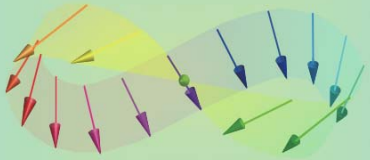
Introductory Nanotechnology
~ Basic Condensed Matter Physics ~



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Quick Review over the Last Lecture

3 states of matters :

	solid	liquid	gas
density	( )	( )	( )
ordering range	( )	( )	
rigid time scale	( )	( )	

4 major crystals :

soft solid

( ) ( ) ( )

( )

Contents of Introductory Nanotechnology

First half of the course :

Basic condensed matter physics

1. Why *solids* are *solid* ?
2. What is the *most common atom* on the earth ?
3. How does an electron travel in a material ?
4. How does lattices vibrate thermally ?
5. What is a *semi*-conductor ?
6. How does an electron tunnel through a barrier ?
7. Why does a magnet attract / retract ?
8. What happens at interfaces ?

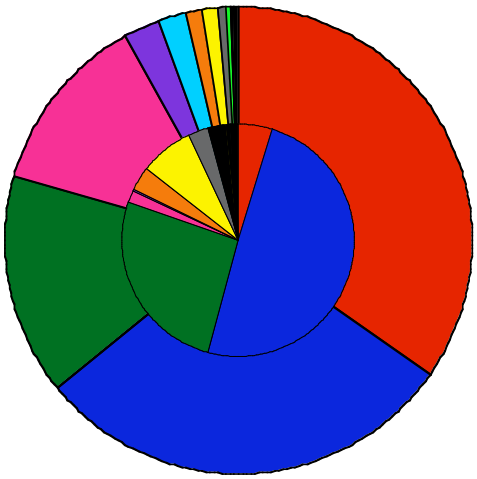
Second half of the course :

Introduction to nanotechnology (nano-fabrication / application)

What Is the Most *Common Atom* on the earth?

- Phase diagram
- Free electron model
- Electron transport
- Degeneracy
- Electron Potential
- Brillouin Zone
- Fermi Distribution

Abundance of Elements in the Earth



Mason (1966)

Only surface 10 miles (Clarke number)

Can We Find So Much around Us ?

” Civilization" Today

-based products around us :

Buildings
(reinforced concrete)

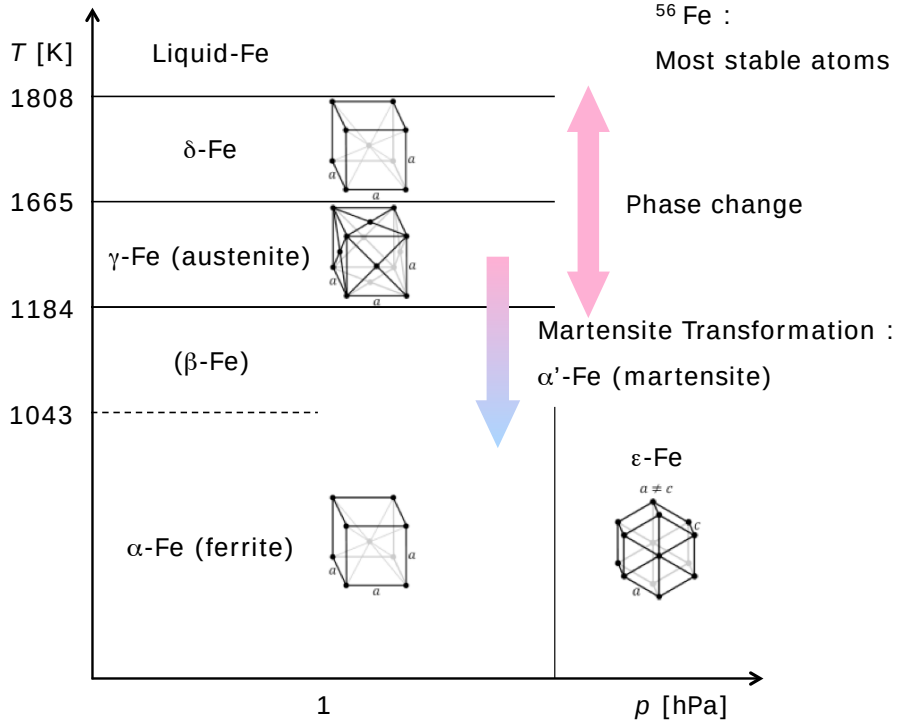
Bridges

Qutb Minar :
Pure pillar (99.72 %), which has never rusted since AD 415.

