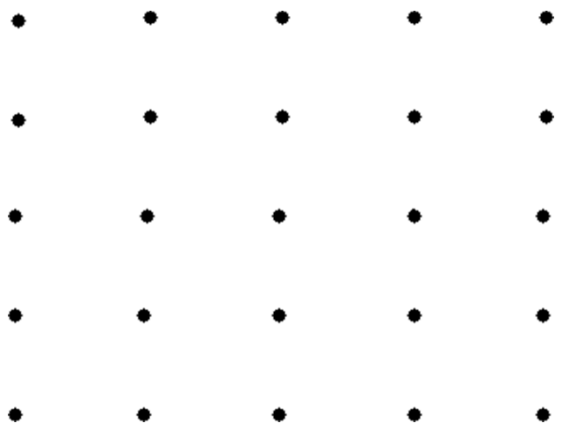
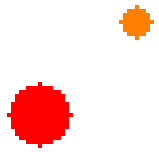
DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

Concept of phonons
Concept of Brillouin Zone (1D)
Lecture 8

A **lattice** is a hypothetical regular and periodic arrangement of points in space. It is used to describe the structure of a crystal. Two-dimensional lattice may look like below:

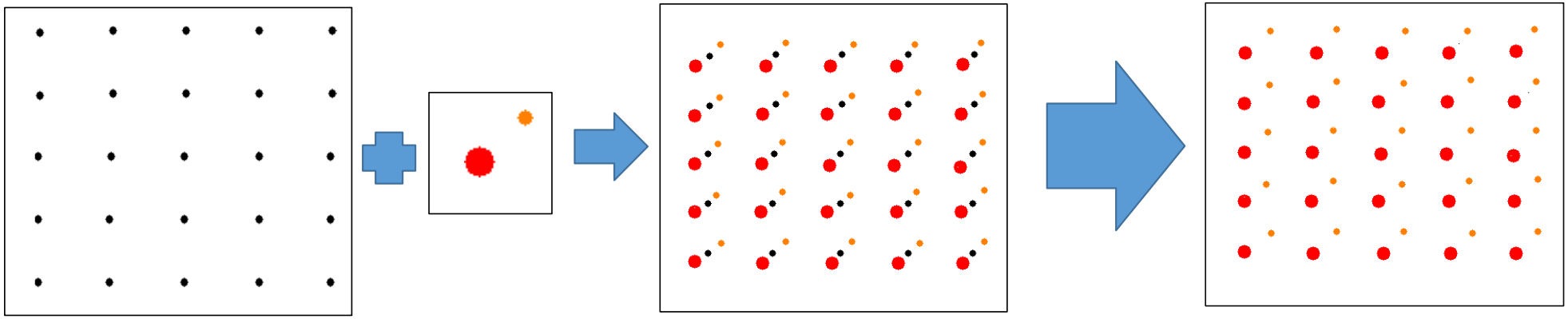


A **basis** is a collection of atoms in particular fixed arrangement in space. We could have a basis of a single atom as well as a basis of a complicated but fixed arrangement of hundreds of atoms. A basis of two atoms inclined at a fixed angle in a plane is shown below:



Let us now attach **the basis to each lattice point** (in black) as follows.

Now, remove the lattice points in black (remember that the lattice is an abstract entity). See the result as below

