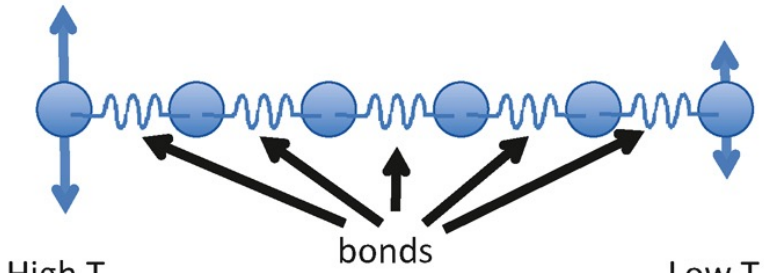
Lecture 10 (week 10: 29 April 2025)

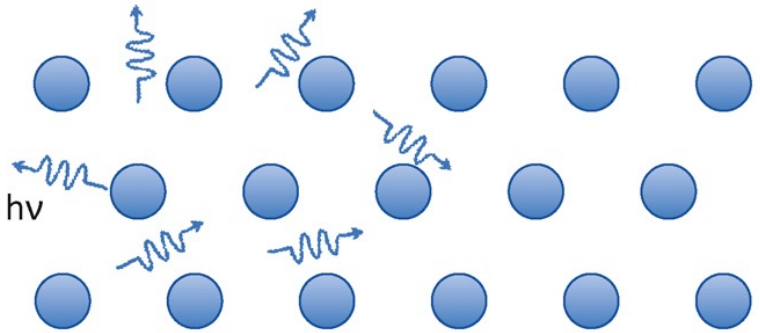
Thermal and electrical conduction – part II: practical aspects and mechanisms

Thermal conductivity: mechanisms

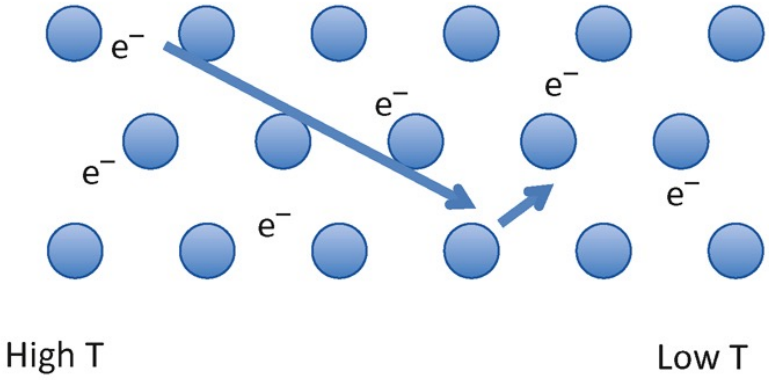
PHONONS



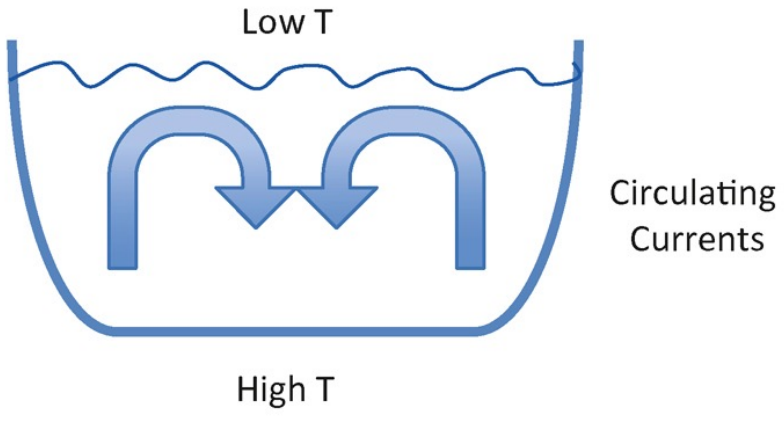
PHOTONS



FREE ELECTRONS



CONVECTION



Thermal conductivity

Thermal transport is defined by heat flux (J/m^{2}s) $$h_i = -k_{ij} \frac{\partial T}{\partial x_j}$$

There are 4 key mechanisms that contribute to the thermal conductivity:

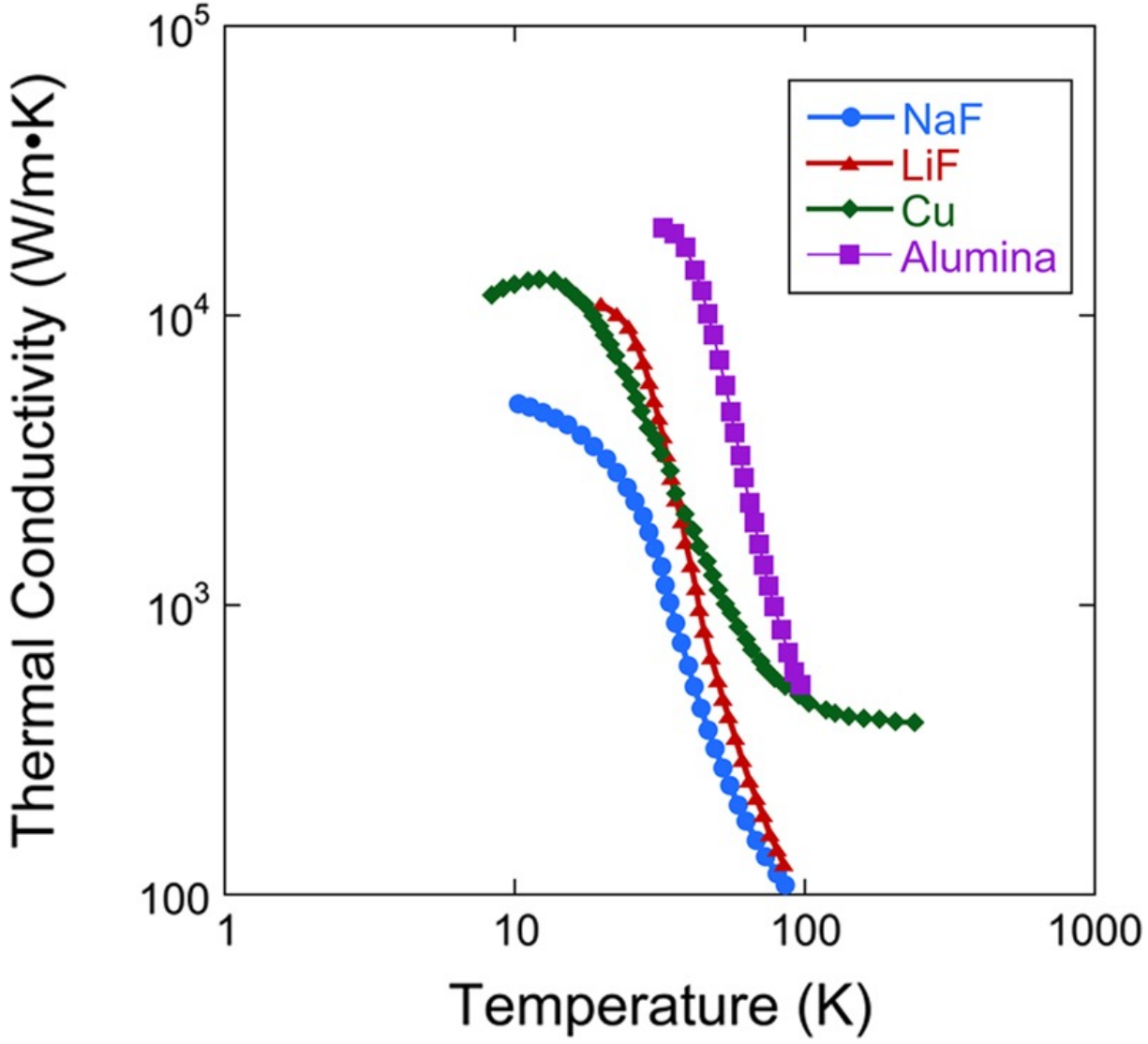
- Phonons – quantized lattice vibrations, or other collective vibrations in solids

- Mobile charge carriers (electrons) transport heat

- Photons emitted from the hot section of material are absorbed by the cooler part

- Convection – circulating currents in liquids or gases transport heat

Thermal conductivity vs temperature



When the phonon contribution to the thermal conductivity dominates:

- thermal conductivity decreases with the temperature increase (phonon-phonon scattering)

- Alumina has strongest thermal conductivity (strongest bonds)

Copper has free electrons – the contribution of electrons to thermal conductivity above 100K results in a saturation of the curve

Thermal conductivity of some materials at 300K, J/(s cm K)

