Lectures on Materials Science - Material properties

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Parts of the script are adopted from
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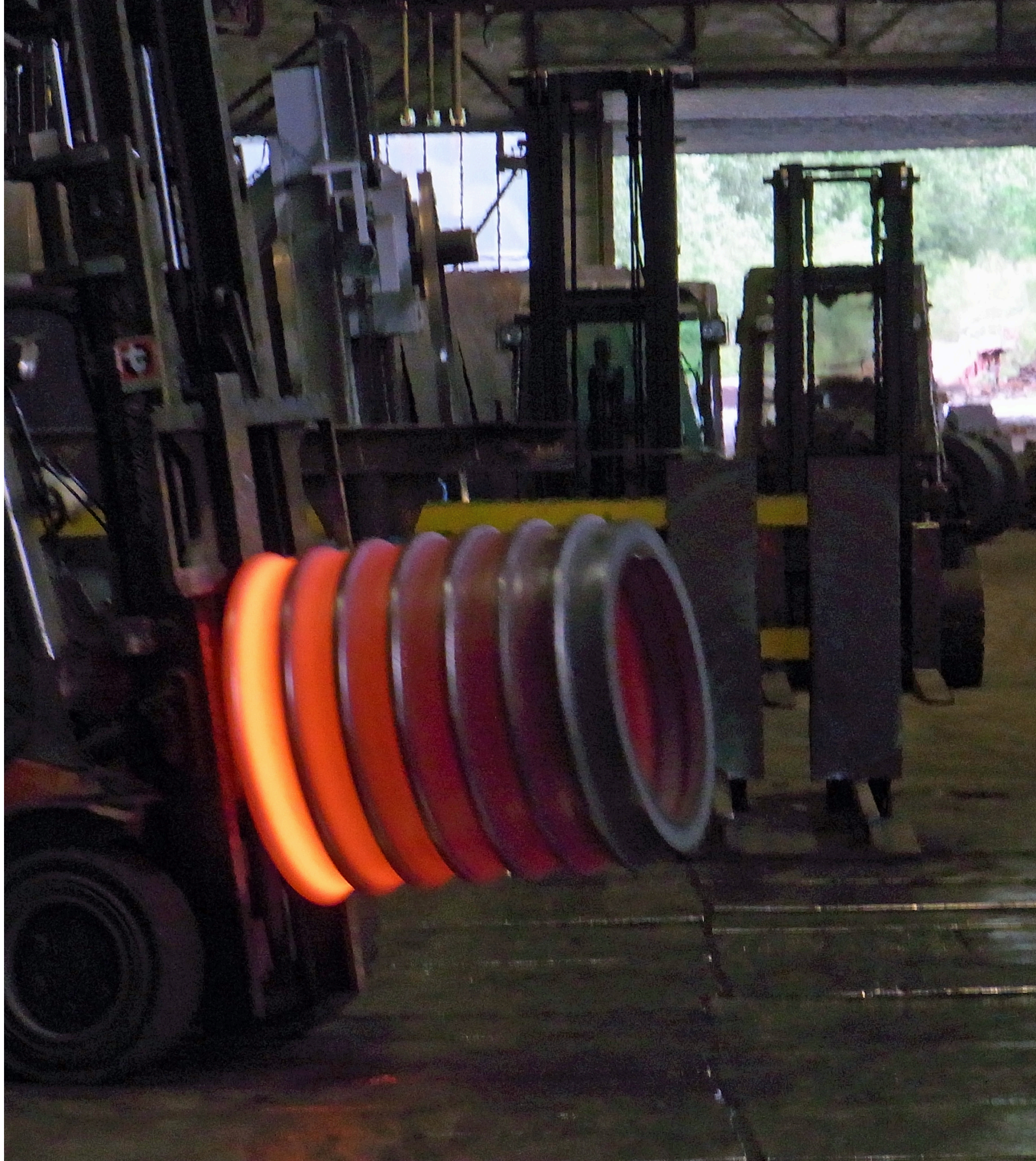