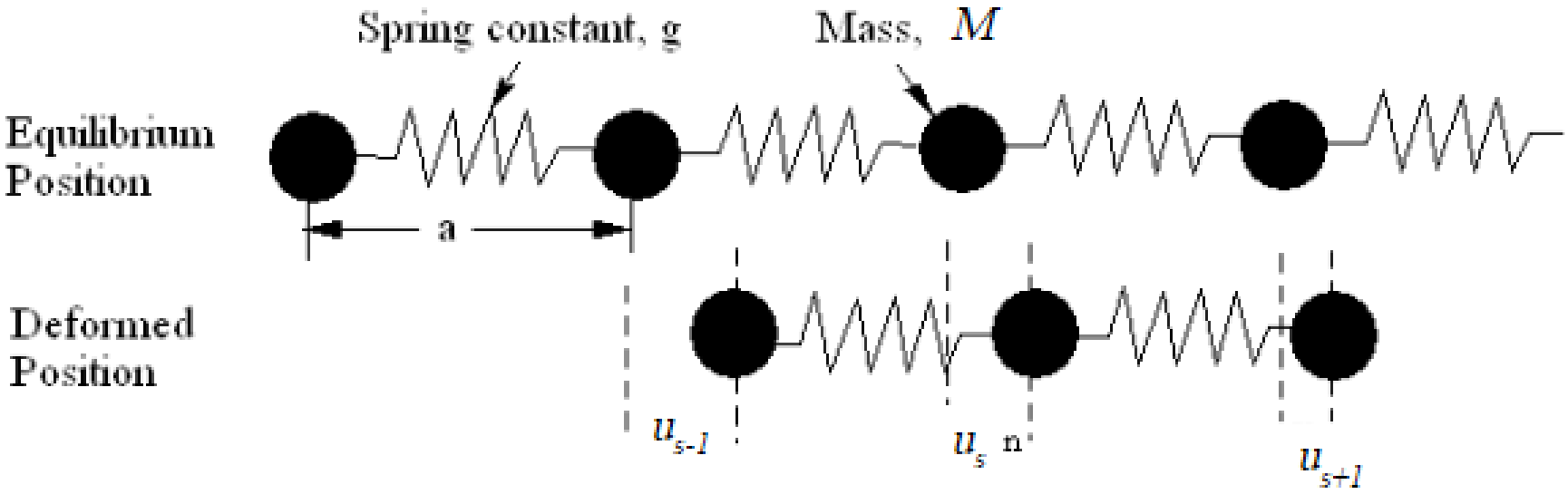


We have got the actual two-dimensional crystal in real space. So, we may write:

