

- 1 Binding types
- 2 Crystal lattices
- 3 Lattice vibrations
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### Solids: Lattice vibrations

- Vibrational modes and phonons
- Brillouin and Raman scattering
- Inelastic neutron scattering
- Heat capacity of the crystal lattice
- Umklapp scattering

#### thermal conductivity of silicon



thermal conductivity

$$\vec{j} = -\kappa \nabla T$$



temperature gradient  $\nabla T$ 



The figure shows the thermal conductivity of silicon.

The formula outlined in red gives the definition of thermal conductivity.

When a temperature gradient is applied to a crystal, energy flows from the warm side to the cold side, i.e. in the opposite direction to the temperature gradient.

The energy flow  $\vec{j}$  is the energy density e times the energy flow velocity, i.e.  $\vec{j} = e\vec{v}$  and  $e = \partial E/\partial V$ .

The energy flow is measured in W/m<sup>2</sup>.

If the temperature difference is not too great, the energy flow  $\vec{j}$  is proportional to the temperature gradient  $\nabla T$ .

The constant of proportionality  $\kappa$  is the thermal conductivity.

- If there are no conduction electrons, the thermal energy is transported exclusively by phonons from areas of higher to lower temperature
- The flow of energy due to a temperature gradient is proportional to and opposite to the temperature gradient

$$\vec{j} = -\kappa \nabla T$$

Phonons are necessary for the transport of thermal energy. Therefore

 $\kappa 
ightarrow 0$  if T 
ightarrow 0

Phonons are scattered on impurities and grain-boundaries → the transport of thermal energy is diffusive



Silicon is a semiconductor, i.e. a very poor conductor with a low thermally activated conductivity.

The transport of thermal energy is dominated by the excitation of phonons.

Since more phonons are excited on the warm side of the sample than on the cold side, there is a net phonon flow from the warm to the cold side.

The phonons do not propagate undisturbed through the crystal lattice, but are scattered at impurities and imperfections in the crystal lattice, so that the energy transport through phonons has a diffusive character.

## Comment 2

Since the number of phonons decreases with decreasing temperature, it is plausible that the thermal conductivity decreases with decreasing temperature.

However, the thermal conductivity of silicon does not increase steadily with increasing temperature.

The thermal conductivity reaches a maximum at temperatures around 50 K and then decreases with increasing temperature.

The reason for the maximum is that at higher temperatures the phonons are not only scattered from lattice defects, but also from the lattice vibrations themselves.

Although the law of conservation of energy prevents most phonon-phonon scattering processes, phonon-phonon scattering becomes more common with increasing temperature.

phonon-phonon scattering at high temperatures

 $\hbar\omega(\vec{q}_1) + \hbar\omega(\vec{q}_2) = \hbar\omega(\vec{q}_3)$  and  $\vec{q}_1 + \vec{q}_2 + \vec{K} = \vec{q}_3$ 



Comment 1

### Umklapp scattering 3

The first formula gives the energy conservation law for the collision of two phonons that merge to a single new phonon.

The total energy before and after the scattering event must be the same.

The second formula gives the law of conservation of momentum, which in a crystal lattice can also contain a vector of the reciprocal lattice.

Since the momentum of a phonon is a crystal momentum, any vector of the reciprocal lattice can be added without changing the momentum of the phonon.

The figure shows the addition of the momenta of two phonons.

#### Comment 2

The addition of  $\vec{q}_1$  and  $\vec{q}_2$  results in the blue vector  $\vec{q}'_3$ , the tip of which protrudes into the neighboring Brillouin zone.

The addition of the reciprocal lattice vector  $\vec{K} = -\vec{b}_1 - \vec{b}_2$  brings the momentum of the phonon  $\vec{q}'_3$  in the neighboring Brillouin zone back into the original Brillouin zone.

The momentum of the associated phonon is  $\vec{q}_3$ , which points exactly in the opposite direction to  $\vec{q}'_3$ .