* Corresponding pages on the web.

Major Phases of Fe

Fe changes the crystalline structures with temperature / pressure :



^{56}Fe :

Most stable atoms in the universe.

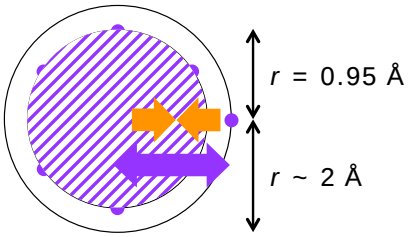
Phase change

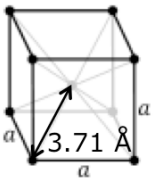
Martensite Transformation :

α’-Fe (martensite)

Electron Transport in a Metal

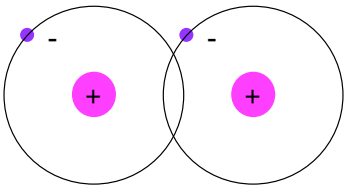
Free electrons :





Na bcc :

a = 4.28 Å



3s electrons move *freely* among Na^+ atoms.

Uncertainty principle :

$\Delta x \Delta p \geq \hbar$ (x : position and p : momentum)

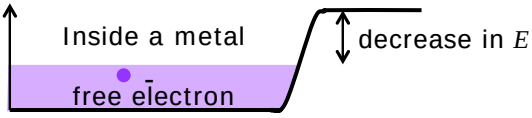
When a 3s electron is confined in one Na atom ($\Delta x \approx r$) :

$$p \approx \Delta p \approx \hbar / r$$

$$E = p^2/2m = (\hbar/r)^2/2m = \hbar^2/2mr^2$$ (m : electron mass)

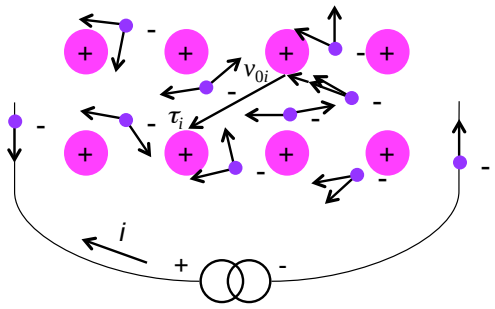
For a free electron, $r \rightarrow$ large and hence $E \rightarrow$ small.

Effective energy for electrons



Free Electron Model

Equilibrium state :



Free electrons :

mass m, charge $-q$ and velocity v_i

Equation of motion along $\boldsymbol{E}$:

$$m\frac{dv_i}{dt} = -q\boldsymbol{E}$$

Average over free electrons :

drift velocity : v_d

For each free electron :

thermal velocity (after collision) : v_{0i}

acceleration by $\boldsymbol{E}$ for τ_i

$$v_i = v_{0i} = -\frac{q}{m}\boldsymbol{E}\tau_i$$

Average over free electrons :

collision time : τ

$$v_d = -\frac{q\tau}{m}\boldsymbol{E}$$

Using a number density of electrons n, current density $\boldsymbol{J}$:

$$\boldsymbol{J} = (-v_d)qn = q^2\frac{n}{m}\boldsymbol{E}\tau$$

Free Electron Model and Ohm's Law

Ohm's law :

$$V = iR = i\frac{\rho\ell}{S} \quad \text{For a small area :} \quad \Delta V = \Delta i\rho\frac{\Delta\ell}{\Delta S} \rightarrow \frac{\Delta V}{\Delta\ell} = \rho\frac{\Delta i}{\Delta S} \rightarrow \boldsymbol{E} = \rho\boldsymbol{J}$$

where ρ : electric resistivity (electric conductivity : σ = 1 / ρ)