lattice + basis = crystal

Crystal Vibration of a Monoatomic Linear Chain

Longitudinal wave of a 1-D Array of Spring Mass System



u_s: displacement of the s^{th} atom from its equilibrium position

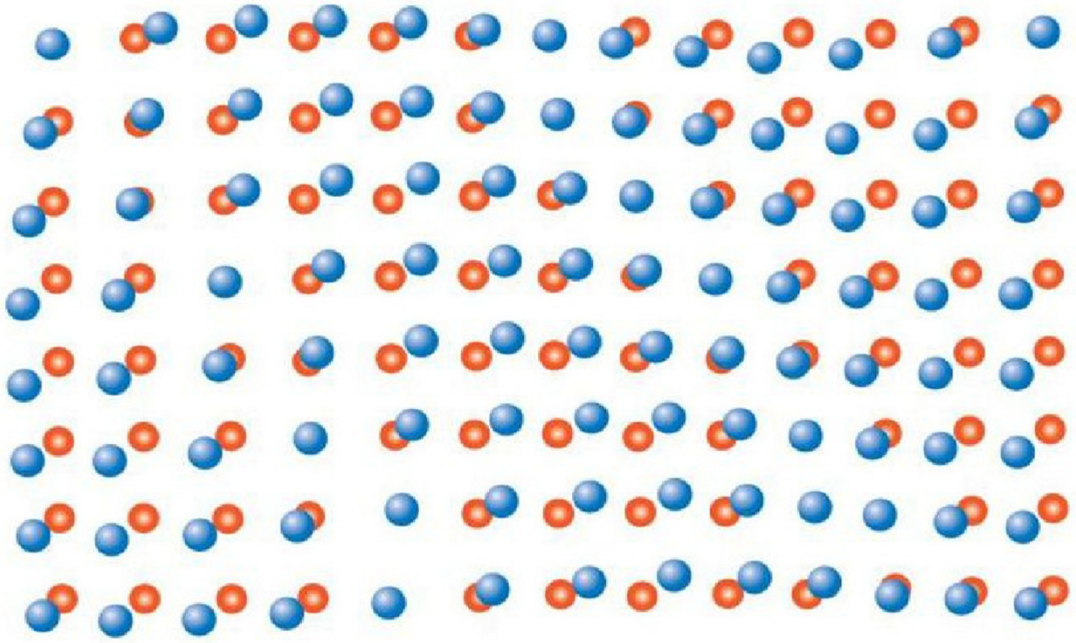
CONCEPT OF PHONONS

- Any solid crystal consists of atoms bound into a specific repeating three- dimensional spatial pattern called a lattice.
- Here the atoms behave as if they are connected by tiny springs, their own thermal energy or outside forces make the lattice vibrate.
- This generates mechanical waves that carry heat and sound through the material.
- *A packet of these waves can travel throughout the crystal with a definite energy and momentum, so in quantum mechanical terms the waves can be treated as a particle, called a phonon.*
- **A phonon is a definite discrete unit or *quantum* of vibrational mechanical energy, just as a photon is a quantum of electromagneticor light energy.**

Concept of Phonons

Atomic Vibrations

Atomic vibrations are in the form of lattice waves or phonons



Normal lattice positions for atoms

Positions displaced because of vibrations

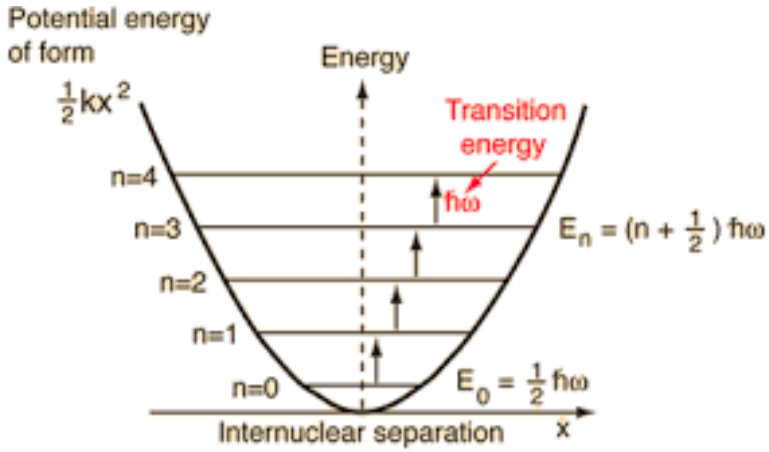
Adapted from Fig. 17.1

Phonon:

A photon is the smallest unit of light. Similarly, for sound, the smallest unit is called phonon. In a lattice structure, vibrations are created by atoms. **The quantized, lowest state energy of vibration is called phonon.**

❖Atoms were considered as **rigid**, with atoms stuck in their lattice. In reality, atoms can be considered as simple harmonic oscillators. **The harmonic oscillator has a ground state energy and an associated vibrational mode even at 0 ° K.**

The quantum harmonic oscillator is one of the foundation problems of quantum mechanics. It can be applied rather directly to the explanation of the vibration spectra of diatomic molecules but has implications far beyond such simple systems.



Quantum Harmonic Oscillator

❖It is named phonons because at high energy levels long wavelength phonons give rise to sound. **According to quantum mechanics, similar particles have wave nature, waves must also have particle nature. So, phonon is also treated as quasi particle. Similar to particles, these waves can carry throughout the crystal, heat, energy and momentum**.

❖In solid state physics, the elementary particles are electrons and phonons. The arrangement of the electrons will help determine material's electrical properties whereas the speed of sound through material and heat required to change its temperature is given by phonons. Another important application of phonons is in the field of superconductivity, **where the electrical resistance of certain materials become zero near absolute zero.**

❖In ordinary crystals, there is a loss of energy as heat as the electrons collide with impurities. But in superconductors, at low temperatures, they tend to attract slightly because of phonons. Now the movement occur as a coherent group thus minimizing energy loss.

❖Phonons also have important application in detectors like Cryogenic Dark Matter Search, which aim to detect even the slightest vibration in a crystal lattice caused by even a single phonon.