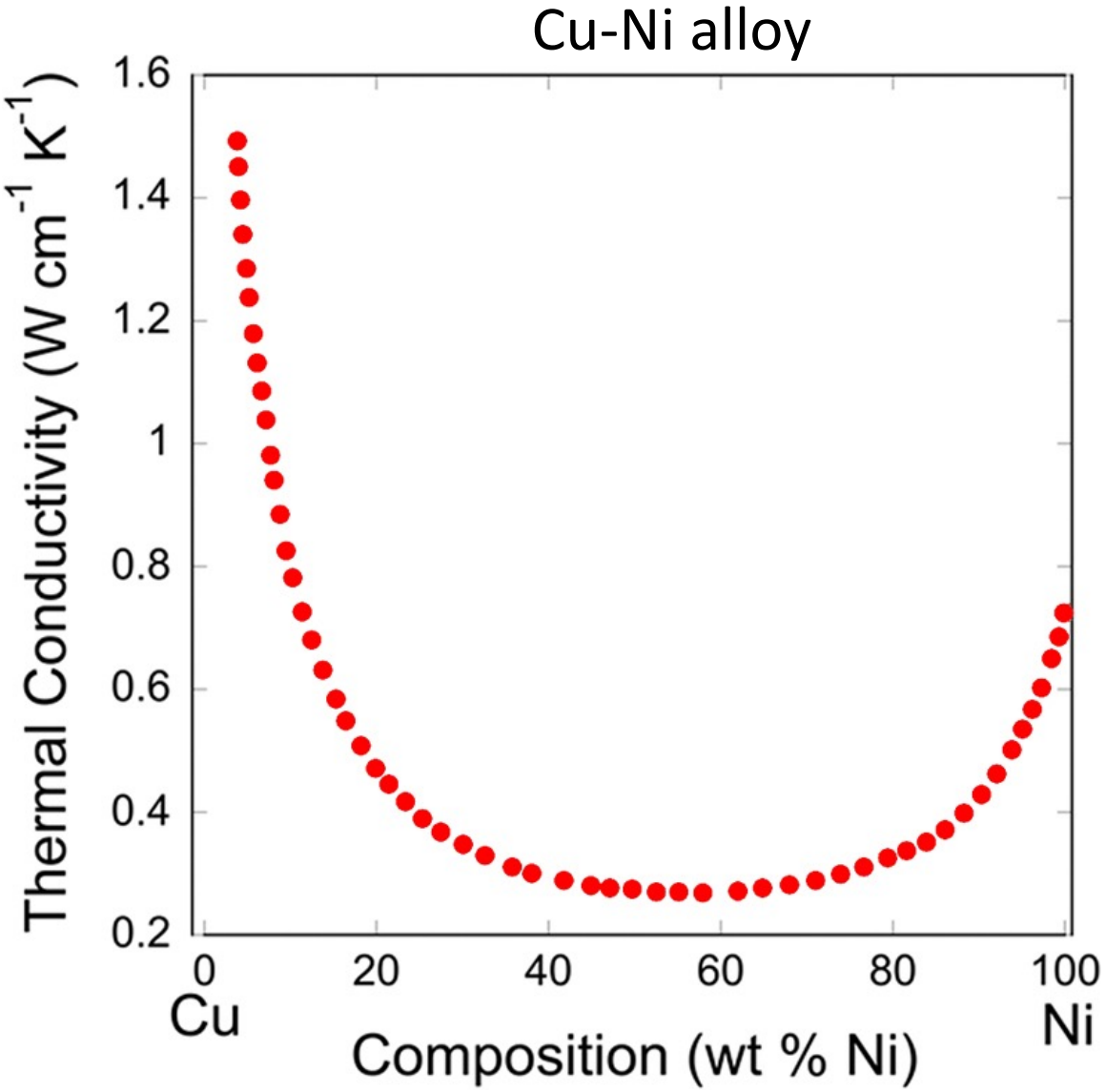
Diamond	9
Silicon	1.48
Germanium	0.599
Aluminum	2.37
Copper	3.98
Gold	3.15
Silver	4.27
Iron	0.803
Platinum	0.714
Tungsten	1.78
Graphite	
parallel to layers	20
perpendicular to layers	0.095
Alumina	
Single crystal	0.46
Polycrystal	0.36
Beryllia	2.72
Magnesia	0.60
AlN	3.21

- diamond-silicon-germanium (same colomn): longer and weaker bond = weaker thermal conduction

- diamond, beryllia, aluminum nitride are excellent thermal conductors (all three are considered as replacement for alumina in electronic packaging

AlN and BeO are binary compounds with particularly high thermal conductivity: strong bonding and similar atomic masses (vibrations better propagate along lattice when the mass contrast is small)

Thermal conductivity in the alloy systems: a strong effect of disorder



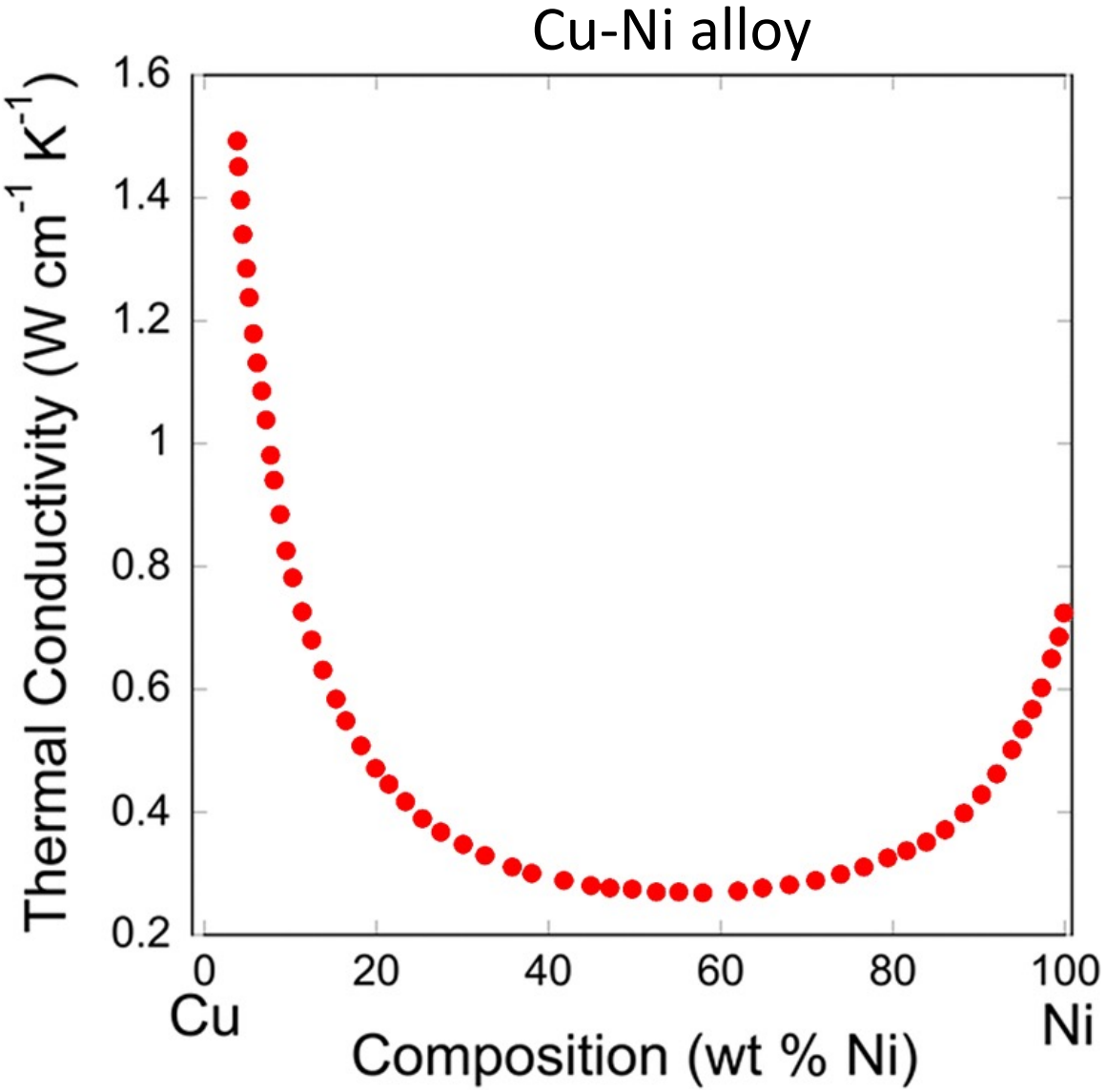
- any lattice disorder impacts phonon scattering

- Cu and Ni alloy form a perfect substitutional solid solution, the sample is a single phase across the entire phase diagram