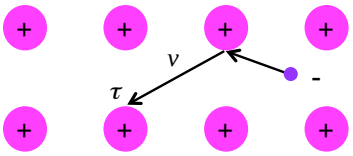
By comparing with the free electron model :

$$\boldsymbol{J} = q^2\frac{n}{m}\boldsymbol{E}\tau$$

$$\sigma = \frac{1}{\rho} = q^2\frac{n}{m}\tau$$

Relaxation Time

Resistive force by collision :



Equation of motion :

with resistive force mv/τ

$$m\frac{dv}{dt} = -qE - \frac{m}{\tau}v$$

For the initial condition :

v = 0 at t = 0

$$v = -\frac{q\tau}{m}E\left[1-\exp\left(-t/\tau\right)\right]$$

For a steady state (t >> τ),

$$v = -\frac{q\tau}{m}E$$

τ : collision time

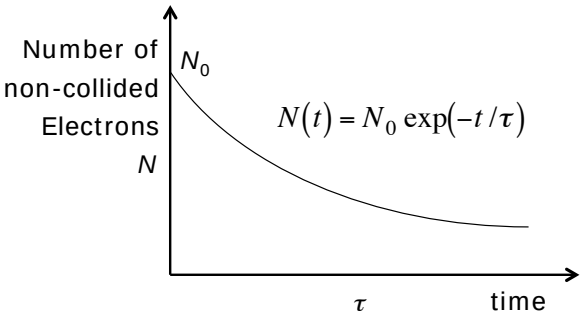
If E is removed in the equation of motion :

$$m\frac{dv}{dt} = -\frac{m}{\tau}v$$

For the initial condition :

$v = v_d$ at t = 0

$$v = v_d\exp\left(-t/\tau\right)$$



τ : relaxation time = $\langle t \rangle$

Mobility

Equation of motion under $\boldsymbol{E}$:

$$m\frac{dv}{dt} = -qE$$

For an electron at $\boldsymbol{r}$,

collision at t = 0 and $\boldsymbol{r} = \boldsymbol{r}_0$ with v_0

$$\boldsymbol{r} - \boldsymbol{r}_0 = \boldsymbol{v}_0 t + \frac{1}{2}\frac{(-q)\boldsymbol{E}}{m}t^2$$

Here, ergodic assumption :

temporal mean = ensemble mean

therefore, by taking an average over non-collided short period,

$$\langle \boldsymbol{r} - \boldsymbol{r}_0 \rangle = \langle \boldsymbol{v}_0 t \rangle + \frac{-q\boldsymbol{E}}{2m}\langle t^2 \rangle$$

Since t and v_0 are independent,

$$\langle \boldsymbol{v}_0 t \rangle = \langle \boldsymbol{v}_0 \rangle \langle t \rangle$$

Here, $\langle \boldsymbol{v}_0 \rangle$ = 0, as v_0 is random.

Also,

$$\langle t^2 \rangle = \int_0^\infty \frac{t^2}{\tau}\exp\left(-\frac{t}{\tau}\right)dt = 2\tau^2$$

Accordingly,

$$\langle \boldsymbol{r} - \boldsymbol{r}_0 \rangle = \frac{-q\boldsymbol{E}}{m}\tau^2$$