After this scattering event, the energy flows in the opposite direction.

Such scattering events are the reason that the thermal conductivity decreases again at higher temperatures after the maximum.



This explanation was given by Rudolf Peierls in 1929.

Peierls wrote, "...I used the German term Umklapp (flip-over) and this rather ugly word has remained in use...."

The umklapp scattering obviously hinders the transport of thermal energy and therefore leads to a reduction in thermal conductivity at high temperatures.

Although Rudolf Peierls was not awarded the Nobel Prize, he is very famous.

E.g. the building housing the sub-department of Theoretical Physics at the University of Oxford is formally named the Sir Rudolf Peierls Centre for Theoretical Physics.



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# Ohm's Law

### Electrons in crystal lattices

#### Electric conductivity and Ohm's law

- Drude model
- Sommerfeld model
- Bloch waves
- Energy bands and Fermi surfaces
- Photoemission Spectroscopy
- Electron dynamics and Electron hole bands
- Semiconductors
- Ferromagnetism
- Superconductivity

#### Most elements are metals at room temperature



Comment 1

## Electric conductivity and Ohm's law 1

Most elements of the periodic table form electrically conductive solids.

The only exception are the noble gases, which form insulating crystals held together by van der Waals forces.

In addition, the diatomic covalently bonded molecules of hydrogen, nitrogen, oxygen, fluorine and chlorine form insulating crystals at low temperatures due to the van der Waals force.

A notable exception is helium.

Helium atoms do not form molecules and condense at 4.2 K (<sup>4</sup>He) and 3.2 K (<sup>3</sup>He), respectively.

## Comment 2

Condensed helium forms a quantum liquid that remains liquid down to absolute zero.

The other elements marked in green form covalently bonded nonmetals.

The electric conductivity is poor.

These elements form semiconductors or semi-metals.



The drift velocity of the charge carriers results from the acceleration of the charges through the electric force  $m\vec{a} = q\vec{E}$  during the mean free time  $\tau$ 

$$\vec{v} = \frac{q}{m} \tau \vec{E}$$
  $\rightarrow$  electric mobility  $\mu : \vec{v} = \mu \vec{E}$ 

If the electric potential energy within a conductor depends on the location, then the charge carriers flow from the locations with high potential energy to locations with low potential energy.

The charge carriers gain kinetic energy

An electric field acts in the electric conductor, which accelerates the charge carriers.

Due to collisions with imperfections in the conductor, the charge carriers transfer part of the kinetic energy gained to the material of the conductor.

Between the collisions, the charge carriers move undisturbed and gain kinetic energy.

### Comment 1

The impact frequency is characterized by the reciprocal of the mean free flight time.

The mean free flight time determines the drift speed that the charge carriers can reach in the conductor.

The drift speed is superimposed on the "actual speed" of the charge carriers. The "actual speed" of the charge carriers is determined on the one hand by the thermal energy and on the other hand by quantum physics. The "actual speed" averages to zero, so that no electric current flows when no electric field is applied.

Since the drift speed is proportional to the electric field, the electric mobility  $\mu$  is defined:  $\vec{v} = \mu \vec{E}$ .

## Comment 2



Charge density

$$\rho = \frac{1}{V} \sum_{i} q_i$$

Charge that flows through the area A in the time interval  $\Delta t$ 

 $\Delta \mathbf{Q} = \boldsymbol{\rho} \, \mathbf{v} \, \mathbf{A} \, \Delta t$ 

electric current

$$I = \frac{\Delta \mathbf{Q}}{\Delta t} = \rho \, v \, A$$

electric current density

It makes sense to define a charge density in terms of the density of charge carriers and the charge they carry.

The charge that can flow through a cross-sectional area A during a time interval  $\Delta t$  can be easily calculated using the charge density and the drift velocity of the charge carriers.

The equation underlined in red formulates the relationship between the charge  $\Delta Q$  that flows through the cross-section *A* per unit of time and the charge density and the drift velocity.

