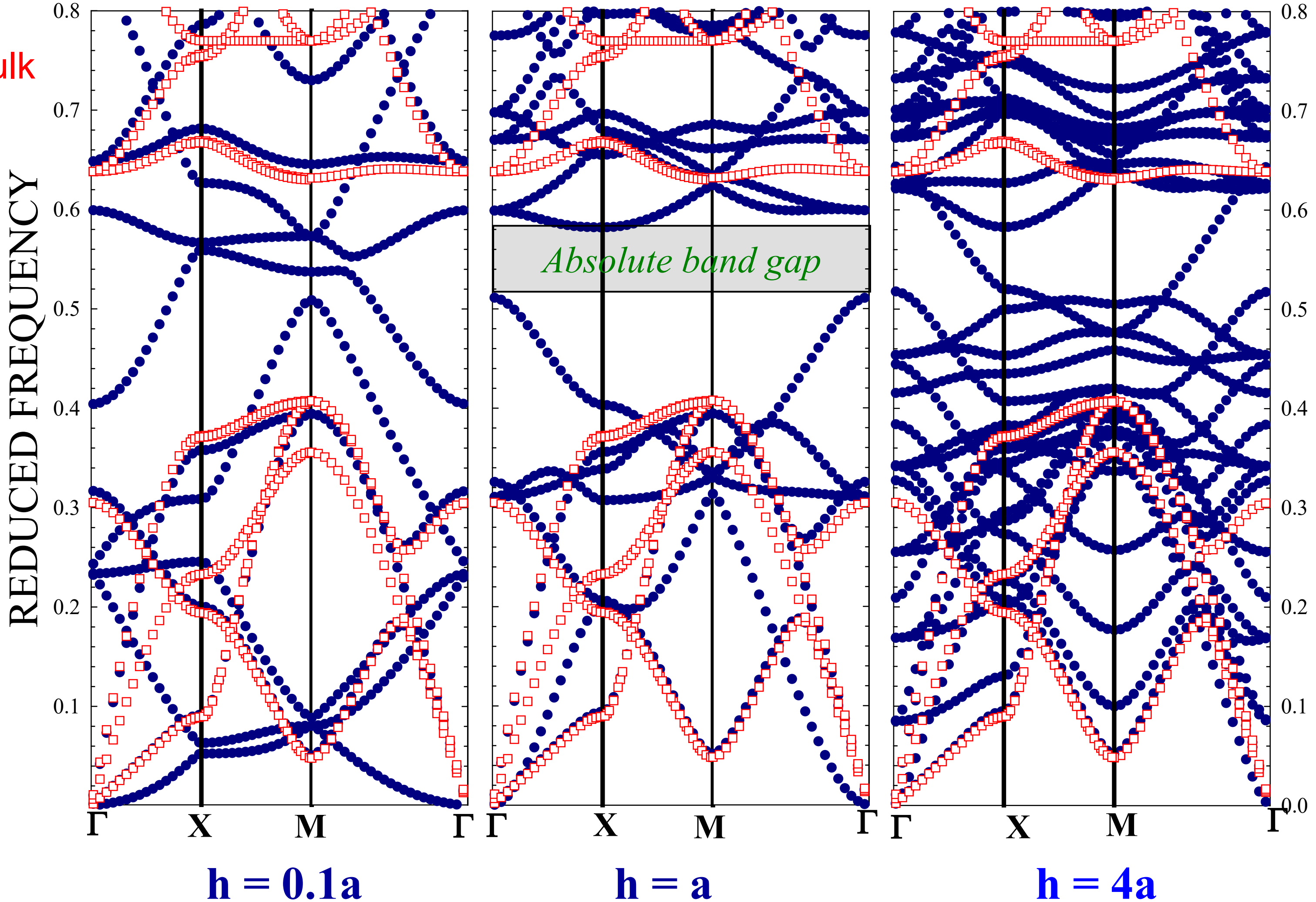
Method suitable only for array of voids inserted in a solid matrix

SQUARE ARRAY OF HOLES DRILLED IN A STEEL PLATE ($f = 0.70$)

□ : PWE band structure of the bulk PC

● : PWE band structure of the PC plate

Existence of an absolute band gap if the thickness h_2 is of the same order of magnitude as the lattice parameter *a*, typically h_2 between *0.5a* and *1.5a*.



