1.What is dispersion relation

Tutorial 3

- In science and technology, dispersion relations describe the effect of dispersion in a medium on the properties of a wave propagating in that medium.
- A dispersion relation relates the wavelength (λ) or wavenumber (k) of a wave to its frequency (ω). (From this relation, the phase velocity and the group velocity of the wave can be derived, which then determine the refractive index of the medium).

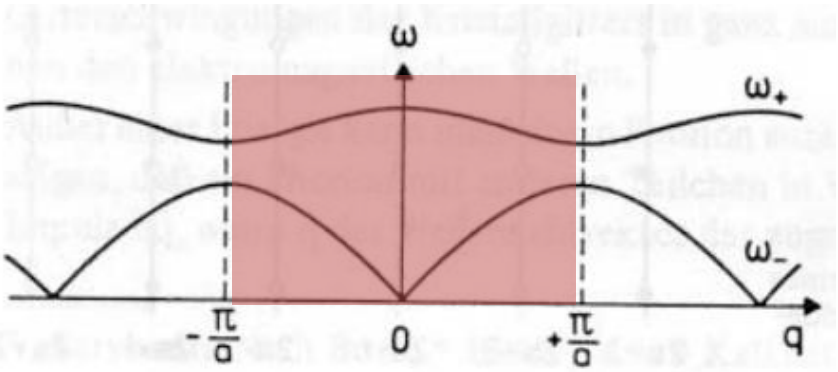
Homework: Why are natural oscillations also called normal modes?
;-) This does not happen by chance. There is a physical and mathematical reason for it!

2. What is a phonon?

- A phonon is the quantum mechanical description of an elementary oscillatory motion, in which a lattice of atoms or molecules oscillates uniformly at a single frequency.
- In classical mechanics, this is called natural oscillation (normal mode). Natural oscillations are important, because any lattice vibration can be considered as a superposition of these elementary vibrations (Fourier analysis).
- Natural oscillations in classical mechanics are wave-like phenomena, phonons also have particle-like properties, in a way related to the wave-particle duality of quantum mechanics.

3. Draw the phonon dispersion relation and identify its components for a crystal with 2 atoms in the base.

- On what parameters does this dispersion relation depend? Identify them. What is **f** and where does it come from?
- What is the red marked area?

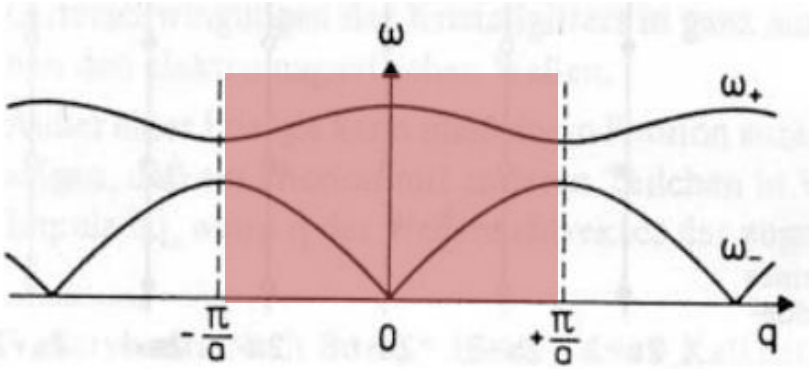


$$\omega^2 = f\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm f\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4}{M_1 M_2} sin^2 \frac{qa}{2}}$$

Answer:

M_1 and M_2 : mass of the atoms
q: wavevector
a: lattice constant
f: spring constant and comes from the semiclassical model of coupled oscillators, which is used to describe the oscillations of the crystal

The first Brillouin zone, on which we have based the entire analysis due to the periodic nature of the crystal can be reduced and simplified.



Optical branch

Acoustic branch

Acoustic branch:

- Begins at $q = 0$ and $\omega = 0$.
- With increasing q the frequency increases in a linear fashion called acoustic, it corresponds to elastic waves or sound.