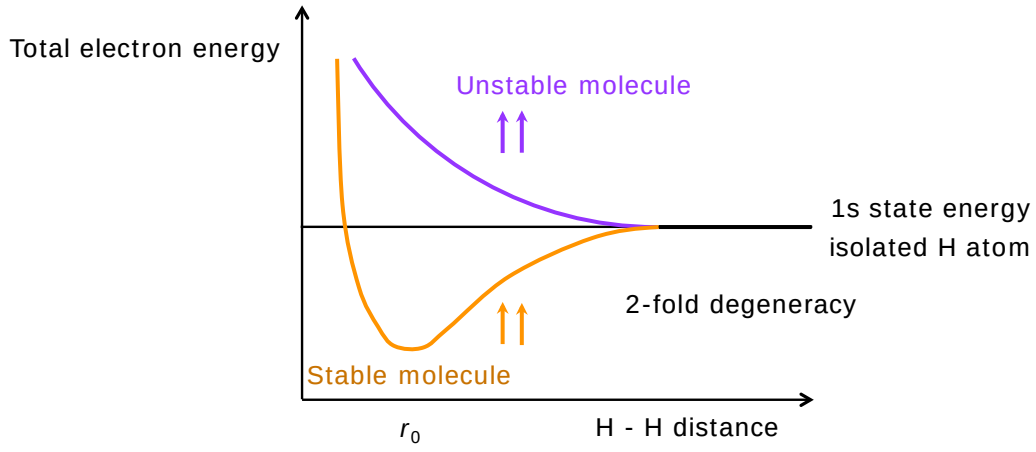
$$\frac{\langle \boldsymbol{r} - \boldsymbol{r}_0 \rangle}{\tau} = \frac{-q\tau}{m}\boldsymbol{E} = v_\mathrm{d}$$

Finally, $v_\mathrm{d} = -\mu\boldsymbol{E}$ is obtained.

$\mu = q\tau / m$: mobility

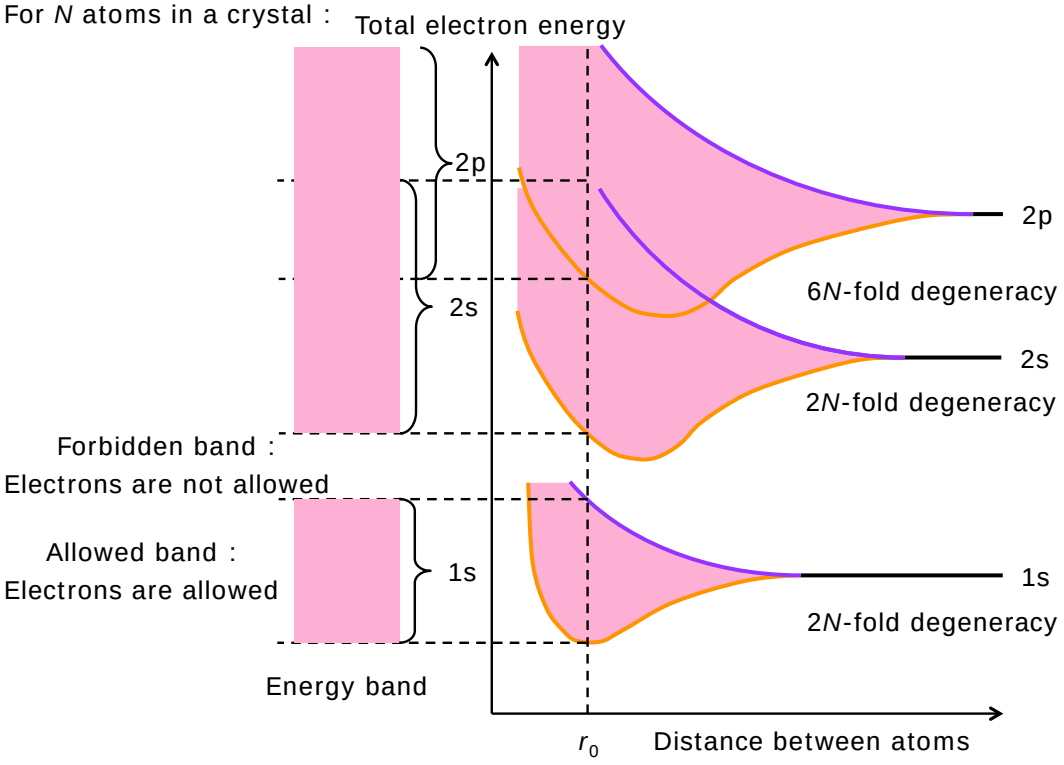
Degeneracy

For H - H atoms :