The electric current is defined as the quotient of the charge  $\Delta Q$  and the time interval  $\Delta t$ .

The product of the charge density  $\rho$  and the drift velocity of the charge carriers results in the current density *j*.

#### Comment 1

## Comment 2

Note that the sign of the charge does not affect the electric current *I* and the electric current density  $j = \rho v$ .

Negative carriers have a negative charge density and a drift velocity opposite to that of positive carriers.

Therefore the product  $\rho \cdot v$  is independent of the sign of the charge carriers.

#### Hans Christian Ørsted 1820



(Oerstedversuch.mp4)

In 1826, Georg Ohm was the first to systematically investigate the relationship between electric current and the potential difference between the ends of a conductor.

To measure the strength of the electric current, he used an effect discovered by Hans Christian Ørsted in 1820.

Magnetic needles that are close to a conductor can change orientation when an electric current flows through the conductor.

If the magnetic needle is attached to the end of a torsion thread, even small electric currents can be measured very sensitively.

The video shows the Ørsted experiment.

### Comment 1

## Comment 2

In 1826, finding a suitable current or voltage source was a major problem for Georg Ohm.

The electrochemical batteries of that time were gassing and bubbling, causing the voltage and current to fluctuate wildly.

Under such conditions, the current cannot be measured with a magnetic needle.

#### Thomas Johann Seebeck discovered the thermoelectric voltage in 1821





(Thermospannung.mp4)

Comment 1

### Electric conductivity and Ohm's law 5

Finally, Georg Ohm used thermocouples for his measurements.

The video shows the generation of a voltage with a thermocouple.

Johannes Seebeck discovered in 1821 that the charge carriers diffuse from the warm to the cold end of a conductor when there is a temperature difference.

Johannes Seebeck discovered that the diffusion of charge carriers depends on the type of metal.

If the connection point between two wires made of different metals is heated, the charge carriers can diffuse to the wire ends at different speeds.

Comment 2

## Electric conductivity and Ohm's law 5

The charge accumulates at different levels at the ends of the wires, so that a voltage builds up between the contacts, which can drive an electric current.

In the video, the symmetric combination BAB was chosen to show that the sign of the voltage reverses when the other junction is heated.

When several thermocouples are connected in series, the thermal voltages add up.

A constant electric current can be driven by a temperature gradient with a thermocouple.

Ohm's law (1826)

The electric current density j is proportional to the electric field strength E

$$j = \sigma E$$

 $\sigma$  is the conductivity of the metal and with I = jA and  $U = E\ell$ 

$$I = jA = \frac{A}{\ell}\sigma E\ell \quad \rightarrow \quad I = GU \quad \text{or} \quad U = RI \quad \text{with} \quad R = G^{-1}$$
electric conductance *G* and resistance *R*
$$G = \frac{A}{\ell}\sigma \qquad \text{and} \qquad R = \frac{\ell}{A}\rho \quad \text{and} \quad \rho = \sigma^{-1}$$

Comment 1

## Electric conductivity and Ohm's law 6

Georg Ohm's measurements showed that the electric current density in a metal is proportional to the electric field strength.

Although this result seems very plausible, it took ten years for Ohm's law to become generally accepted.

The first formula outlined in red gives Ohm's law.

 $\sigma$  is the electric conductivity of the metal.

Multiplying the current density by the cross-sectional area of the wire gives the electric current *I* and multiplying the electric field strength by the length  $\ell$  of the wire gives the electric voltage *U*.

This results in the second formula outlined in red: The electric current is proportional to the applied voltage.

The proportionality constant *G* is the electric conductance.

The greater the conductivity  $\sigma$  and the larger the cross-section A of the wire, the greater the conductance G.

The longer the wire, the smaller the conductance.

The formula underlined in red summarizes this relationship.

The third formula, outlined in red, is probably the best-known version of Ohm's law.

The resistance *R* is the reciprocal of the conductance *G* and the resistivity  $\rho$  the reciprocal of the conductivity  $\sigma$ .

