

# Course Plan

## STANDARD PENSUM

|  |        |
|--|--------|
| 24.02 – Introduction + Crystal structures-----           | (DONE) |
| 02.03 – Reciprocal space + Form & Structure Factor ----- | (DONE) |
| 09.03 – Scattering theory -----                          | (DONE) |
| 16.03 – Crystal binding energies-----                    | (DONE) |
| 23.03 – Lattice vibrations -----                         | (DONE) |
| 06.04 – Phonons measurements -----                       | (DONE) |
| 13.04 – Phonons specific heat-----                       | (DONE) |
| 20.04 – Free electron gas -----                          | (DONE) |
| 27.04 – Band structure -----                             | (DONE) |
| 04.05 – Fermi surfaces -----                             | (DONE) |
| 11.05 – Semiconductors                                   |        |

## BONUS PENSUM

|   |  |
|---|--|
| 18.05 – Magnetism                                     |  |
| 25.05 – Superconductivity + Charge density wave order |  |
| 01.06 – Repetition + Examples of Exam Questions       |  |

09.06 & 10.06 ORAL **EXAM (Room: Y-36-H-48)**

# Fermiology - continued

## 1. Summary of last lecture

Tight-binding Model

Quantum Oscillation experiments

Exercises of this week

## 2. Measurements of Fermi surfaces

Fermi surface area

Multi band

Electronic mass

## 3. Hall effect

Electron concentration

Electron / hole like carriers

## 4. Semimetals and Semi-conductors

# Summary of previous lecture

## (1) Tight-binding Model:

### **Exercise 1** *Tight binding model*

In the lecture, we derived the tight-binding expression for a two-dimensional square lattice:

$$\epsilon_k = -\epsilon_0 - 2t[\cos(k_x a) + \cos(k_y a)] \quad (1)$$

(a) Plot, using your favourite computer program, (1) the full three-dimensional band structure  $\epsilon_k$  versus  $k_x$  and  $k_y$ , (2) the band structure along the zone diagonal  $k_x = k_y$ , and (3) the Fermi surface ( $\epsilon_k = \epsilon_F$ ) for systems with  $\mu = \epsilon_F$  having the values  $-\epsilon_0$  and  $-\epsilon_0 \pm 2t$  [Hint: Set  $t = 1$  meaning that  $\epsilon_k$  is plotted in units of  $t$  and set  $\epsilon_0 = 0$ ].

(b) In the lecture, we developed the tight binding only to first order. Let's include second order terms. We define  $t'$  as the integral over next-nearest neighbours that are given by  $R_m = \{\pm a, \pm a\}$  and  $\{\pm a, \mp a\}$ . Show that the tight-binding dispersion becomes:

$$\epsilon_k = -\epsilon_0 - 2t[\cos(k_x a) + \cos(k_y a)] - 4t'[\cos(k_x a) \cos(k_y a)] \quad (2)$$

(c) Let's say that  $\mu = -\epsilon_0 - 0.87t$ . Compare the Fermi surfaces for  $t' = 0$  and  $t' = -0.2t$ .

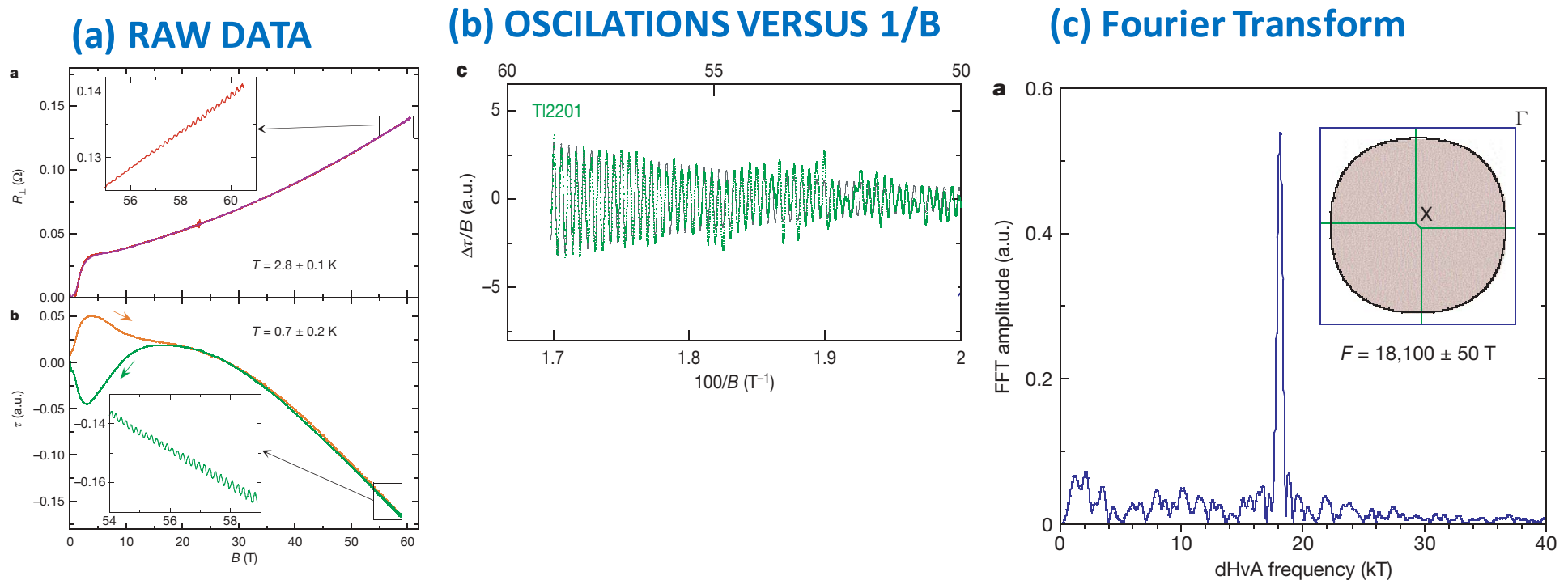
# Summary of previous lecture

## (1) Quantum Oscillation experiments:

### **Exercise 2** *Quantum oscillations on quasi two-dimensional systems*

In  $\text{Ti}_2\text{Ba}_2\text{CuO}_{6+\delta}$ , quantum oscillations with a frequency of  $F = 18.1 \text{ kT}$  are observed (B. Vignolle et al., Nature **455**, 952-955 (2008)).

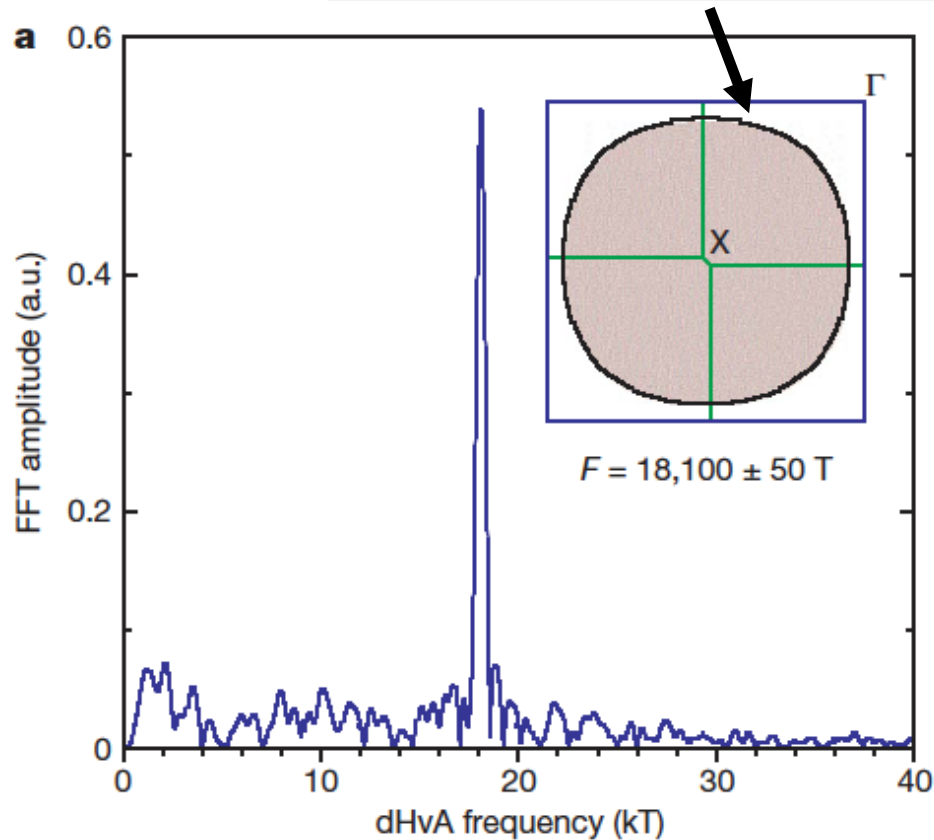
- Use the Onsager relation ( $S = 2\pi \frac{eF}{h}$ ) to calculate the Fermi surface area.
- If we assume a circular Fermi surface shape what is the Fermi momentum?



# Fermi surface: $\text{Ti}_2\text{Ba}_2\text{CuO}_{6+y}$ (Ti2201)

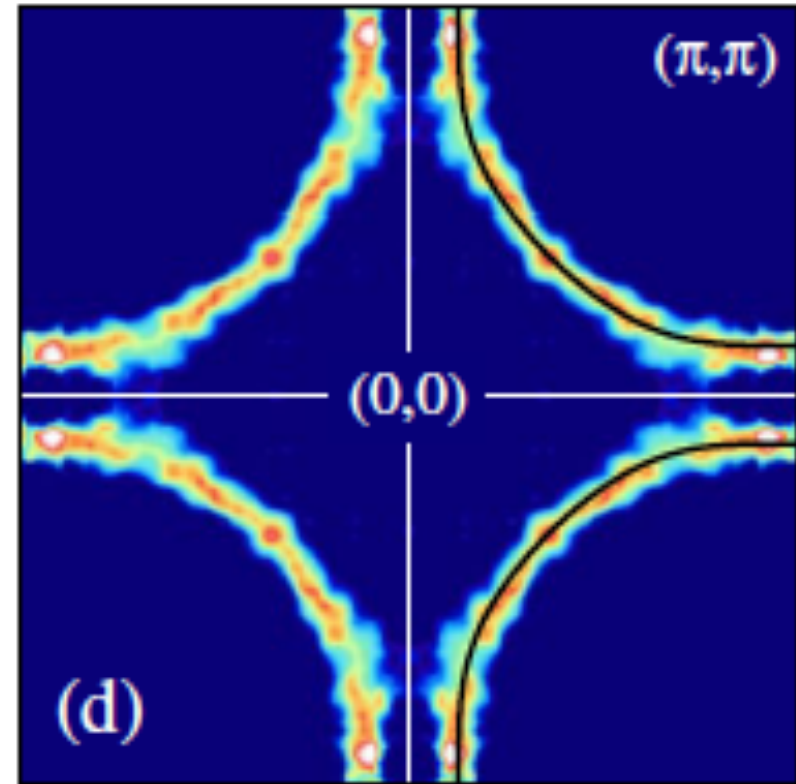
*ARPES vs Quantum Oscillations*

## Band Structure Calculations



Nature 455, 952 (2008)

