ENGINEERING PHYSICS VNT-3ELECTRICAL CONDUCTION IN METALS

Vibha Masti

Feedback/corrections: vibha@pesu.pes.edu

Solids / will be studing

- · crystalline & amorphous
- · amorphous: ordering of atoms is short range
- · crystalline: periodic arrangement of atoms in lattice is long-range.

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$\Theta \oplus \Theta \oplus$	

Crystalline Solids

Monovalent copper



- for monovalent copper, no of free e = 1028
- · e will move with thermal velocity

$$\langle V_{\text{thermal}} \rangle = 0 \Rightarrow \text{no current}.$$

· only drift velocity can give rise to current cemp)

Three Models to Explain Electrical Conduction

D Classical Free Electron Theory CCFET)

- · Also called Drude Lorentz Model
- 2) Quantum Free Electron Theory
 - · Sommerfield Model
- 3) Kronig-Penney Model

CEEI

Assumptions

1. Electrons in metals treated as gas molecules (free electron gas)



 $\frac{3kT}{2} = \frac{1}{2}mv_{m}^{L}$

 $V_m = \sqrt{\frac{3k!}{m}}$

- $\langle V_n \rangle = 0 = 0$ no unrent
- 2-Average behaviour of electron Cvelocity, energy) is studied using classical statistics (MV statistics)

(other statistics: Bose-Einsten, Formi - Dirac)

- integral spin 1/2 integral spin
- 3. e⁻e⁻ interactions and e⁻ +ve ionic core interaction neglected,
- 4 e treated as free particles (constant potential)

Expression for Electrical conductivity

n, e 1 no of free e

E=V/d Volts/m



e will drift in the direction opposite to E



Demerits or Failures of CFET

1. Dependence of 5 on n

Model	Experimental Results
Al Cu trivalent monovalent	conductivity of cu> conductivity of Al
a-Dependence of σ on Model	temperature.
$\sigma = \frac{ne^2}{m_e} \left(\frac{\lambda}{v_m}\right)$	$\nabla \propto \frac{1}{T}$
$V_{m} = \sqrt{\frac{3kT}{me}}$ $\overline{\sigma} = \frac{ne^{2}\lambda}{\sqrt{3kTme}}$	

3.	Elect	ronic	Sp	ecifi	c H	eat

Model	Experimental Results
$U = N \frac{3}{2} kT$	
$(C_V)_{ele} = \frac{du}{dt} = N \frac{3}{2}k$	actual observed value not independent of term perceturce
independent of temp.	value ~100 times less
when calculated, 2	for M, Ag, Cu etc.
orders of magnitude higher	

Mattheisen's Rule (Variation of resistivity with T)





As temp increases, area of cross-section increases

 $A = \pi f^2$ + r = amplitude

Collisions increase, A decreases





- · correction to Drude model
- · Given by Sommerfield

Assumptions

1. c⁻ are treated as quantum particles as they show quantum behaviour

Classes of Quantum Particles

1. Bosons particles with integral spin eg: photons Bose particles go to highly occupied state

2. Fermions

- particles with yz integral spin
 eg: electrons (±1/2)
 Fermions obey Paulis exclusion principle

Fermi particles are identical and indistinguishable Max 2 particles in one energy state

Pauli's Exclusion Principle

No two electrons can occupy the same quantum state in a given energy state

2 et can be accomodated in one energy state.

2. Fermions follow Fermi-Dirac statistics

$$F(E) = \frac{1}{1 + e^{\frac{E \cdot E_E}{kT}}}$$

- 3. e⁻-e⁻ interactions and e⁻ tre ionic hole interactions neglected
- 4 et is a free particle moving in constant potential cquantum free electron gas)



The highest occupied energy level at T=OK is called the fermi level.

me energy of the e at that level is called fermi energy

At T=OK, all levels above the fermi level are empty.

Probability of occupation of e in different energy states given by Fermi-Dirac statictics (fermi factor)

$$F(E) = \frac{1}{1 + e \frac{E - E_F}{kT}}$$
fermi
factur

value of F(E) in different cases

Case 1: E C EF at T= O K

$$F(E) = \frac{1}{1 + e^{-\infty}}$$

F(E) = 1

100% occupation below Fermi level (for E < E_F)

Case 2: E > E = at T = OK

$$F(E) = \frac{1}{1 + e^{\infty}}$$

F(E) = 0

0% occupation above Fermi level (for E>EF)

Case 3: E=EF at T>OK

 $F(E) = \frac{1}{1+e^{\circ}}$

F(E) = 1/2

- · at T>OK, EF is no longer the highest occupied level
- 50% occupation at EF
 At max, 50% of e can occupy higher levels than EF

Variation of Fermi Factor as a function of Temperature



From the graph, it is clear that, given thermal energy, all free e cannot conduct.