Optical branch:

- Has a non-zero frequency at zero q
- The frequency of the vibrations lies in infrared region which is the reason for referring to this branch as optical.

The gap (forbidden band) between the optical and acoustic branches is the region where frequencies are not allowed to propagate. **The width of this forbidden band depends on the difference of the masses of the two atoms.**

4. How many phonon modes can be expected for a crystal with $p > 2$ atoms?

a) Perform the calculation for $p = 2$ and 3

b) How many modes do you expect to see in the dispersion relation of Si, Ge and GaAs? Why?

Answer:

a) The number of modes is calculated using the following relationships:
   - 3D crystal with p atoms in the basis → phonon branches and polarization
   - In total, 3p phonon branches:
     - 3 acoustic (2 transversal and 1 longitudinal)
     - 3(p-1) optical with: 2(p-1) transversal and (p-1) longitudinal modes

b) They all have 3 acoustic and 3 optical (2TO+1LO) modes.

5. The following figures show the phonon dispersion relations of GaAs and InP and the corresponding densities of states (DOS).

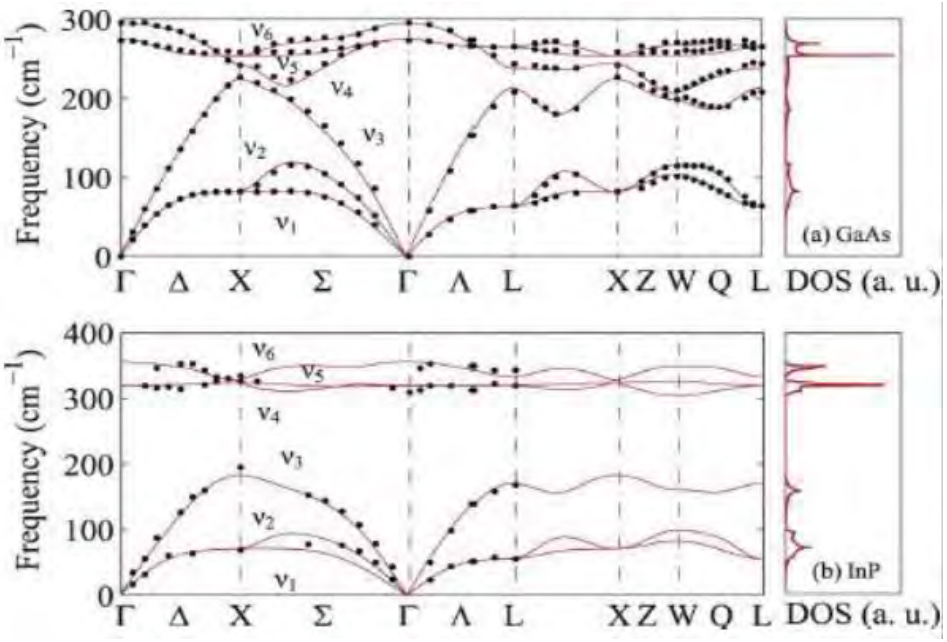
a) Identify the branches you observe in the figure. Did you expect this result? Why?

b) Why is the gap between optical and acoustic modes different for the two semiconductors? Use the information in the periodic table of elements to estimate the difference.

c) How is the density of states DOS related to the dispersion relations?

d) What part of the dispersion relation is detected by Raman spectroscopy?

e) What are the Roman capital letters? What are the Greek letters?



Answer:

a) 3 optical on top (ν_4, ν_5, ν_6) & 3 acoustic (ν_1, ν_2, ν_3). Yes, because both semiconductors have 2 atoms in the base.

b) Homework!

c) In general, the DOS is proportional to the inverse of the slope of the dispersion relation. The flatter the band is, the greater the density of states, which is consistent with what we observe in the figure.

d) Raman spectroscopy can only cover a narrow region around the center of the Brillouin zone Γ and detect there only phonons with ω > 0 (optical phonons).