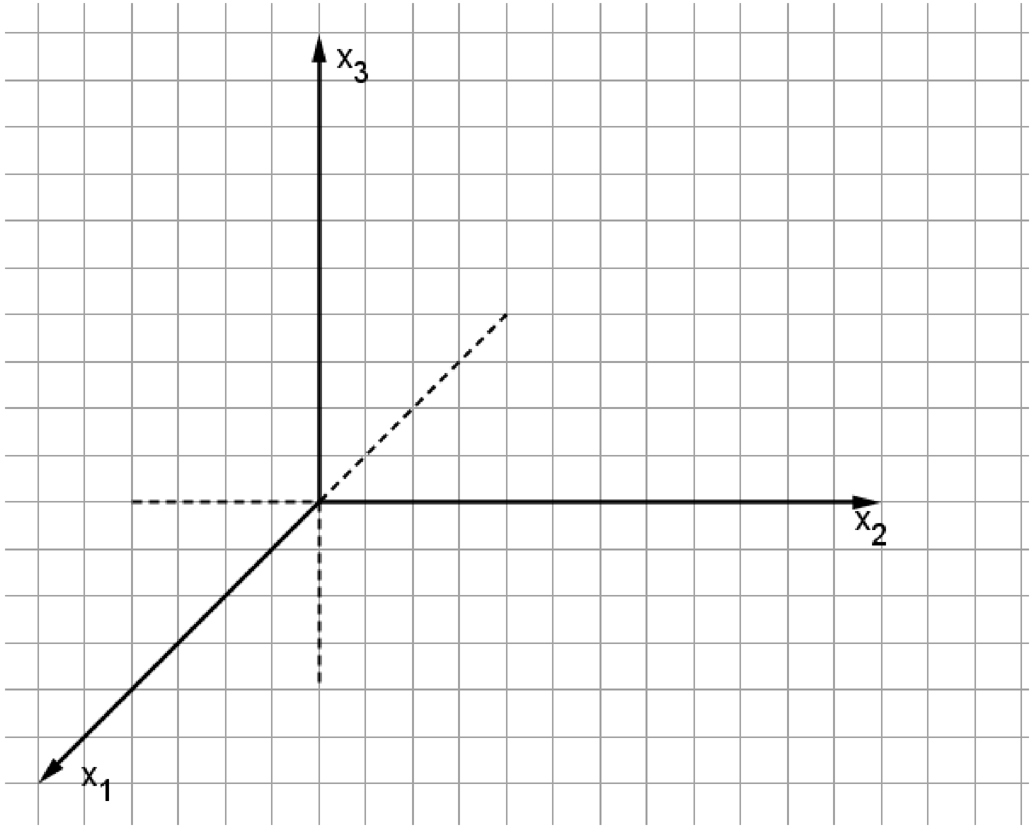
Topics

Material Properties

- What are material properties?

Symmetry

- Isotropy
- Transverse Isotropy
- Orthotropy
- …
- Anisotropy



Mechanical Properties

- **Reversible** deformation, where immediately or after a certain time following the application of external load, the deformed material returns to its original shape: elastic and viscoelastic deformation.
- **Irreversible (permanent)** deformation, where the shape change remains even after the external load is removed: plastic and viscous deformation.
- Fracture, i.e., separation of the material caused by the formation and propagation of cracks.

Simulation Example

External Link

Reminder: Concept of Stress - Strain

- Geometry-independent characteristics
- How can one determine a characteristic that is defined solely by the material?
- Example: Density

Elasticity

- Reversible, energy-preserving
- Hooke's Law 1D

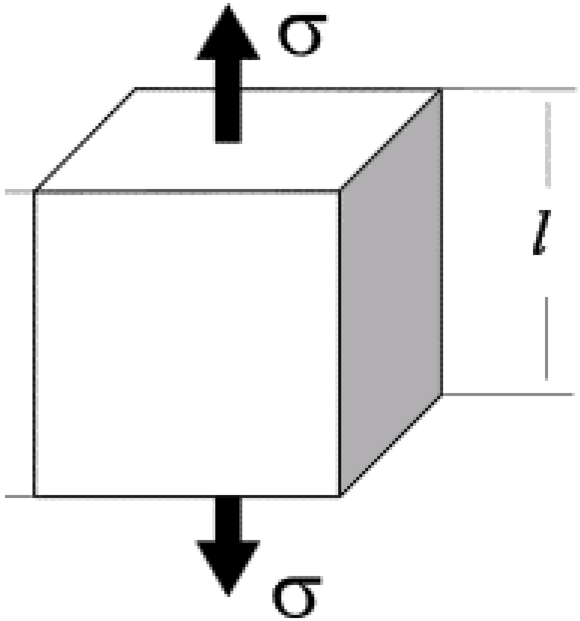
  Normal stress $\sigma = E\varepsilon$

  Shear stress $\tau = G\gamma$
- Hooke's Law 2D or 3D

  $\boldsymbol{\sigma} = \mathbf{C}\boldsymbol{\varepsilon}$

Basics

- Normal strain [-]
  $\varepsilon_{mechanical} = \frac{l-l_0}{l_0}$
- Normal stress $\left[\frac{N}{m^2}\right]$, $[Pa]$
  $\sigma = \frac{F}{A} = E\varepsilon$
  E - Elastic modulus, Young's modulus $\left[\frac{N}{m^2}\right]$