Quantum Oscillation (QO) experiments

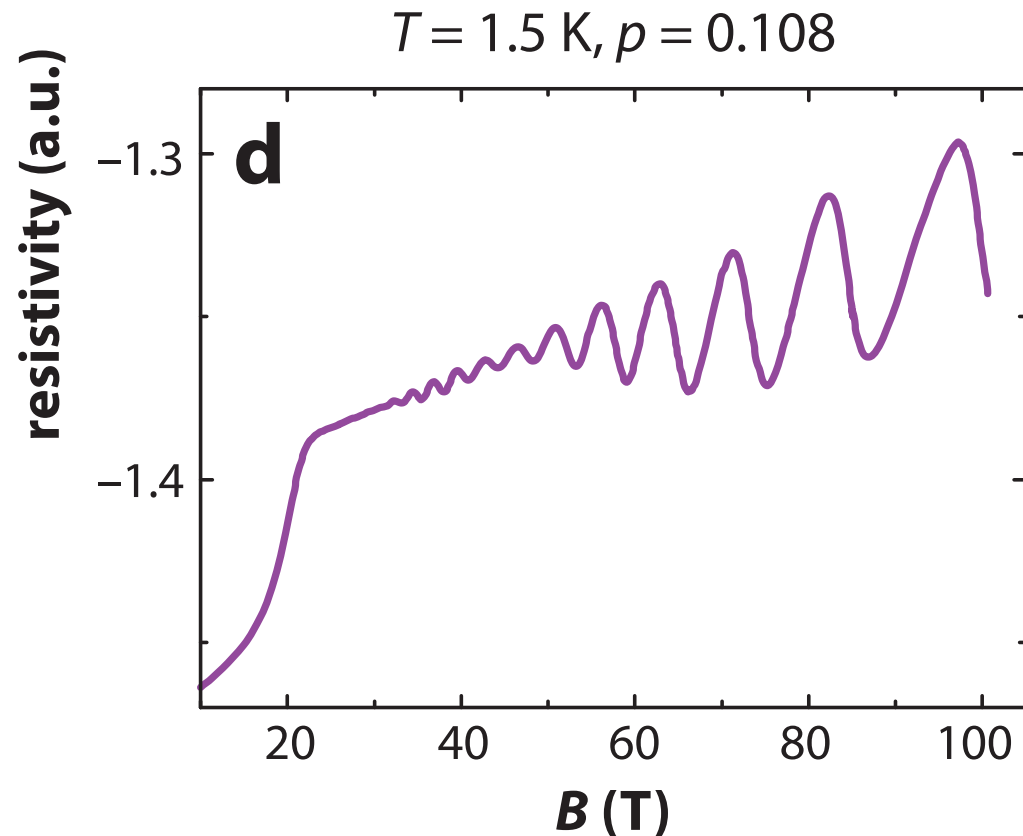


PRL 95, 077001 (2005)

Data taken @ Swiss Light Source

Angle-resolved Photo-Emission Spectroscopy (ARPES)

# QUANTUM OSCILLATIONS:



OSCILLATION AMPLITUDE

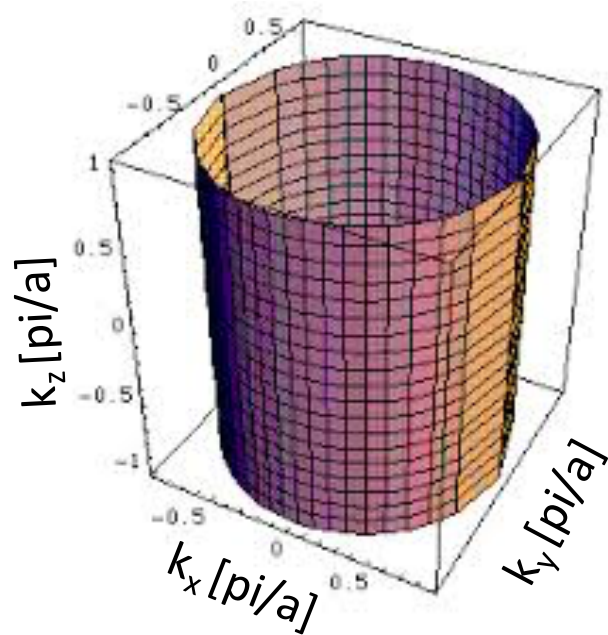
$$\propto e^{\left(\frac{-\pi\hbar k_F}{eB\ell}\right)}$$

Where  $\ell$  = mean free path

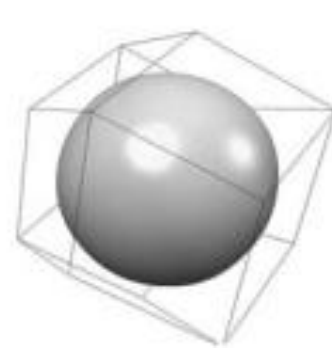
Resistivity measurement of a high-temperature superconductor:  $\text{YBa}_2\text{Cu}_3\text{O}_{6.51}$  (YBCO)

<http://www.annualreviews.org/doi/pdf/10.1146/annurev-conmatphys-030212-184305>

# Fermi surface - Dimension



2D cylindrical  
Fermi Surface

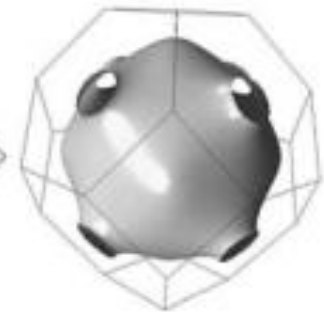


Potassium

3D spherical  
Fermi Surface



Lithium



Copper

3D spherical +  
some structure  
Fermi Surface

# Fermi surface – Gold and Copper

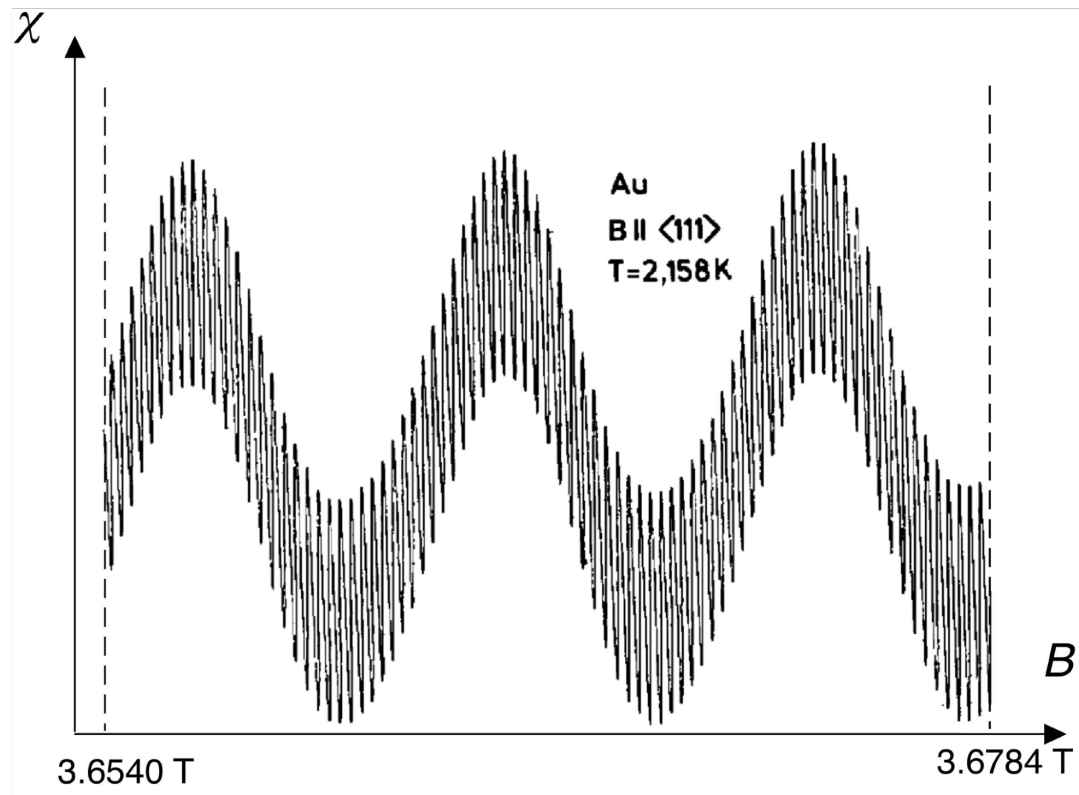
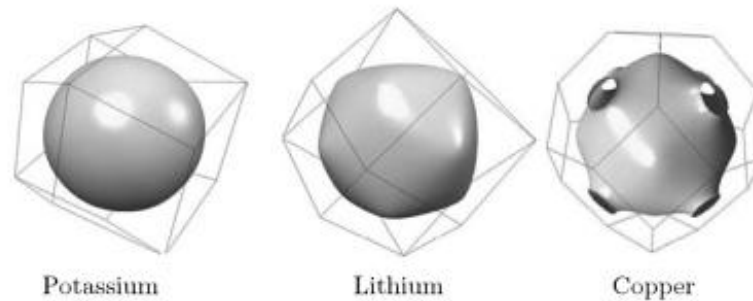
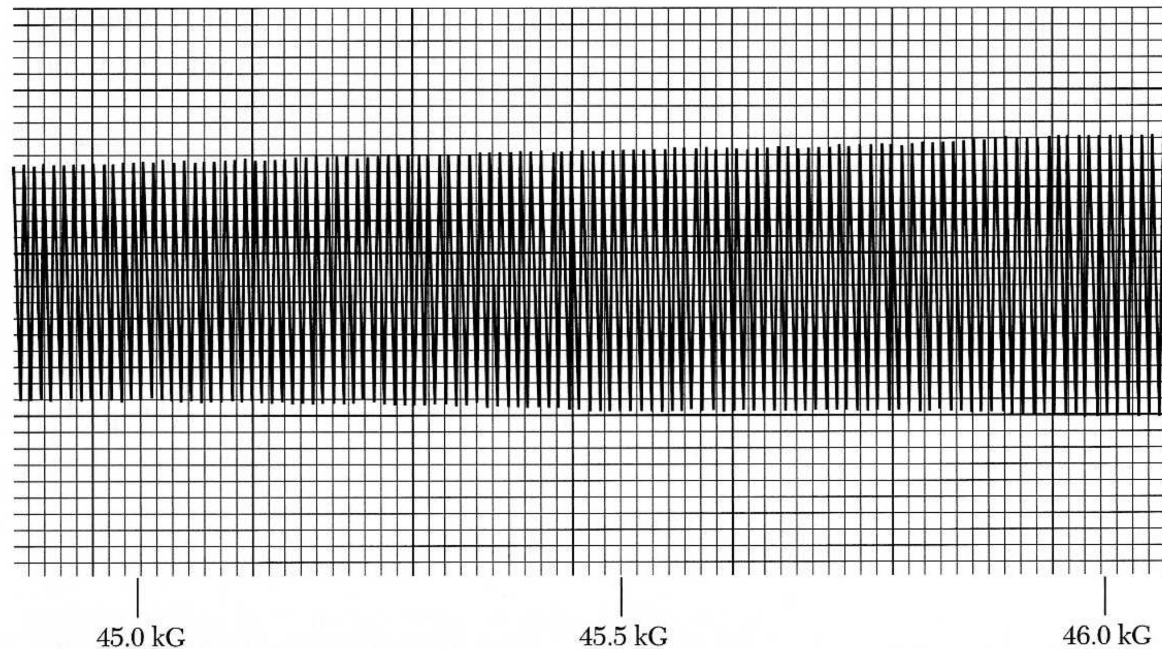


Figure 1: The spin susceptibility of gold in a magnetic field.

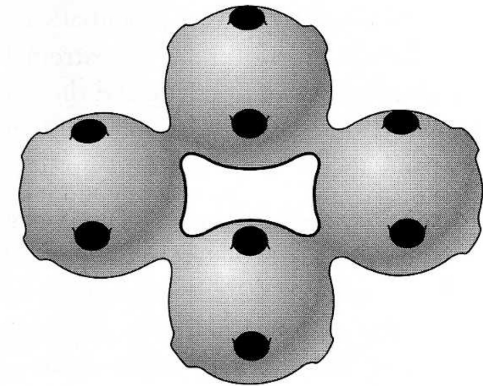




# QUANTUM OSCILLATIONS: Gold



**Figure 31** De Haas-van Alphen effect in gold with  $\mathbf{B} \parallel [110]$ . The oscillation is from the dog's bone orbit of Fig. 30. The signal is related to the second derivative of the magnetic moment with respect to field. The results were obtained by a field modulation technique in a high-homogeneity superconducting solenoid at about 1.2 K. (Courtesy of I. M. Templeton.)



**Figure 30** Dog's bone orbit of an electron on the Fermi surface of copper or gold in a magnetic field. This orbit is classified as holelike because the energy increases toward the interior of the orbit.

