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:

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

(a) Plot, using your favourite computer program, (1) the full three-dimensional band structure ϵ_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 ϵ_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:

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

(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:

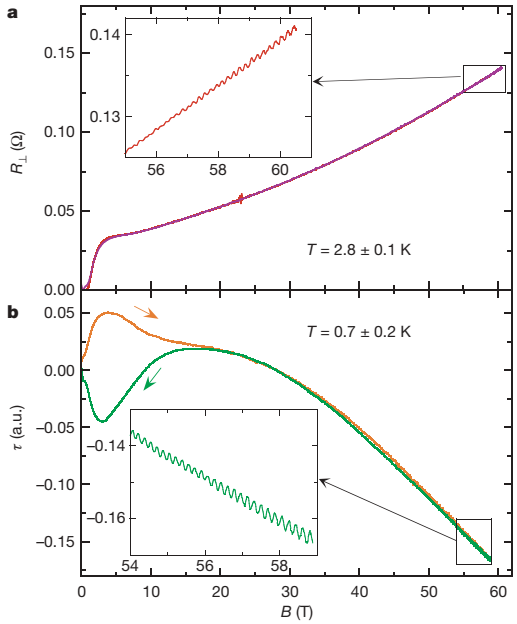
Exercise 2 *Quantum oscillations on quasi two-dimensional systems*

In $Tl_2Ba_2CuO_{6+\delta}$, quantum oscillations with a frequency of $F = 18.1\,\mathrm{kT}$ are observed (B. Vignolle et al., Nature **455**, 952-955 (2008)).

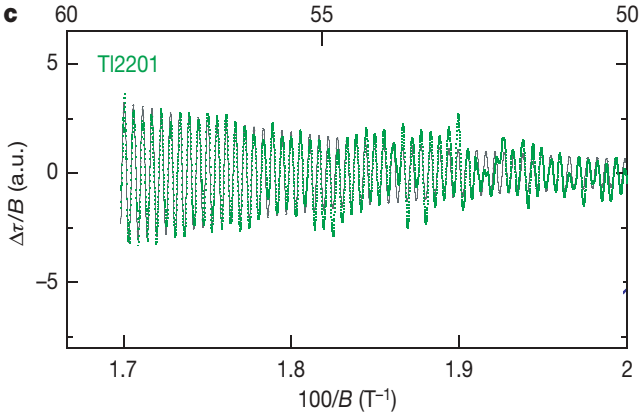
(a) Use the Onsager relation ($S = 2\pi\frac{eF}{\hbar}$) to calculate the Fermi surface area.

(b) If we assume a circular Fermi surface shape what is the Fermi momentum?

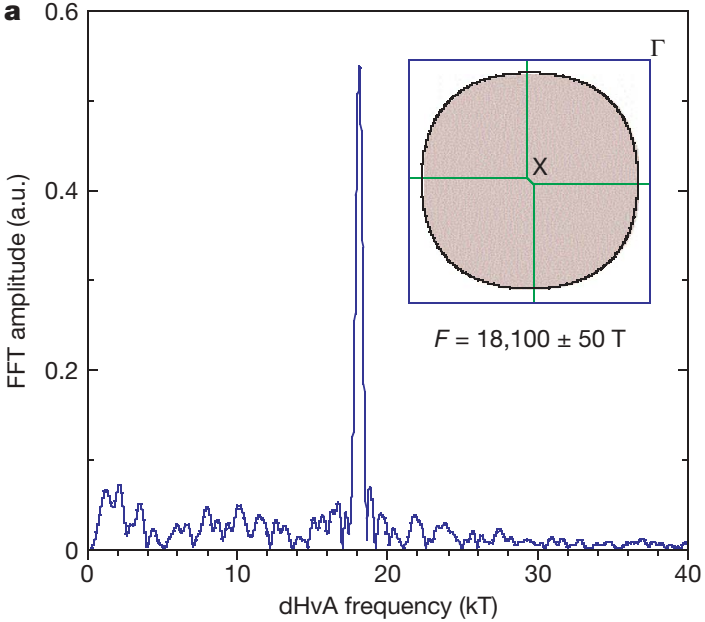
(a) RAW DATA



(b) OSCILATIONS VERSUS 1/B



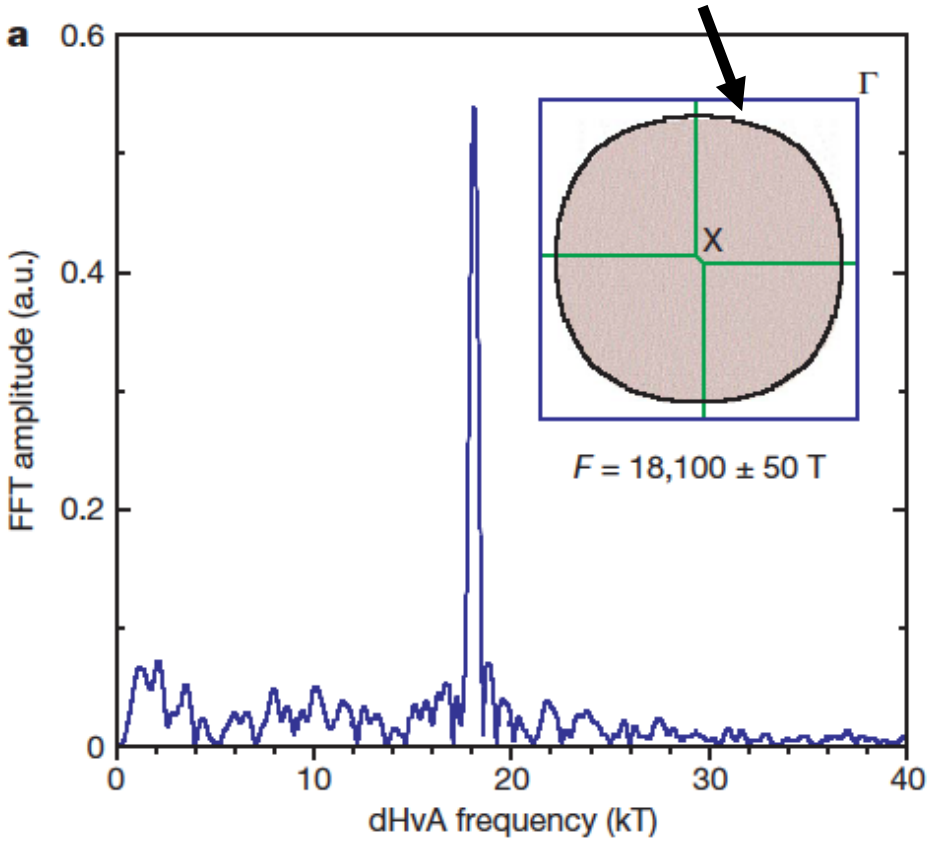
(c) Fourier Transform



Fermi surface: $Tl_2Ba_2CuO_{6+y}$ (Tl2201)

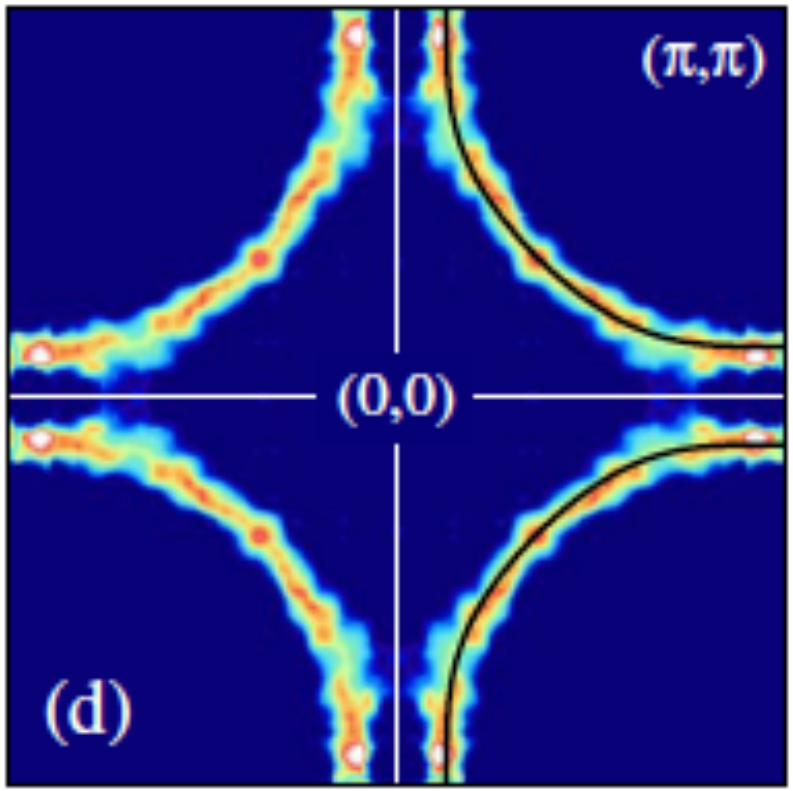
ARPES vs Quantum Oscillations

Band Structure Calculations



Nature 455, 952 (2008)

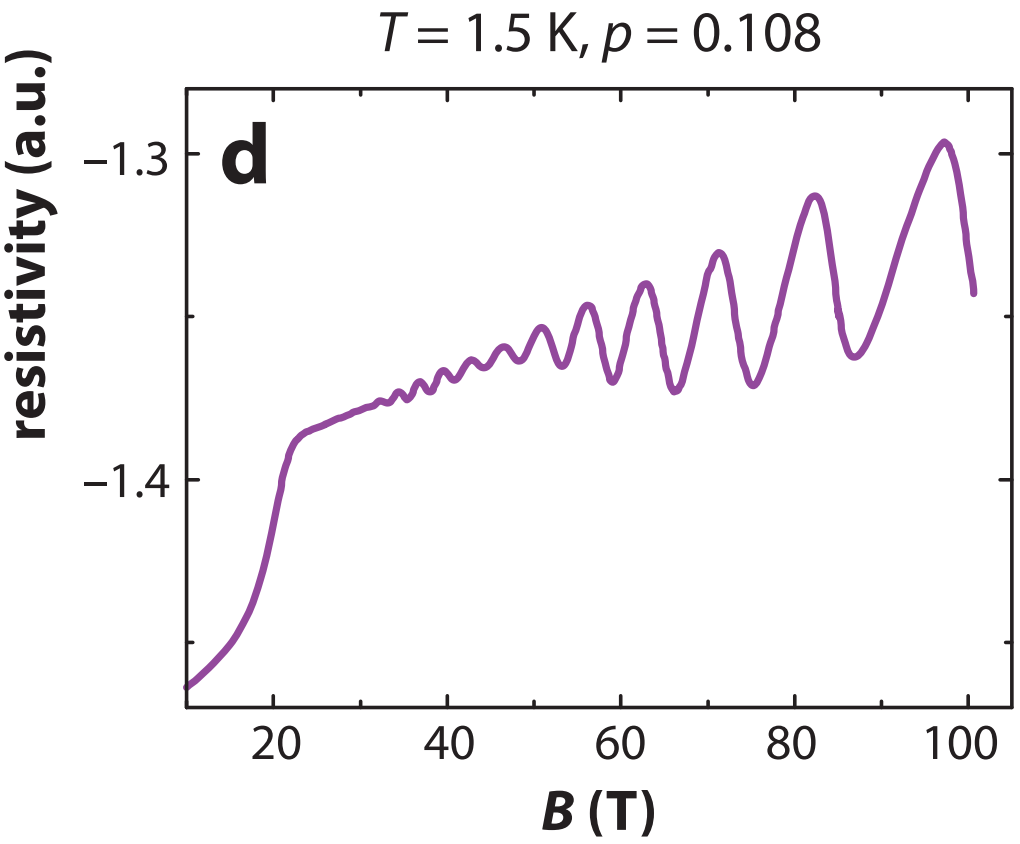
Quantum Oscillation (QO) experiments



PRL **95**, 077001 (2005)
Data taken @ Swiss Light Source

Angle-resolved Photo-Emission Spectroscopy (ARPES)