Only a fraction of et close to the fermi level can conduct total free et

$$Neff = N \frac{k_{BT}}{E_{F}}$$

According to quantum (Sommerfields) meory, all free eare not conduction e-

Example: EF (cu) = 7eV

If innermost et to be conduction et, neff = N

T_E≈ 81000 K (Fermi Temperature)

At such high temperatures, metals are liquid (impractical)

It is the temperature at which all e are above EF.

Fermi temperature is the temperature required to remove the last e below the Fermi level Conly theoretically possible)

BI. Find the temperatures at which the occupancy of an energy state 0.3 eV above the Fermi level has an occupancy probability of 0.01

$$F(E) = \frac{1}{1 + e^{\frac{E - E_E}{k_s T}}}$$

$$0.01 = \frac{1}{1 + e^{\frac{0.3eV}{k_T}}}$$

$$100 - 1 = e^{\frac{0.3eV}{k_T}}$$

$$4.595 = \frac{0.3eV}{k_T}$$

T = 757.6 K

Q2. Calculate the Fermi factor of an energy state 0.01 eV below the Fermi level at T= 500 K.

$$F(E) = 1 = 0.558$$

 $1 + e^{-0.01eV}$

Density of states * SO Pillai solid state

3D Solids

No of available energy states within a given energy interval E to E+dE

gle) dE or Dle) de

consider a conducting ube Cubic crystal a=b=cand $\alpha = \beta = \gamma = 90^{\circ}$



We have 10²⁶ particles in a box (SWE)
 We think of the e- as waves in a box (quantised energy)

 $E_{n} = \frac{(n_{2}^{2} + n_{y}^{2} + n_{z}^{2})h^{2}}{8ml^{2}}$

$\Psi_{n} = \sqrt{\frac{2}{L}} \sin\left(\frac{n_{\chi}\pi\chi}{L}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{n_{\chi}\pi\chi}{L}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{n_{\chi}\pi\chi}{L}\right)$

(stable only when $\psi_2, \psi_y, \psi_z \neq 0$)

Phase Space

To accomodate 1026 electrons



We consider a radius R corresponding to all states with energy E and a sphere of radius RtdR with energy EtdE

volume = no. of whes = no. of points = no. of states

... volume=no. of states

In phase space, equation of sphere

$R^2 = n_1^2 + n_2^2 + n_2^2$ (three axes)

 $E = \frac{R^2 h^2}{8mL^2}$

 $R^2 = \frac{8EmL^2}{h^2}$; $R = \sqrt{8Em} \frac{L}{h}$; $dR = \frac{L}{8} \frac{8Em}{h} \frac{1}{2} \frac{1}{16}$

No of energy states between E and E+dE = volume of R+dR - volume of R

= UTR dR

 $= \frac{T}{2} \left(\frac{8mL^2E}{h^2} \right) \left(\frac{L}{h} \sqrt{8m} \frac{L}{2} \right) dE$

 $= \frac{\pi}{2} \left(\frac{8m^{2}E}{2k^{3}} \sqrt{8m} \right) dE$

 $= \frac{\pi}{2} \left(\left(\frac{8mL^2}{h^2} \right)^{3/2} \frac{\sqrt{c}}{2} \right) dE$

 $= \frac{T1}{4} \left(\frac{8mL^2}{h^2} \right)^{3/2} f = d =$

Each state actually can accomp date à distinct electron states due to spir quantum number CPauli Exclusion Principle)





AS ET, GLE)?

variation of Density of States as a function of E



No of energy states up to an energy E

$$N = \int_{a}^{b} \frac{\pi}{a} \left(\frac{8m}{b^{2}}\right)^{3/2} \sqrt{E} dE$$

$$= \frac{\pi}{2} \left(\frac{8m}{h^2} \right)^{3/2} \left[\frac{2}{3} E^{3/2} \right]_{0}^{6}$$

$$N = \frac{\pi}{3} \left(\frac{8m}{h^2}\right)^{3/2} E^{3/2}$$

No of energy states upto fermi level

$$N_{F} = \prod_{3}^{F_{F}} \left(\frac{8 \text{ m}}{h^{2}}\right)^{3/2} \left(F_{F}\right)^{3/2} \qquad \text{per unit}$$

At T=O, all energy states below EF are occupied.