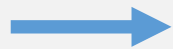
# Fermiology - continued

## 1. Summary of last lecture

Tight-binding Model  
Quantum Oscillation experiments  
Exercises of this week

## 2. Measurements of Fermi surfaces

Fermi surface area



Multi band

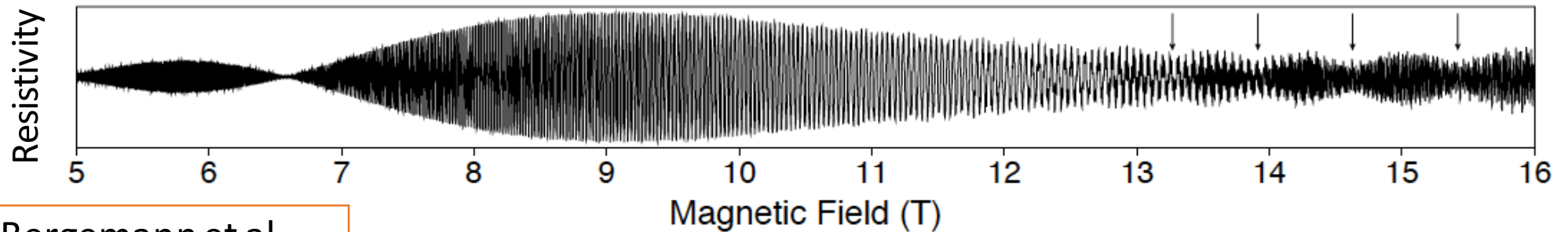
Electronic mass

## 3. Hall effect

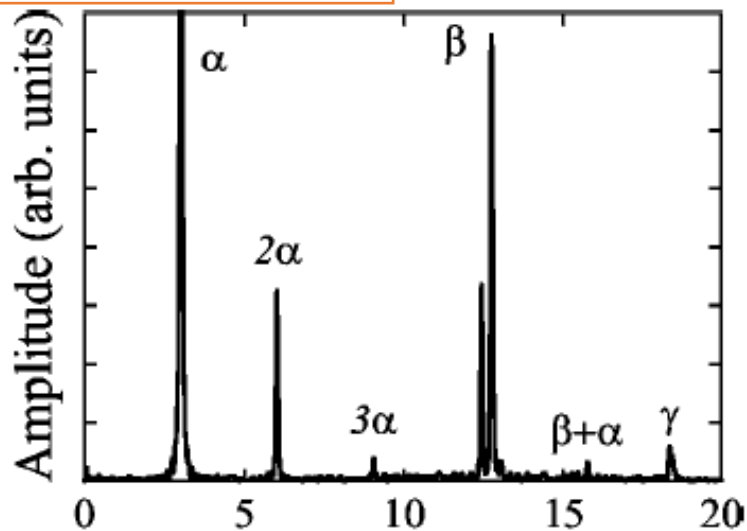
Electron concentration  
Electron / hole like carriers

## 4. Semimetals and Semi-conductors

# Multi – band metals: $\text{Sr}_2\text{RuO}_4$

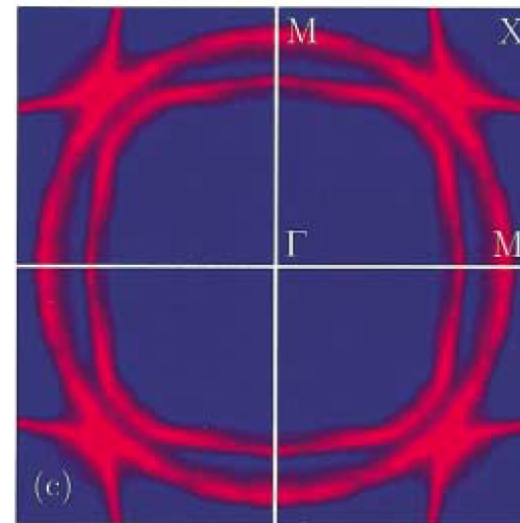


Bergemann et al,  
PRL 84, 2662 (2000)



A.P. Mackenzie et al,  
JPSJ 67, 385 (2003)

Quantum Oscillation (QO) experiments



A. Damascelli et al,  
PRL 85, 5194 (2000)

Angle-resolved Photo-Emission Spectroscopy  
(ARPES)

# Fermiology - continued

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Tight-binding Model

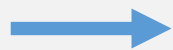
Quantum Oscillation experiments

Exercises of this week

## 2. Measurements of Fermi surfaces

Fermi surface area

Multi band



Electronic mass

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Electron concentration

Electron / hole like carriers

## 4. Semimetals and Semi-conductors

# QUANTUM OSCILLATIONS:

*Temperature dependence*

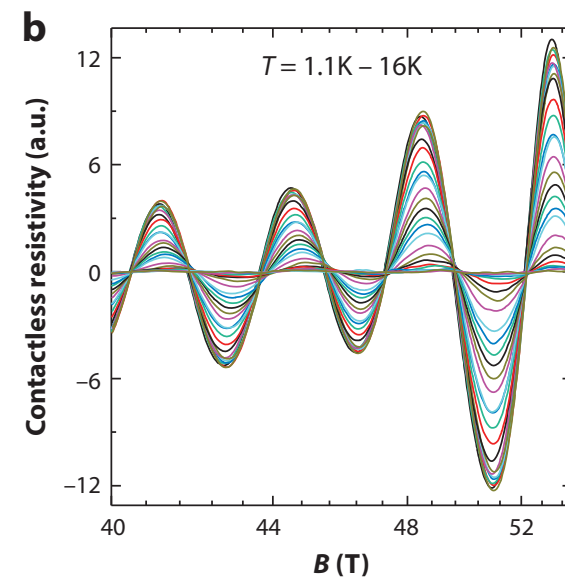
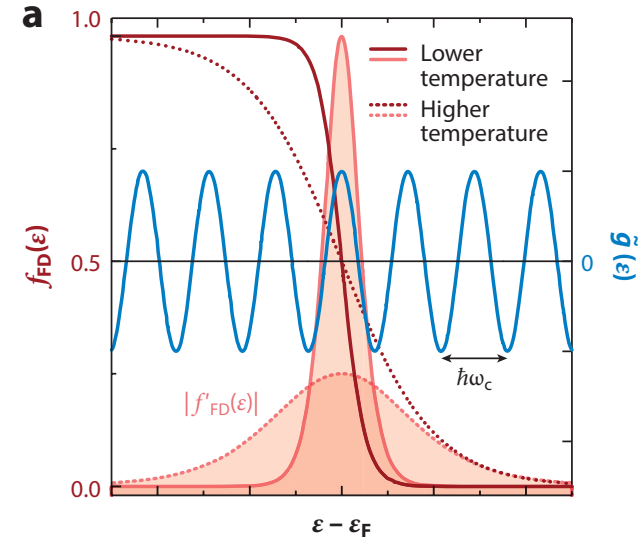
Thermal Condition:

$$\hbar\omega_c > k_B T$$

Landau level splitting > thermal energy

$$\omega_c = \frac{eB}{m}$$

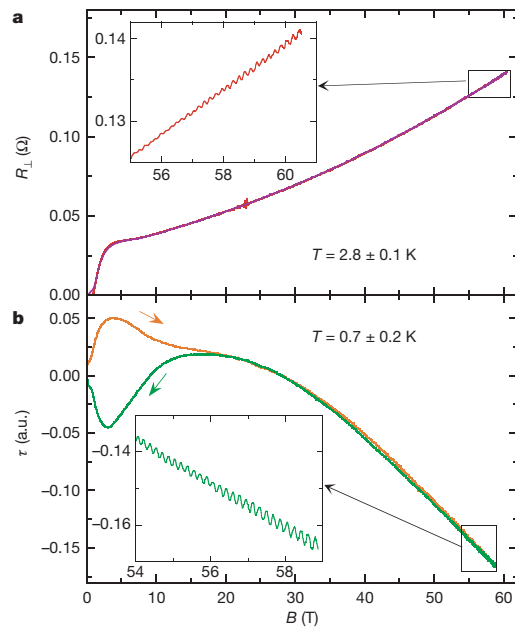
Temperature dependence of the oscillatory amplitude yield information about the electronic mass.



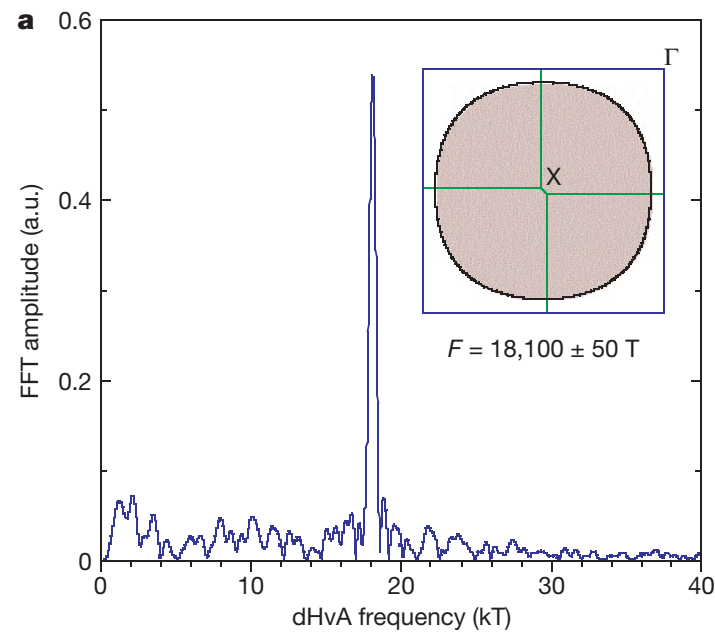
# Electronic Mass

## (1) Quantum Oscillation experiments:

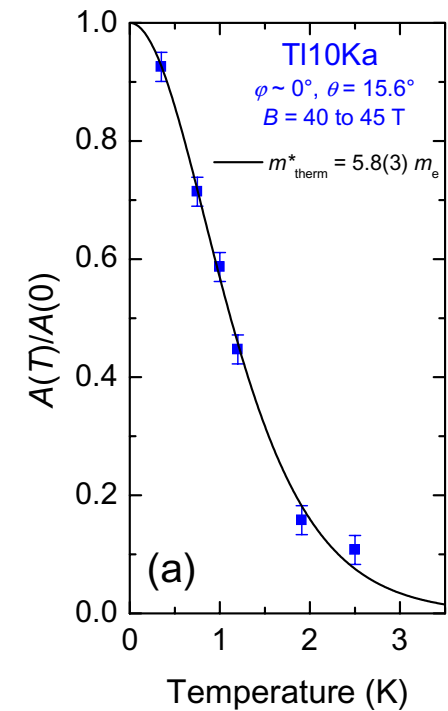
(a) RAW DATA



(b) Fourier Transform



(c) T-dependence



# Electronic Mass: Specific heat

## Exercise 1 *Electronic specific heat in two dimensions*

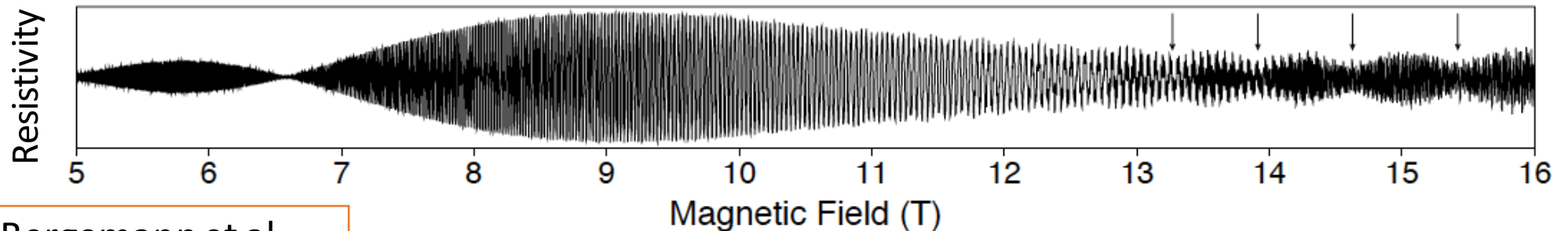
Layered crystal structures often have electronic structures that can approximately be considered two-dimensional. The high-temperature superconductor  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$  is one such example.

(a) The electronic heat capacity is given by  $C_{\text{el}} = \gamma T$ . Show that in two dimensions the Sommerfeld parameter  $\gamma$  can be written as  $\gamma = \frac{A\pi k_{\text{B}}^2}{3\hbar^2} m$  where  $m$  is the electronic mass and  $A$  is the total area. What is the unit of  $C_{\text{el}}$ ? Hint: Use  $C_{\text{el}} = \frac{1}{3}\pi^2 D(\epsilon_{\text{F}})k_{\text{B}}^2 T$  and derive the density of state (DOS) in two dimensions.