QUANTUM OSCILLATIONS:



OSCILLATION AMPLITUDE

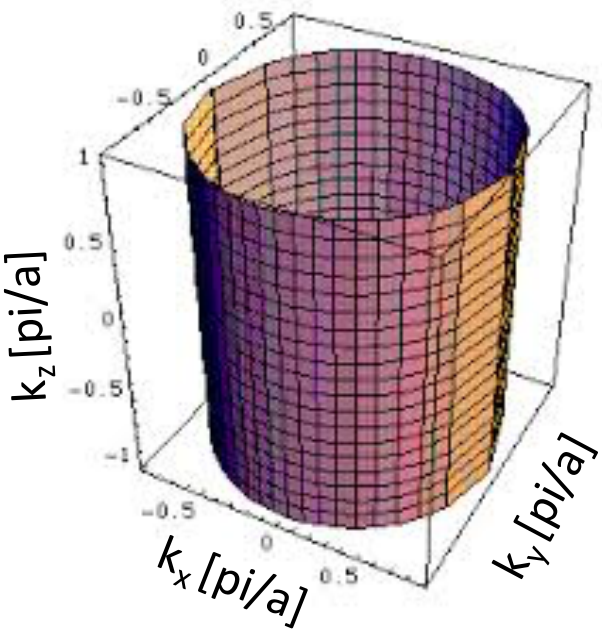
$$\propto \; e^{\left(\frac{-\pi\hbar k_F}{eB\ell}\right)}$$

Where ℓ = mean free path

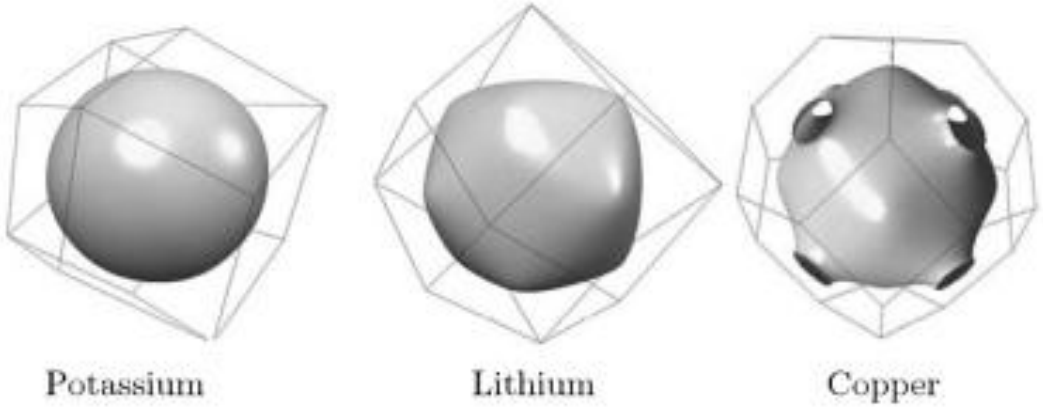
Resistivity measurement of a high-temperature superconductor: $YBa_2Cu_3O_{6.51}$ (YBCO)

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

Fermi surface - Dimension



2D cylindrical
Fermi Surface



3D spherical
Fermi Surface

3D spherical +
some structure
Fermi Surface

Fermi surface – Gold and Copper

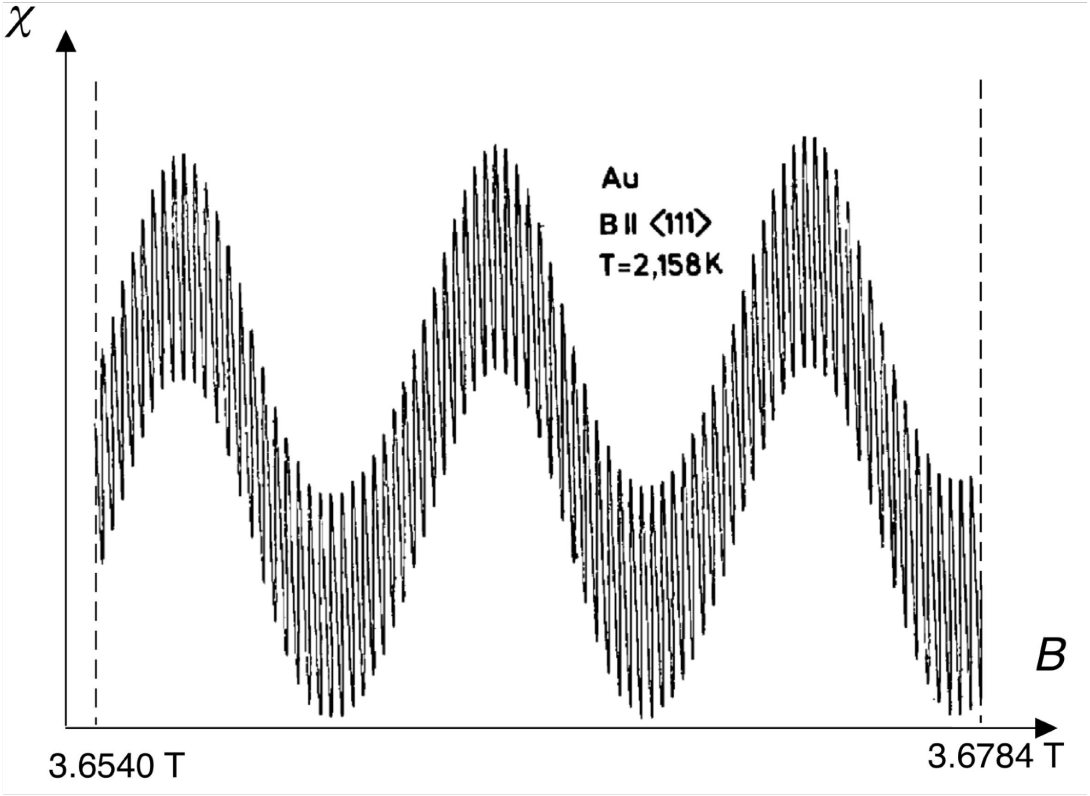


Figure 1: The spin susceptibility of gold in a magnetic field.

QUANTUM OSCILLATIONS: Gold

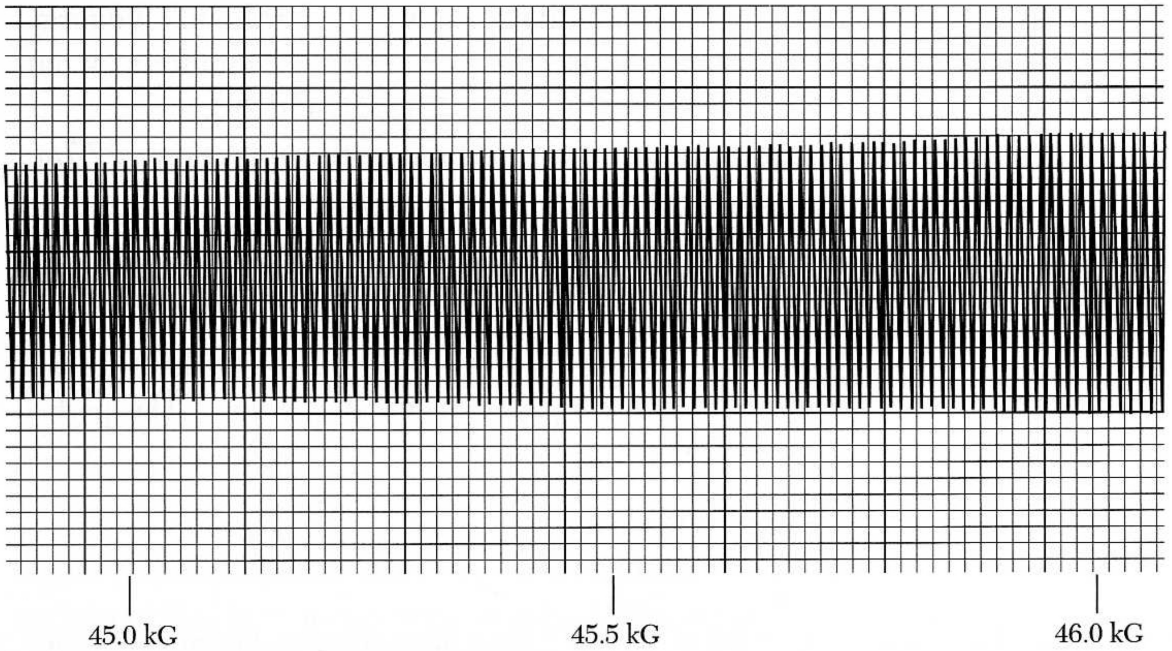


Figure 31 De Haas-van Alphen effect in gold with **B** ∥ [110]. The oscillation is from the dog's bone orbit of Fig. 30. The signal is related to the second derivative of the magnetic moment with respect to field. The results were obtained by a field modulation technique in a high-homogeneity superconducting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

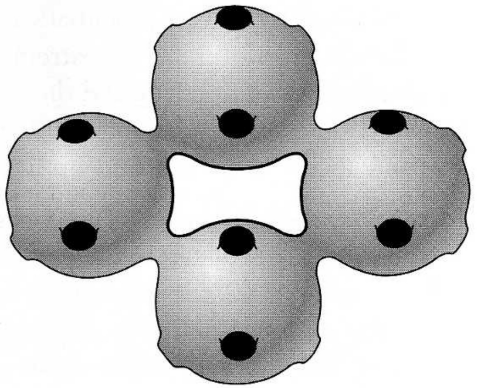


Figure 30 Dog's bone orbit of an electron on the Fermi surface of copper or gold in a magnetic field. This orbit is classified as holelike because the energy increases toward the interior of the orbit.

