Further Adventures in k-space

Why Reciprocal (k) Space?

Bloch Wavefunctions

The Reciprocal Lattice

The Reciprocal Unit Cells (Brillouin Zones)

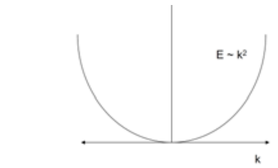
Their Use in Band Diagrams

Fermi Surfaces

Charles Kittel, *Introduction to Solid State Physics* (Wiley: New York, 1996).
P. M. Chaikin & T. C. Lubensky *Principles of Condensed Matter Physics* (Paperback), Cambridge Univ. Press, 2000)

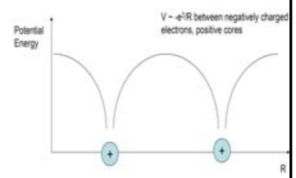
Origin of Band Gaps

Free e- model:
E = hv = $(\hbar k)^2/2m$
where $k^2 = k_x^2 + k_y^2 + k_z^2$



The free e- wavefunctions are plane waves:
$\Psi_k(r)$ = exp (ikr)
with momentum $p = \hbar k$
k can have any value for a free e-

What happens when a periodic potential is added?
i.e., with a lattice distance a



Bloch Wavefunction

A Bloch wavefunction or Bloch state, named after Felix Bloch, describes a particle (usually, an electron) placed in a periodic potential (e.g., a crystal).

$\Psi_k(r)$ = exp(ikr) * U(x)
where U(x) is a periodic function
that matches the periodic potential (i.e. U(x+a)=U(x))

Bloch's theorem: all eigenfunctions for a periodic potential can be written as the product of a plane wave and a function with the translation symmetry of the lattice, i.e., a periodic function, $U_{nk}(r)$.

Charles Kittel, *Introduction to Solid State Physics* (Wiley: New York, 1996).
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Reciprocal Space (aka k-space) Description of a Crystal

For electrons in extended solids,
the Bloch wavefunction is distributed throughout the crystal,
the position of the electrons are highly delocalized.

Therefore, the momentum of an electron (in the crystal) is well defined (Uncertainty Principle).

Therefore, it is convenient to consider a space where "momentum" axes replace x,y,z: This is "k-space" or RS.

The Reciprocal Lattice has a k-space unit cell that fully reconstructs the entire reciprocal space via only translations
(just as the real space unit cell reconstructs the entire crystal via only translations). This k-space unit cell is the Brillouin Zone.

Note that the k-space (Reciprocal Space) unit cell maintains the same symmetry as the real space unit cell.

Brillouin Zone

In the propagation of any type of wave motion (electronic wavefunctions, phonons, etc.) through a crystal lattice, the frequency is a periodic function of some wave vector **k**.

Brillouin Zone is defined as a "Wigner-Seitz primitive cell in the reciprocal lattice".

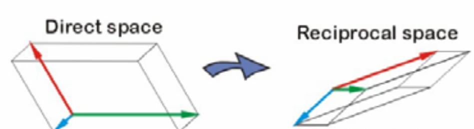
The first Brillouin Zone exhibits all wavevectors, k, which can be Bragg-reflected by a crystal.

The Brillouin Zones represent "special" points in k-space that reflect the underlying symmetry of the crystal.

These represent the "limiting" cases of different MO mixings of the local MO that go into forming the structure of the bands.

Charles Kittel, *Introduction to Solid State Physics* (Wiley: New York, 1996).
P. M. Chaikin & T. C. Lubensky *Principles of Condensed Matter Physics* (Paperback), Cambridge Univ. Press, 2000)

Direct space to reciprocal space



$\bar{r} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$ $\bar{H} = hb_1 + kb_2 + lb_3$

$$\vec{a}_i \bullet \vec{b}_j^* = 2\pi\delta_{ij}$$

$\delta_{ij} = 1$ if i=j
0 if i≠j

Real (direct) space — Reciprocal space

Note: The real space and reciprocal space vectors are not necessarily in the same direction

Reciprocal Space (aka k-space) Description of a Crystal

Given a real space lattice vector $\vec{R} = n_1a_1 + n_2a_2 + n_3a_3$

then we can define a reciprocal lattice vector $\vec{G} = hb_1 + kb_2 + lb_3$

$\vec{G} \bullet \vec{R} = 2\pi n$ where n is an integer.