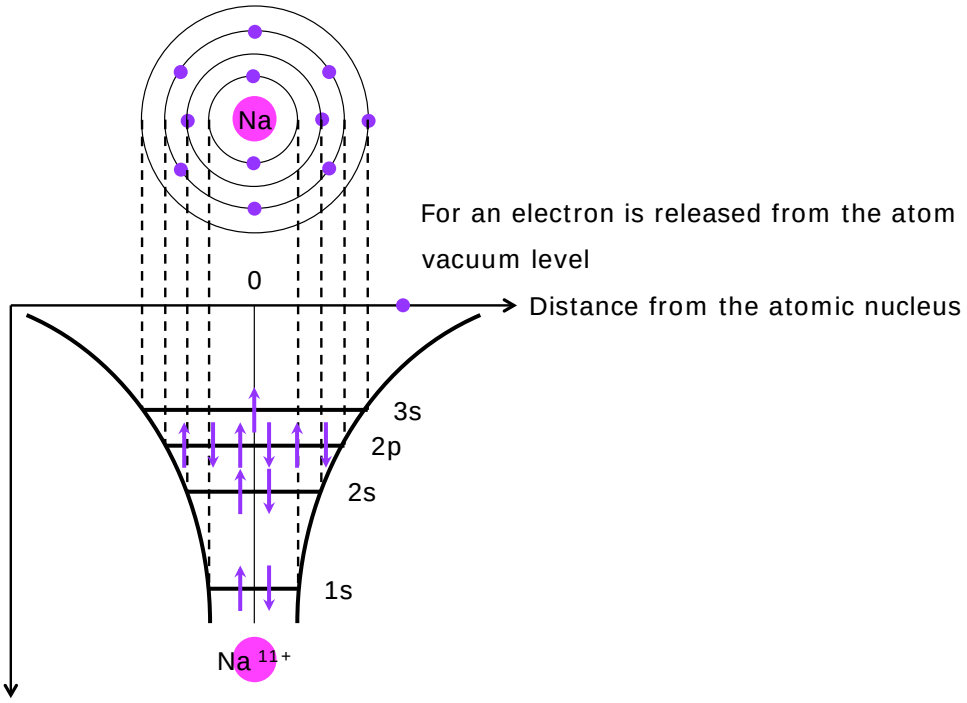
Energy Bands in a Crystal

For *N* atoms in a crystal :



Electron Potential Energy

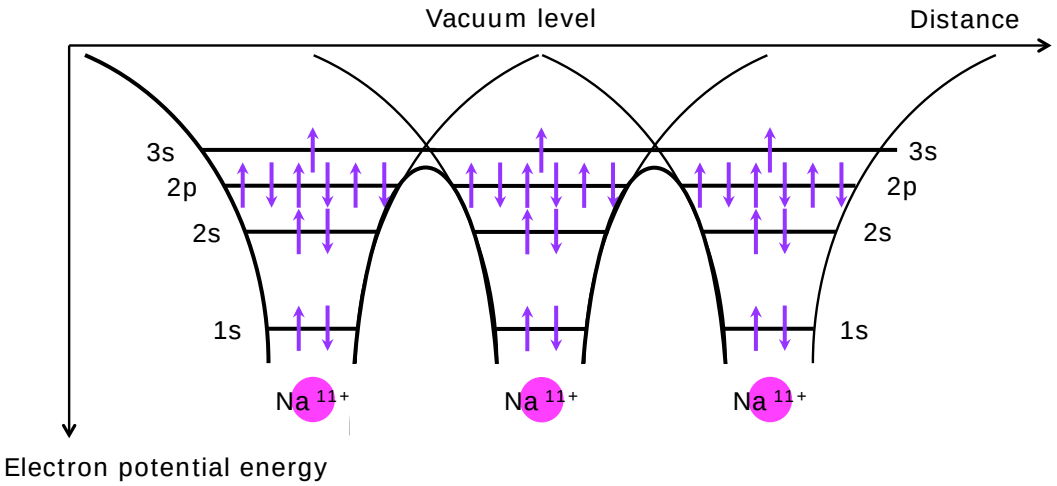
Potential energy of an isolated atom (*e.g.*, Na) :