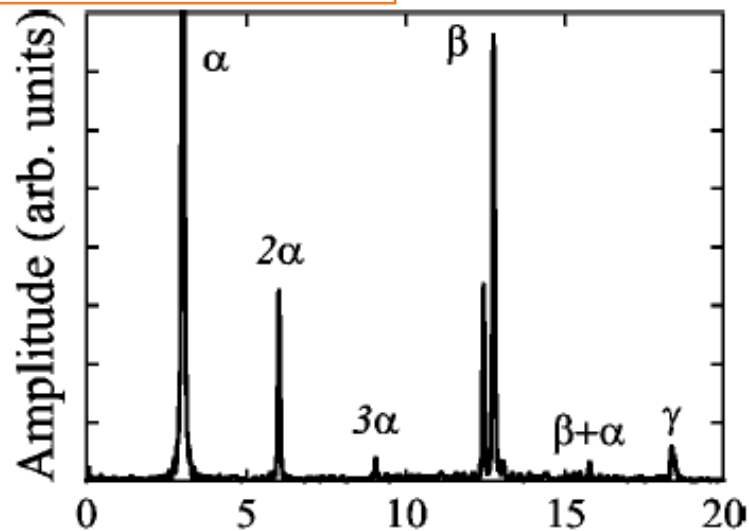
(b) The crystal structure of  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$  consists of stacked layers of  $\text{CuO}_2$ . Within a layer, the  $\text{CuO}_2$  forms a square lattice with a Cu-O lattice distance of  $a = 3.8 \text{ \AA}$ . The sample area can thus be written as  $A = a^2 N$  where  $N$  is the number of Cu-O squares. The electronic **specific** heat capacity is measured in units  $\text{J mol}^{-1} \text{K}^{-1}$ . Show that  $\gamma = \frac{N_{\text{A}} a^2 \pi k_{\text{B}}^2}{3\hbar^2} m$  where  $N_{\text{A}}$  is the Avogadro number.

(c)  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$  is observed to have the Sommerfeld parameter  $\gamma = 6 \text{ mJ mol}^{-1} \text{K}^{-2}$ . Using the result of (b), what is the electronic mass  $m$  for  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$ ? How does it compare to the free electron mass?

# Multi – band metals: $\text{Sr}_2\text{RuO}_4$



Bergemann et al,  
PRL 84, 2662 (2000)



A.P. Mackenzie et al,  
JPSJ 67, 385 (2003)

TABLE II. Summary of quasiparticle parameters of  $\text{Sr}_2\text{RuO}_4$ .

| Fermi-surface sheet                      | $\alpha$ | $\beta$      | $\gamma$     |
|--|----------|--------------|--------------|
| Character                                | Holelike | Electronlike | Electronlike |
| $k_F$ ( $\text{\AA}^{-1}$ ) <sup>a</sup> | 0.304    | 0.622        | 0.753        |
| $m^*$ ( $m_e$ ) <sup>b</sup>             | 3.3      | 7.0          | 16.0         |

A.P. Mackenzie et al,  
RMP 75, 657 (2003)

Quantum Oscillation (QO) experiments



# Multi – band metals: $\text{Sr}_2\text{RuO}_4$

## Heat Capacity

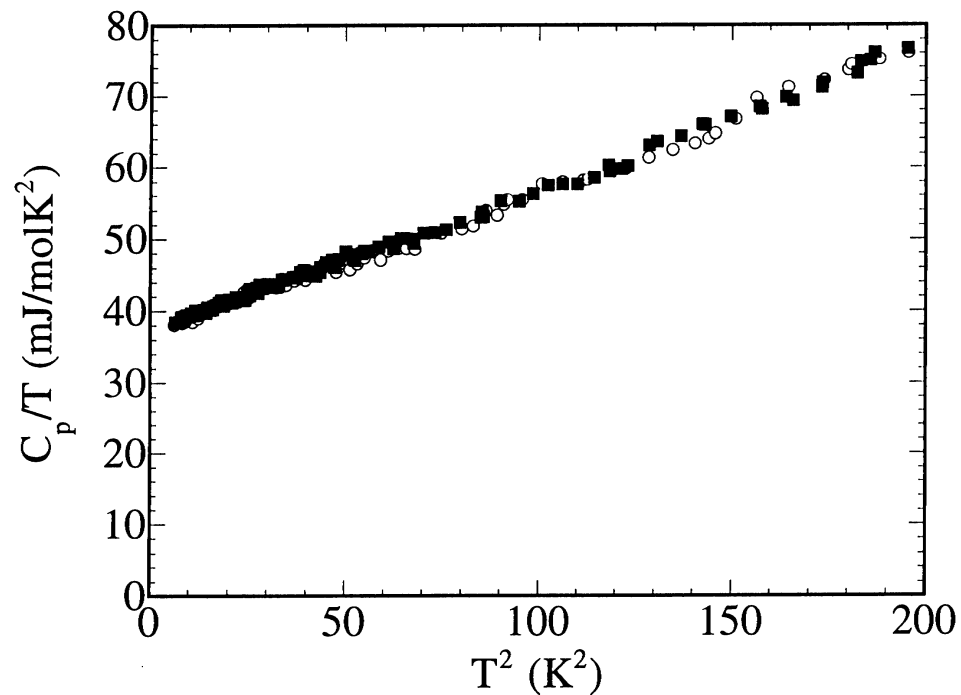


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Multi band

Electronic mass

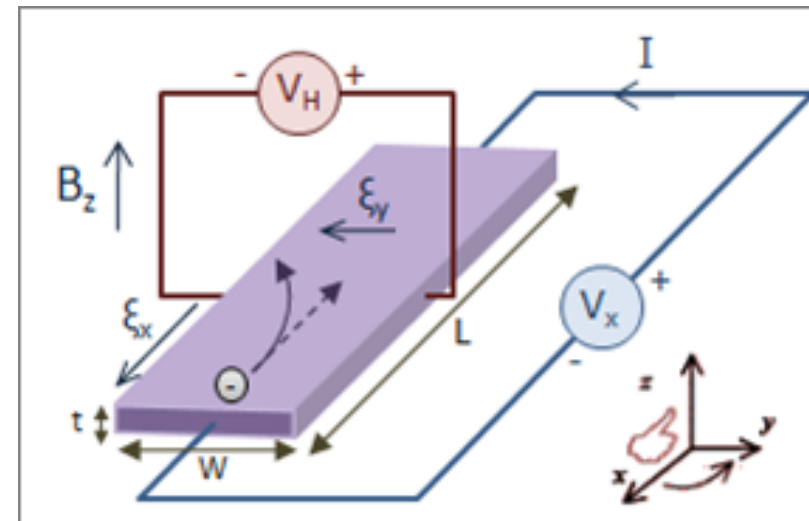
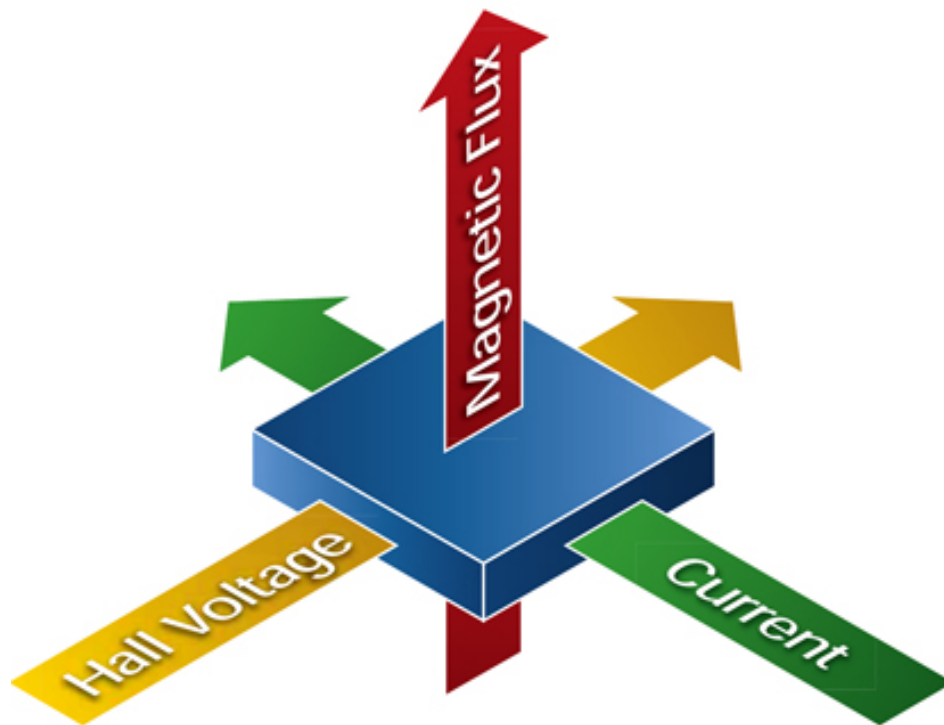
## 3. Hall effect