. no of e present = energy states below EF

n→ electron density electrons per unit volume

· n= NF

Electron Density

 $n = \frac{\pi}{3} \left(\frac{8m}{h^{2}}\right)^{3/2} E_{f}^{3/2}$

03. If Er of Lu= 7eV, find & concentration of Lu

 $n = \frac{\pi}{3} \left(\frac{8m}{h^2} \right)^{3/2} (Te)^{3/2}$

 $n = 8.411 \times 10^{28} \text{ m}^{-3}$

 $\theta_4 = n_{Ag} = 5.211 \times 10^{21} \text{ m}^{-3} E_{p} = 7$

 $n = \frac{11}{3} \left(\frac{8m}{k^2}\right)^{3/2} (E_p)^{3/2}$

 $\left(\frac{3n}{\pi}\right)^{a/3}\frac{h^2}{8m} = E_F$

e_F = 5.09 eV

Variation of Number Density as a function of Temperature



Average Energy of Electron at T= OK

average energy = { no of electrons x energy

total no. of electrons

$$\int_{1}^{E_{\rm F}} g(E) dE E = \int_{1}^{E_{\rm F}} \left(\frac{\pi}{2}\right) \left(\frac{8m}{k^2}\right)^{3/2} E E dE$$

$$\langle E \rangle = 0 = 0$$

 $\int_{1}^{k_{\mathrm{f}}} \left(\frac{\pi}{2}\right) \left(\frac{8m}{h^{2}}\right)^{3/2} \text{ for } \mathrm{d} \mathrm{e}$

 $\langle E \rangle = \left(\frac{3}{5} \frac{E^{5/2}}{E^{3/2}} \right)^{E_{\rm F}} = \frac{3}{5} E_{\rm F}$

On Find the average energy of Ag e (EF=55eV)

< => = 3 EF = 3.3 eV

Merits of QFET

1 Dependence of σ on n



nal > non

MAL = 2.34 n cm

$$\left(\frac{\lambda_F}{V_F}\right) \approx 3.14 \left(\frac{\lambda_F}{V_F}\right)_{AL}$$

In accordance with experiment

2 Electronic specific heat

$$(Cv)_{ele} = \frac{du}{dT}$$

$$U = n_{eff} = \frac{3}{2} k_B T$$

$$= N \frac{k_B T}{E_F} = \frac{3}{2} k_B T$$

$$U = \frac{3}{2} N \frac{k_B^2}{E_F} T^2$$

$$U = \frac{3}{2} N \frac{k_B^2}{E_F} T^2$$

$$Cv)_{ele} = \frac{du}{dT} = 3 N \frac{k_B^2}{E_F} T$$

(Cv)ele for Lu is 12666 Jug lit which is in accordance with experimental results.

06. $(E_{\rm F})_{14} = 7eV$, $n = 6.28 \times 10^{28} \text{ m}^{-3}$, find (Lv)ele at T = 300 k $(C_{\rm v})_{\rm ele} = \frac{3 \times 8.28 \times 10^{28} \times 10^{28$

3. Dependence of σ on T

- · With increase in temperature, the area of cross-section of each of the positive ionic core increases, which means the amplitude of vibrations increases
- · Mis gives rice to more electronic collisions
- · merefore, mean free path reduces.

$$\lambda_F \propto \frac{1}{T}$$

 $\sigma \propto \frac{1}{T}$

Relationship between mermal and Electrical conductivity

Weidemann - Franz Law

K: thermal conductivity o: electrical conductivity

$$K = \frac{1}{3} \frac{(L_v)_{ele}}{V} \quad \forall_F \lambda$$

$$\sigma = \frac{ne^2 \gamma}{m}$$

Modified Electronic Specific Heat Equation

$(Cv)ele = \frac{T^2}{2} N \frac{k_B^2 T}{E_F}$

Plugging in values



$$\sigma = \frac{ne^2 z}{m}$$

Relationship

$$\frac{K}{D} = \frac{\pi^2}{3e^2} \quad k_B^2 T = \text{constant at } T$$

For any metal at a given temperature, the value of $\frac{k}{\sigma}$ is constant

$$\frac{k}{\sigma} = \frac{\Pi^2}{3e^2} k_8^2 T$$

$$\frac{k}{\sigma} = LT$$

$$\frac{k}{\sigma} = LT$$

$$\frac{1}{\sigma} = LT$$

$$\frac$$

Demerits of QFET

1. Generally, metals exhibit -ve Hall coefficient, but certain metals like Zn, Cd exhibit tve Hall coefficient.

This model could not account for this.