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \bullet a_2 \times a_3} \quad b_2 = 2\pi \frac{a_3 \times a_1}{a_1 \bullet a_2 \times a_3} \quad b_3 = 2\pi \frac{a_1 \times a_2}{a_1 \bullet a_2 \times a_3}$$

unit cell vol.

a_1, a_2 and a_3 are the vectors in the real space lattice.

b_1, b_2 and b_3 are the vectors of the reciprocal lattice (k-space).

Reciprocal lattice to SC lattice

- The primitive translation vectors of any simple cubic lattice are:
  $\vec{a}_1 = a\vec{x}$ $\vec{a}_2 = a\vec{y}$ $\vec{a}_3 = a\vec{z}$
- Using the definition of reciprocal lattice vectors:

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \bullet a_2 \times a_3} \quad b_2 = 2\pi \frac{a_3 \times a_1}{a_1 \bullet a_2 \times a_3} \quad b_3 = 2\pi \frac{a_1 \times a_2}{a_1 \bullet a_2 \times a_3}$$

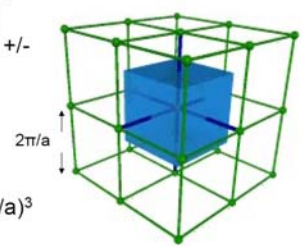
- We get the following primitive translation vectors of the reciprocal lattice:
  $\vec{b}_1 = (2\pi/a)\vec{x}$ $\vec{b}_2 = (2\pi/a)\vec{y}$ $\vec{b}_3 = (2\pi/a)\vec{z}$

This is another cubic lattice of length 2π/a

Reciprocal lattice to SC lattice

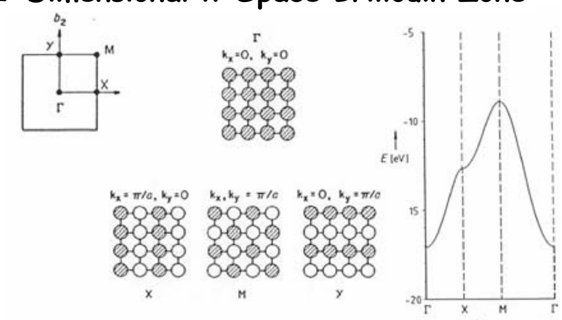
The boundaries of the first Brillouin zone are the planes normal to the six reciprocal lattice vectors +/- $\vec{b}_1$, +/- $\vec{b}_2$, +/- $\vec{b}_3$ at their midpoints:

+/- (π/a)



The length of each side is 2π/a and the volume is $(2\pi/a)^3$

2-Dimensional k-Space Brillouin Zone

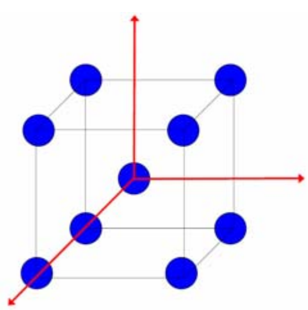


$\Gamma = (k_x=0, k_y=0, k_z=0)$ $X = (\pi/a, 0, 0)$

$M = (\pi/a, \pi/a, 0)$ $Y = (0, \pi/a, 0)$

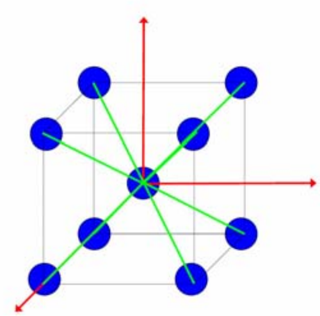
$R = (\pi/a, \pi/a, \pi/a)$ $Z = (0, 0, \pi/a)$