Phonons and Photons

PHONONS

- Quantized normal modes of lattice vibrations. The energies & momenta of phonons are quantized

$$E_{phonon} = \frac{h\nu_s}{\lambda}$$

$$p_{phonon} = \frac{h}{\lambda}$$

Phonon wavelength:

$\lambda_{phonon} \approx a_0 \approx 10^{-10}$ m

PHOTONS

- Quantized normal modes of electromagnetic waves. The energies & momenta of photons are quantized

$$E_{photon} = \frac{hc}{\lambda}$$

$$p_{photon} = \frac{h}{\lambda}$$

Photon wavelength (visible):

$\lambda_{photon} \approx 10^{-6}$ m

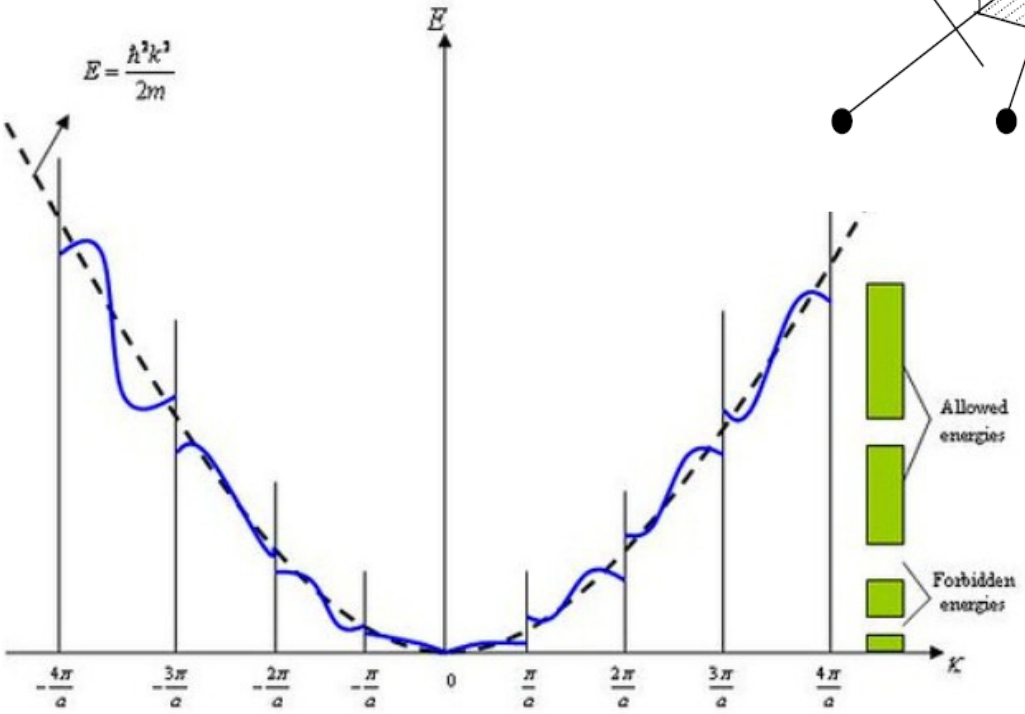
Concept of Brillouin zone

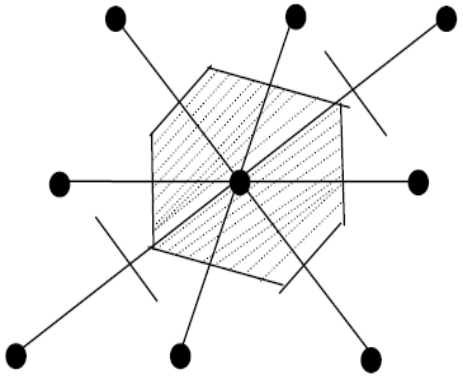
- The different Brillouin zones correspond to primitive cells of a different type that come up in the theory of electronic levels in a periodic potential.