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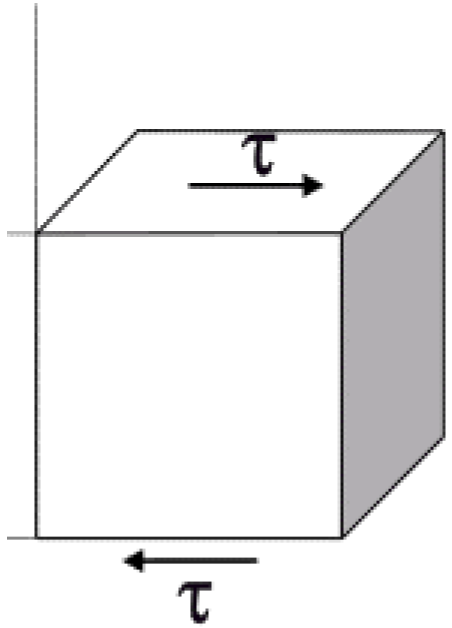
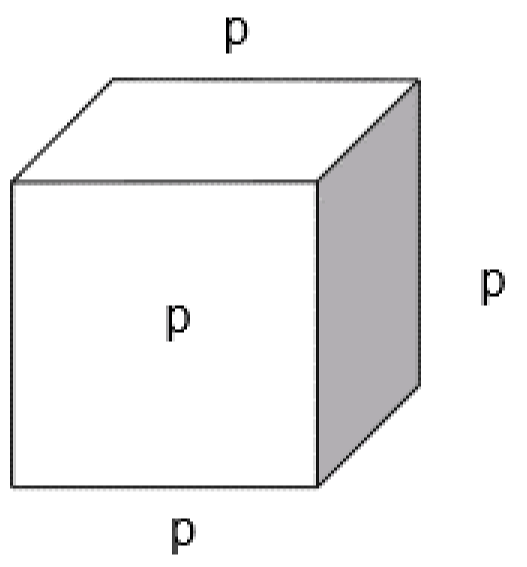
Basics

- Shear strain [-]
  $\varepsilon = \frac{1}{2}(\frac{u_x}{l_0} + \frac{u_y}{b_0}) = \frac{\gamma}{2}$
- Shear stress $\left[\frac{N}{m^2}\right]$, $[Pa]$
  $\tau = \frac{F_s}{A} = G\gamma$
- Normal and shear stresses are not compatible, leading to the concept of equivalent stresses -> Engineering Mechanics
- G - Shear modulus $\left[\frac{N}{m^2}\right]$



Basics

- Poisson's ratio [-]
  $\nu = -\frac{\varepsilon_y}{\varepsilon_x}$
  for homogeneous materials $0 \leq \nu \leq 0.5$
  for heterogeneous materials, other configurations are possible
- Bulk modulus $K = \frac{E}{3(1-2\nu)}$
- Shear modulus $K = \frac{E}{2(1+\nu)}$



Material Examples

Material	E [GPa]	G [GPa]	$\nu [-]$
Unalloyed steel	200	77	0.30
Titanium	110	40	0.36
Copper	120	45	0.35
Aluminum	70	26	0.34
Magnesium	45	17	0.27
Tungsten	360	130	0.35
Cast iron with lamellar graphite	120	60	0.25
Brass	100	35	0.35

Stiffness

- How are material properties related to stiffness?