Reciprocal Space (aka k-space) Description of a Crystal example: Body Centered Cubic Reciprocal Lattice



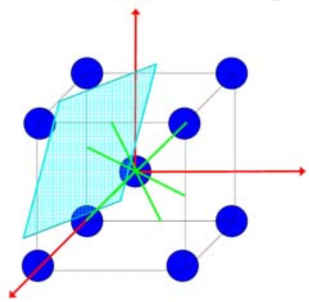
Reciprocal Space (aka k-space) Description of a Crystal example: Body Centered Cubic Reciprocal Lattice

Connect an arbitrary lattice point to all of its nearest neighbors (green lines)...



Reciprocal Space (aka k-space) Description of a Crystal
example: Body Centered Cubic Reciprocal Lattice

...construct the perpendicular bisectors to all of these lines. The 1st Brillouin Zone is the volume enclosed within this region.



Reciprocal Space (aka k-space) Description of a Crystal
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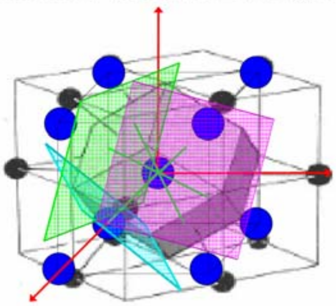
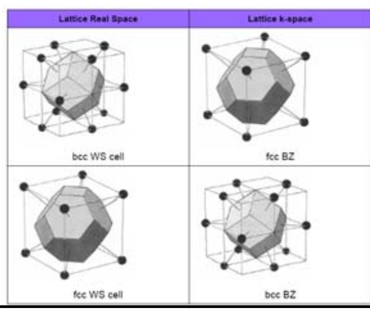


Reciprocal Space

The reciprocal space for a simple cubic lattice is simple cubic, and for HCP is HCP, but the other cubic lattice (BCC, FCC) are less obvious:

The BCC and FCC lattices are Fourier transforms of one another.



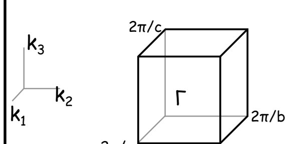
Reciprocal Space (aka k-space) Description of a Crystal

Most important k-space points:

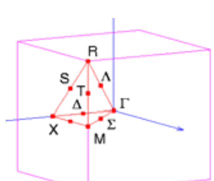
- Γ-point is the center of crystal momentum space (k-space) at k=0.
- X-point is the edge of the first Brillouin zone (π/L edge) of crystal momentum space (k-space) in the <100> direction.
- L-point is the edge of the first Brillouin zone (π/L edge) of crystal momentum space (k-space) in the <111> direction.

Reciprocal Space Description of an Orthorhombic Cell

http://cst-www.nrl.navy.mil/bind/kpts/index.html



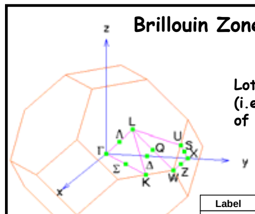
reciprocal vectors
b1 = (2π/a, 0, 0)
b2 = (0, 2π/b, 0)
b3 = (0, 0, 2π/c)



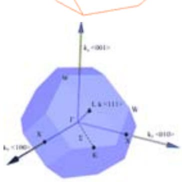
Most important k-space points (k_1, k_2, k_3):

- Γ: (0,0,0). Wavefunction all in phase.
- X: (1/2, 0, 0)-the edge of the first Brillouin zone

Brillouin Zone For The Fcc Unit Cell



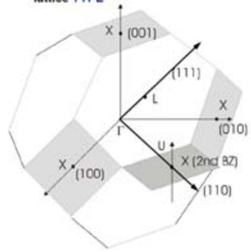
Lots of labels for specific points in k-space (i.e., in phase vs. out of phase in each dimension of the reciprocal space, etc.)