J.O. Vasseur *et al.*, Phys. Rev. B 77, 085415 (2008)

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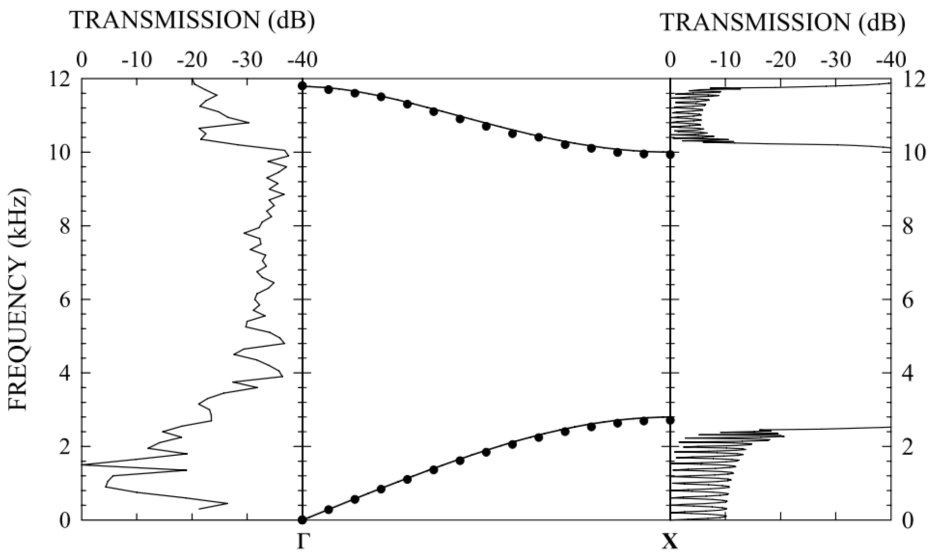
D) COMMENTS

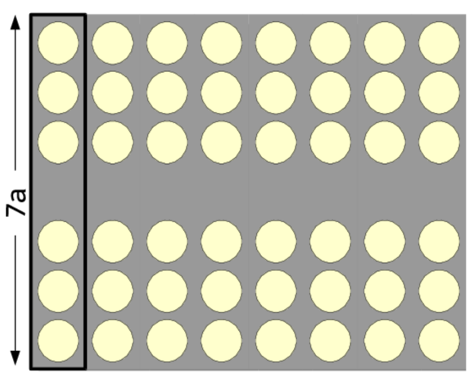
I) Supercell together with the PWE method may allow to consider defective phononic crystal ⇒ Phononic crystal with rectilinear defect (waveguide)