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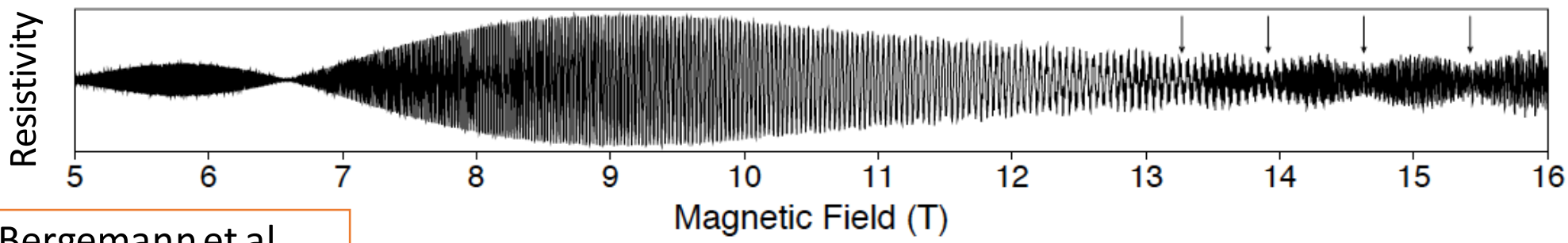
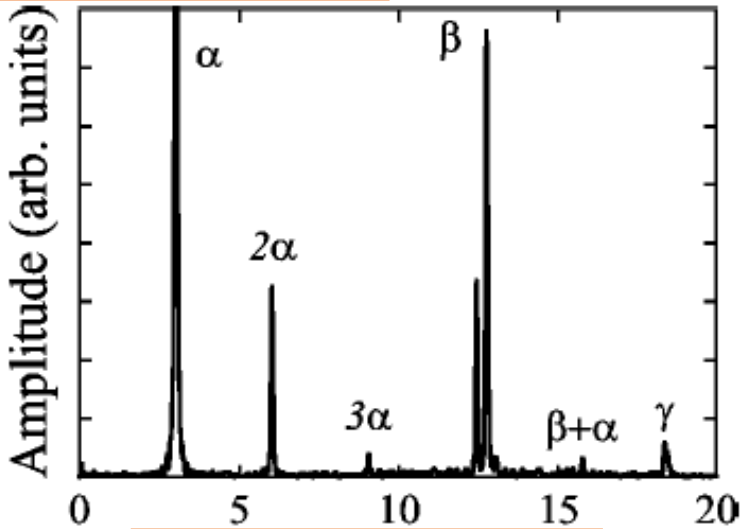
Multi – band metals: Sr_2RuO_4

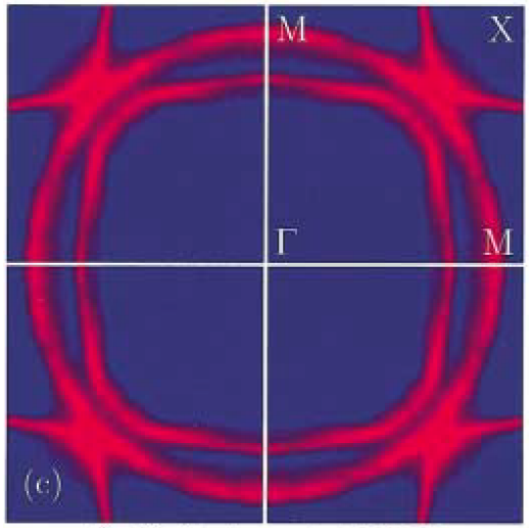


Bergemann et al,
PRL 84, 2662 (2000)



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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QUANTUM OSCILLATIONS:

Temperature dependence

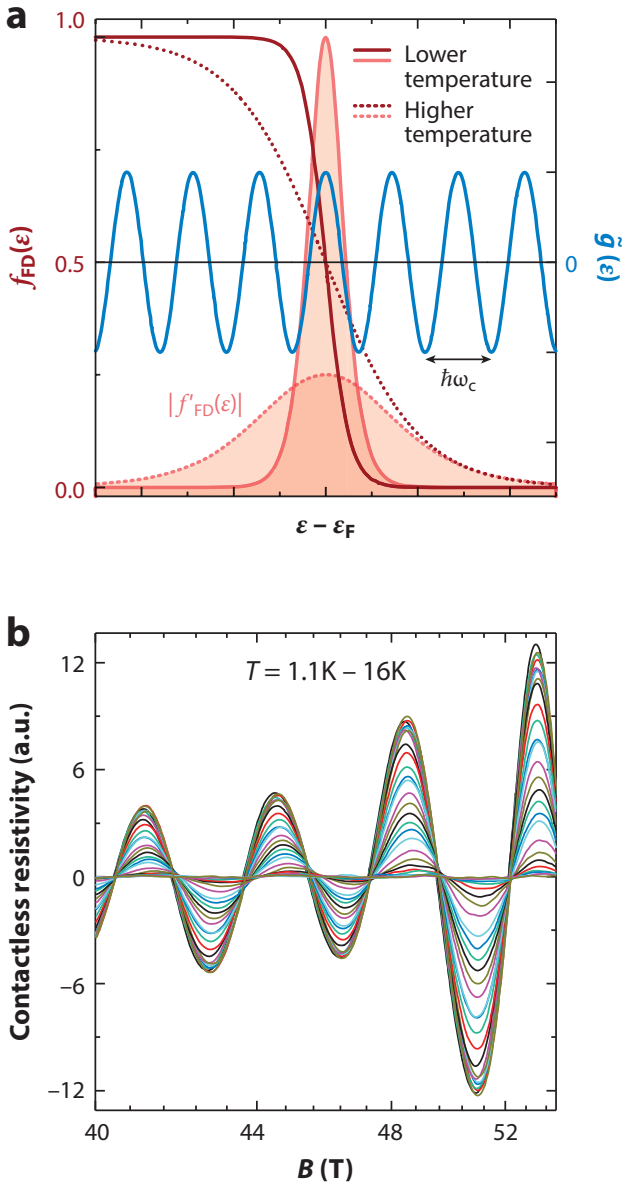
Thermal Condition:

$$\hbar\omega_c > k_B T$$

Landau level splitting > thermal energy

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

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

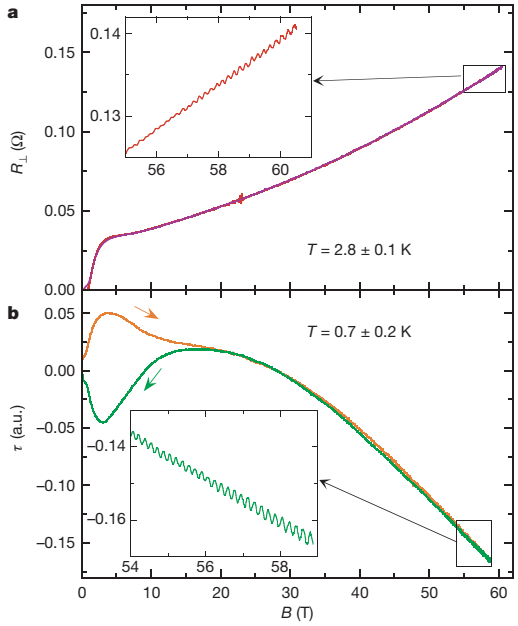


annurev-conmatphys-030212-184305

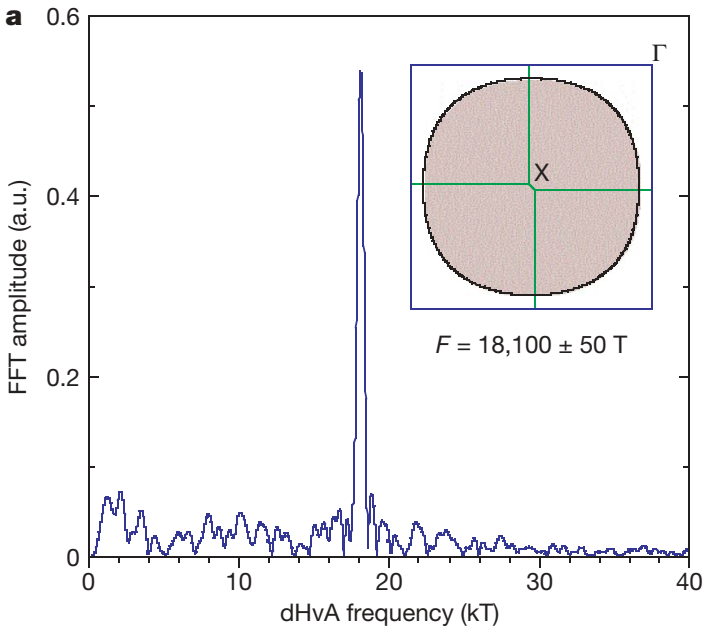
Electronic Mass

(1) Quantum Oscillation experiments:

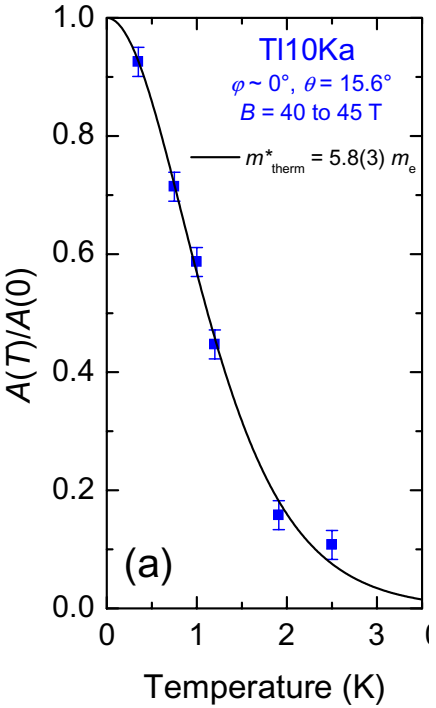
(a) RAW DATA



(b) Fourier Transform



(c) T-dependence



Electronic Mass: Specific heat

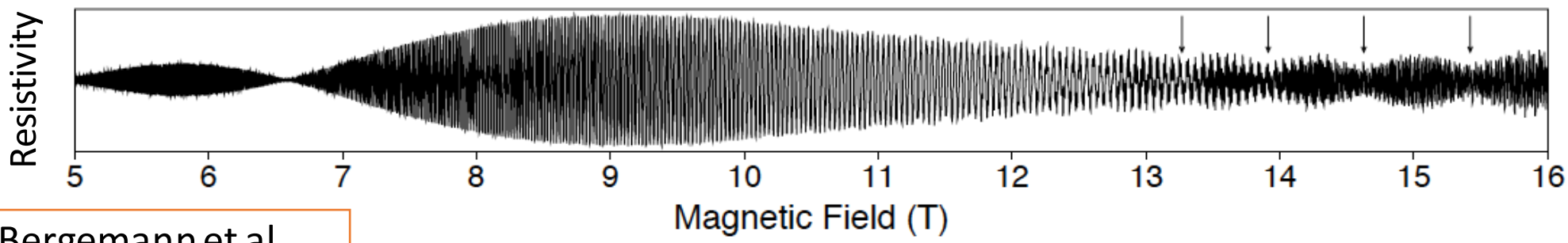
Exercise 1 *Electronic specific heat in two dimensions*
Layered crystal structures often have electronic structures that can approximately be considered two-dimensional. The high-temperature superconductor $Tl_2Ba_2CuO_{6+\delta}$ is one such example.