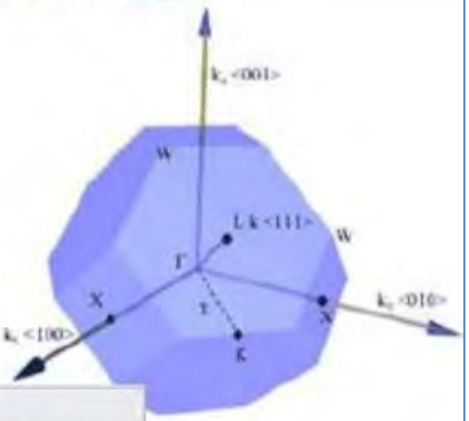
e)

Brillouin zone of Silicon (fcc)

Γ – center of the Brillouin zone

Greek letters – high symmetry points and lines inside Brillouin zone

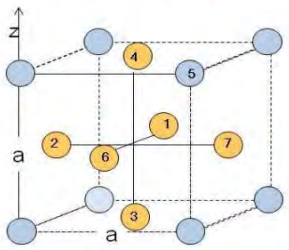
Roman letters - points on the surfaces of the Brillouin zone



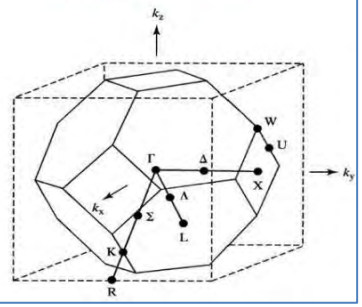
Face-centered cubic	
K	Middle of an edge joining two hexagonal faces
L	Center of a hexagonal face
U	Middle of an edge joining a hexagonal and a square face
W	Corner point
X	Center of a square face

Brillouin Zone in *Real* FCC Lattices …

Real Space FCC (for Si, Ge, GaAs)



Reciprocal Lattice



6. Determine the reciprocal lattice vectors:

a) of the primitive cubic lattice.

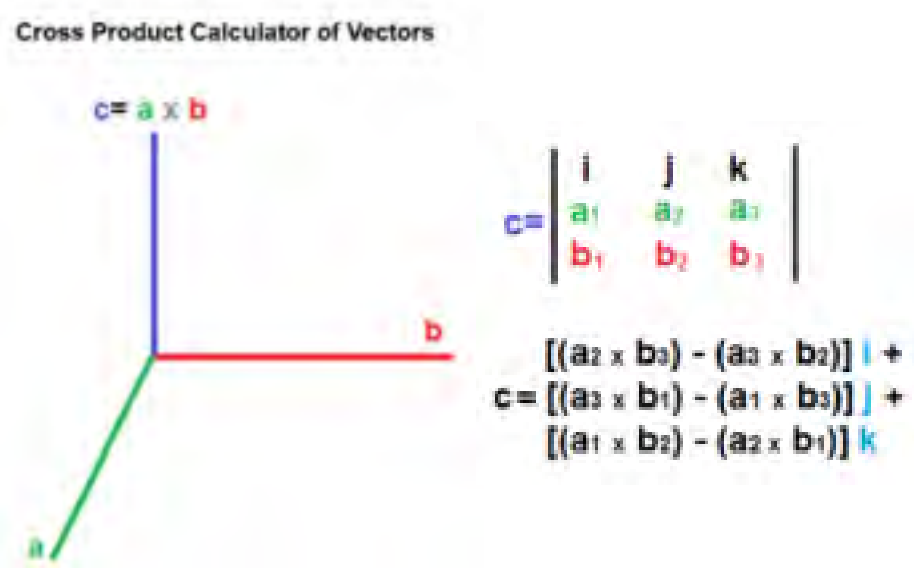
b) of the face-centered cubic lattice.

c) of the cubic space-centered lattice. (Homework)

d) Consider the results, what do you conclude?

e) What are the names of these structures in reciprocal space.

Remember that you have 2 possibilities to perform this calculation. Choose the one that you prefer, but the result should be the same.



See the following concepts:

- Dot product of vectors
- Cross product of vectors.