- However, the thermal conductivity shows a sharp decrease in the center section

- The phonons are scattered when they encounter a small change of the periodic potential due to substitution of Cu for Ni

Thermal conductivity in the alloy systems: a strong effect of disorder



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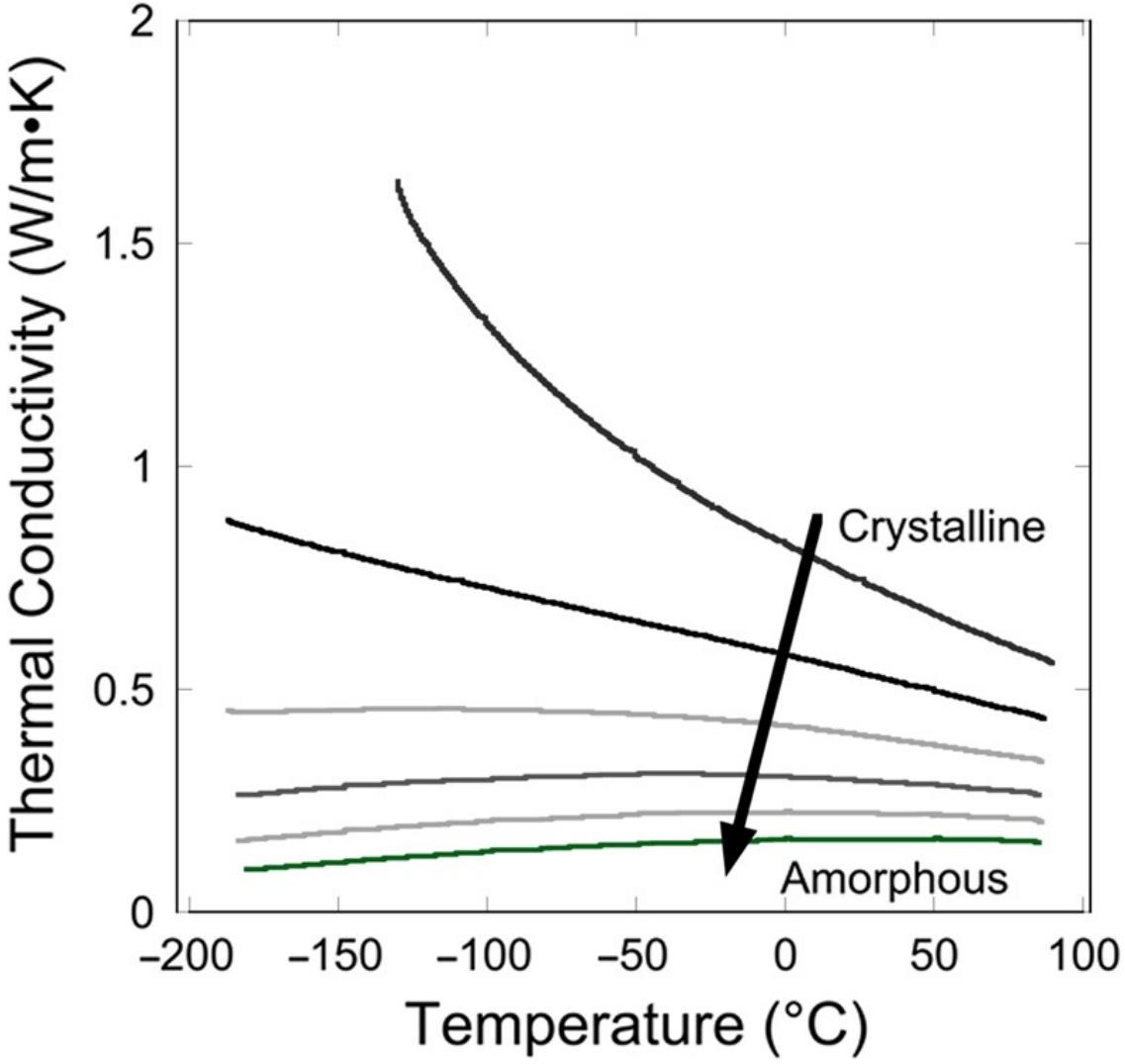
Thermal conductivity vs. degree of crystallinity: polymers

Typical changes of thermal conductivity in a polymer with crystallinity of 100%, 80%, 60%, 40%, 20%, 0%



- crystalline polymers like high-density polyethylene, polypropylene, PVDF show high thermal conductivity

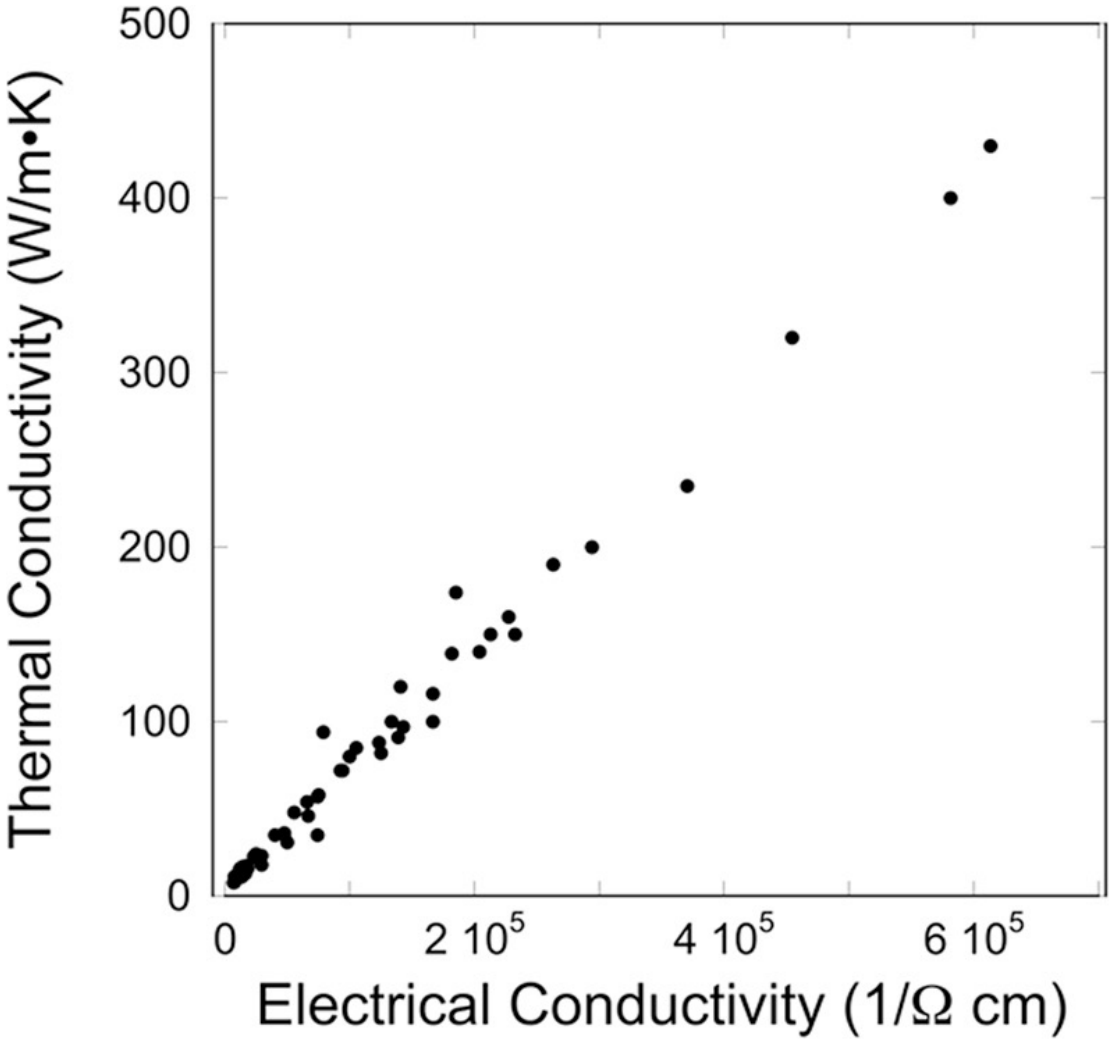
- the thermal conductivity decreases dramatically with the degree of crystallinity decrease

- in stretched polymers the thermal conductivity is higher in the direction of elongation (parallel to the covalently bonded backbone

- Van der Walls bonds = lower thermal conductivity

Electric conductors at the temperatures around 300K or higher: thermal conductivity vs electric conductivity