Electron concentration

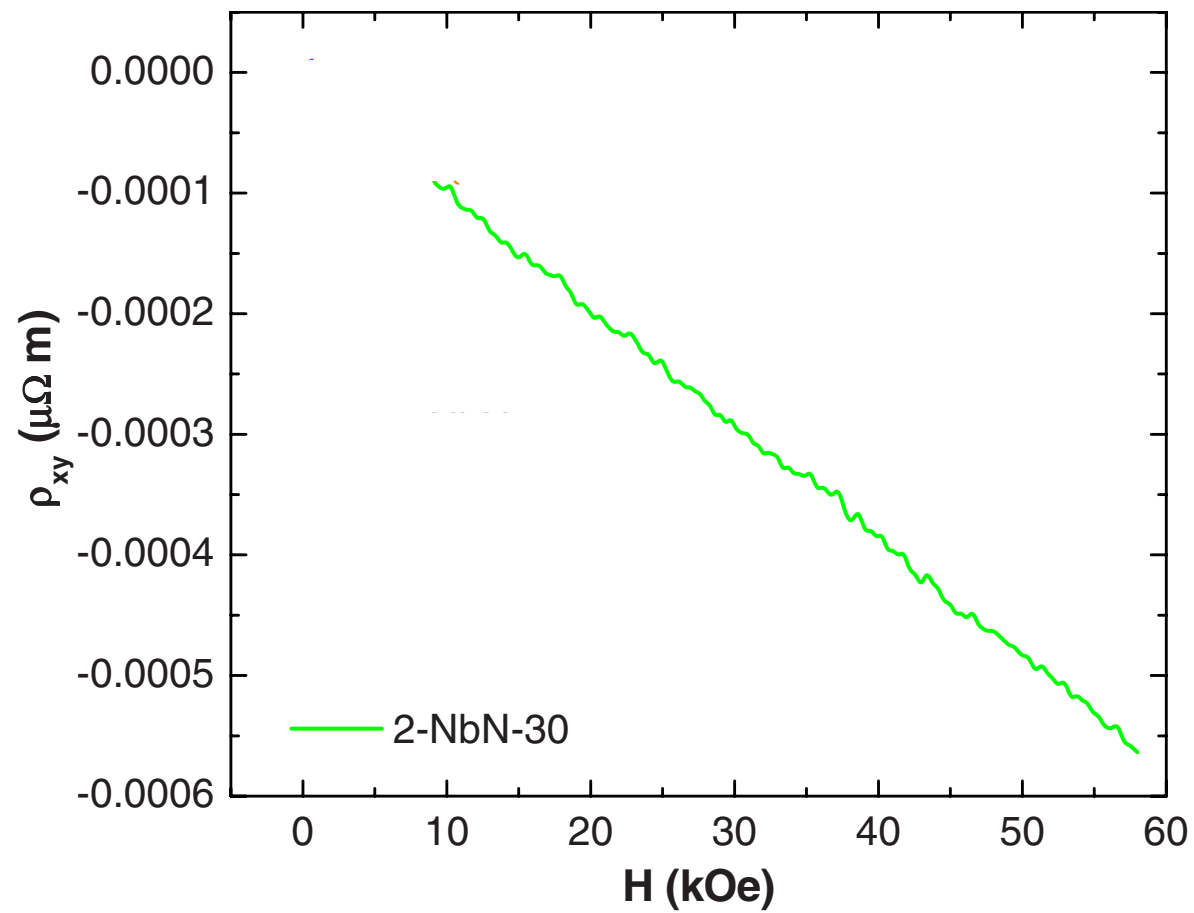
Electron / hole like carriers

## 4. Semimetals and Semi-conductors

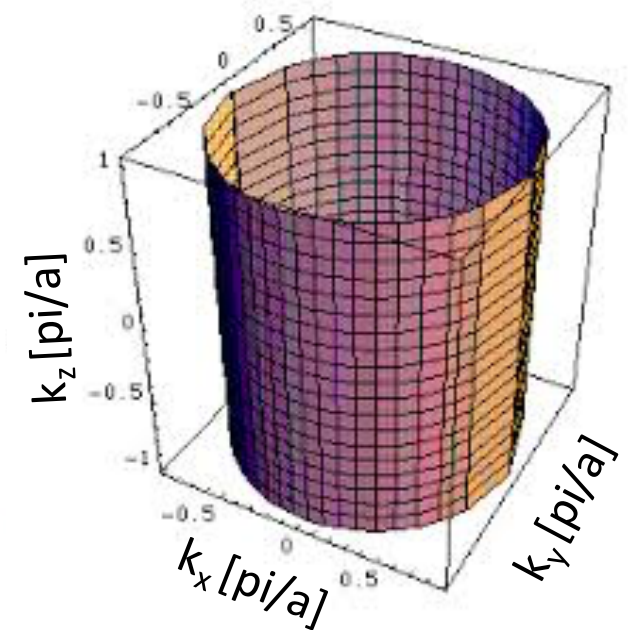
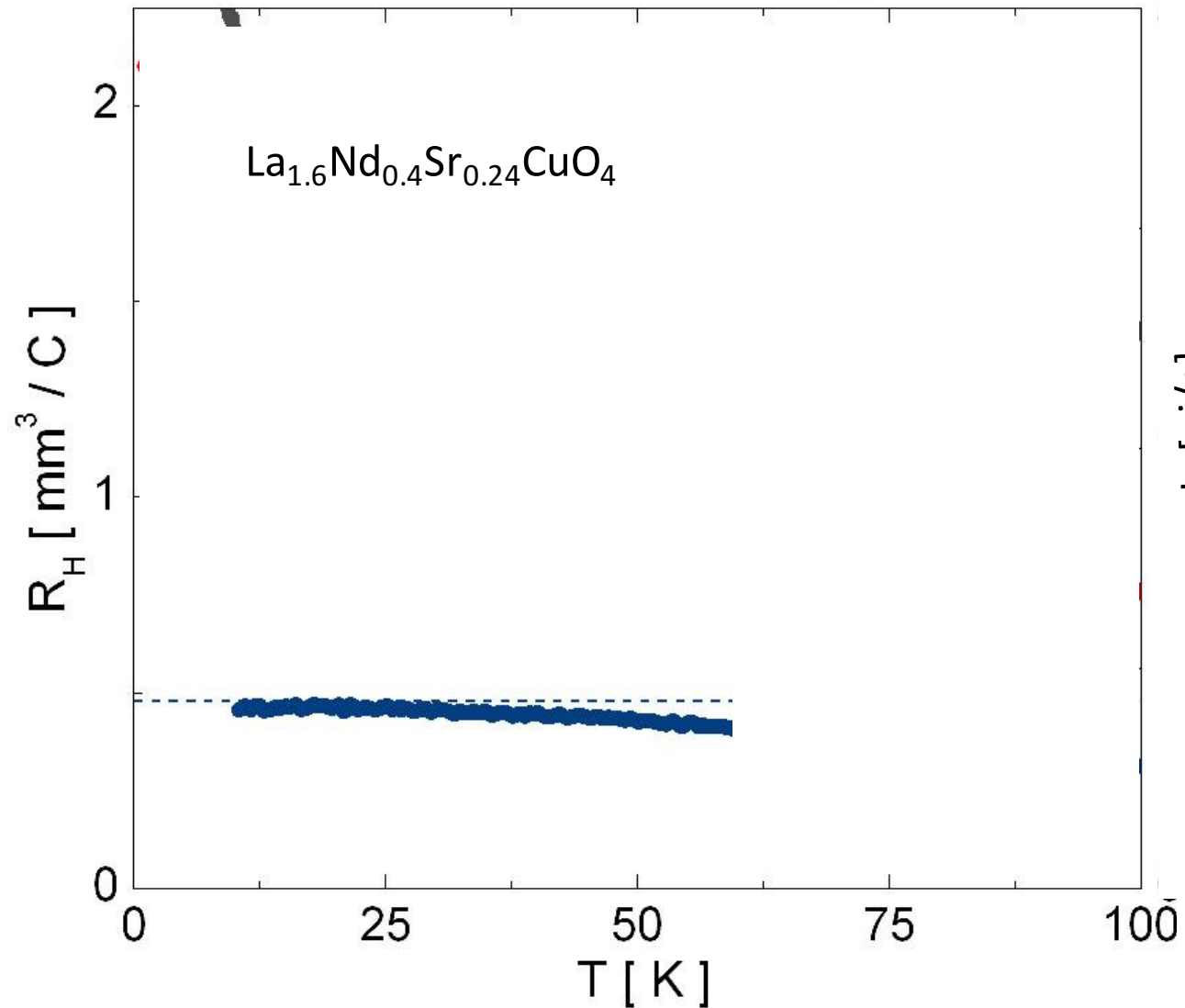
# Hall effect:



# Hall effect: Niobium

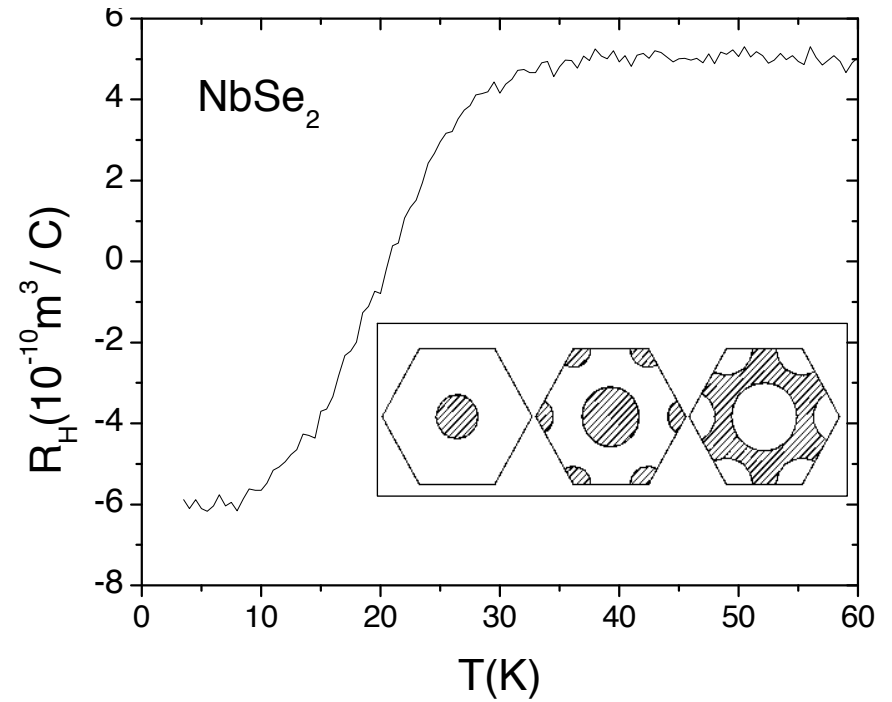
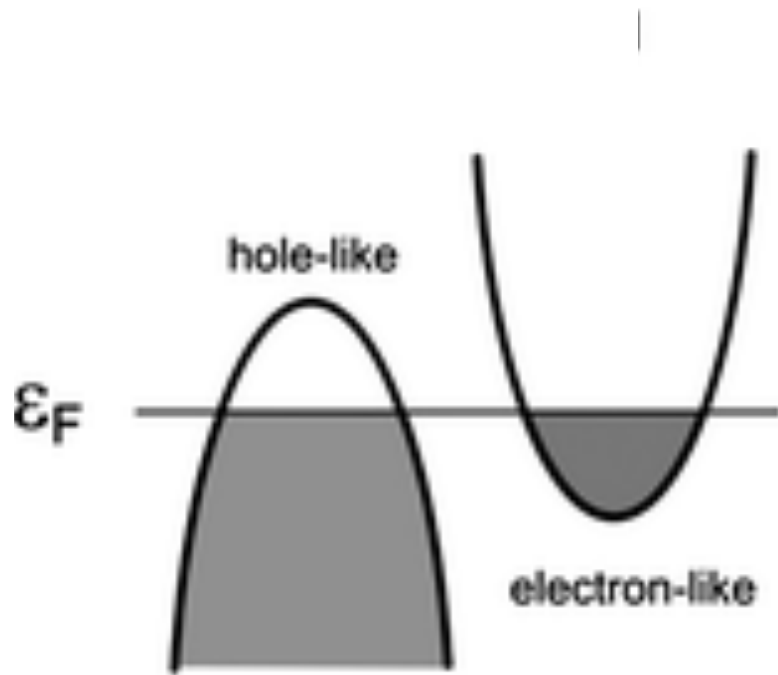