Answer (6a&d):

Steps (general):

1. Lattice vectors of the direct lattice: $\begin{cases} \overrightarrow{a_1} = a\hat{x} \\ \overrightarrow{a_2} = a\hat{y} \\ \overrightarrow{a_3} = a\hat{z} \end{cases}$

2. General expression for the reciprocal lattice vectors.

   a. Volume of the unit cell

$$V = \overrightarrow{a_1} \cdot (\overrightarrow{a_2} \times \overrightarrow{a_3})$$

3. Reciprocal lattice vectors: $\begin{cases} \overrightarrow{b_1} = (2\pi/V)\overrightarrow{a_2} \times \overrightarrow{a_3} \\ \overrightarrow{b_2} = (2\pi/V)\overrightarrow{a_3} \times \overrightarrow{a_1} \\ \overrightarrow{b_3} = (2\pi/V)\overrightarrow{a_1} \times \overrightarrow{a_2} \end{cases}$

Simple cubic structure

1. $\begin{cases} \overrightarrow{a_1} = a\hat{x} \\ \overrightarrow{a_2} = a\hat{y} \\ \overrightarrow{a_3} = a\hat{z} \end{cases}$

2. $$V = \overrightarrow{a_1} \cdot (\overrightarrow{a_2} \times \overrightarrow{a_3})$$
$$= a\hat{x} \cdot (a\hat{y} \times a\hat{z})$$
$$= a^3$$

3. $\begin{cases} \overrightarrow{b_1} = (2\pi/a)\hat{x} \\ \overrightarrow{b_2} = (2\pi/a)\hat{y} \\ \overrightarrow{b_3} = (2\pi/a)\hat{z} \end{cases}$

The cubic lattice is still cubic, but with dimensions changed by a factor of $2\pi/a$.

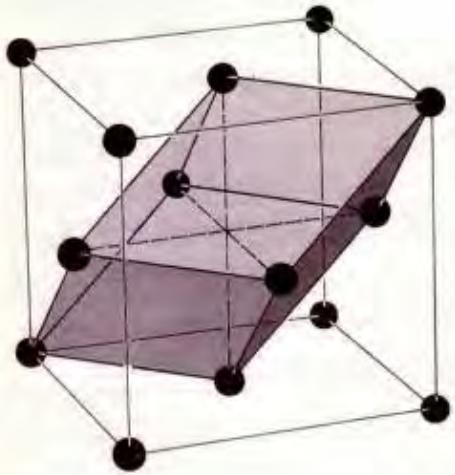
Answer (6b&d):

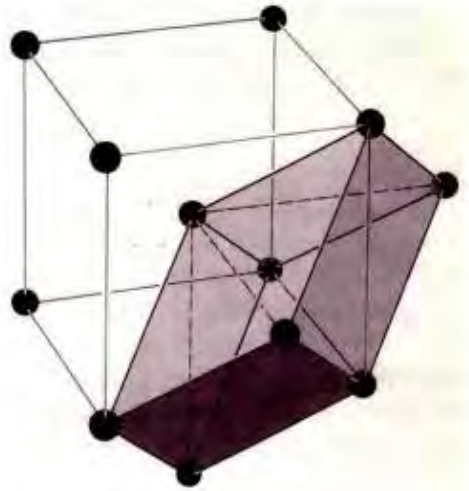
Homework (6c&d)

The reciprocal lattice vectors of face-centered cubic lattice are:

$$\begin{cases} \vec{a}_1 = \frac{1}{2}a(\hat{x}+\hat{y}) \\ \vec{a}_2 = \frac{1}{2}a(\hat{y}+\hat{z}) \\ \vec{a}_3 = \frac{1}{2}a(\hat{z}+\hat{x}) \end{cases}$$

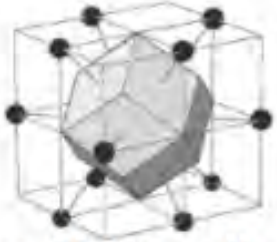
$$\begin{cases} \vec{b}_1 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}) \\ \vec{b}_2 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z}) \\ \vec{b}_3 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z}) \end{cases}$$





Conclusion: the same observation as before applies, the lengths change by a factor of $2\pi/a$ and the primitive vectors of the face-centered structure are transformed into the primitive vectors of the space-centered structure in the reciprocal space converted!