Elemental metals: thermal conductivity vs electric conductivity

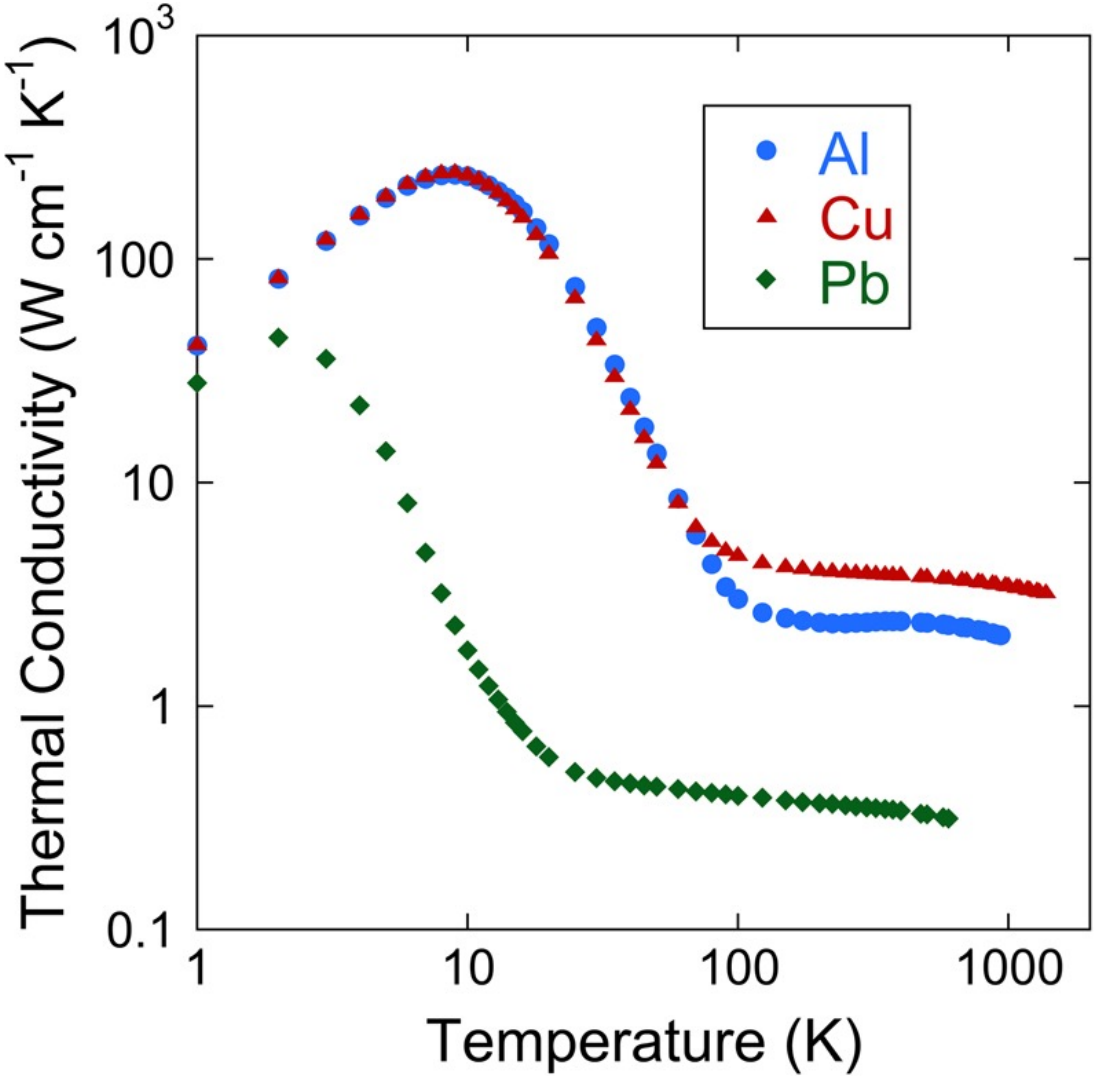


- when the thermal conductivity has a significant contribution from mobile electrons, there is a linear dependence between ***k*** and σ

- this linear relation is known as Weidemann-Franz law

Thermal conductivity of metals: electron and phonon contributions

thermal conductivity vs temperature for Al, Cu, Pb



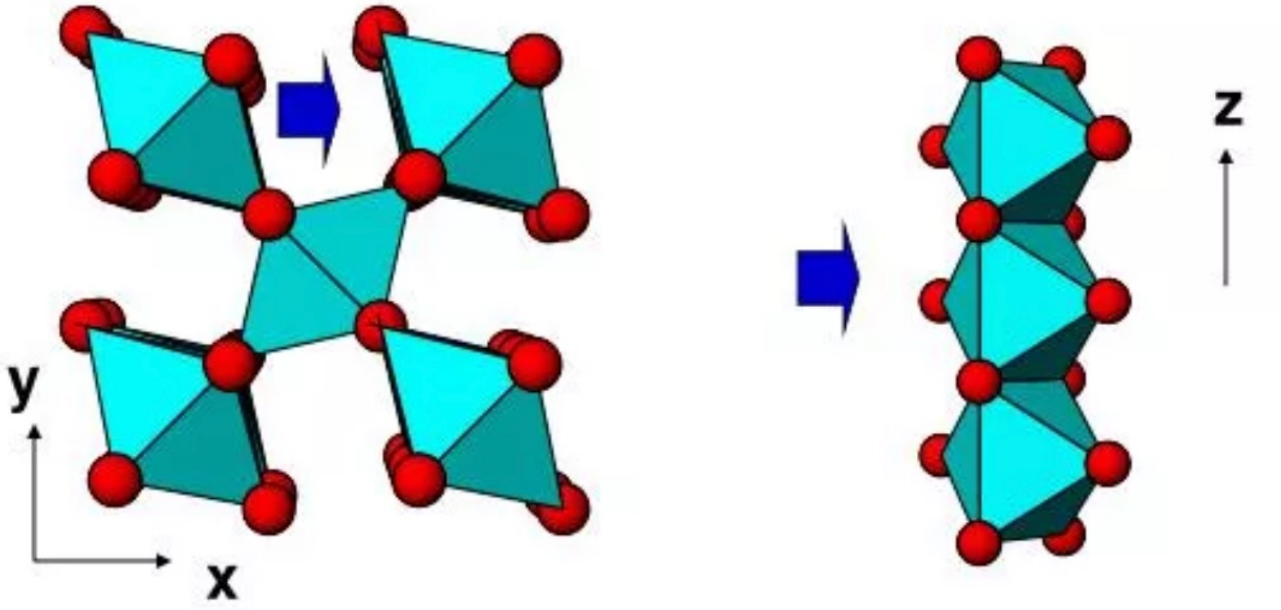
- electron and phonon contributions both play a role in thermal transport in metals, but their relative importance depends on temperature range

- lower temperature = higher phonon contribution

- temperature dependence of thermal conductivity signals the crossover between the two predominant mechanisms of thermal conductivity

Thermal conductivity: anisotropy

Rutile



• Along Z there is edge sharing of polyhedra, which brings the Ti atoms closer together. In the X-Y plane, there is only corner sharing. This facilitates phonon transport of heat parallel to the c direction. Thus, $k_{33} > k_{11}$ at temperatures where phonons dominate the thermal conductivity.

• Ceramics: As a first approximation, a weighted average can be utilized, so that the polycrystalline ceramic from a tetragonal point group would be $(2\ k_{11} + k_{33})/3$.

In a polycrystalline ceramic, there is more scattering of the phonon contribution to thermal conductivity at the **grain boundaries**. The polycrystalline ceramic may then have a lower thermal conductivity than the weighted average.