Label	Cartesian Coordinates	Lattice Coordinates	Range
Γ	**(0 , 0 , 0)**	**0**	**Point**
Δ	(0 , 2 π x/a , 0)	½ x ($\mathbf{b}_1$ + $\mathbf{b}_3$)	0 < x < 1
X	**(0 , 2 π/a , 0)**	**½ (b_1 + b_3)**	**Point**
Z	(½ x π/a , 2 π/a , 0)	½ $\mathbf{b}_1$ + ¼ x $\mathbf{b}_2$ + ¼ (2+x) $\mathbf{b}_3$	0 < x < 1
W	(π/a , 2 π/a , 0)	½ $\mathbf{b}_1$ + ¼ $\mathbf{b}_2$ + ¾ $\mathbf{b}_3$	Point
Q	(π/a , (2 - x) π/a , x π/a)	½ $\mathbf{b}_1$ + ¼ (1 + x) $\mathbf{b}_2$ + ¼ (3 - x) $\mathbf{b}_3$	0 < x < 1
L	**(π/a , π/a , π/a)**	**½ b_1 + ½ b_2 + ½ b_3**	**Point**
Λ	(x π/a , x π/a , x π/a)	½ x $\mathbf{b}_1$ + ½ x $\mathbf{b}_2$ + ½ x $\mathbf{b}_3$	0 < x < 2
Σ	(2 π x/a , 2 π x/a , 0)	½ x $\mathbf{b}_1$ + ½ x $\mathbf{b}_2$ + x $\mathbf{b}_3$	0 < x < ¾
K = U	($^3/_2$ π/a , $^3/_2$ π/a , 0)	$^3/_8$ $\mathbf{b}_1$ + $^3/_8$ $\mathbf{b}_2$ + ¾ $\mathbf{b}_3$	Point
S	(2 π x/a , 2 π x/a , 0)	½ x $\mathbf{b}_1$ + ½ x $\mathbf{b}_2$ + x $\mathbf{b}_3$	¾ < x < 1
X'	(2 π/a , 2 π/a , 0)	½ $\mathbf{b}_1$ + ½ $\mathbf{b}_2$ + $\mathbf{b}_3$	Point

Crystal Diffraction in Many Directions

- In a THREE dimensional crystal the Brillouin zones are more COMPLICATED since diffraction is now possible in all THREE directions
- The resulting Brillouin zone is thus THREE dimensional, and also depends on the lattice TYPE



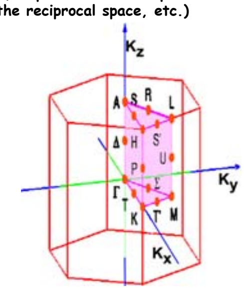
FIRST BRILLOUIN ZONE OF THE FACE-CENTERED CUBIC LATTICE

This is the BZ for all diamond and Zinc-blende materials (C, Si, Ge, GaAs, InAs, CdTe, etc.

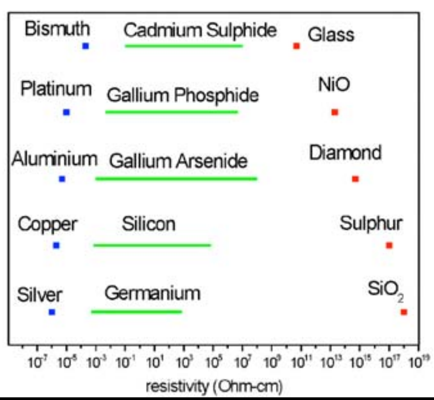
There are 8 hexagonal faces (normal to [111]) and 6 square faces (normal to [100]). The sides of each hexagon and square are equal.