Electron potential energy : $V = -A / r$

Periodic Potential in a Crystal

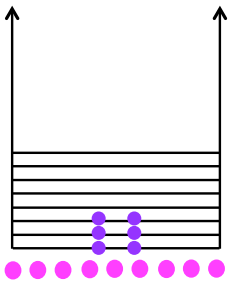
Potential energy in a crystal (*e.g.*, *N* Na atoms) :



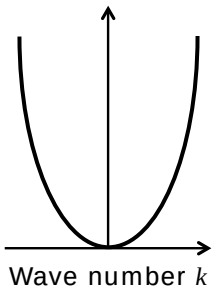
- Potential energy changes the shape inside a crystal.
- 3s state forms *N* energy levels → Conduction band

Free Electrons in a Solid

Free electrons in a crystal :



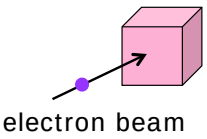
Total electron energy



Wave / particle duality of an electron :

Wave nature of electrons was predicted by de Broglie,

and proved by Davisson and Germer.



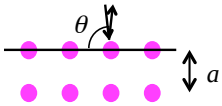
	Particle nature	Wave nature
Kinetic energy	$mv^2/2$	$h\nu = \hbar\omega$
Momentum	mv	$h/\lambda = \hbar k$

$\lambda = \dfrac{h}{p} = \dfrac{h}{mv}$ (h : Planck's constant)

$\hbar = h/2\pi,\ \omega = 2\pi\nu,\ k = 2\pi/\lambda$

Brillouin Zone

Bragg's law : $n\lambda = 2d\sin\theta$



For θ ~ 90° (π / 2),

$n\lambda \approx 2a$

Therefore, no travelling wave for

$$k = \frac{2\pi}{\lambda} = \frac{n\pi}{a} \qquad n = 1, 2, 3, \ldots$$

→ Forbidden band

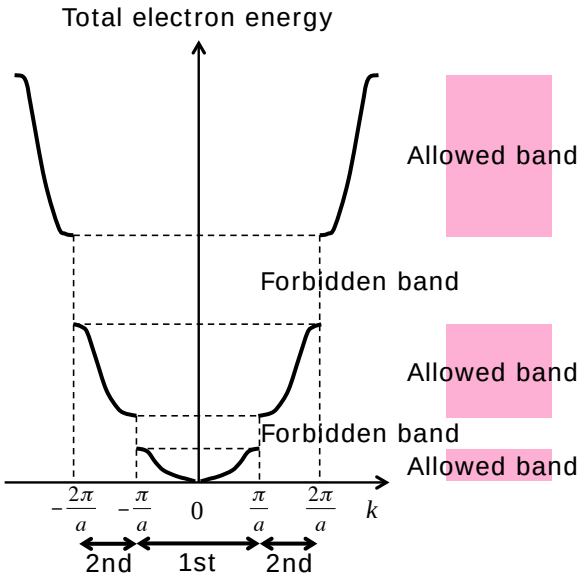
Allowed band :