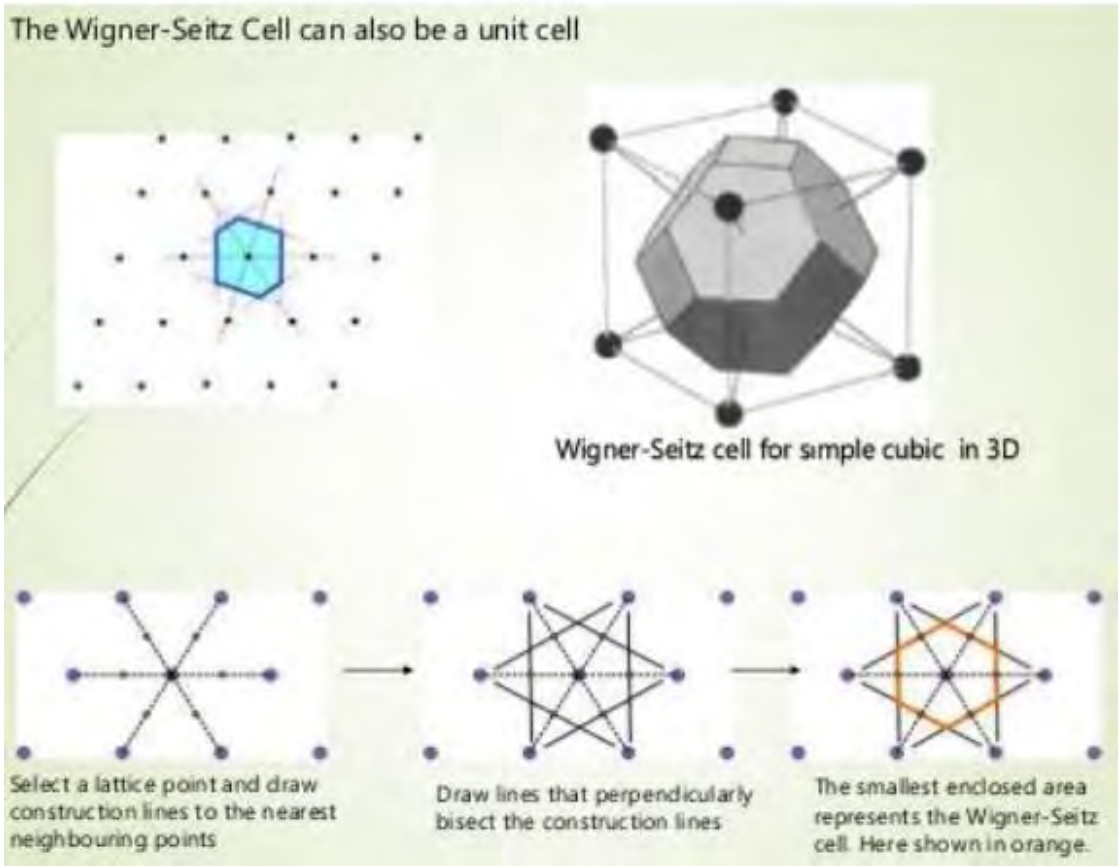
Answer (6e):

Lattice Real Space	Lattice K-space
 bcc WS cell	 bcc BZ (fcc lattice in K-space)
 fcc WS cell	 fcc BZ (bcc lattice in K-space)

- ✓ The WS cell of bcc lattice in real space transforms to a Brillouin zone (BZ) in a fcc lattice in reciprocal space;
- ✓ The WS cell of a fcc lattice transforms to a Brillouin zone of a bcc lattice in reciprocal space!!!