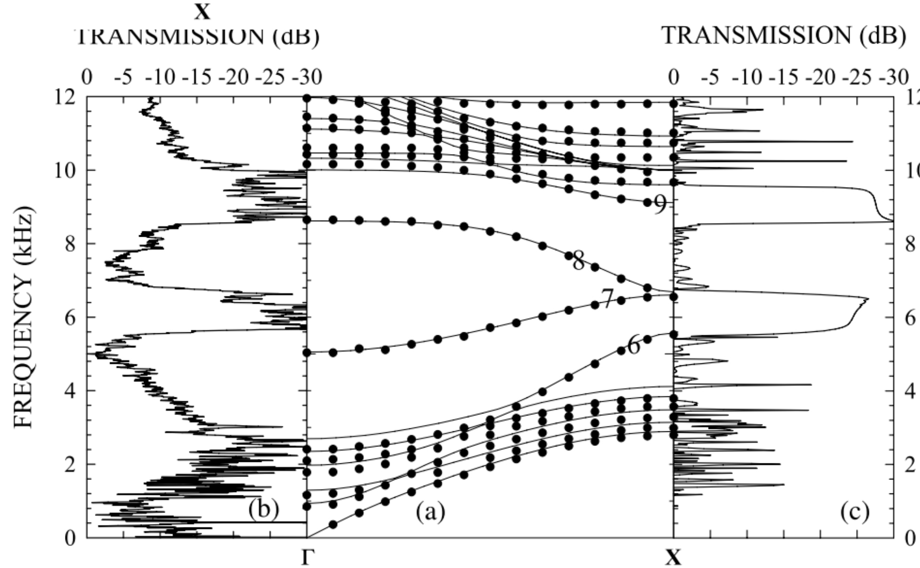


<u>Middle panel</u> : PWE Band structure (unit cell and inclusions assumed perfectly rigid) along the ΓX direction for a square array of PVC cylinders in air

<u>Left Panel</u> : Experimental transmission coefficient

<u>Right Panel</u> : Calculated (FDTD) transmission coefficient





<u>Middle panel</u> : PWE Band structure(super-cell = 1x7 unit cells) along the ΓX direction

⇒ Waveguide modes inside the band gap of the perfect phononic crystal

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II) Eigenvector associated with some eigenvalue ?

$$\omega^2 \overleftrightarrow{B}.\vec{U}_{\vec{K}} = \overleftrightarrow{A}.\vec{U}_{\vec{K}} \quad (1)$$