Reciprocal Space For HCP is HCP

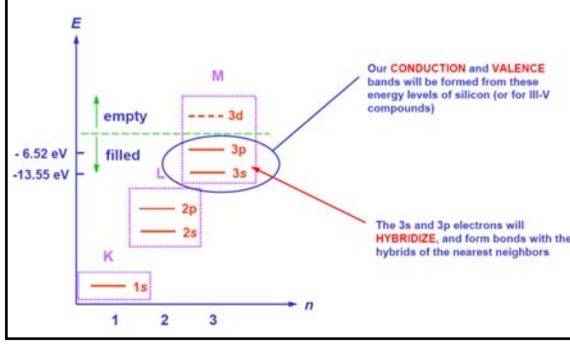
Lots of labels for specific points in k-space
(i.e., in phase vs. out of phase in each dimension of the reciprocal space, etc.)



Metals vs. Semiconductors: Resistivity



Band Structure of Silicon



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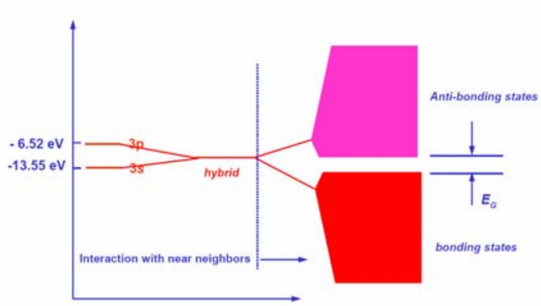

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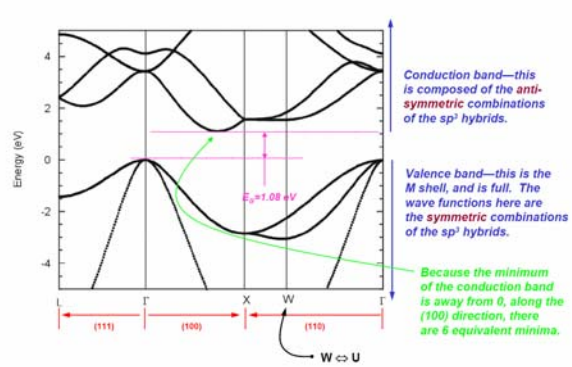


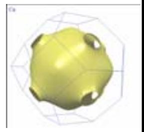
Metals and Semiconductors

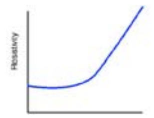
Metals are defined by the presence of a Fermi surface (Boundary between filled and unfilled states in k-space at 0 K).

Infinitesimally small energy difference between filled and unfilled bands.

Electrons are free to move.

Resistivity falls on cooling as lattice vibrations freeze out.





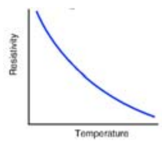
Semiconductors:

No free electrons at 0 K.

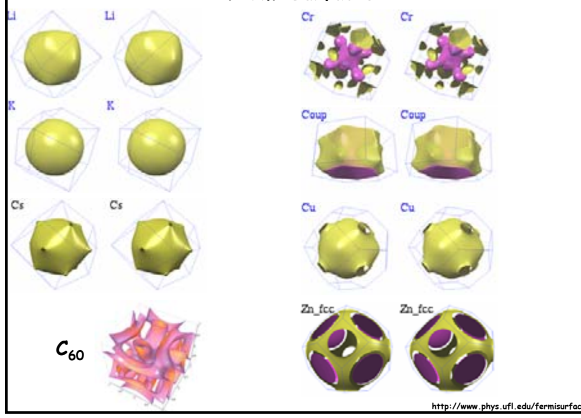
Energy gap between filled and unfilled states.

Conduction relies on thermally activated carriers: resistivity increases on cooling as there are fewer carriers.

No Fermi surface (due to gap).



Fermi Surfaces



http://www.phys.ufl.edu/fermisurface/