### Comment 2

If there is one type of charge carriers in a conductor with the charge q and the density n = N/V, then the current density is  $j = \rho v$ 

$$j = q \frac{N}{V} v$$

with the drift speed  $v = \frac{q}{m}\tau E = \mu E$  and Ohm's law

$$j=qrac{N}{V}rac{q}{m} au E$$
 and  $j=\sigma E$ 

electric conductivity

$$\sigma = rac{q^2}{m}rac{N}{V}\cdot au$$
 and  $\sigma = qrac{N}{V}\mu$   $(\mu = rac{q}{m} au)$ 

Comment 1

## Electric conductivity and Ohm's law 7

If the charge carrier density is known, the mean free time  $\tau$  of the charge carriers can be derived from the electric conductivity.

Inserting the formula for the drift velocity into the formula for the current density *j* results in Ohm's law and from it the formula for the electric conductivity, outlined in red.

The mean free time  $\tau$  can be calculated from the electric conductivity.

The mean free time and the electric field strength can then be used to calculate the drift velocity if the mass of the charge carriers is known.

It should be noted that the drift velocity is not the "actual speed" of the charge carriers.

The charge carriers can move back and forth at high speed without an electric current flowing.

The drift velocity is the average of all charge carrier velocities and is caused by the electric field.

The mean free time between two collisions can therefore not provide any information about the microscopic movement and the "actual speed" of the charge carriers.

The formula outlined in red is therefore completely general and independent of any microscopic theory of the charge carriers.

#### Comment 2

	valency	<i>N/V</i> [cm <sup>-3</sup> ]	<i>ρ</i> [nΩ· m]	μ [m <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> ]	au [10 <sup>-15</sup> s]
Li	1	$4.70\cdot 10^{22}$	92.8	1.43·10 <sup>−3</sup>	7.96
Rb	1	$1.15\cdot 10^{22}$	128.0	4.25·10 <sup>-3</sup>	23.6
Cu	1	$8.45\cdot 10^{22}$	16.8	4.40·10 <sup>-3</sup>	24.5
Au	1	$5.90\cdot 10^{22}$	22.1	4.79·10 <sup>−3</sup>	26.6
Ве	2	$24.20\cdot 10^{22}$	36.0	7.17·10 <sup>−3</sup>	4.0
Zn	2	$13.10\cdot10^{22}$	59.0	0.81·10 <sup>-3</sup>	4.5
AI	3	$18.06 \cdot 10^{22}$	26.5	1.31·10 <sup>-3</sup>	7.25
Pb	4	$13.20\cdot10^{22}$	208.0	0.23·10 <sup>-3</sup>	1.3

The table gives the valence, electron density, specific resistance, electric mobility and the mean free flight time for some metals.

The drift speed of the electrons can be calculated with the mobility.

If a voltage of 100 V is applied to a 1 meter long cable, the electric field strength is 100 V/m.

At this electric field strength, the drift velocity for all metals is less than 1 m/s.



#### Summary of Ohm's law





#### Drift velocity

#### The drift velocity of the charge carriers is in the range of 1 m/s

#### Collision rate

 $\tau^{-1} \approx 10^{15} \, \mathrm{s}^{-1}$  (frequency of visible and UV light!)

Comment

## Electric conductivity and Ohm's law 9

Noteworthy are two results that follow from Ohm's law.

The drift velocity of the charge carriers is extremely small and is only a few cm/s.

The collision rate of charge carriers is extremely high.

 $\tau^{-1}$  is in the frequency range of light in the visible and ultraviolet range of the electromagnetic spectrum.

# Revision

## Summary in Questions

- 1. What is the basic idea of the Drude model of metallic conductivity?
- 2. Calculate the drift velocity of conduction electrons in copper when a voltage of 220 V is applied to a wire 1 m long.
- 3. What does Ohm's law say?
- 4. Write down the formula for electric conductivity. What does the parameter  $\tau$  mean?