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

(b) The crystal structure of $Tl_2Ba_2CuO_{6+\delta}$ consists of stacked layers of CuO_2. Within a layer, the CuO_2 forms a square lattice with a Cu-O lattice distance of $a = 3.8\,\text{Å}$. 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 $\mathrm{J\,mol^{-1}\,K^{-1}}$. Show that $\gamma = \frac{N_{\mathrm{A}} a^2 \pi k_{\mathrm{B}}^2}{3\hbar^2} m$ where N_{A} is the Avogadro number.

(c) $Tl_2Ba_2CuO_{6+\delta}$ is observed to have the Sommerfeld parameter $\gamma = 6\,\mathrm{mJ\,mol^{-1}\,K^{-2}}$. Using the result of (b), what is the electronic mass m for $Tl_2Ba_2CuO_{6+\delta}$? How does it compare to the free electron mass?

Multi – band metals: Sr_2RuO_4



Bergemann et al,
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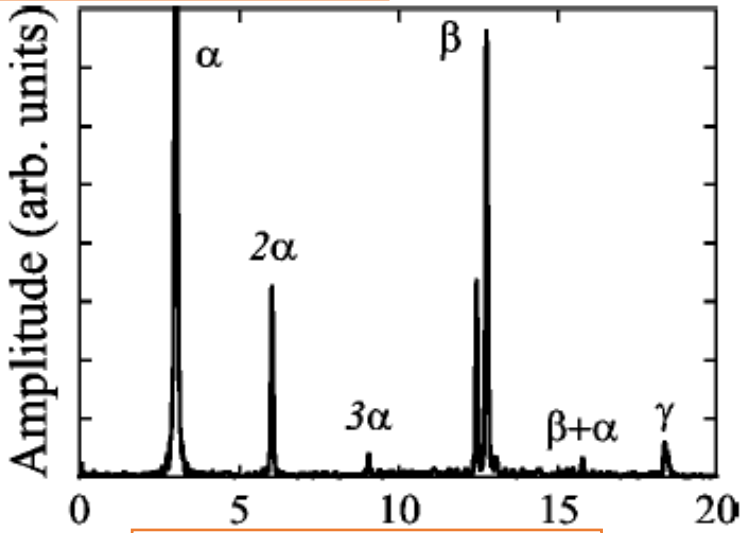


A.P. Mackenzie et al,
JPSJ 67, 385 (2003)

TABLE II. Summary of quasiparticle parameters of Sr_2RuO_4.

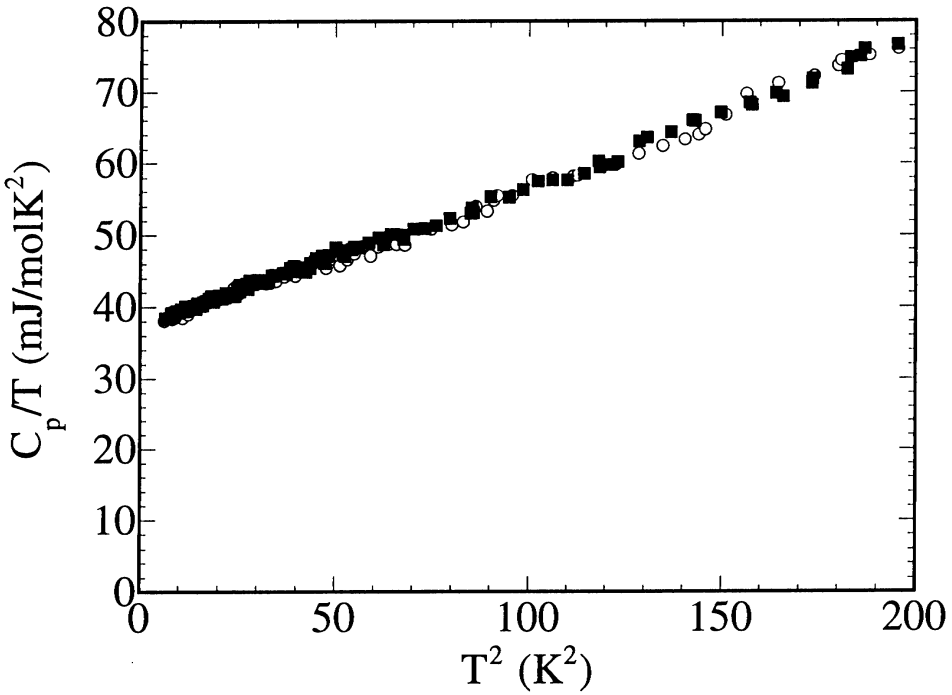
Fermi-surface sheet	α	β	γ
Character	Holelike	Electronlike	Electronlike
k_F (Å^{-1})[a]	0.304	0.622	0.753
m^* (m_e)[b]	3.3	7.0	16.0

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

Quantum Oscillation (QO) experiments

Multi – band metals: Sr_2RuO_4

Heat Capacity



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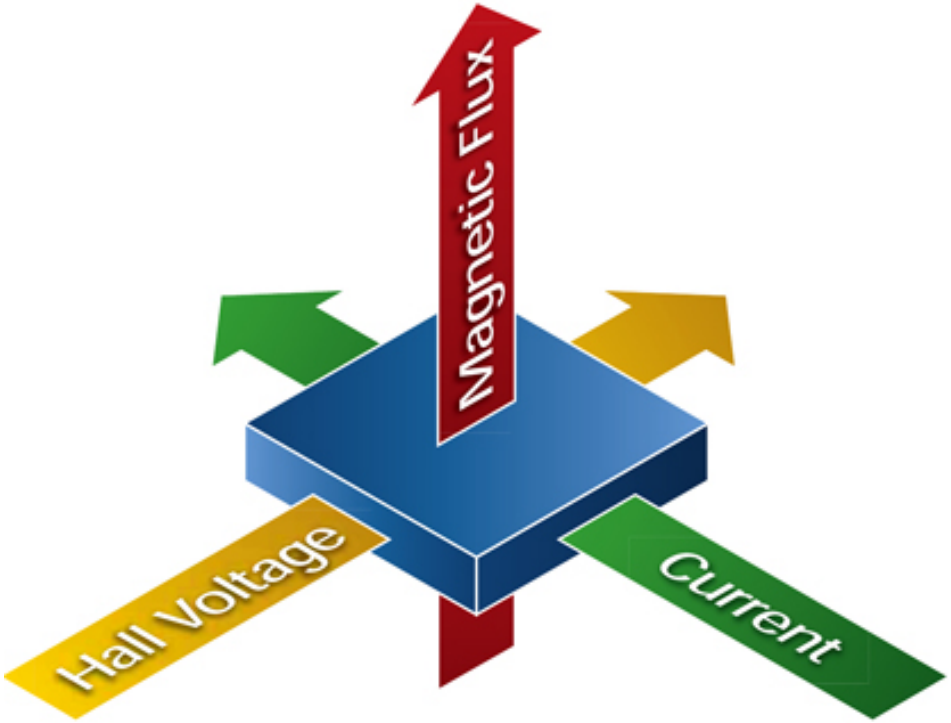
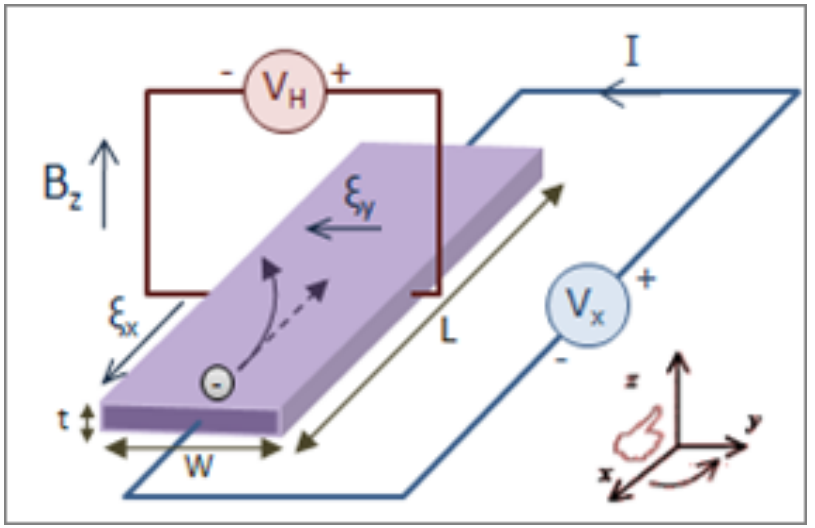
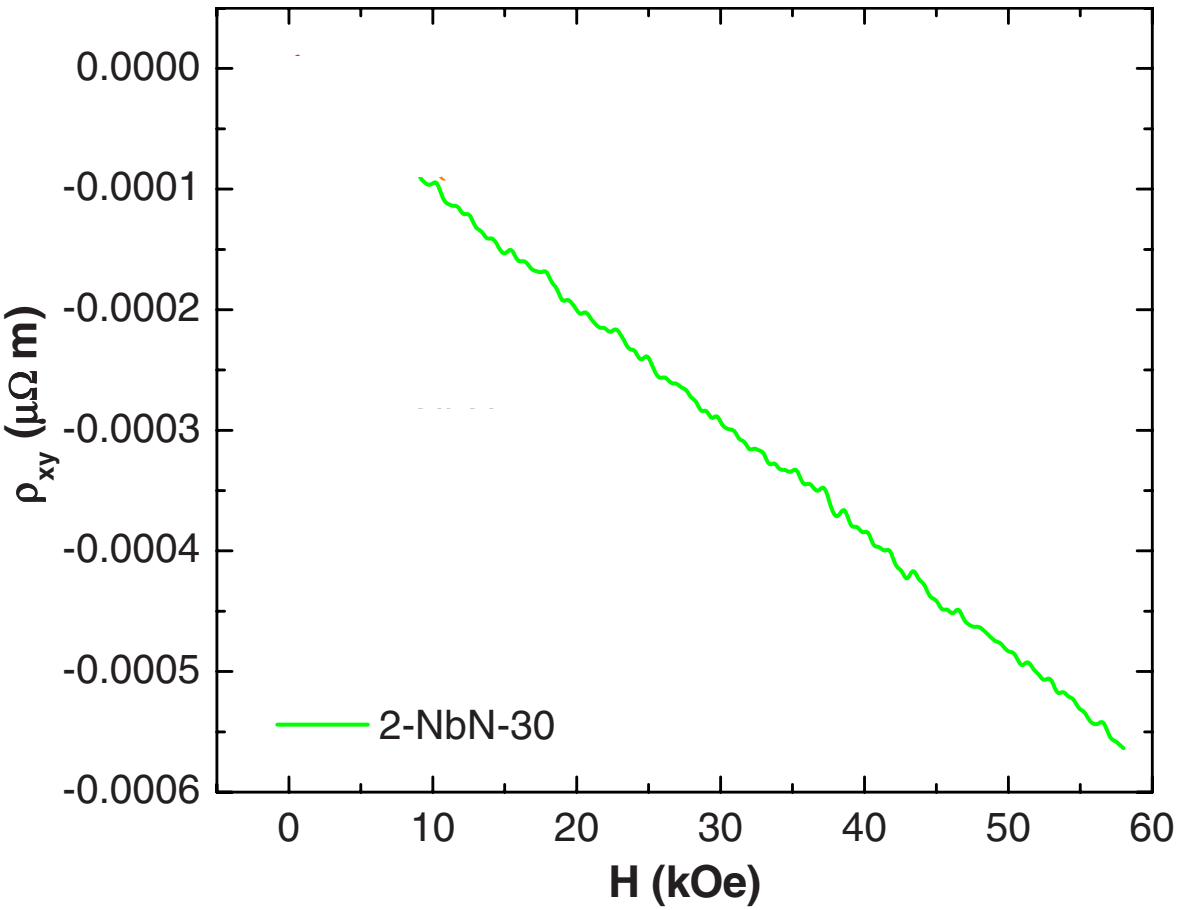
Hall effect:



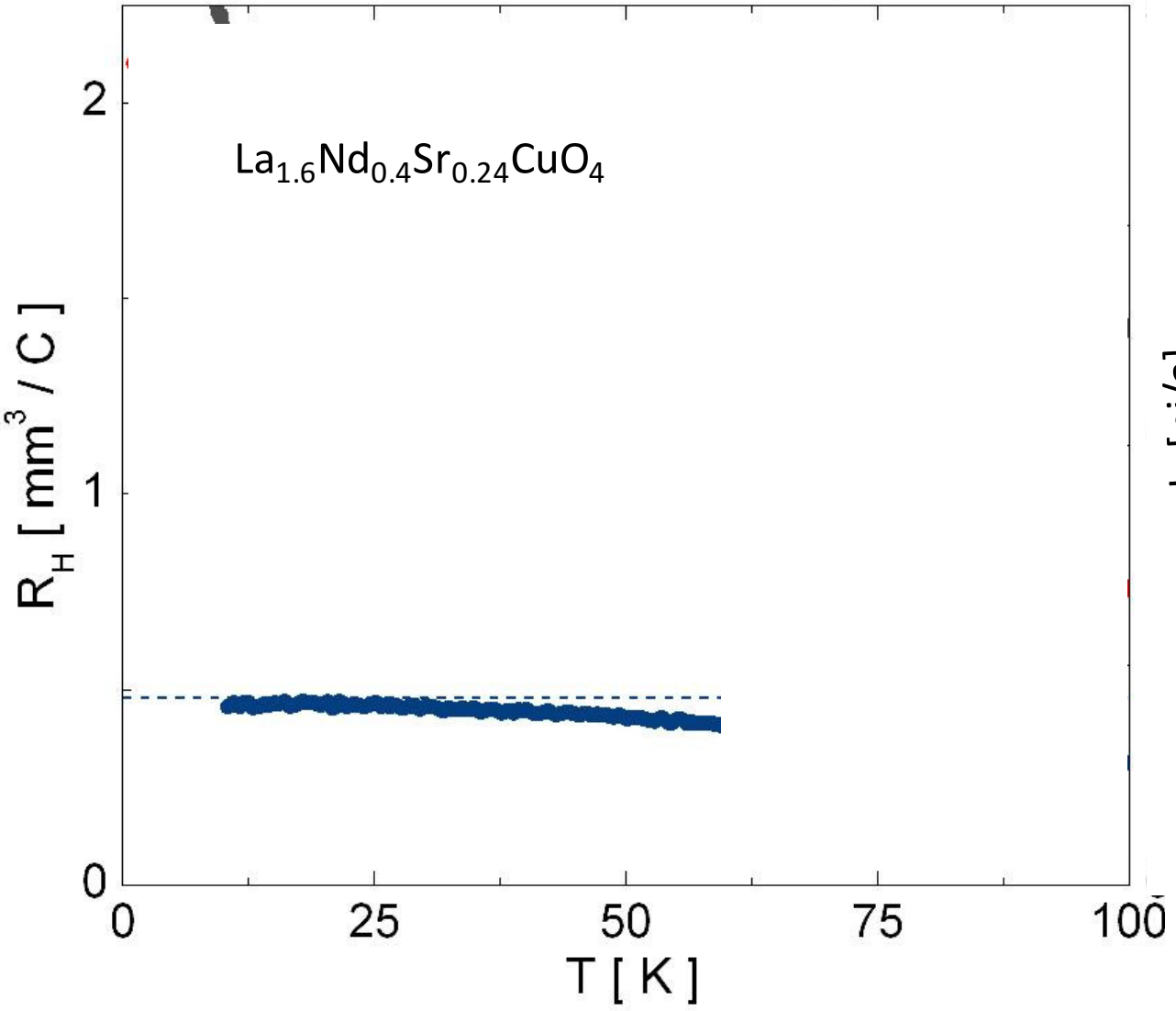


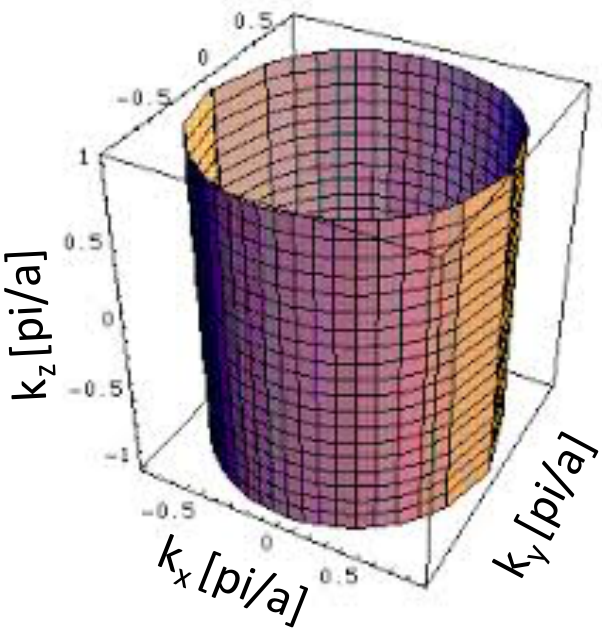
Hall effect: Niobium



Phys. Rev. B **77**, 214503 – Published 4 June 2008

Hall effect: Temperature dependence

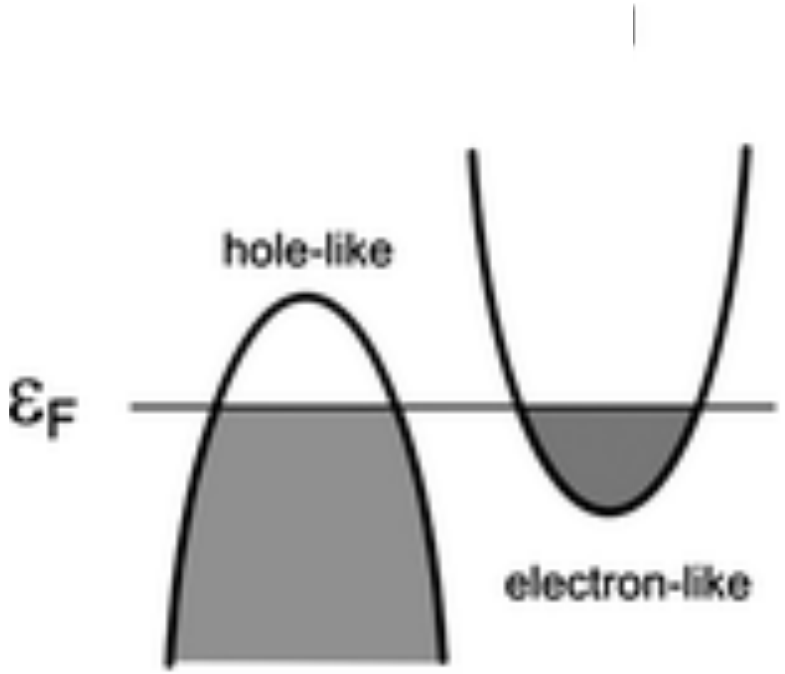


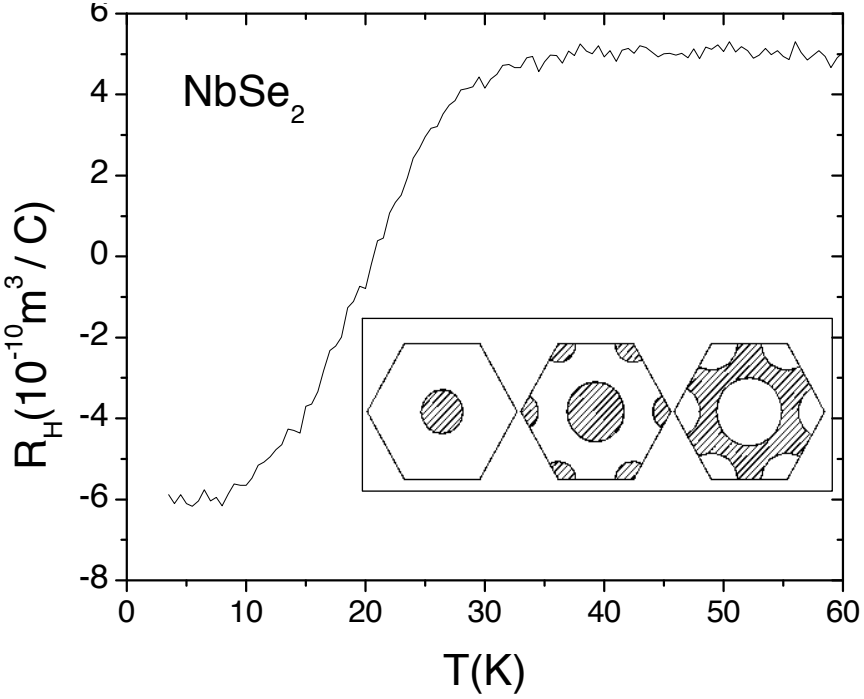


2D cylindrical
Fermi Surface

Daou et al., Nature Physics 2009

Sign of the Hall Coefficient R_H





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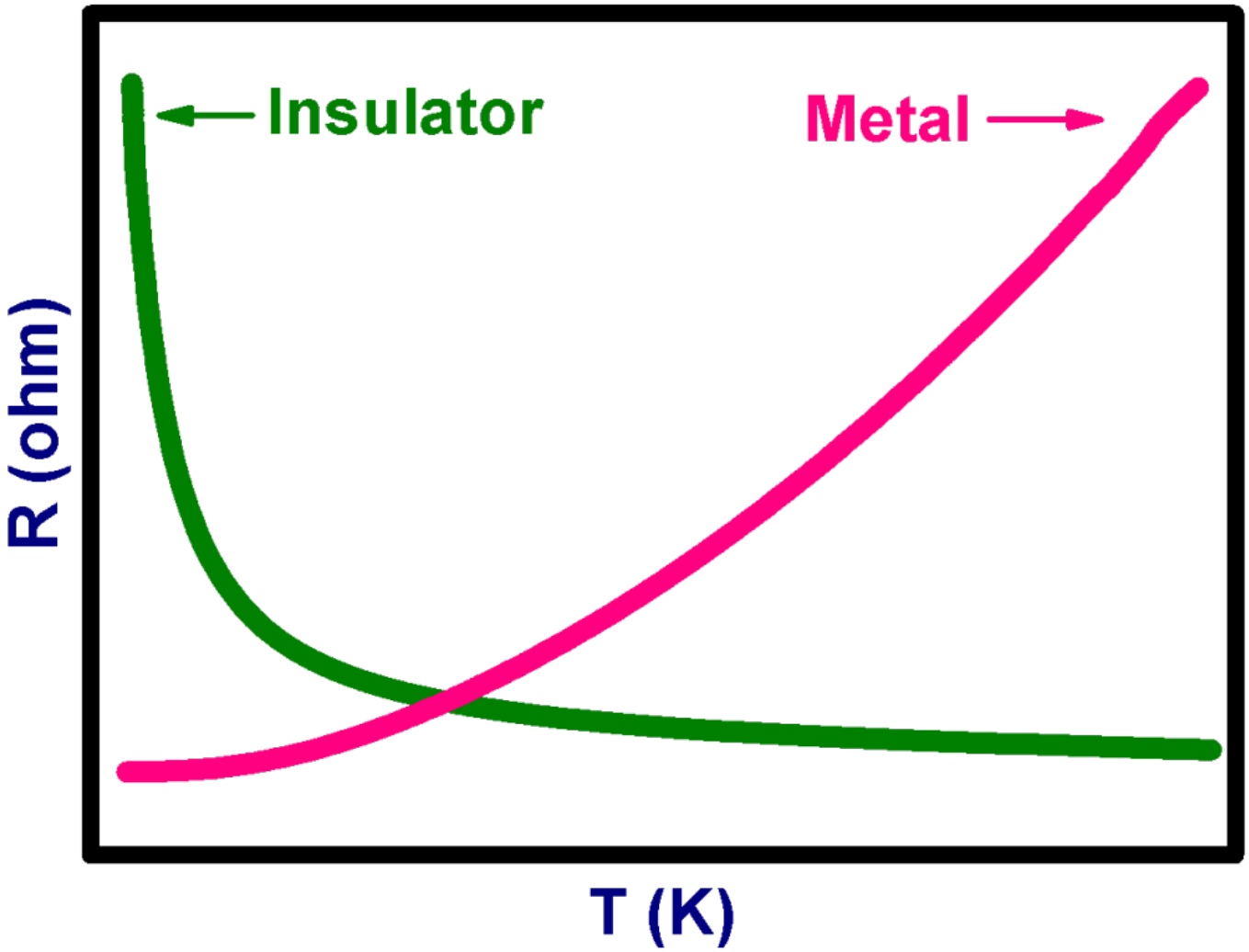