Image reference

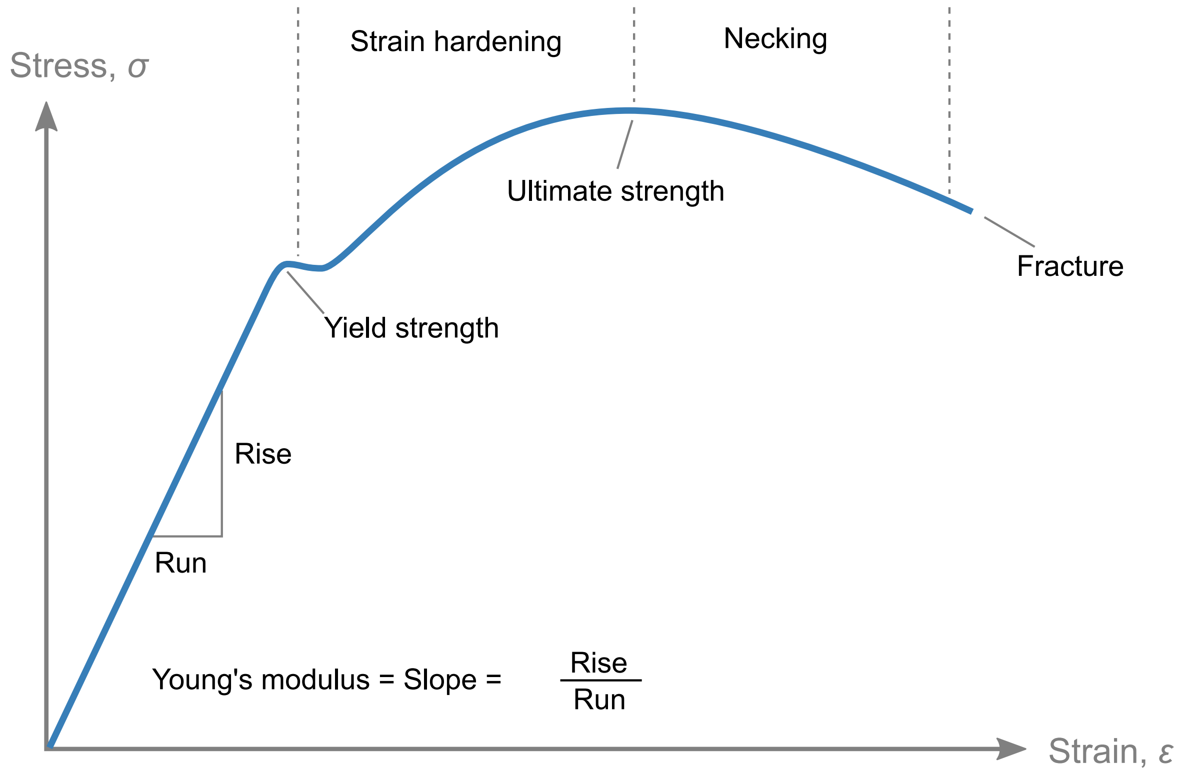
Reminder: Strength

The strength of a material describes its ability to withstand mechanical loads before failure occurs and is expressed as mechanical stress $[N/m^2]$. Failure can involve **unacceptable deformation**, particularly **plastic (permanent) deformation**, or **fracture**.

> Important: Strength $\neq$ Stiffness

Reminder: Stress-Strain relation in a ductile material

Datasheet

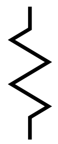


Viscous Behavior

- Reversible
- Time-dependent

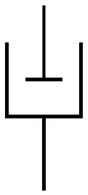
Spring model $\sigma = E\epsilon$

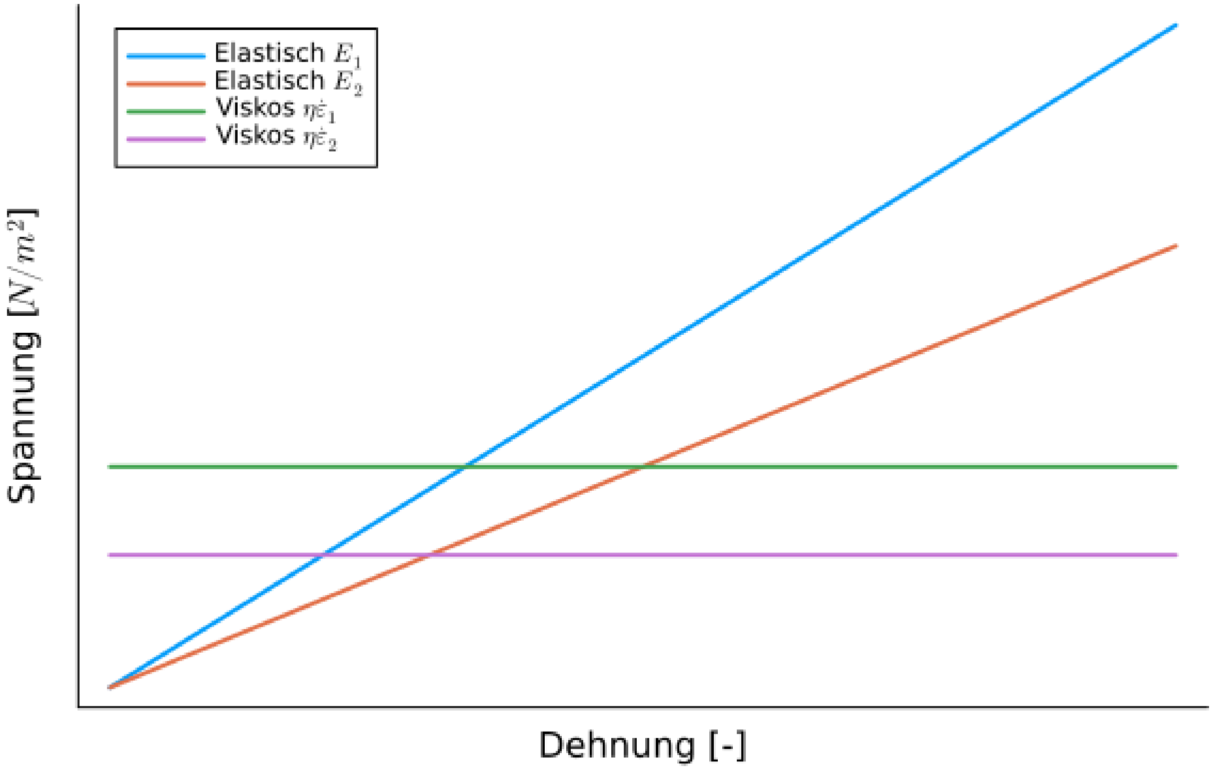
- Elastic component
- Represented by spring elements