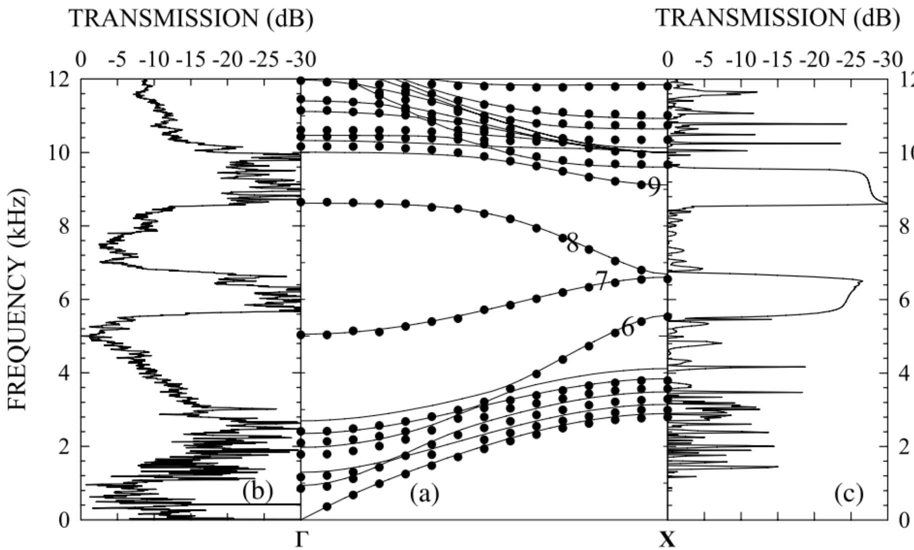
and

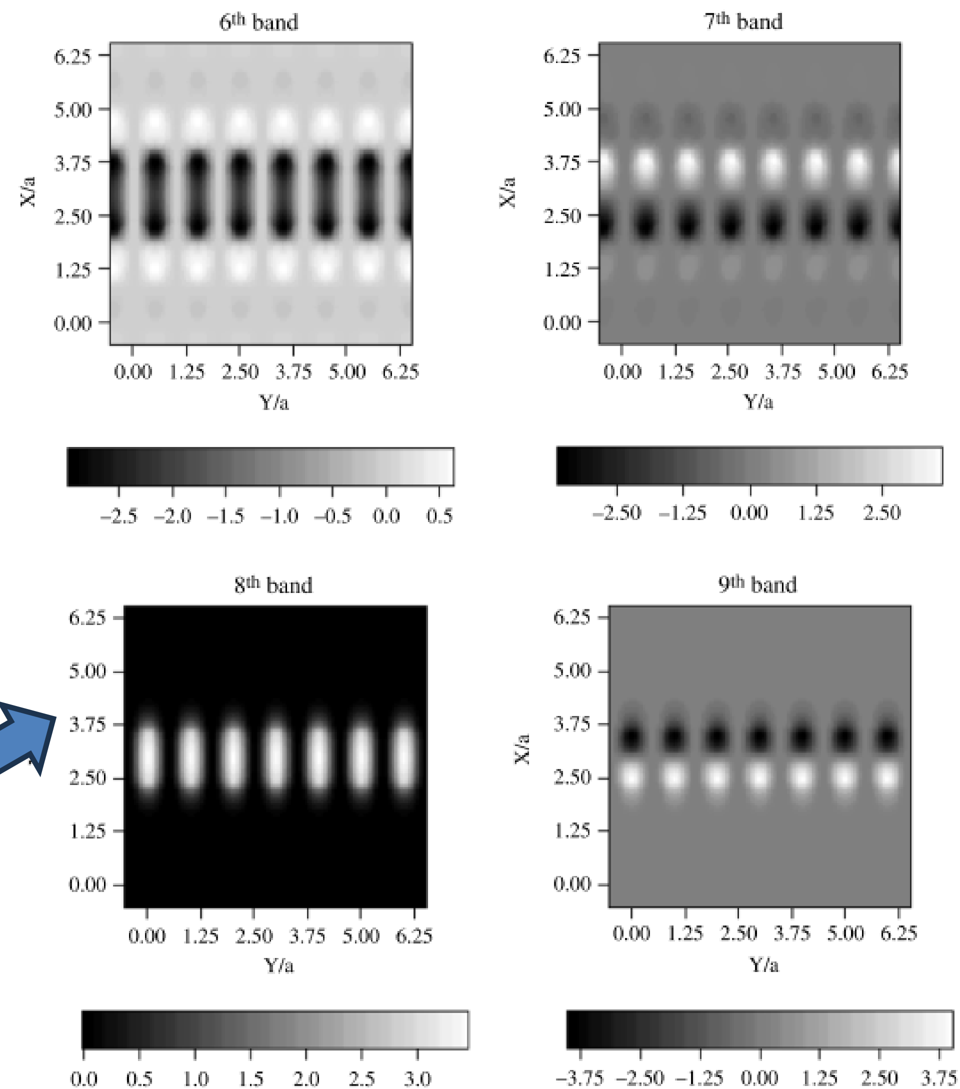
$$\vec{u}(\vec{r},t) = e^{i(\vec{K}.\vec{r}-\omega t)} \sum_{\vec{G}} \vec{U}_{\vec{K}}(\vec{G}) e^{i\vec{G}\cdot\vec{r}} \quad (2)$$

→ For some eigenvalue ω and for a chosen $\vec{K}$, eigenvector $\overrightarrow{U_{\vec{K}}}$ can be computed

→ From Equation (2), the displacement field $\vec{u}(\vec{r})$ associated with eigenvalue ω and eigenvector $\overrightarrow{U_{\vec{K}}}$ can be computed at some time (t=0!)

→ This may give some interesting informations about the symmetry of the mode, the way the mode propagates inside the structure, …





Pressure field calculated with the PWE method at X point

7th and 9th bands do not have the right symmetry for being excited by an incident longitudinal wave in air and they do not contribute to the transmission⇔ Deaf modes

Modes associated with the 6th and 8th bands are rather well confined inside the waveguide ⇔ Guided modes

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CONCLUSION

The PWE method is a useful and « ancient » tool for investigating properties of periodic structures such as phononic crystals but it presents some restrictions ….


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