Metals and insulators: Resistivity



Conduction Electron Concentration

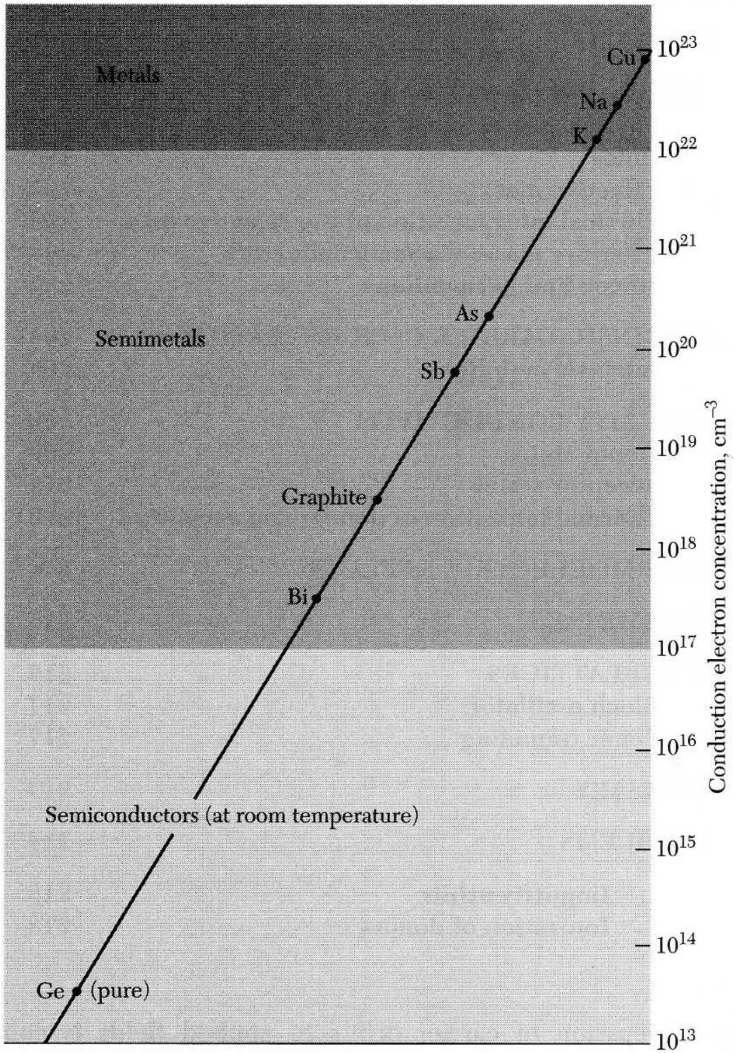
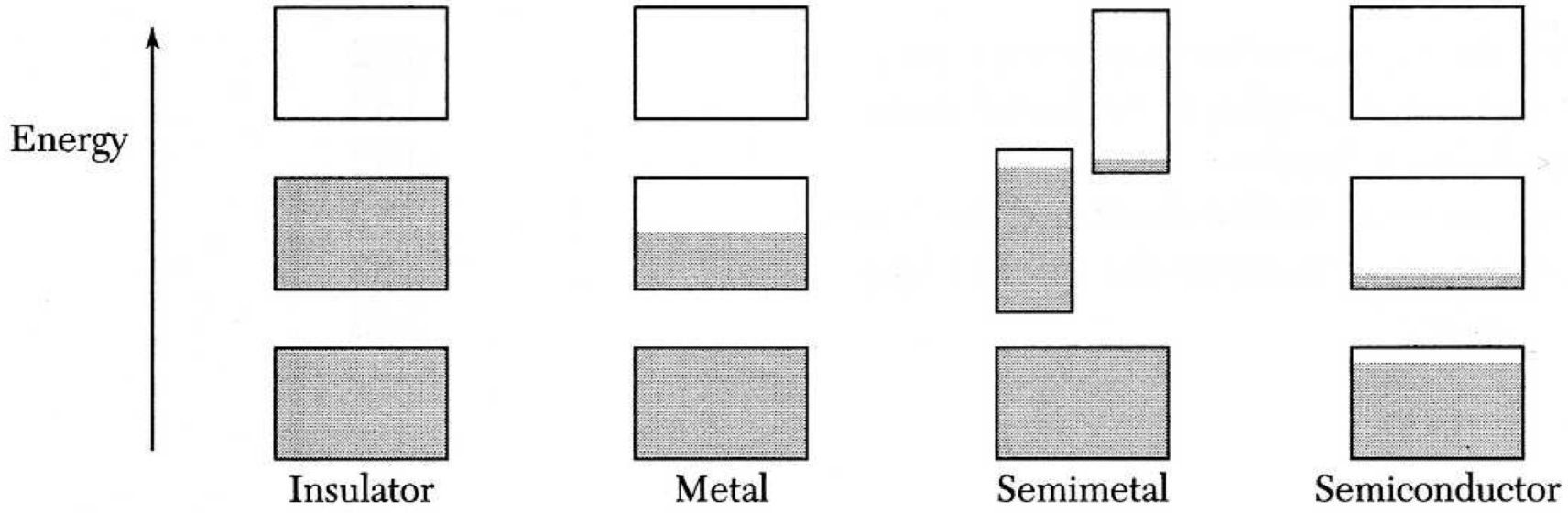
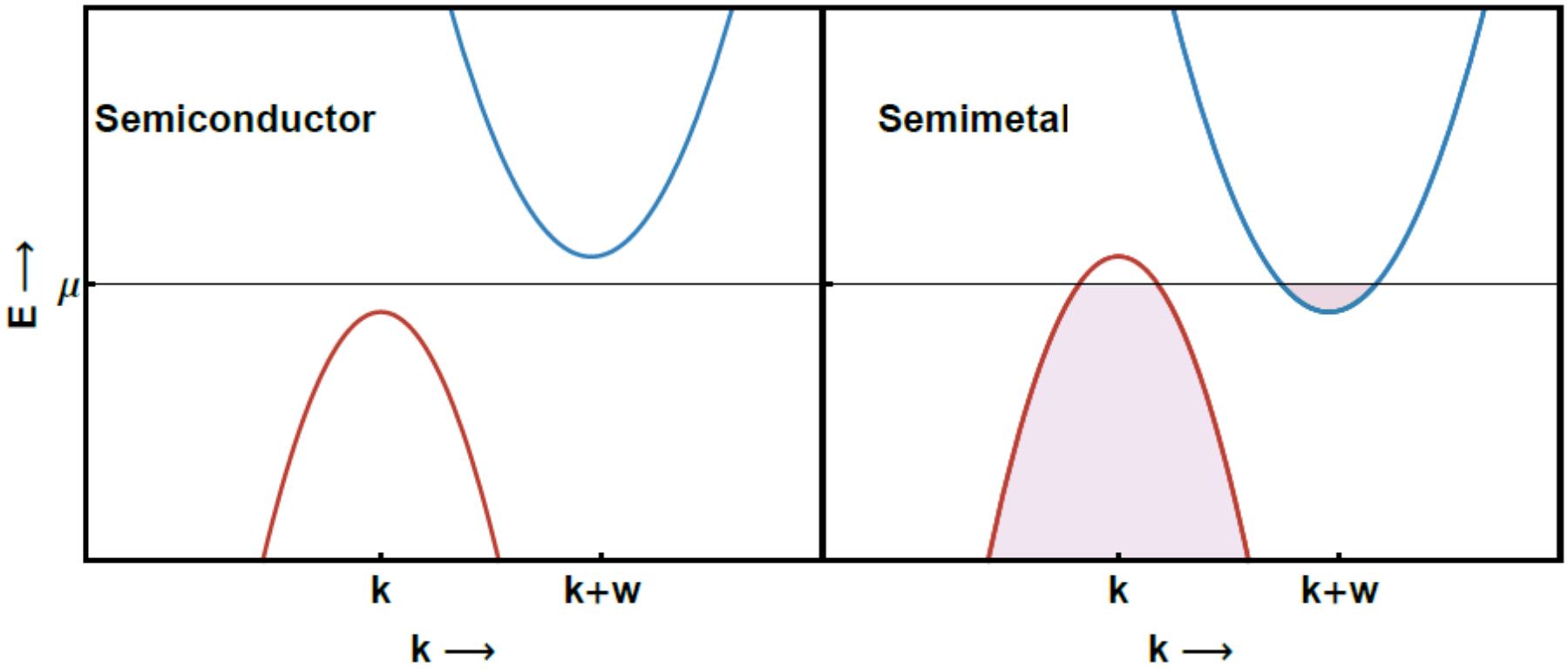


Figure 1 Carrier concentrations for metals, semimetals, and semiconductors. The semiconductor range may be extended upward by increasing the impurity concentration, and the range can be extended downward to merge eventually with the insulator range.