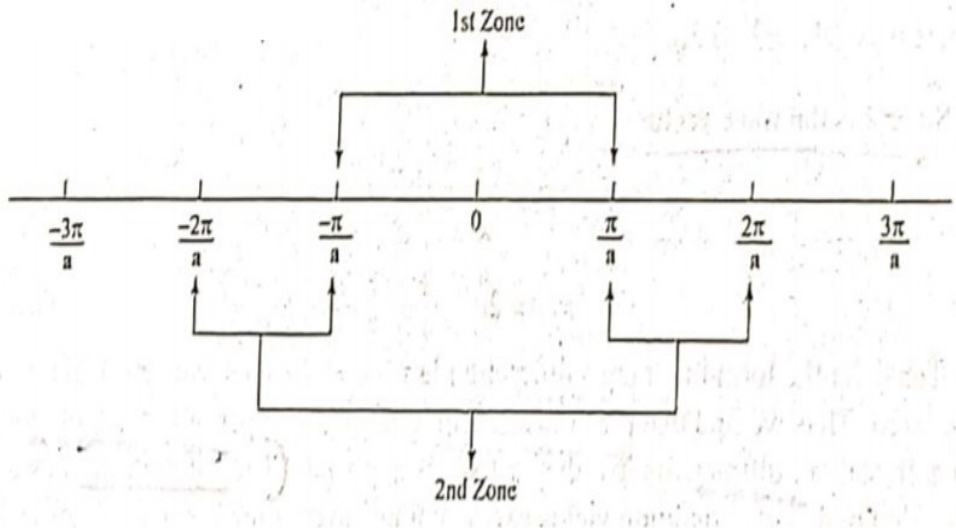
- The first Brillouin zone is considered as the Wigner-Seitz (WS) primitive cell in the reciprocal lattice. In other words, the first Brillouin zone is a geometrical construction to the WS primitive cell in the k-space.

- In a direct lattice, the procedure of drawing a WS cell is as follows:

- Draw lines to connect a given lattice points to all nearby lattice points.
  - i) Draw lines to connect a given lattice points to all nearby lattice points.
  - ii) Draw new lines or plane at the mid point and normal to the lines in(i) .
  - iii) The smallest volume enclosed in this way is the WS primitive cell.


E
$E = \frac{\hbar^2 k^2}{2m}$
Allowed energies
Forbidden energies
K
$-\frac{4\pi}{a}$
$-\frac{3\pi}{a}$
$-\frac{2\pi}{a}$
$-\frac{\pi}{a}$
0
$\frac{\pi}{a}$
$\frac{2\pi}{a}$
$\frac{3\pi}{a}$
$\frac{4\pi}{a}$




1st Zone
$\frac{-3\pi}{a}$
$\frac{-2\pi}{a}$
$\frac{-\pi}{a}$
0
$\frac{\pi}{a}$
$\frac{2\pi}{a}$
$\frac{3\pi}{a}$
2nd Zone

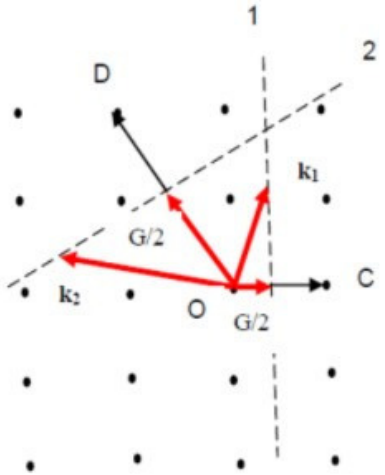
Construction of a Wigner-Seitz cell in the reciprocal lattice (called first Brillouin zone):

To construct the first Brillouin zone, we need to find the link between the incident beam (like electron or neutron or phonon beam) of wave vector k and the reciprocal lattice vector G . This relation may be found as

[for example, an x-ray beam in the crystal will be diffracted if its wave vector k has the magnitude and direction required by this latter relation].

$$;\vec{k} \bullet (\frac{\vec{G}}{2}) = (\frac{G}{2})^2$$

Thus the procedure to build up the first Brillouin zone is as follows (see figure 30):



i) Select a vector G from the origin to a reciprocal lattice point.
ii) Construct a plane normal to the vector G at its mid point. This plane forms a part of the zone boundary.
iii) The diffracted beam will be in the direction k -G .
iv) Thus the Brillouin construction exhibits all the wave vectors k which can be Bragg-reflected by the crystal.