$$-\frac{\pi}{a} \le k \le \frac{\pi}{a}$$

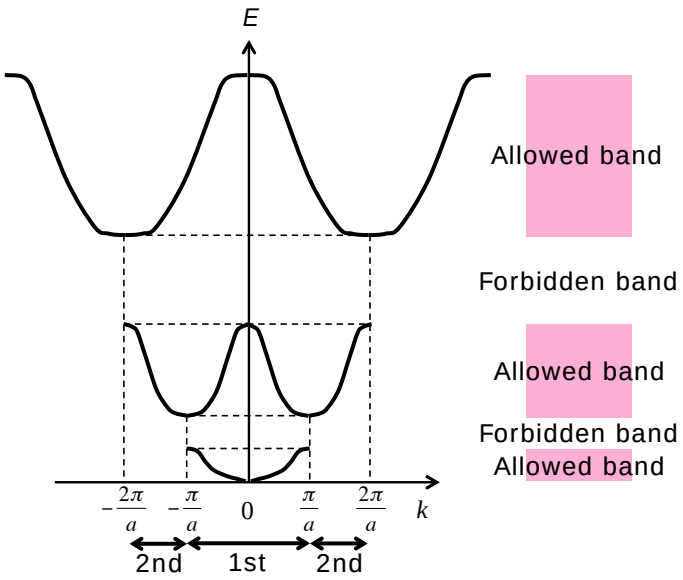
→ 1st Brillouin zone

In general, forbidden bands are

$$k = \frac{2\pi}{\lambda} = \frac{n\pi}{d\sin\theta} \equiv k_n \quad n = 1, 2, 3, \ldots$$



Periodic Potential in a Crystal

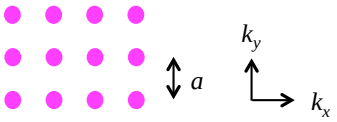


Energy band diagram
(reduced zone)
↔ extended zone

Brillouin Zone - Exercise

Brillouin zone : In a 3d ***k***-space, area where ***k*** ≠ 0.

For a 2D square lattice,



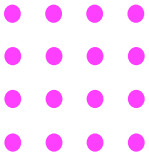
$$k_x n_x + k_y n_y = \frac{\pi}{a}\left(n_x^2 + n_y^2\right)$$

n_x, n_y = 0, ± 1, ± 2, ...

1st Brillouin zone is defined by

n_x = 0, n_y = ± 1 → k_x = ± π/a

n_x = ± 1, n_y = 0 → k_y = ± π/a



Fourier transformation

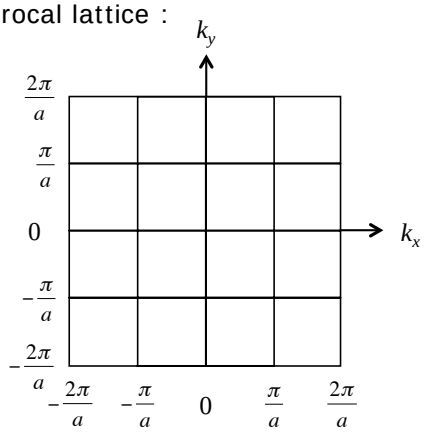
= Wigner-Seitz cell

2nd Brillouin zone is defined by

n_x = ± 1 , n_y = ± 1

→ ± k_x ± k_y = 2π/a

Reciprocal lattice :



3D Brillouin Zone

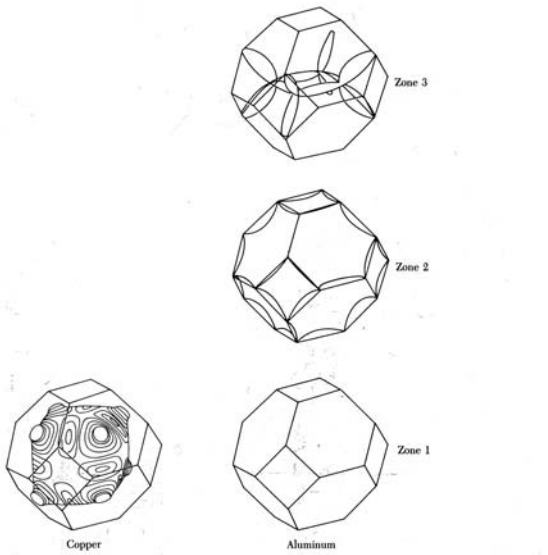
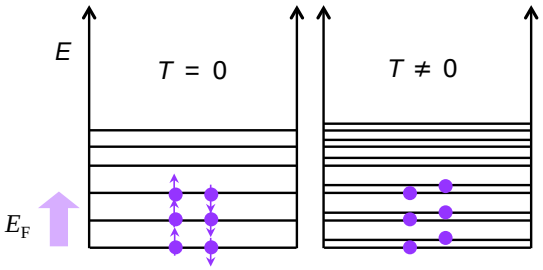


Figure 1 Free electron Fermi surfaces for fcc metals with one (Cu) and three (Al) valence electrons per primitive cell. The Fermi surface shown for copper has been deformed from a sphere to agree with the experimental results. The second zone of aluminum is nearly half-filled with electrons. (A. R. Mackintosh.)