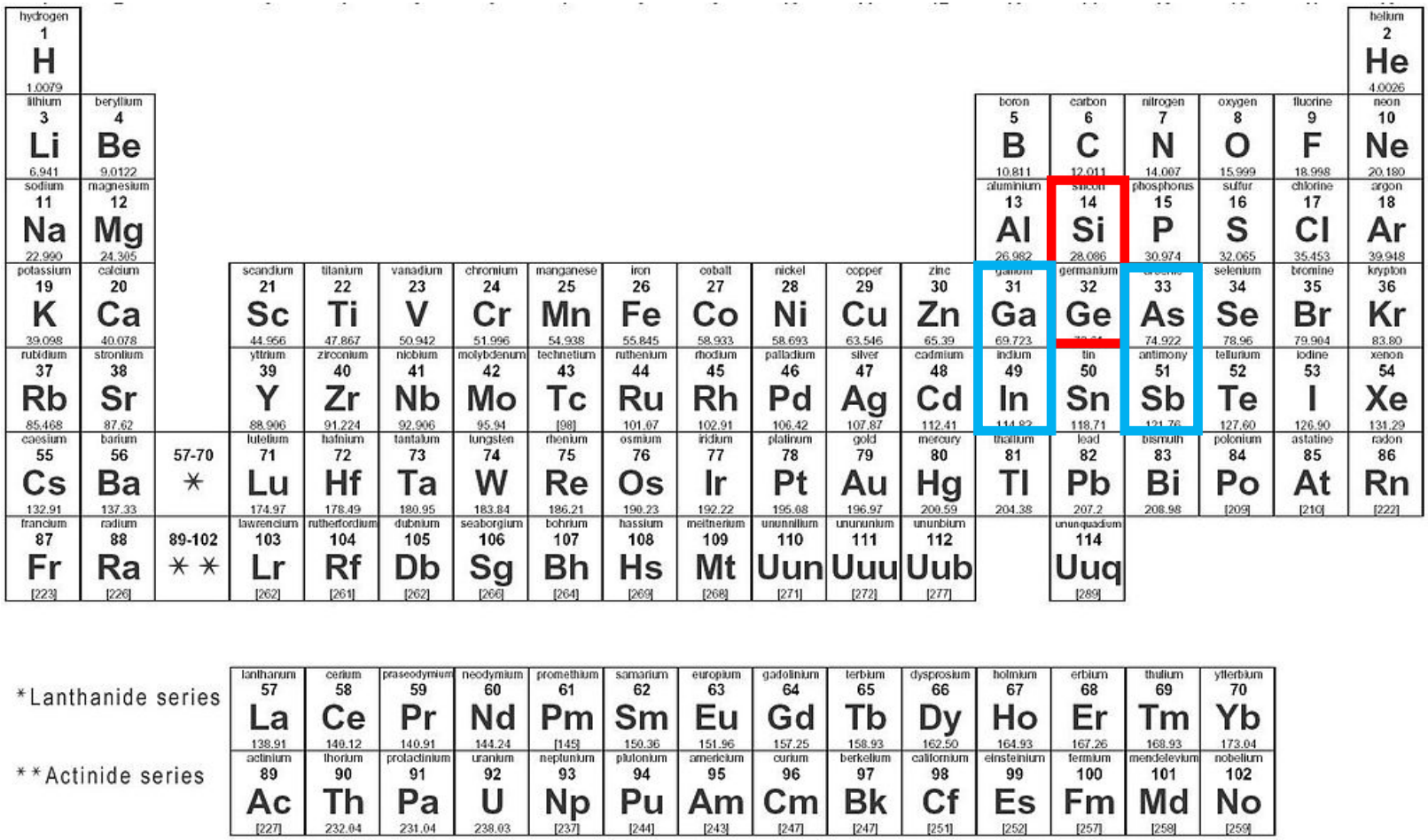
Semimetals & Semiconductors



Semimetals & Semiconductors



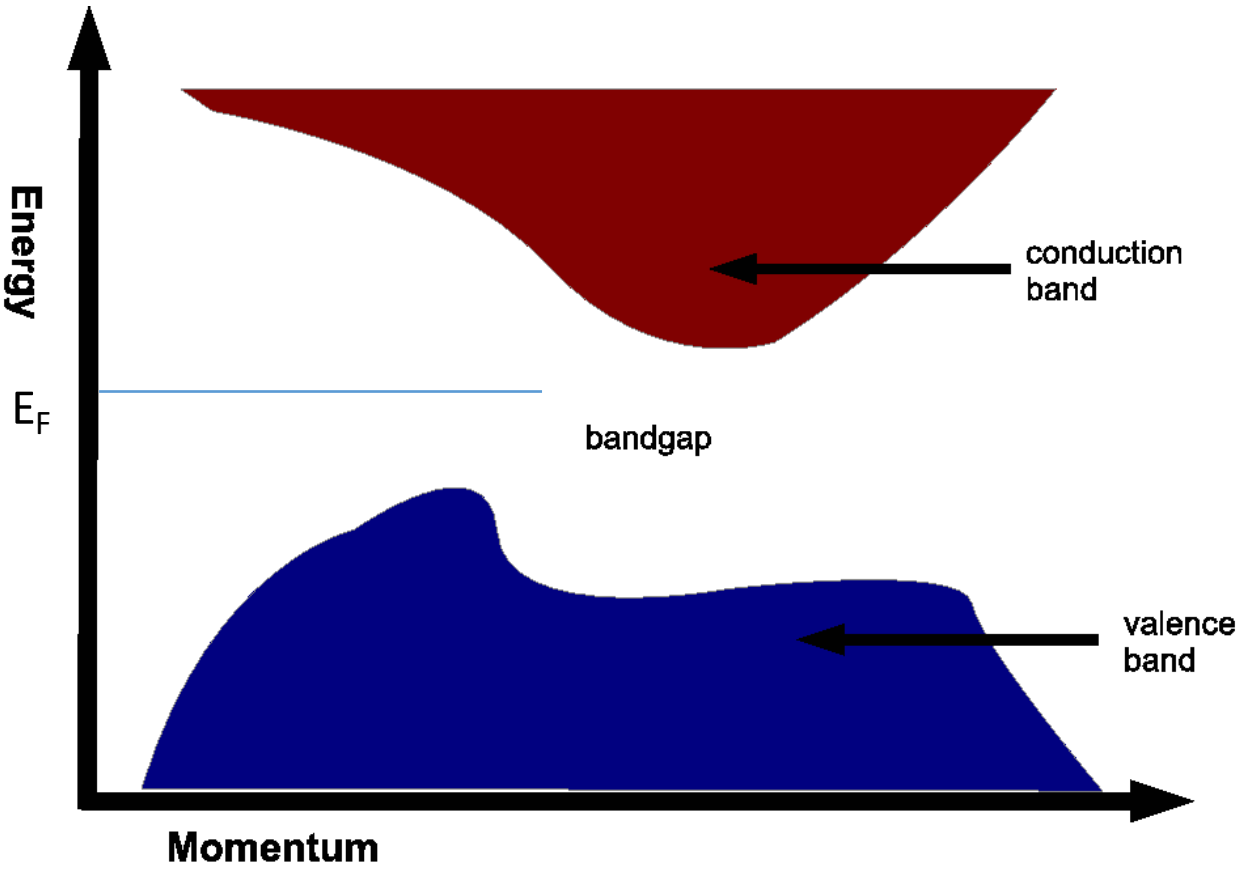
Semiconductor Materials



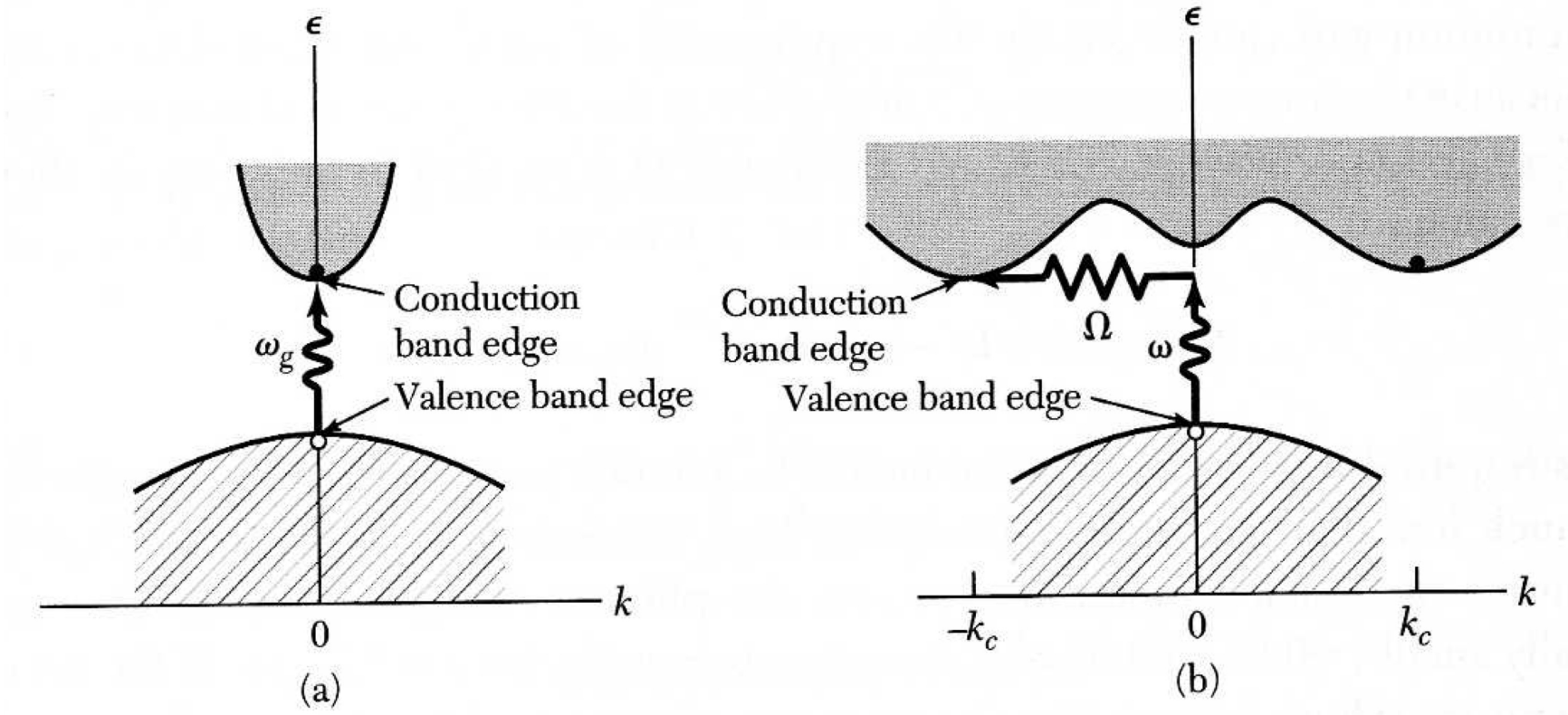
Diamond-type semiconductors

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)

		E_g, eV				E_g, eV	
Crystal	Gap	0 K	300 K	Crystal	Gap	0 K	300 K
Diamond	*i*	5.4		SiC(hex)	*i*	3.0	—
Si	*i*	1.17	1.11	Te	*d*	0.33	—
Ge	*i*	0.744	0.66	HgTe[a]	*d*	−0.30	
αSn	*d*	0.00	0.00	PbS	*d*	0.286	0.34–0.37
InSb	*d*	0.23	0.17	PbSe	*i*	0.165	0.27
InAs	*d*	0.43	0.36	PbTe	*i*	0.190	0.29
InP	*d*	1.42	1.27	CdS	*d*	2.582	2.42