7. What is the Wigner-Seitz cell? How can these cells be drawn? Do they belong to the direct space or to the reciprocal space? What is the relationship between the WZ-cells and the first Brillouin zone?

- The Wigner-Seitz cell, named after Eugene Wigner and Frederick Seitz, is a primitive cell constructed by applying the Voronoi decomposition on a crystal lattice. It is used in the study of crystalline materials in solid-state physics.
- A Wigner-Seitz cell is an example of a primitive cell, which is a unit cell containing exactly one lattice point. For any given lattice, there are a number of possible primitive cells.
- Like the Bravais lattices, they exist both in the direct/real space as well as in reciprocal space. In reciprocal space, they are the Fourier transform of one into the other and vice versa. BUT in reciprocal space they are called Brillouin zones!



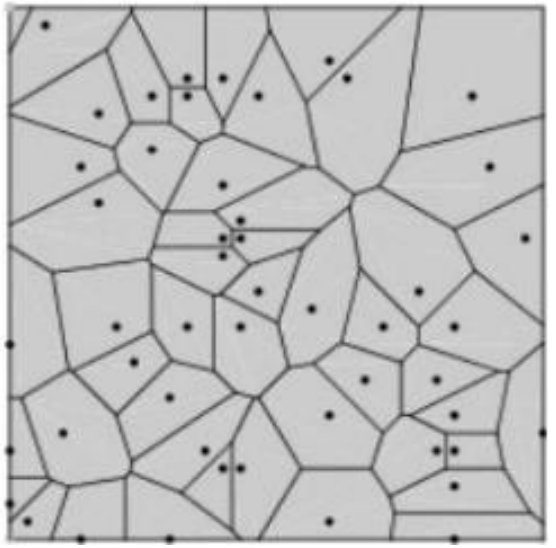
About the Voronoi diagrams

The partitioning of a plane with n points into convex polygons such that each polygon contains exactly one point and each point in a given polygon is closer to its creation point than to any other.

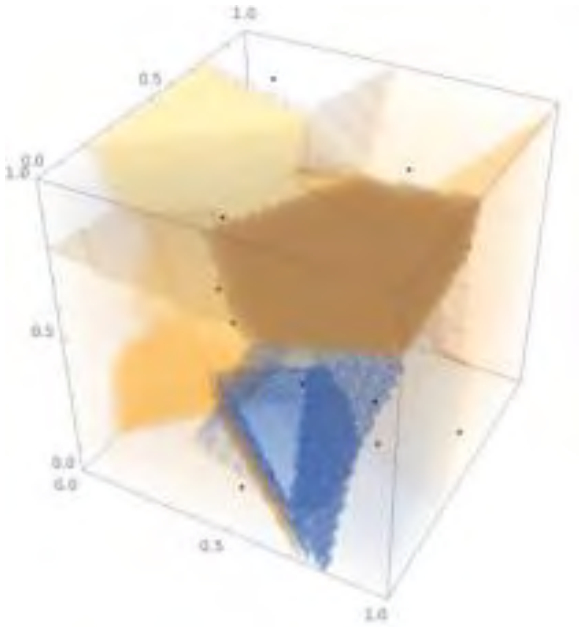
A Voronoi diagram is sometimes called a Dirichlet-tessellation. The cells are called Dirichlet regions, Thiessen polytopes, or Voronoi polygons. Voronoi diagrams were considered as early as 1644 by René Descartes and used by Dirichlet (1850) in the study of positive quadratic forms.

They were also studied by Voronoi (1907), who extended the study of Voronoi diagrams to higher dimensions. They find widespread application in fields such as computer graphics, epidemiology, geophysics, and meteorology. One particularly notable application of a Voronoi diagram was the analysis of the 1854 cholera epidemic in London, in which the physician John Snow found a strong correlation of deaths with proximity to a particular (and infected) water pump in Broad Street.

Find more details here:
https://mathworld.wolfram.com/VoronoiDiagram.html
https://de.wikipedia.org/wiki/Voronoi-Diagramm



2D Voronoi decomposition



3D Voronoi decomposition