Hall effect - later

a This model could not differentiate solide as conductors, semiconductors and insulators

KRONIG-PENNEY MODEL

Assumption

1. Electrons are not free particles; they are partially bounded

Potential 7 0

e⁻ inside the metal is not free; it experiences a periodic potential (series of finite wells and barriers) due to the periodicity of lattice.





Bloch Function

Whenever a particle experiences a periodic potential, the associated wavefunction is given by Bloch function

$$\Psi(x) = V_{k}(x)e^{ikx} \qquad k = \frac{2\pi}{\lambda}$$
$$\Psi(x+a) = V_{k}(x+a)e^{ik(x+a)} \qquad \lambda$$

Vica) is a periodic function with periodicity a

 $V_{\mu}(xta) = V_{\mu}(x)$

For a free particle, E vs K

e can take any value

continuous

k

For a partly free particle, E vs k



merefore, we plug in the Bloch function into the differential equations (1) and (2)

$$\Psi(x) = V_{k} e^{ikx}$$

Differentiating W(x) and using the values in equation (1) and (2) we get two equations

Applying boundary conditions, we get four equations Can also be solved by linear algebra. Creating Eigenvalue Equations

$$\psi(x) = V_{k}(x) e^{ikx} \longrightarrow eigen function$$

Take a translational operator $\hat{\tau}$ such that

$$\hat{T} \psi(x) = V_{\mu}(x+a) e^{i\mu(x+a)}$$

$$= V_{\mu}(x) e^{i\mu x} e^{i\mu a}$$

$$\hat{T} \psi(x) = e^{i\mu a} \psi(x) \longrightarrow eigenvalue$$

$$= e^{i\mu a} \psi(x) \longrightarrow eigenvalue$$

me final solution



From the graph, we notice that discontinuity arises when the y value is ±1

$$P \frac{sin \alpha \alpha}{\alpha \alpha} + \cos \alpha \alpha = \pm 1$$

$$coska = \pm 1$$

$$ha = n\pi$$

Whenever $k = \frac{n\pi}{a}$, gap in energies appears.

Note: K is continuous; no condition for discontinuity x is discontinuous due to condition

a- K Correspondence

$$\alpha^{2} = \frac{\partial ME}{\hbar^{2}} , E = \frac{p^{2}}{\partial M} = \frac{\pi^{2}k^{2}}{\partial M}$$

$$\alpha^{2} = \frac{\partial M}{\hbar^{2}} + \frac{\pi^{2}k^{2}}{\partial M} = \frac{1}{2} + \frac{$$

d & k are physically the same and both represent momentum.

k is called crystal momentum.



2 whenever an e-moves in a solid, it is not free and it undergoes bragg reflection when it encounters the ionic corres.

y becomes discontinuous (particle doesn't exist there)

- 3. There are inner & outer bands; only outermost bands conduct.
- 4. In case of a metal/inductor, the VB and is overlap Contermost band) >> no energy gap (Fermi energy in is)
- 5. In case of semiconductors, the outermost band, mere is a gap of ~3eV between VB and CB (Fermi energy in band gap)
- 6. For insulators, there is a gap of > Jev between VB and CB contermost gap) (Fermi energy in band gap)

Other Conclusions

Extreme cases

Case I



Effective mass

For free particles, true momentum tek = p = mV group velocity $E = \frac{k^2 k^2}{2m}$

For particles in solid Curystal)

group velocity does not change

 $\frac{d^2 E}{dk} = \frac{k^2}{m^*}$

 $m^* = \frac{k^2}{(d^2 \varepsilon/dk^2)} \qquad \sigma = \frac{ne^2 \tau}{m^*}$

The effective mass depends on the curvature of Evs k graph.

Higher is the curvature, lesser will be its effective mass and vice versa



The concept of effective mass is used to study mobility of charge carriers, particularly in semiconductors

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Effective mass of et is the in CB and -ve in VB.

This allows us to view conduction in VB of SC as happening due to the charge carriers, or holes

Effective masses of et in different SC

i) Ge $m_e^* = 0.55 m_o$ $m_h^* = -0.37 m_o$