GaP	*i*	2.32	2.25	CdSe	*d*	1.840	1.74
GaAs	*d*	1.52	1.43	CdTe	*d*	1.607	1.44
GaSb	*d*	0.81	0.68	SnTe	*d*	0.3	0.18
AlSb	*i*	1.65	1.6	Cu_2O	*d*	2.172	—

[a]HgTe is a semimetal; the bands overlap.

Semiconductor gaps versus $k_B T$

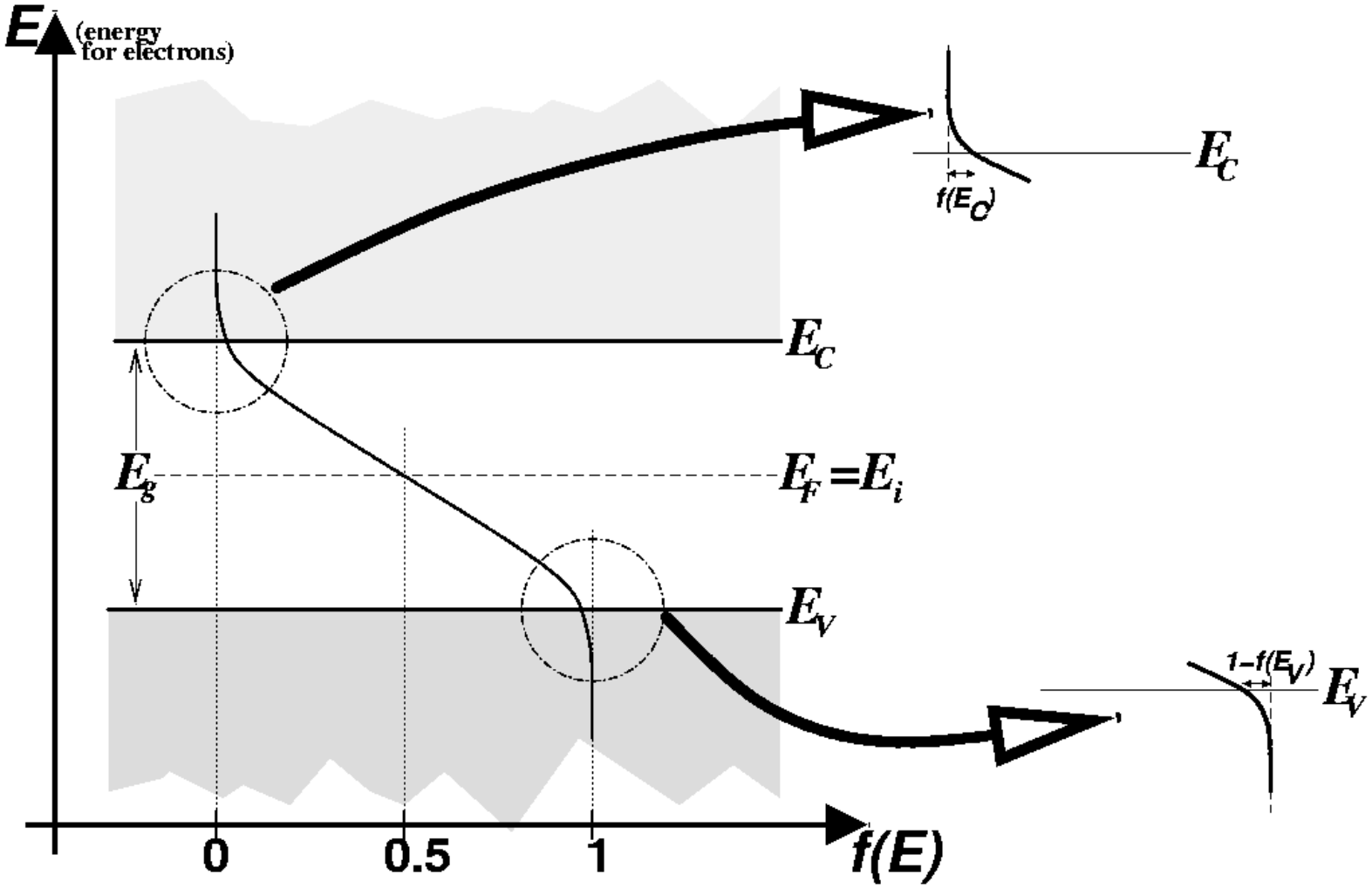
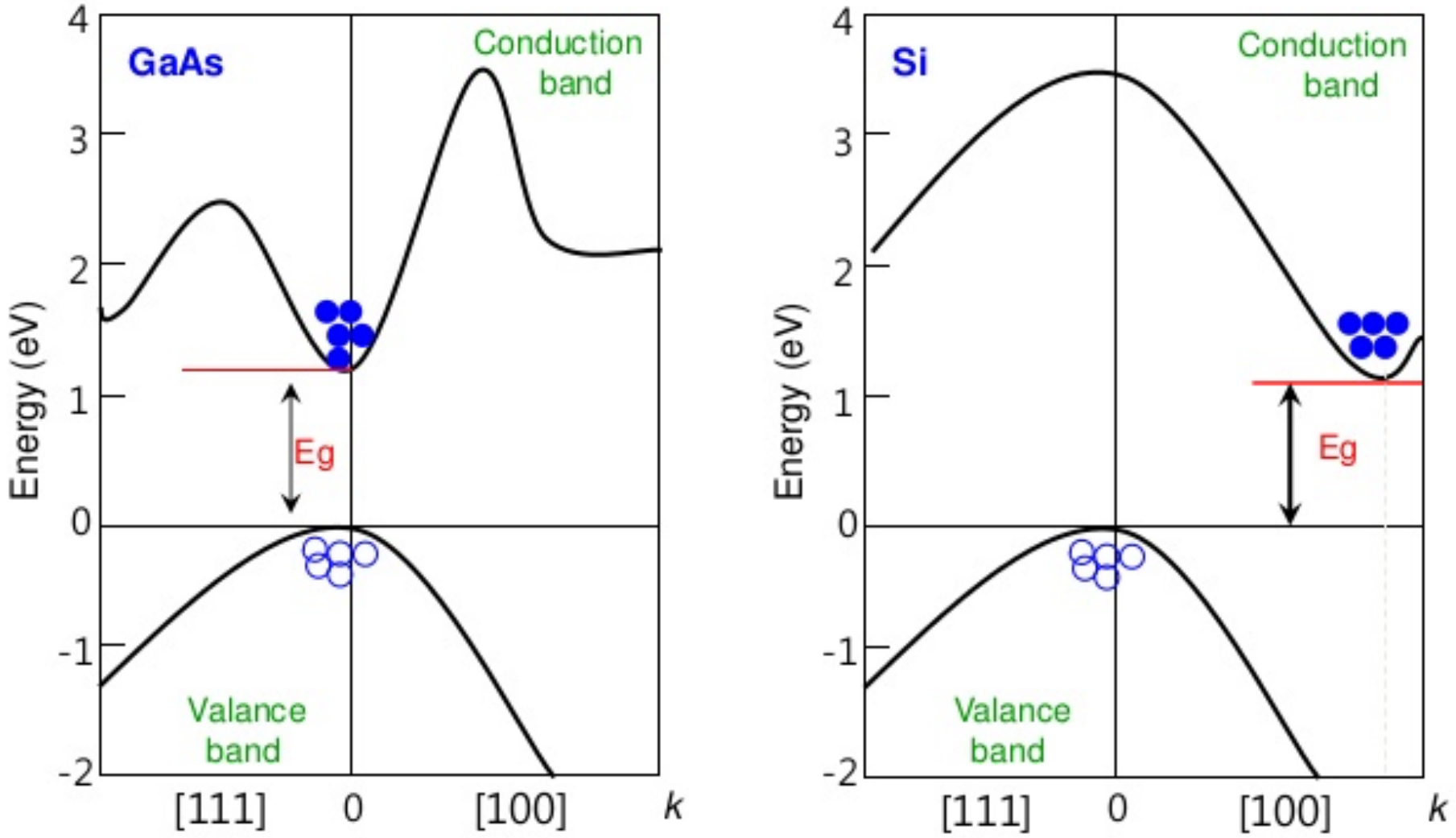


Figure 4:

Band Structure of Semiconductors



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

Electronic masses

Crystal	Electron m_e/m
InSb	0.015
InAs	0.026
InP	0.073
GaSb	0.047
GaAs	0.066
Cu_2O	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 $cm^2/V\text{-}s$

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