# Hall effect: Temperature dependence



2D cylindrical  
Fermi Surface

# Sign of the Hall Coefficient $R_H$



# Fermiology - continued

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Electronic mass

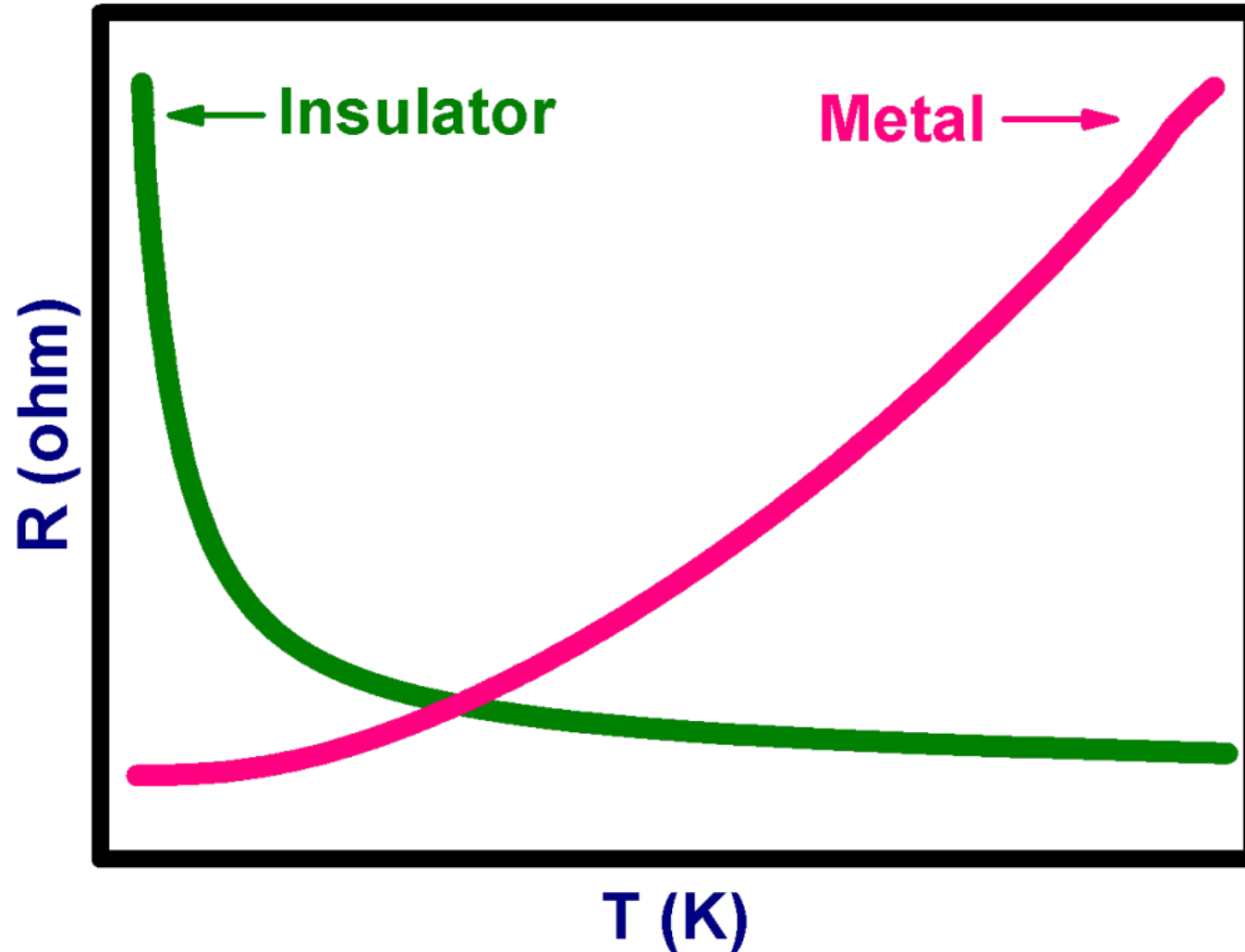
## 3. Hall effect

Electron concentration

Electron / hole like carriers

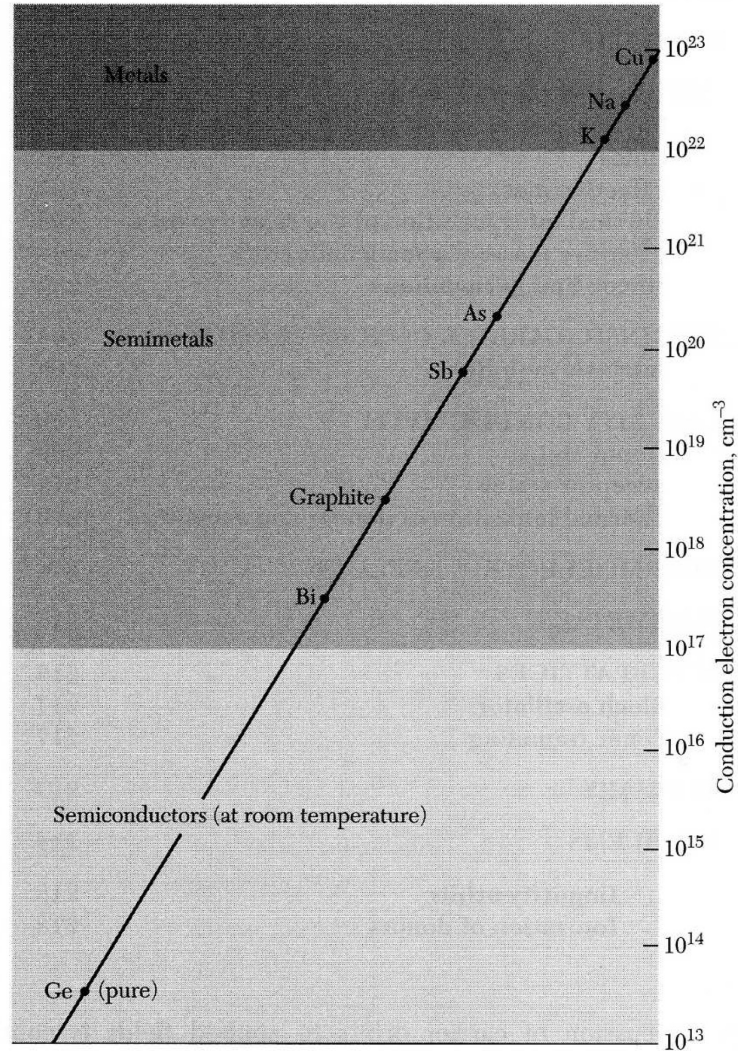
## 4. Semimetals and Semi-conductors

# Metals and insulators: Resistivity



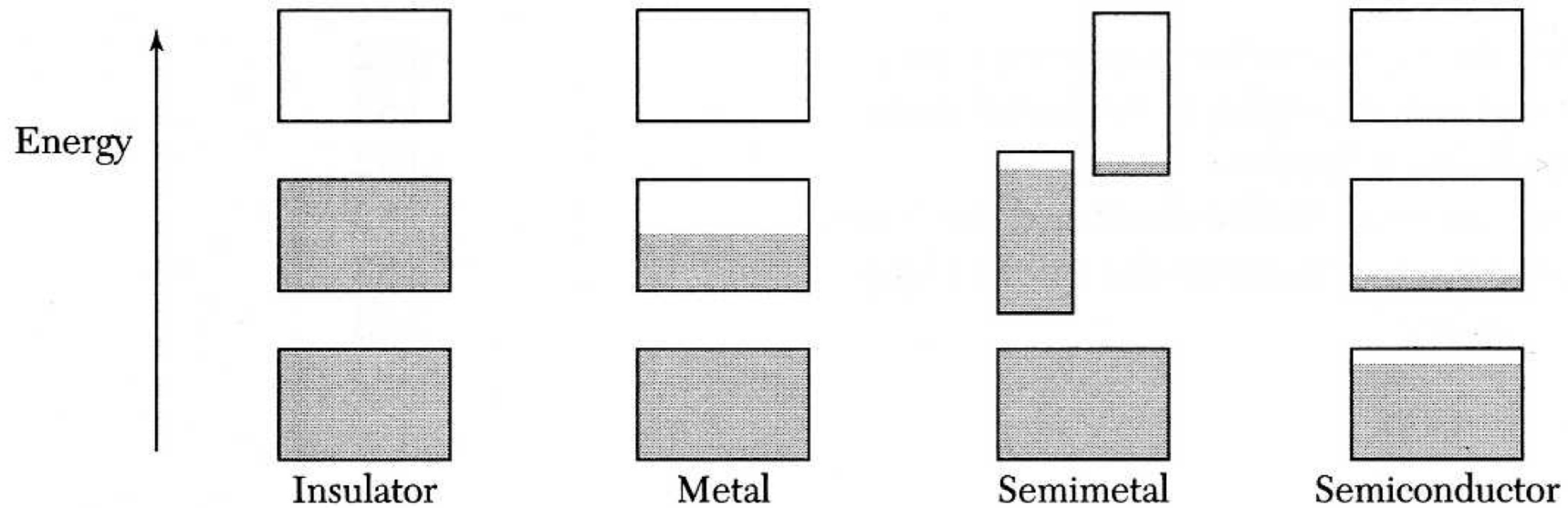


# Conduction Electron Concentration

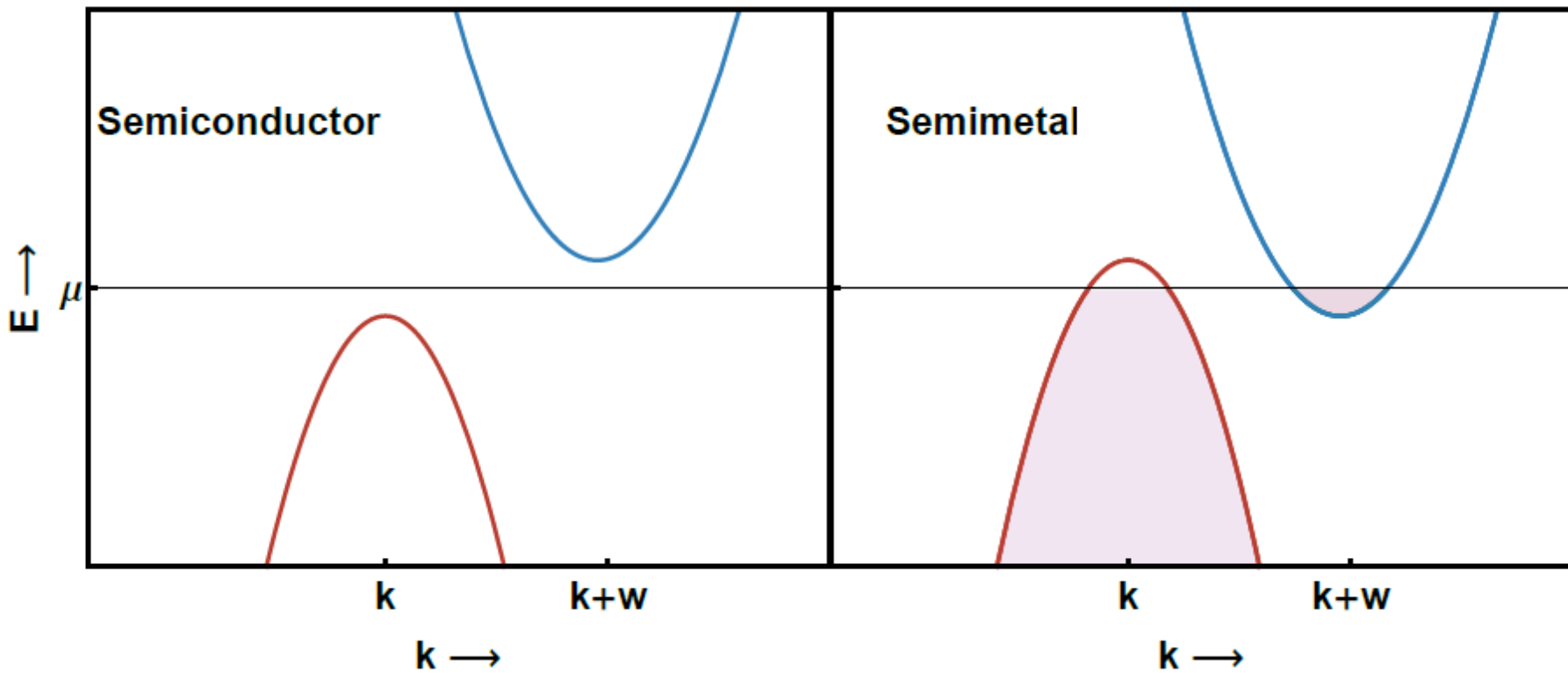


**Figure 1** Carrier concentrations for metals, semimetals, and semiconductors. The semiconductor range may be extended upward by increasing the impurity concentration, and the range can be extended downward to merge eventually with the insulator range.

# Semimetals & Semiconductors



# Semimetals & Semiconductors



# Semiconductor Materials

|                                       |  |   |  |                                       |   |  |  |   |  |                                       |  |                                       |  |   |  |   |  |  |                                    |
|---------------------------------------|--|---|--|---------------------------------------|---|--|--|---|--|---------------------------------------|--|---------------------------------------|--|---|--|---|--|--|------------------------------------|
| hydrogen<br>1<br><b>H</b><br>1.0079   |  |   |  |                                       |   |  |  |   |  |                                       |  |                                       |  |   |  |   |  | helium<br>2<br><b>He</b><br>4.0026     |                                    |
| lithium<br>3<br><b>Li</b><br>6.941    | beryllium<br>4<br><b>Be</b><br>9.0122  |   |  |                                       |   |  |  |   |  |                                       |  |                                       |  | boron<br>5<br><b>B</b><br>10.811        | carbon<br>6<br><b>C</b><br>12.011      | nitrogen<br>7<br><b>N</b><br>14.007     | oxygen<br>8<br><b>O</b><br>15.999      | fluorine<br>9<br><b>F</b><br>18.998    | neon<br>10<br><b>Ne</b><br>20.180  |
| sodium<br>11<br><b>Na</b><br>22.990   | magnesium<br>12<br><b>Mg</b><br>24.305 |   |  |                                       |   |  |  |   |  |                                       |  |                                       |  | aluminium<br>13<br><b>Al</b><br>26.982  | silicon<br>14<br><b>Si</b><br>28.086   | phosphorus<br>15<br><b>P</b><br>30.974  | sulfur<br>16<br><b>S</b><br>32.065     | chlorine<br>17<br><b>Cl</b><br>35.453  | argon<br>18<br><b>Ar</b><br>39.948 |
| potassium<br>19<br><b>K</b><br>39.098 | calcium<br>20<br><b>Ca</b><br>40.078   | scandium<br>21<br><b>Sc</b><br>44.956   | titanium<br>22<br><b>Ti</b><br>47.867      | vanadium<br>23<br><b>V</b><br>50.942  | chromium<br>24<br><b>Cr</b><br>51.996   | manganese<br>25<br><b>Mn</b><br>54.938 | iron<br>26<br><b>Fe</b><br>55.845      | cobalt<br>27<br><b>Co</b><br>58.933     | nickel<br>28<br><b>Ni</b><br>58.693    | copper<br>29<br><b>Cu</b><br>63.546   | zinc<br>30<br><b>Zn</b><br>65.39       | gallium<br>31<br><b>Ga</b><br>69.723  | germanium<br>32<br><b>Ge</b><br>72.64    | arsenic<br>33<br><b>As</b><br>74.922    | selenium<br>34<br><b>Se</b><br>78.96   | bromine<br>35<br><b>Br</b><br>79.904    | krypton<br>36<br><b>Kr</b><br>83.80    |  |                                    |
| rubidium<br>37<br><b>Rb</b><br>85.468 | strontium<br>38<br><b>Sr</b><br>87.62  | yttrium<br>39<br><b>Y</b><br>88.906     | zirconium<br>40<br><b>Zr</b><br>91.224     | niobium<br>41<br><b>Nb</b><br>92.906  | molybdenum<br>42<br><b>Mo</b><br>95.94  | technetium<br>43<br><b>Tc</b><br>[98]  | ruthenium<br>44<br><b>Ru</b><br>101.07 | rhodium<br>45<br><b>Rh</b><br>102.91    | palladium<br>46<br><b>Pd</b><br>106.42 | silver<br>47<br><b>Ag</b><br>107.87   | cadmium<br>48<br><b>Cd</b><br>112.41   | indium<br>49<br><b>In</b><br>114.82   | tin<br>50<br><b>Sn</b><br>118.71         | antimony<br>51<br><b>Sb</b><br>121.76   | tellurium<br>52<br><b>Te</b><br>127.60 | iodine<br>53<br><b>I</b><br>126.90      | xenon<br>54<br><b>Xe</b><br>131.29     |  |                                    |
| caesium<br>55<br><b>Cs</b><br>132.91  | barium<br>56<br><b>Ba</b><br>137.33    | lanthanum<br>57-70<br>*<br>Lu<br>174.97 | hafnium<br>71<br><b>Hf</b><br>178.49       | tantalum<br>72<br><b>Ta</b><br>180.95 | wolfram<br>73<br><b>W</b><br>183.84     | rhenium<br>74<br><b>Re</b><br>186.21   | osmium<br>75<br><b>Os</b><br>190.23    | iridium<br>76<br><b>Ir</b><br>192.22    | platinum<br>77<br><b>Pt</b><br>195.08  | gold<br>78<br><b>Au</b><br>196.97     | mercury<br>79<br><b>Hg</b><br>200.59   | thallium<br>80<br><b>Tl</b><br>204.38 | lead<br>81<br><b>Pb</b><br>207.2         | bismuth<br>82<br><b>Bi</b><br>208.98    | polonium<br>83<br><b>Po</b><br>[209]   | astatine<br>84<br><b>At</b><br>[210]    | radon<br>85<br><b>Rn</b><br>[222]      |  |                                    |
| francium<br>87<br><b>Fr</b><br>[223]  | radium<br>88<br><b>Ra</b><br>[226]     | actinium<br>89-102<br>**<br>La<br>[227] | rutherfordium<br>103<br><b>Rf</b><br>[261] | dubnium<br>104<br><b>Db</b><br>[262]  | seaborgium<br>105<br><b>Sg</b><br>[266] | bohrium<br>106<br><b>Bh</b><br>[264]   | hassium<br>107<br><b>Hs</b><br>[269]   | meitnerium<br>108<br><b>Mt</b><br>[268] | unnilium<br>109<br><b>Uun</b><br>[271] | ununium<br>110<br><b>Uuu</b><br>[272] | unbinium<br>111<br><b>Uub</b><br>[277] | untrium<br>112<br><b>Uuq</b><br>[289] | unquadrium<br>113<br><b>Uuq</b><br>[289] | unpentium<br>114<br><b>Uup</b><br>[289] | unhexium<br>115<br><b>Uuh</b><br>[289] | unseptium<br>116<br><b>Uus</b><br>[289] | unoctium<br>117<br><b>Uuo</b><br>[289] | unennium<br>118<br><b>Uue</b><br>[289] |                                    |