Electric conductivity

- Transport of electrical charge under electric stimuli

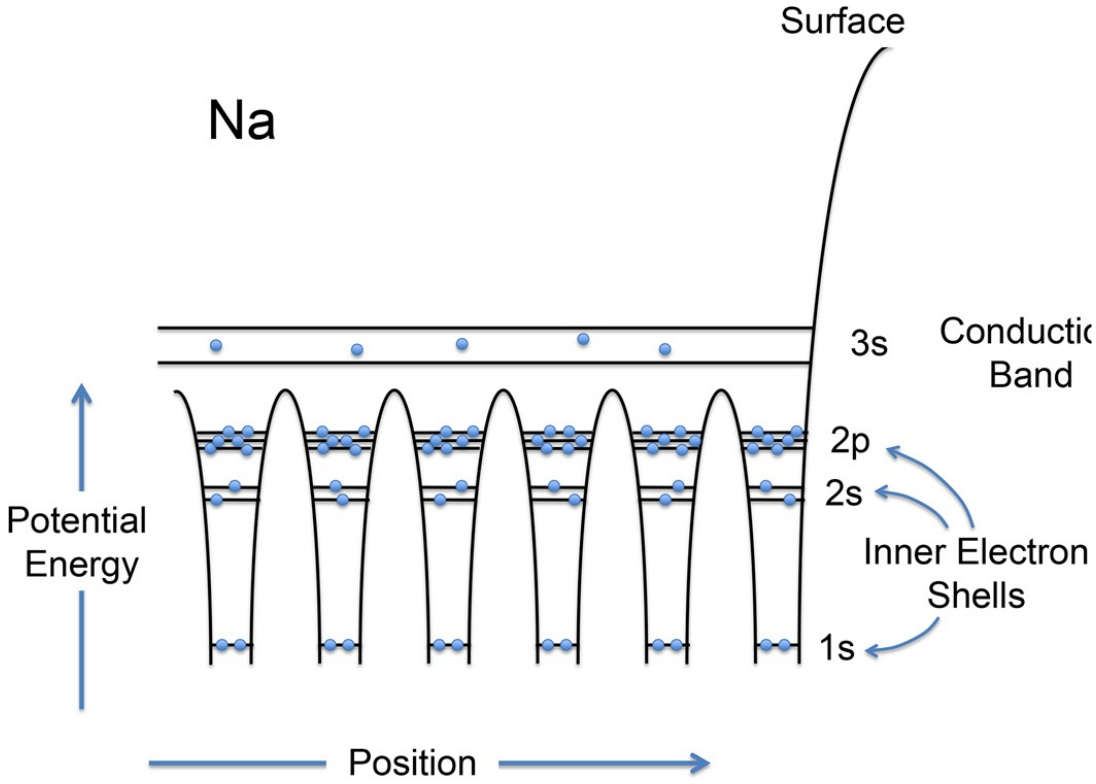
- To analyze conductivity it is essential to understand if we are dealing with metal, semiconductor or insulator

- Nature of charge carriers is also important (electrons, holes, ions)

- Predominant conduction mechanism depends on temperature, frequency and other factors

Metals

- Ion cores that donate electrons to the electron gas (delocalized)
- mobile electrons are available at any temperature
- Band diagram language: valence band is partially filled (often called conduction band)

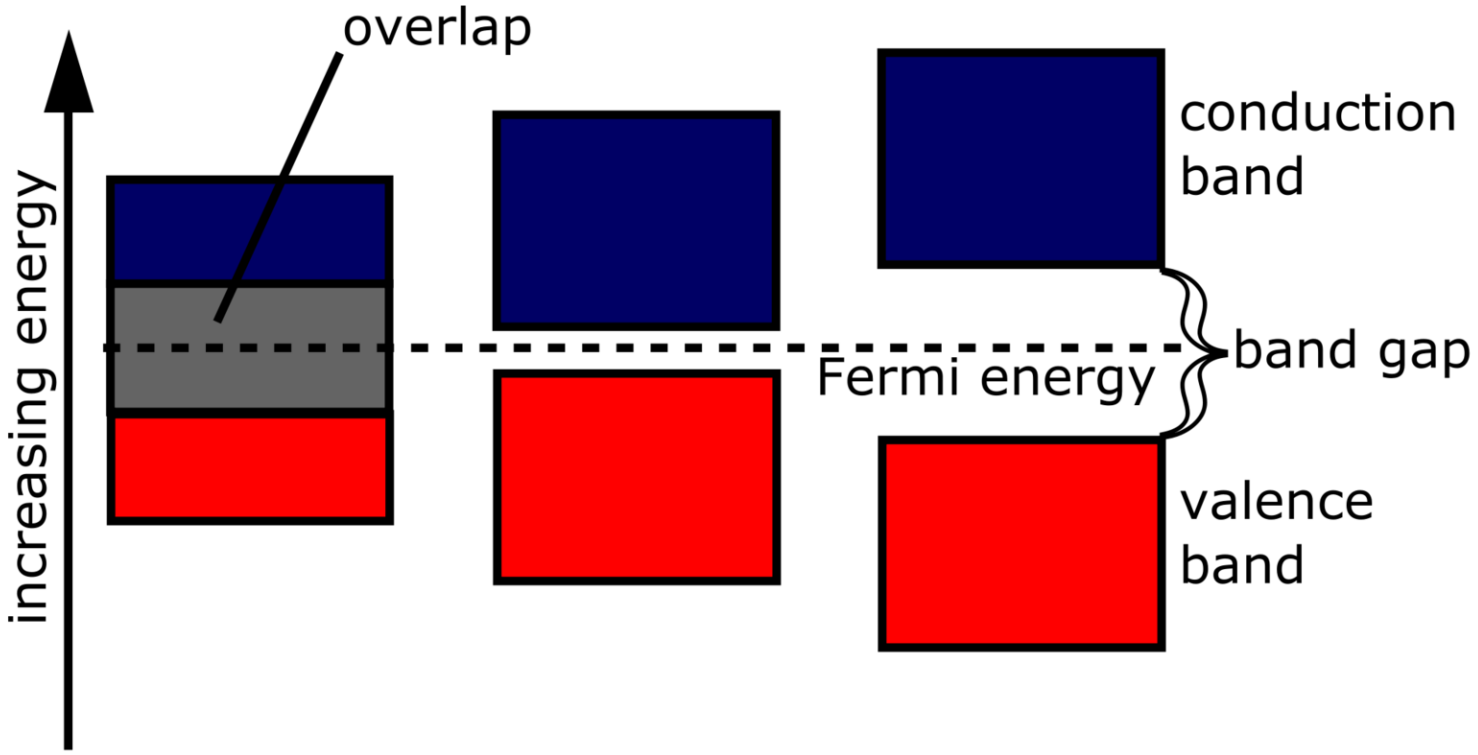


Example of Na atom:

- orbitals that interact with their neighbors split into closely spaced energy levels and become bands of allowed energy separated by energy gaps
- The outermost band originating from the 3s orbitals is partially filled (conduction band)

Metals, semiconductors, insulators

- Ion cores that donate electrons to the electron gas (delocalized)



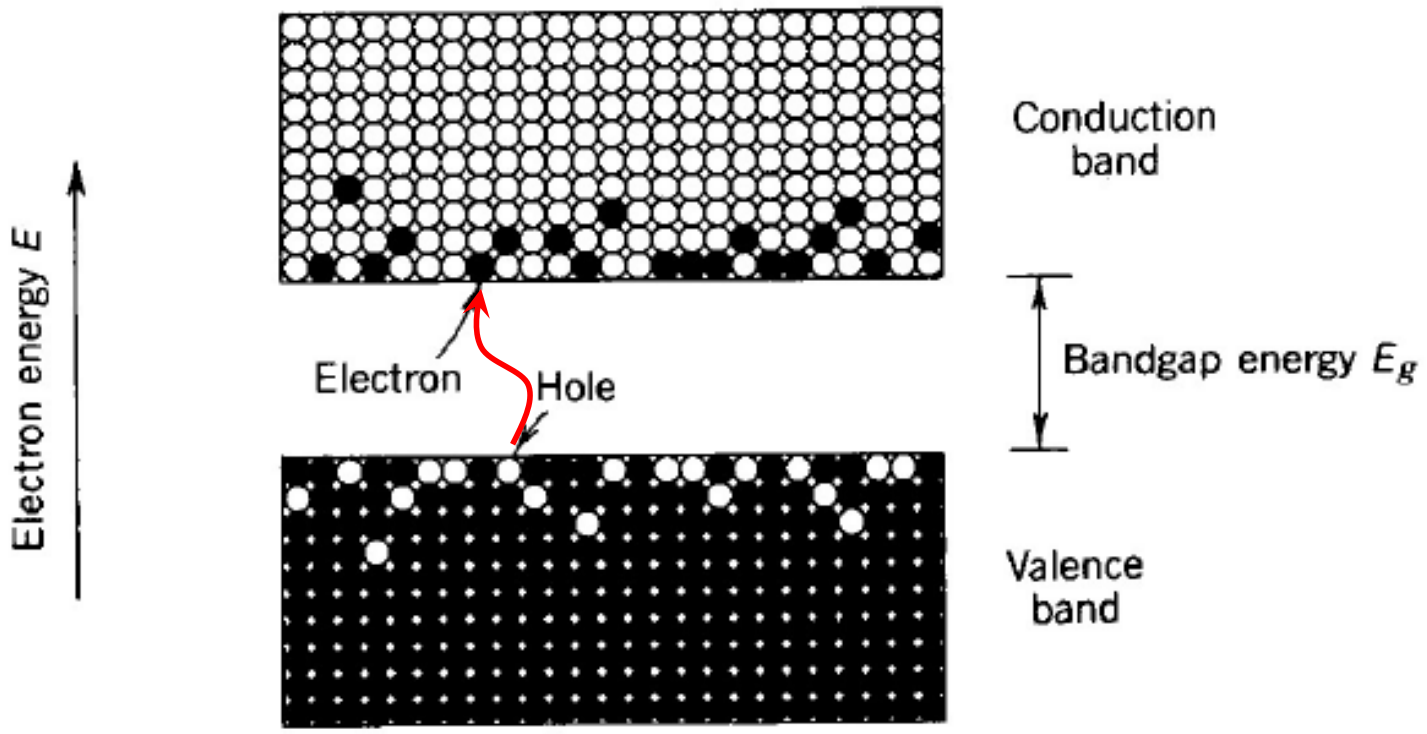
Fermi distribution function

$$f(E) = \frac{1}{1 + e^{\frac{E - E_F}{k_B T}}}$$

- Fermi level E_F in metals separates occupied and empty states (at 0K)
  work function is the energy needed to extract the electron from level E_F to infinity