Important note:

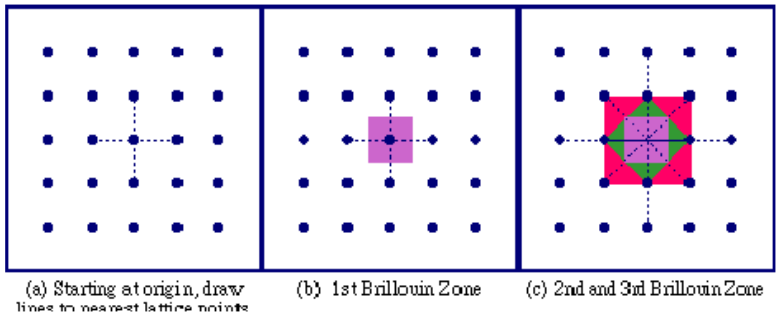
A wave whose wave vector drawn from the origin terminates on any of the planes will satisfy the condition of diffraction. Such planes are the perpendicular bisectors of the reciprocal vectors.

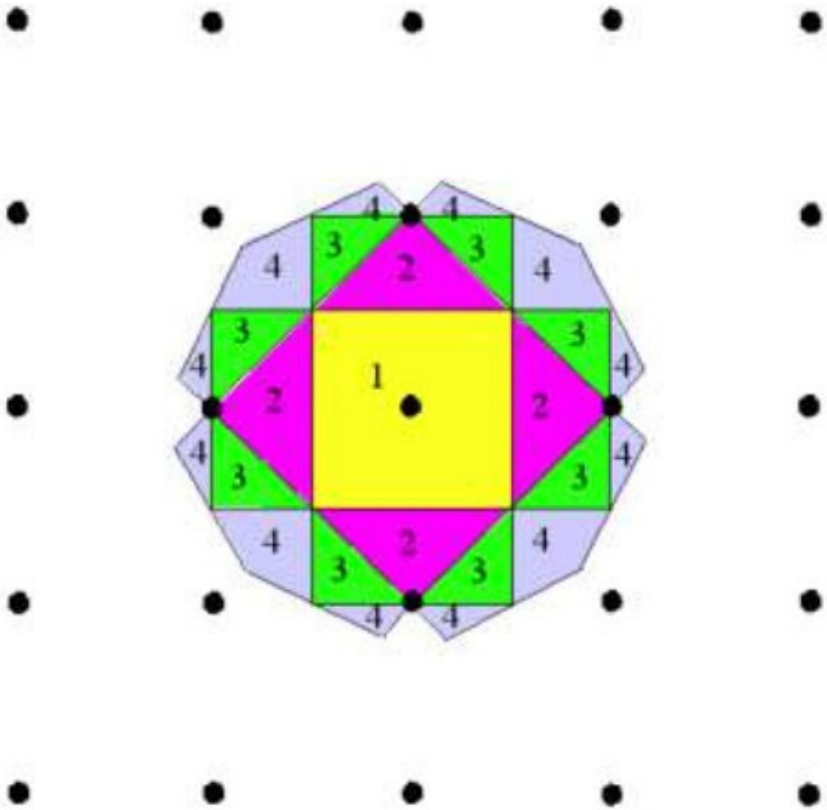
Remarks:

-The planes divide the Fourier space of the crystal into fragments as shown for a square lattice.

- The central square is a primitive cell of the reciprocal lattice. It is a Wigner-Seitz cell of the reciprocal lattice (called the first Brillouin zone).

- The first Brillouin zone is the smallest volume entirely enclosed by the planes.