* C. Kittel, *Introduction to Solid State Physics* (John Wiley & Sons, New York, 1986).

Fermi Energy

Fermi-Dirac distribution :



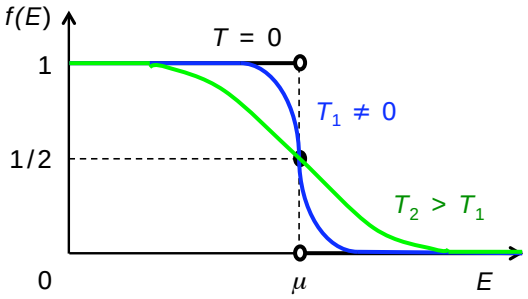
Pauli exclusion principle

At temperature T, probability that one energy state E is occupied by an electron :

$$f(E) = \frac{1}{\exp\left[(E-\mu)/k_B T\right]+1}$$

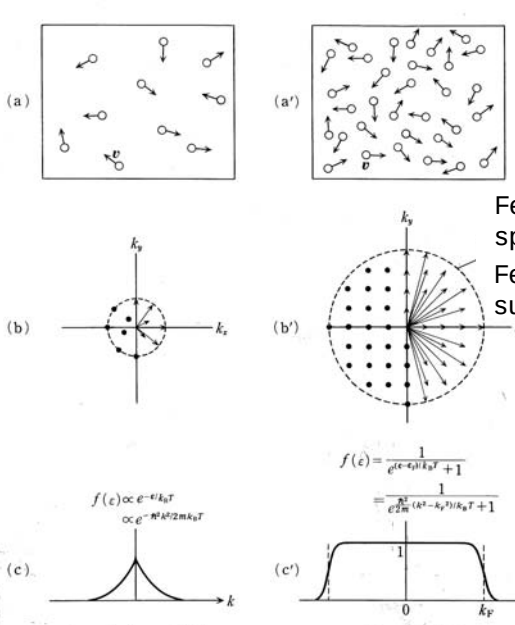
μ : chemical potential
(= Fermi energy E_F at T = 0)

k_B : Boltzmann constant



Fermi-Dirac / Maxwell-Boltzmann Distribution

Electron number density :



Fermi sphere :
sphere with the radius k_F

Fermi surface :
surface of the Fermi sphere

Maxwell-Boltzmann distribution
(small electron number density)

Fermi-Dirac distribution
(large electron number density)

* M. Sakata, *Solid State Physics* (Baifukan, Tokyo, 1989).

Fermi velocity and Mean Free Path

Fermi wave number k_F represents E_F :

Fermi velocity : $v_F = \sqrt{\frac{2E_F}{m}}$

$$k_F = \frac{m}{\hbar} v_F = \frac{\sqrt{2mE_F}}{\hbar}$$

Under an electrical field :

Electrons, which can travel, has an energy of ~ E_F with velocity of v_F

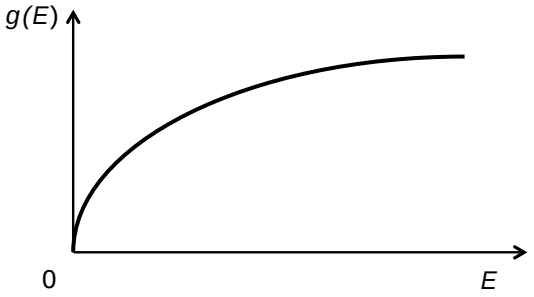
For collision time τ, average length of electrons path without collision is

$\ell = v_F \tau$ Mean free path

Density of states :

Number of quantum states at a certain energy in a unit volume

$$g(E) = 2\frac{1}{(2\pi)^3}\frac{4\pi}{2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}\,dE$$



Density of States (DOS) and Fermi Distribution

Carrier number density n is defined as :

$$n = \int f(E)g(E)dE$$