- In semiconductors/insulators E_F is situated in the forbidden gap

Si and other semiconductors: Bands and Charge Carriers



- At finite temperatures, electrons are promoted from the valence band to the conduction band resulting in electrons in the conduction band and holes in the valence band
- Motion of electrons in the conduction band and holes in the valence band at T>0 K generates electrical current

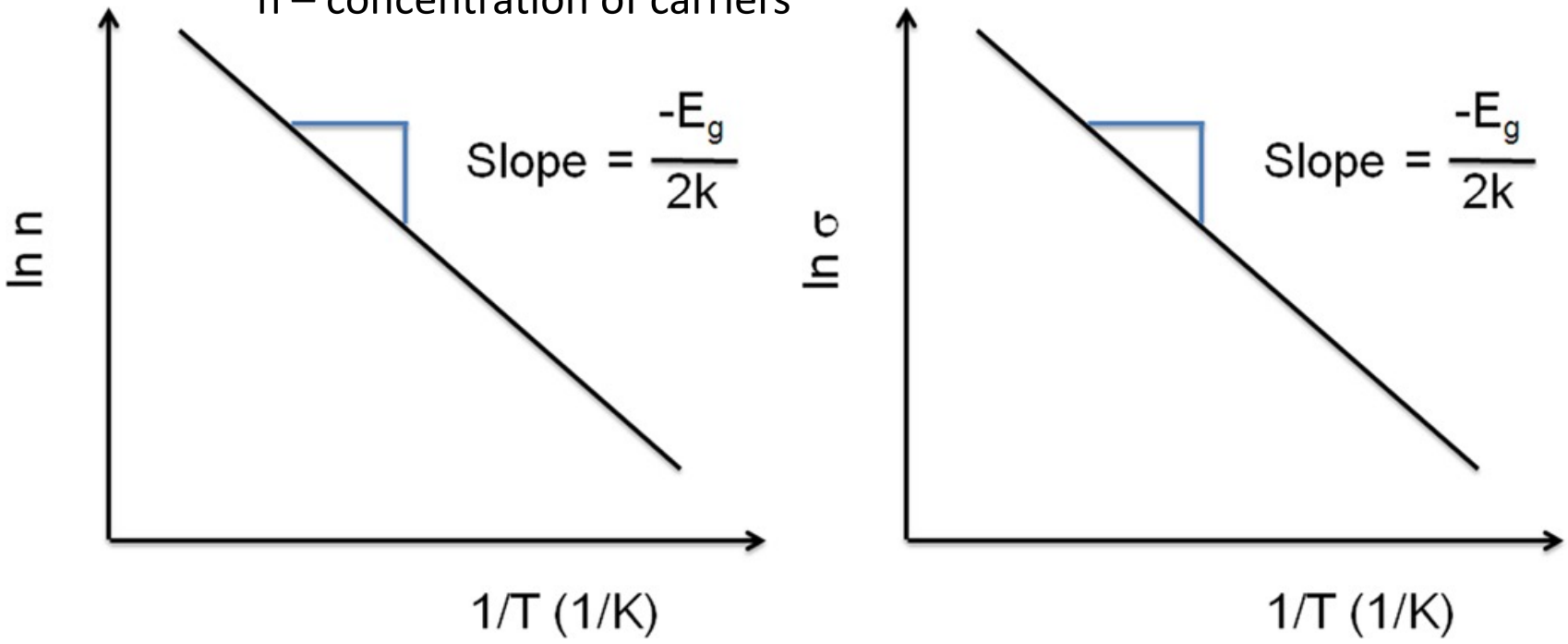
Electrical conductivity in intrinsic (undoped) semiconductors vs. T

n_i is proportional to $exp\left(\frac{-E_g}{2\,KT}\right)$

(Bolzmann approximation)

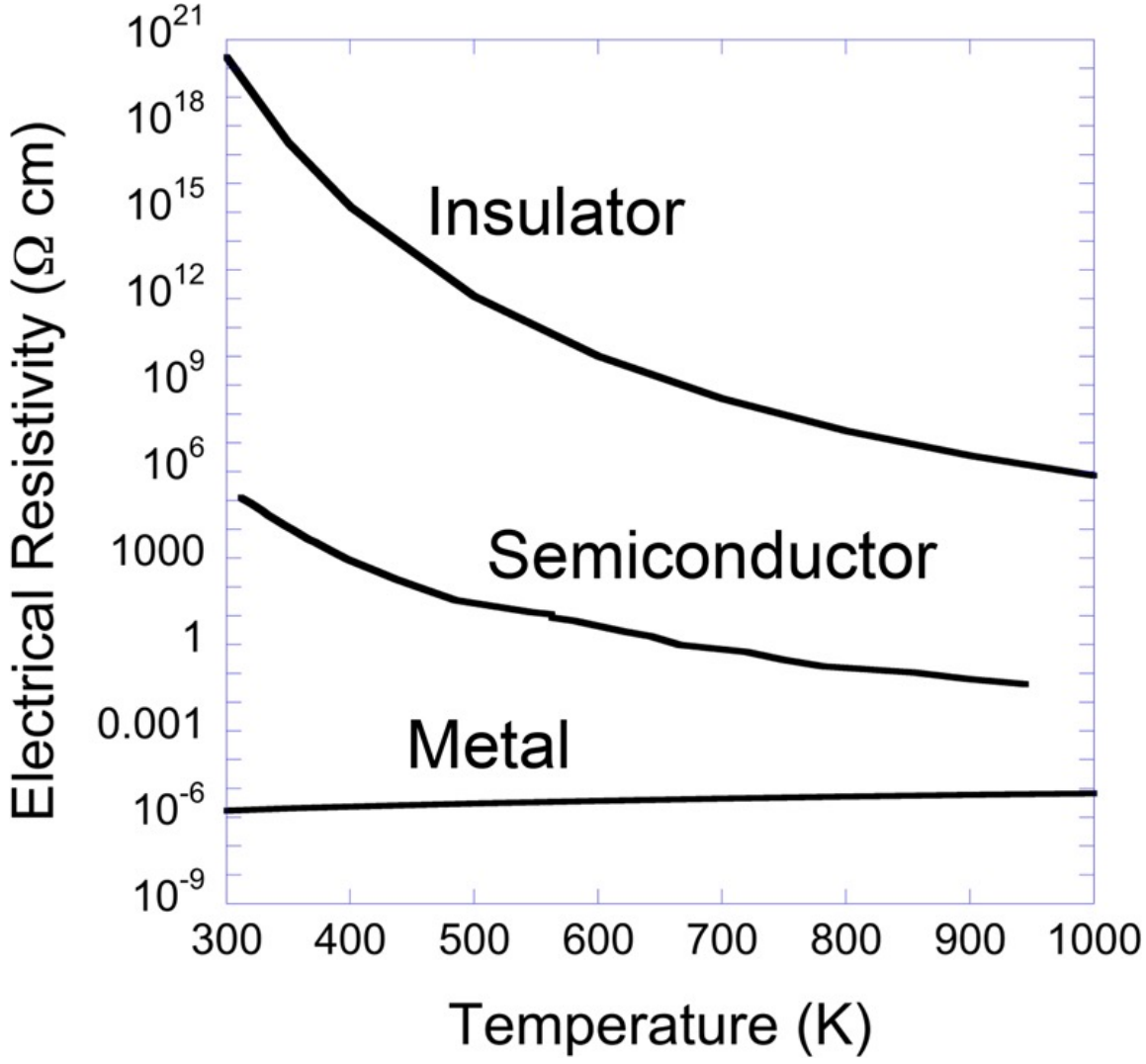
	Germanium	Silicon	Gallium Arsenide
300 K	2.02×10^{13}	8.72×10^{9}	2.03×10^{6}
400 K	1.38×10^{15}	4.52×10^{12}	5.98×10^{9}
500 K	1.91×10^{16}	2.16×10^{14}	7.98×10^{11}
600 K	1.18×10^{17}	3.07×10^{15}	2.22×10^{13}

n – concentration of carriers



Semiconductor	InSb	Ge	Si	GaAs	GaP	ZnSe	Diamond
E_g (eV)	0.18	0.67	1.12	1.42	2.25	2.7	6.0