\* Lanthanide series

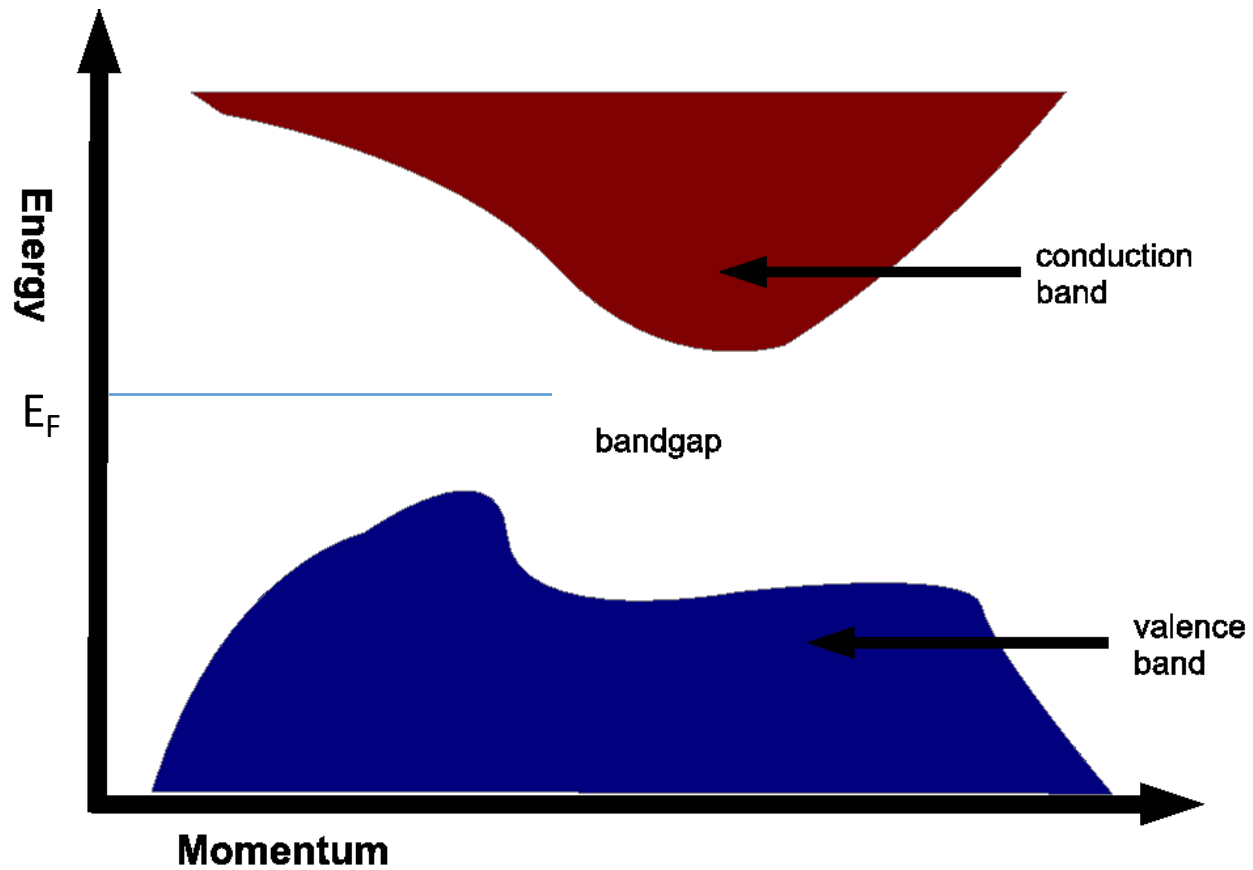
|  |                                      |   |  |  |                                       |                                       |   |                                       |   |   |                                      |  |  |
|--|--------------------------------------|---|--|--|---------------------------------------|---------------------------------------|---|---------------------------------------|---|---|--------------------------------------|--|--|
| lanthanum<br>57<br><b>La</b><br>138.91 | cerium<br>58<br><b>Ce</b><br>140.12  | praseodymium<br>59<br><b>Pr</b><br>140.91 | neodymium<br>60<br><b>Nd</b><br>144.24 | promethium<br>61<br><b>Pm</b><br>[145] | samarium<br>62<br><b>Sm</b><br>150.36 | europium<br>63<br><b>Eu</b><br>151.96 | gadolinium<br>64<br><b>Gd</b><br>157.25 | terbium<br>65<br><b>Tb</b><br>158.93  | dysprosium<br>66<br><b>Dy</b><br>162.50 | holmium<br>67<br><b>Ho</b><br>164.93    | erbium<br>68<br><b>Er</b><br>167.26  | thulium<br>69<br><b>Tm</b><br>168.93     | ytterbium<br>70<br><b>Yb</b><br>173.04 |
| actinium<br>89<br><b>Ac</b><br>[227]   | thorium<br>90<br><b>Th</b><br>232.04 | protactinium<br>91<br><b>Pa</b><br>231.04 | uranium<br>92<br><b>U</b><br>238.03    | neptunium<br>93<br><b>Np</b><br>[237]  | plutonium<br>94<br><b>Pu</b><br>[244] | americium<br>95<br><b>Am</b><br>[243] | curium<br>96<br><b>Cm</b><br>[247]      | berkelium<br>97<br><b>Bk</b><br>[247] | californium<br>98<br><b>Cf</b><br>[251] | einsteinium<br>99<br><b>Es</b><br>[252] | fermium<br>100<br><b>Fm</b><br>[257] | mendelevium<br>101<br><b>Md</b><br>[258] | nobelium<br>102<br><b>No</b><br>[259]  |

\*\* Actinide series

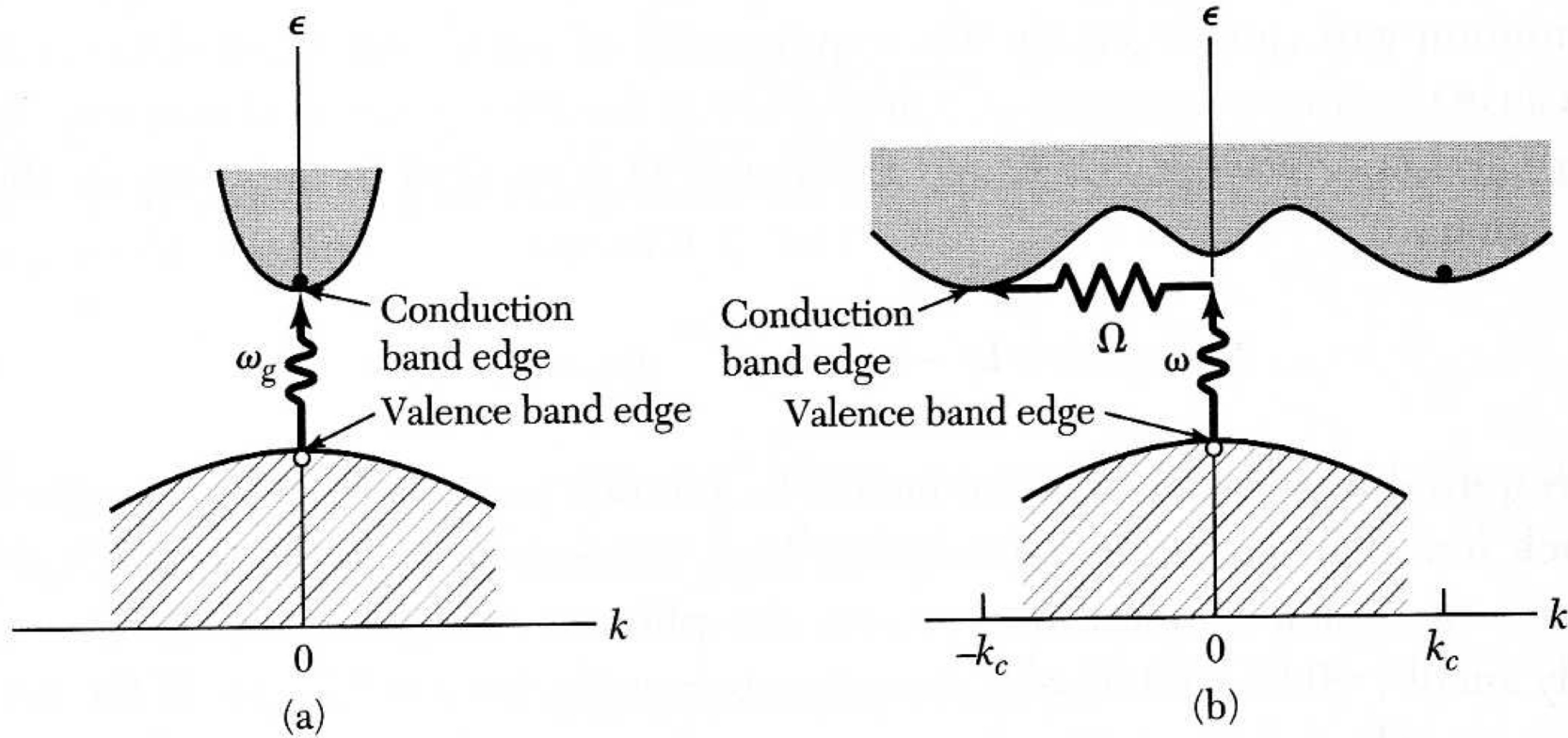
Diamond-type semiconductors

III – V compounds (GaAs, InSb)

# Valence and conduction band



# Direct and indirect gap



# Semiconductor gaps

**Table 1 Energy gap between the valence and conduction bands**  
(*i* = indirect gap; *d* = direct gap)

| Crystal     | Gap      | $E_g$ , eV |       | Crystal           | Gap      | $E_g$ , eV |           |
|-------------|----------|------------|-------|-------------------|----------|------------|-----------|
|             |          | 0 K        | 300 K |                   |          | 0 K        | 300 K     |
| Diamond     | <i>i</i> | 5.4        |       | SiC(hex)          | <i>i</i> | 3.0        | —         |
| Si          | <i>i</i> | 1.17       | 1.11  | Te                | <i>d</i> | 0.33       | —         |
| Ge          | <i>i</i> | 0.744      | 0.66  | HgTe <sup>a</sup> | <i>d</i> | -0.30      |           |
| $\alpha$ Sn | <i>d</i> | 0.00       | 0.00  | PbS               | <i>d</i> | 0.286      | 0.34–0.37 |
| InSb        | <i>d</i> | 0.23       | 0.17  | PbSe              | <i>i</i> | 0.165      | 0.27      |
| InAs        | <i>d</i> | 0.43       | 0.36  | PbTe              | <i>i</i> | 0.190      | 0.29      |
| InP         | <i>d</i> | 1.42       | 1.27  | CdS               | <i>d</i> | 2.582      | 2.42      |
| GaP         | <i>i</i> | 2.32       | 2.25  | CdSe              | <i>d</i> | 1.840      | 1.74      |
| GaAs        | <i>d</i> | 1.52       | 1.43  | CdTe              | <i>d</i> | 1.607      | 1.44      |
| GaSb        | <i>d</i> | 0.81       | 0.68  | SnTe              | <i>d</i> | 0.3        | 0.18      |
| AlSb        | <i>i</i> | 1.65       | 1.6   | Cu <sub>2</sub> O | <i>d</i> | 2.172      | —         |

<sup>a</sup>HgTe is a semimetal; the bands overlap.