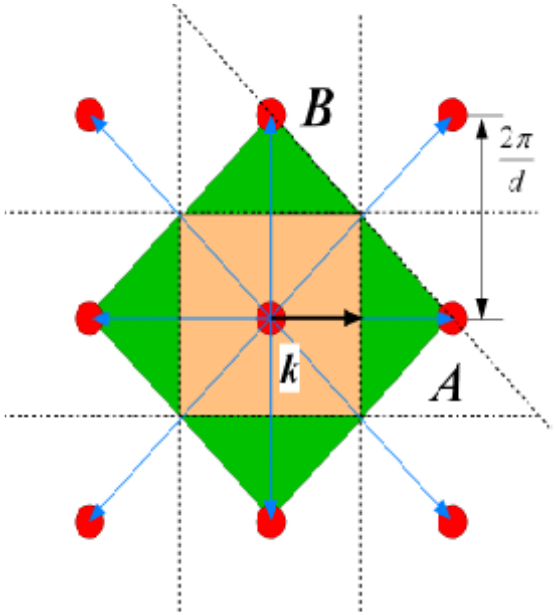


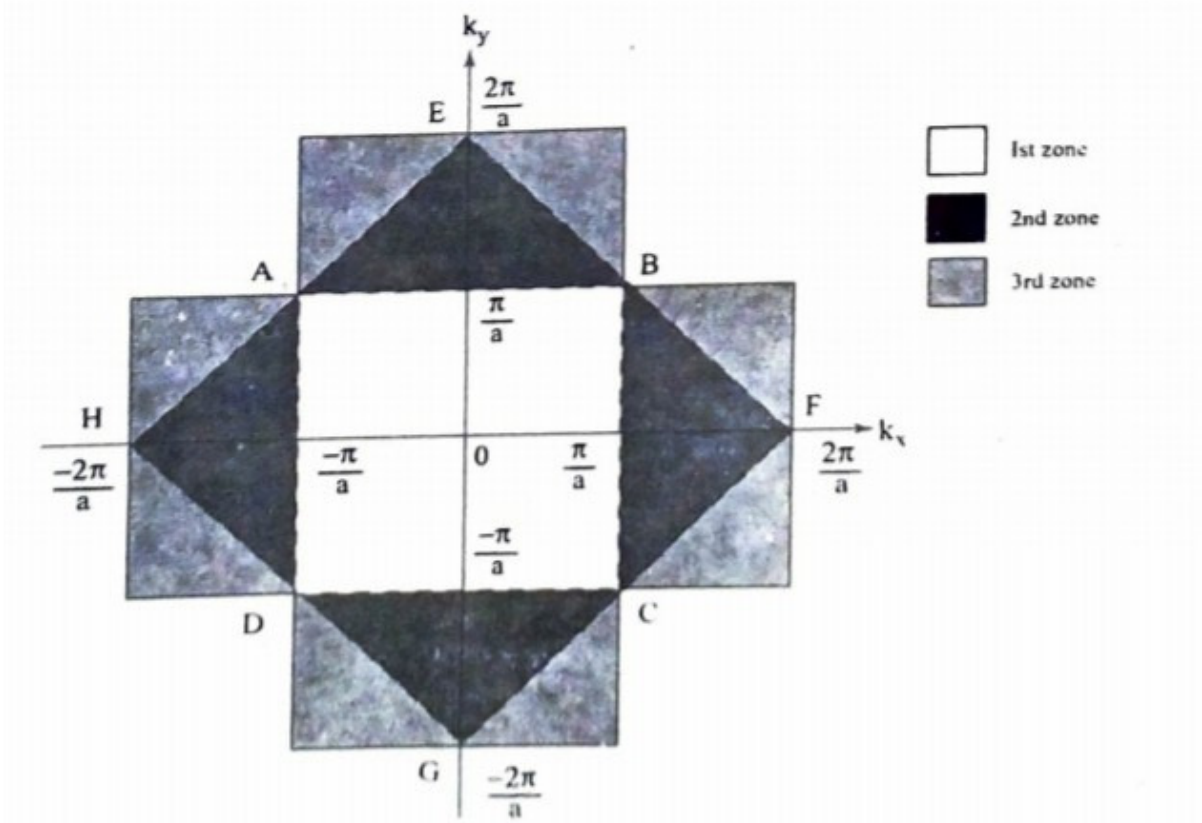
BZ construction

- reciprocal lattice
- bisect vectors to the nearest neighbors
- area defined by bisecting lines represents 1BZ

First Brillouin zone is determined by:

- Select lattice point and draw a line segment to all neighbouring lattice points (blue).
- Draw center normal planes (black, dotted). In 2D they are lines.
- The bounded area closest to the selected point is 1. Brillouin zone (orange).
- The next area (going over one line only) is 2. Brillouin zone (green).





The first three Brillouin Zones for a two dimensional square lattice.

Conclusion:

Wigner-Seitz cell: smallest possible primitive cell, which consist of one lattice point and all the surrounding space closer to it than to any other point. The construction of the W-S cell in the reciprocal lattice delivers the first Brillouin zone (important for diffraction)

The importance of Brillouin zone:

The Brillouin zones are used to describe and analyze the electron energy in the band energy structure of crystals.