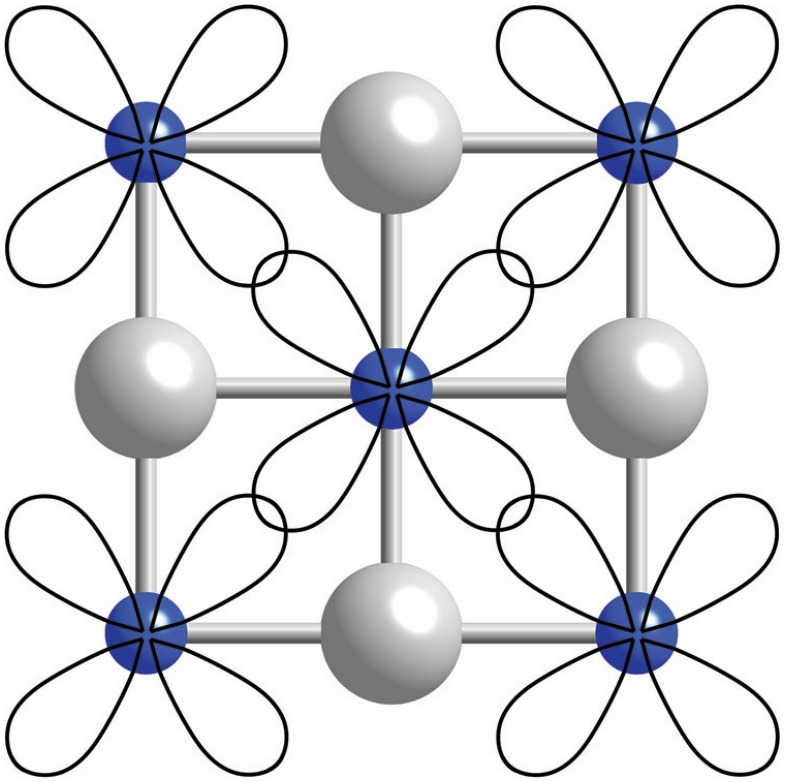
Electrical conductivity: metals, semiconductors, insulators



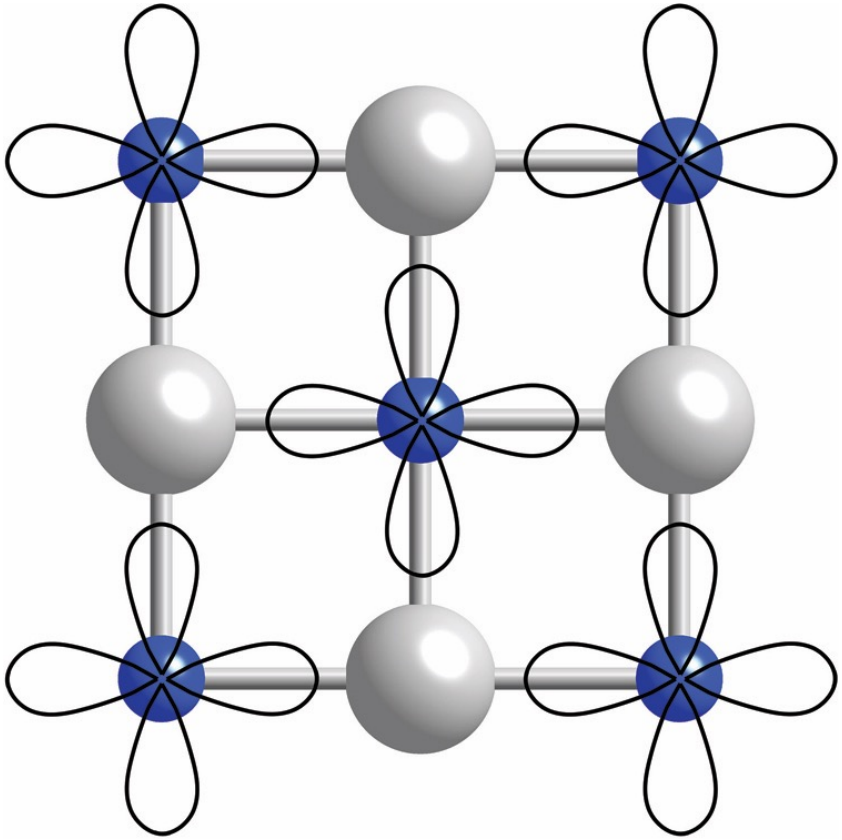
Metals (unlike semiconductors/insulators) typically show a resistivity increase with the temperature

Metallic conduction from compounds including non-metals

TiO (metallic conductor)



NiO (insulator)



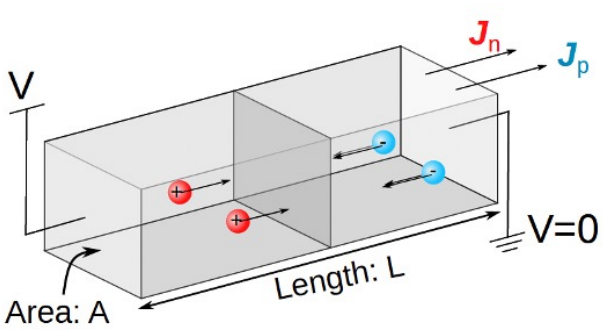
In TiO metallic conduction originates from overlapping diorbitals that form partially filled conduction band. In NiO d-orbitals stay localized

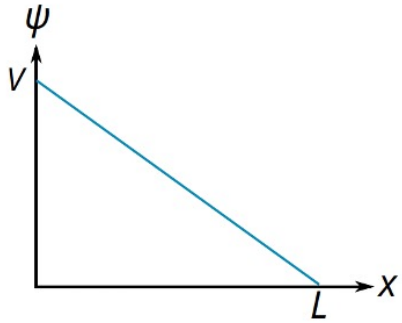
Models of electrical conductivity

- Model of Drude (1902): electrons represented with spheres which follow classical mechanics
- Hopping conduction in insulators/semoconductors
- Energy band model (1935): electrons are quantum objects interacting with the medium but do not affect the medium or other electrons (passive electrons)
- BCS model (Bardeen, Cooper and Schrieffer;1962): electrons are quantum objects which interact with the environment (medium in which they move) and with other electrons.
- Ionic conductivity
- ...

Electrical conduction: Drude model

- a widely used classical model of charge transport
  Works well for describing conductivity in semiconductors & metals



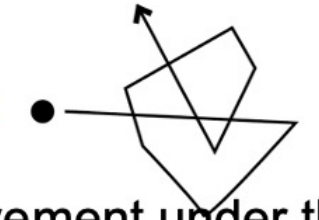


Constant voltage V

Uniform electric field E = V/L

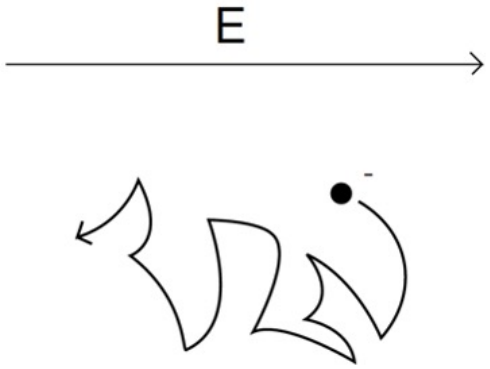
stochastic, time between scuttering events τ_c, $\lambda = v_{th}\tau_c$
mean free path λ depends on the thermal velocity

- Types of movement:
  - Thermal:



  - Drift: movement under the external electric field

Electrical conduction: Drude model - 2

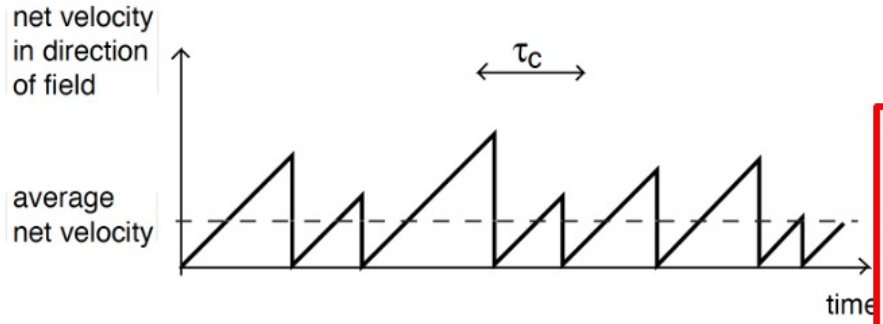


$$E \equiv electric\ field\ [V/cm]$$

$$F = \pm qE$$ *The net force acting on charge carrier*

$$v(t) = at = -\frac{qE}{m_n}t$$ *For electrons*

$$v(t) = \frac{qE}{m_p}t$$ *For holes (holes also have effective mass)*



Drift velocity:

$$\overline{v} = v_d = \pm\frac{qE}{2m_{n,p}}\tau_c = \pm\frac{q\tau_c}{2m_{n,p}}E$$

$$v_{dn} = -\mu_n E$$

$$v_{dp} = \mu_p E$$

$$\mu_{n,p} = \frac{q\tau_c}{2m_{n,p}} \equiv mobility\ [cm^2/V \cdot s]$$

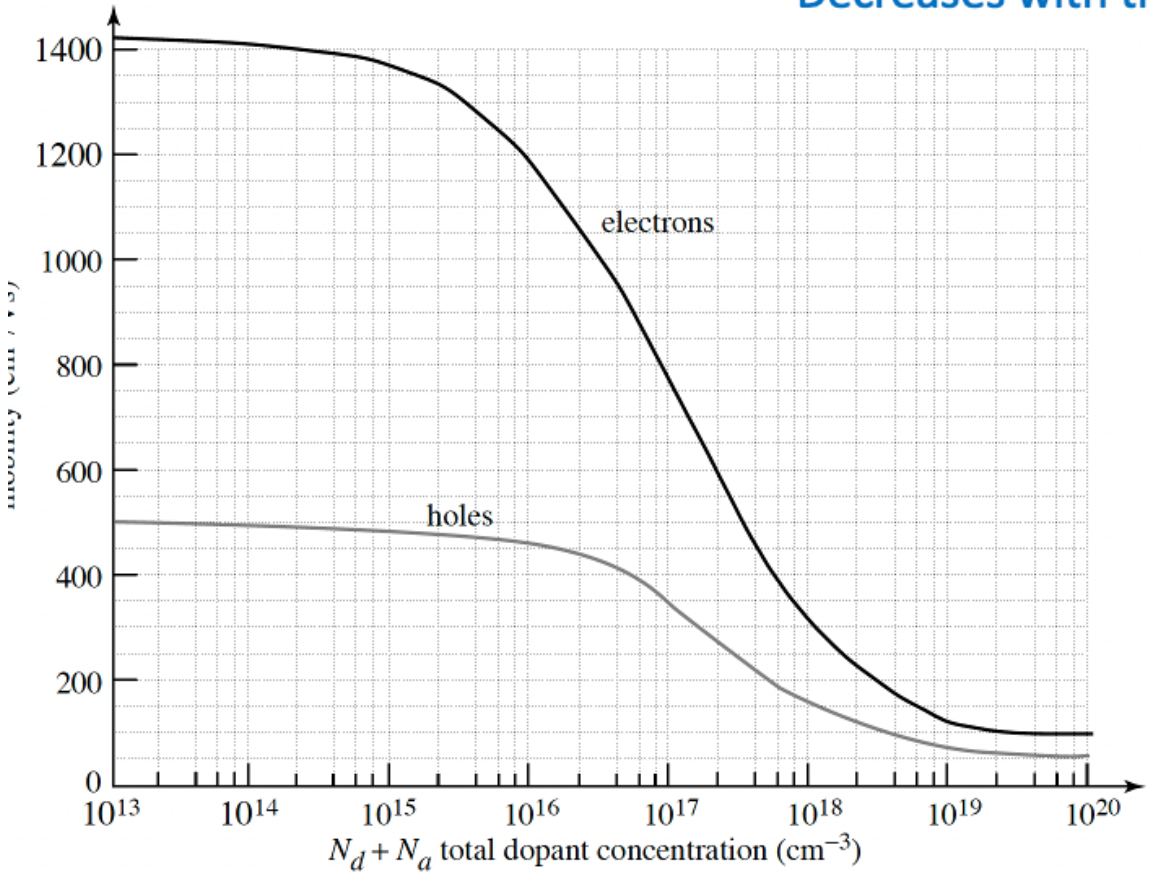
Electrical conduction: Drude model - 3

$$v_{dn} = -\mu_n E$$

$$v_{dp} = \mu_p E$$

$$\mu_{n,p} = \frac{q\tau_c}{2m_{n,p}} \equiv mobility\ [cm^2/V \cdot s]$$

Mobility is measure of *ease* of carrier drift
- Increases with longer time between collisions
- Decreases with the higher effective mass



Mobility for Si at 300K

mobility depends on doping

Holes are "heavier" than electrons

$$\tau_c \simeq 10^{-14} \sim 10^{-13}\ s \ \ll 1\text{ps}$$

$$v_{th} \simeq 10^7\ cm/s$$

$$\Rightarrow \lambda \simeq 1 \sim 10\ nm$$

Electrical conduction: Drude model - 4

Drift current density:

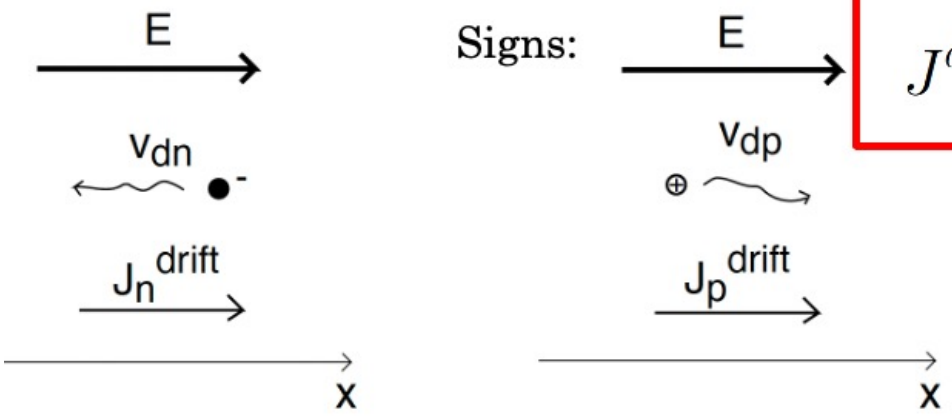
∝ carrier drift velocity

∝ carrier concentration

∝ carrier charge

$$J_n^{drift} = -qnv_{dn} = qn\mu_n E$$

$$J_p^{drift} = qpv_{dp} = qp\mu_p E$$



$$J^{drift} = J_n^{drift} + J_p^{drift} = q(n\mu_n + p\mu_p)E$$

Ohm's law:

$$J = \sigma E = \frac{E}{\rho}$$

$\sigma \equiv conductivity\ [\Omega^{-1} \cdot cm^{-1}]$

$\rho \equiv resistiviy\ [\Omega \cdot cm]$

$$\rho = \frac{1}{\sigma} = \frac{1}{q(n\mu_n + p\mu_p)}$$

Drude model for conductivity – simple relations, numbers

Ohm's law: $\boldsymbol{J} = \sigma \boldsymbol{E}$ where $\boldsymbol{J}$ is the current density, E is the electric field and σ is the conductivity. In microscopic terms,

$\sigma = nq\mu$ where μ is mobility of charge carriers.

$$\overline{v} = v_d = \pm\frac{qE}{2m_{n,p}}\tau_c = \pm\frac{q\tau_c}{2m_{n,p}}E \qquad \mu_{n,p} = \frac{q\tau_c}{2m_{n,p}} \equiv mobility\ [cm^2/V \cdot s]$$

Si at 300K: what is the mean free path?

$\tau_c \simeq 10^{-14} \sim 10^{-13}\ s \ll 1\text{ps}$

$v_{th} \simeq 10^7\ cm/s$

$\Rightarrow \lambda \simeq 1 \sim 10\ nm$

Electron mobility at 300K:
Si (300K) – about 1000 $cm^2/V\ s$
Metals like Cu, Ag – 30-50 $cm^2/V\ s$
GaAs - 10000 $cm^2/V\ s$

Ionic conducton - <1 $cm^2/V\ s$
GaAs/AlGaAs 2D gas:
Mobility below 4K can be 10^6-10^7 $cm^2/V\ s$

Limitations of the classic theory (Drude model)

- Drude model is a useful and important tool for understanding/describing charge transport, however, it has limitations
- Electrons are considered classic particles (like a gas), and their wave nature is not taken into account – problems at short distances
- Ballistic transport (small number of scattering events) is described differently
- Transport through barriers e.g. tunneling is described differently
- Transport at high electric fields may not be accurately described with Drud etheory
- The concept of electron/hole mobility is widely used in semiconductor device physics, very often, the mobility is considered as an empirical parameter (without any relation with electron/hole mass)