# Semiconductor gaps versus $k_B T$

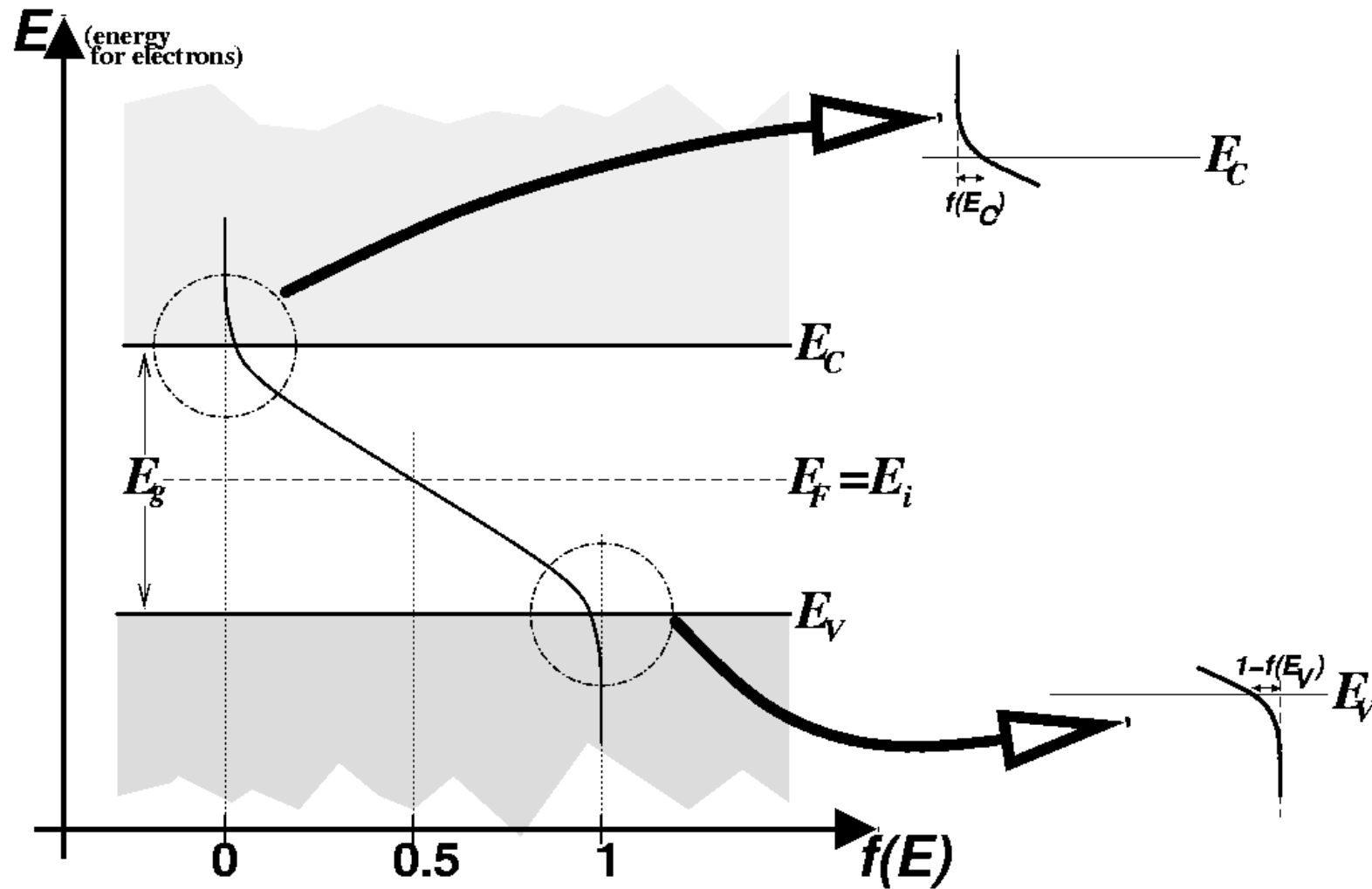
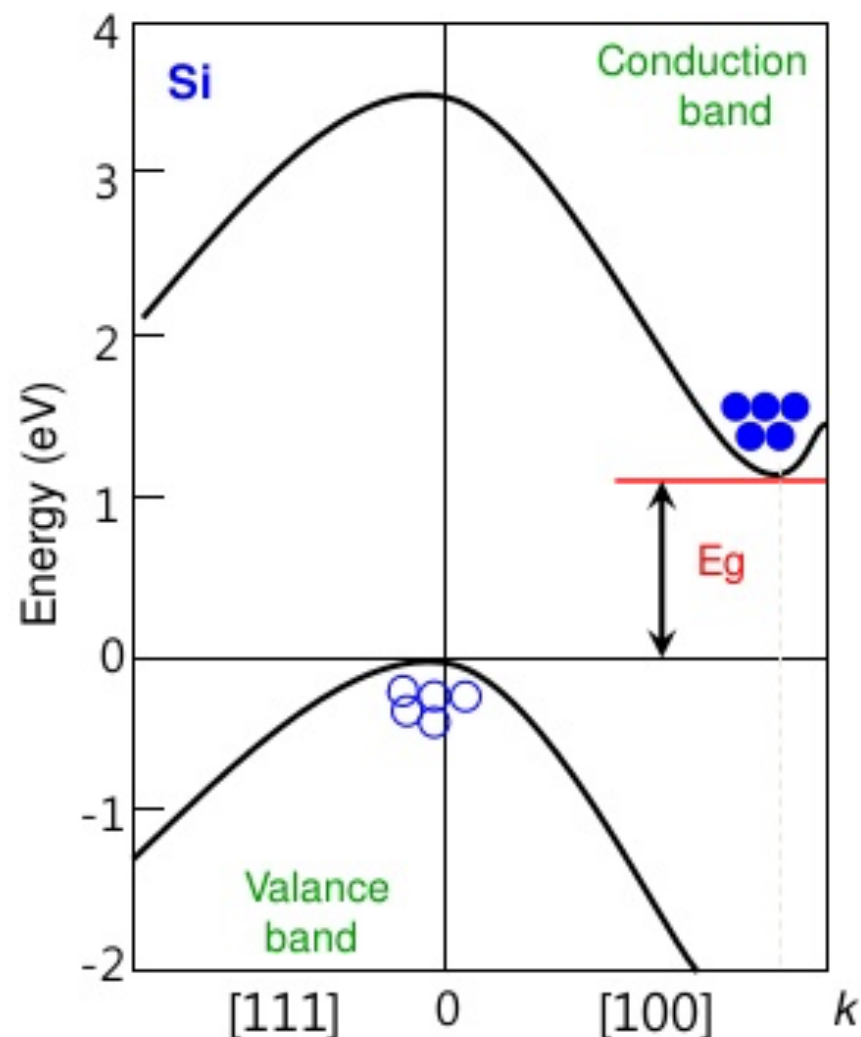
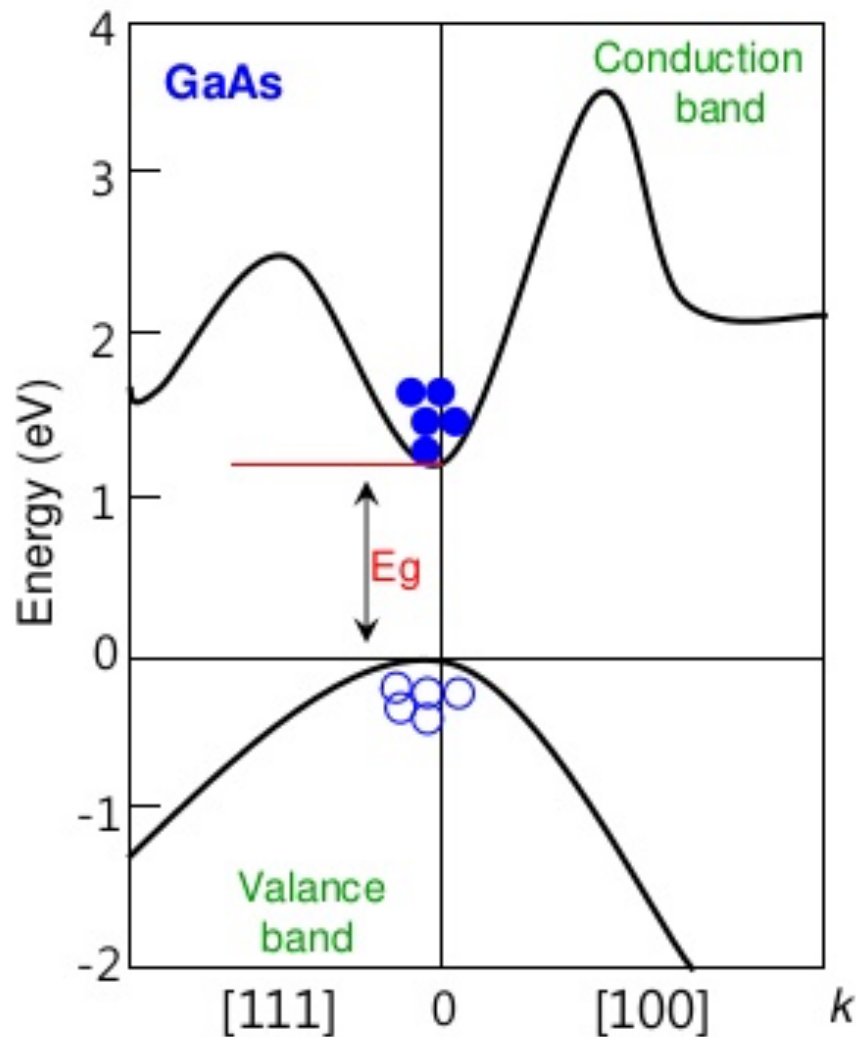


Figure 4:



## Band Structure of Semiconductors



Energy band structures of **GaAs** and **Si**

# Electronic masses

| Crystal           | Electron<br>$m_e/m$ |
|-------------------|---------------------|
| InSb              | 0.015               |
| InAs              | 0.026               |
| InP               | 0.073               |
| GaSb              | 0.047               |
| GaAs              | 0.066               |
| Cu <sub>2</sub> O | 0.99                |

Text added after the lecture.

Reading Kittel more careful, it seems that following notation is adopted.

$m$  = is the free electron mass.

$m_e$  = effective crystal electron mass

The fact that the electron mass is lighter in semiconductors is confirmed on the following link.

<https://www.youtube.com/watch?v=cdirek91Hto>

<http://ecee.colorado.edu/~bart/book/effmass.htm>

# Electronic mobility

**Table 3 Carrier mobilities at room temperature, in  $\text{cm}^2/\text{V}\cdot\text{s}$**

| Crystal | Electrons | Holes | Crystal     | Electrons | Holes |
|---------|-----------|-------|-------------|-----------|-------|
| Diamond | 1800      | 1200  | GaAs        | 8000      | 300   |
| Si      | 1350      | 480   | GaSb        | 5000      | 1000  |
| Ge      | 3600      | 1800  | PbS         | 550       | 600   |
| InSb    | 800       | 450   | PbSe        | 1020      | 930   |
| InAs    | 30000     | 450   | PbTe        | 2500      | 1000  |
| InP     | 4500      | 100   | AgCl        | 50        | —     |
| AlAs    | 280       | —     | KBr (100 K) | 100       | —     |
| AlSb    | 900       | 400   | SiC         | 100       | 10–20 |