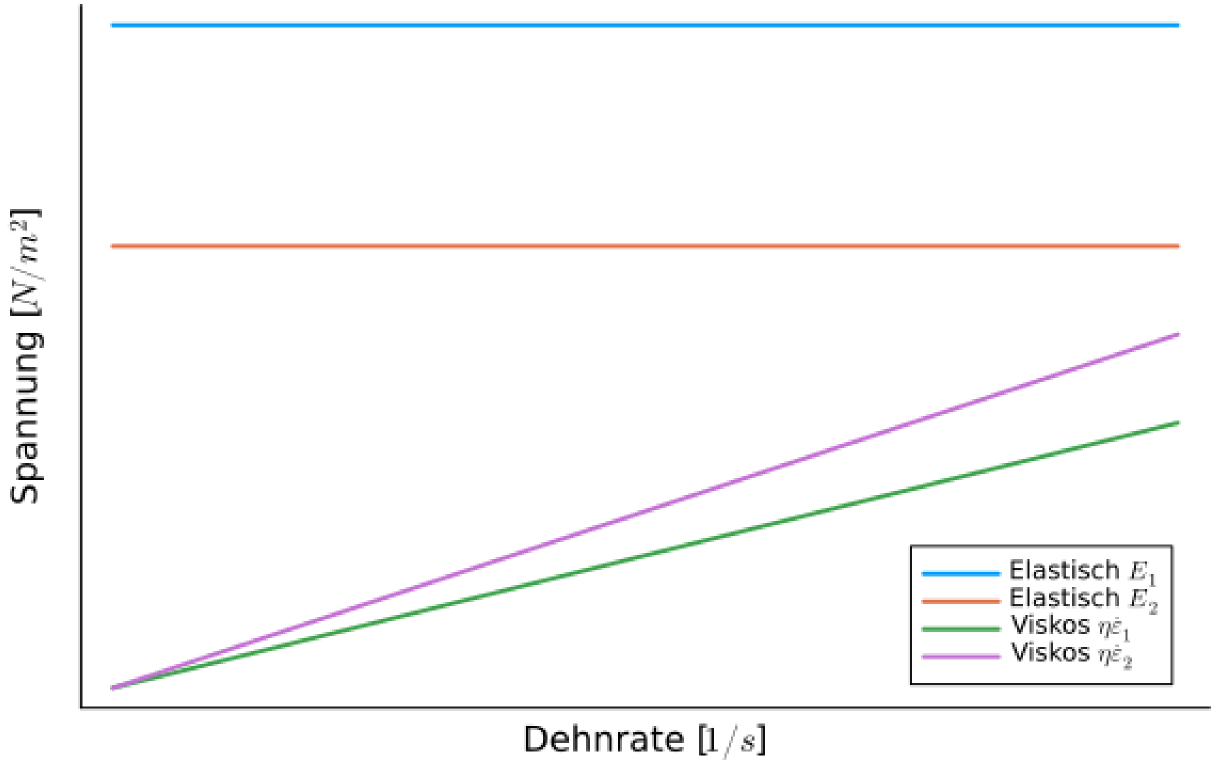


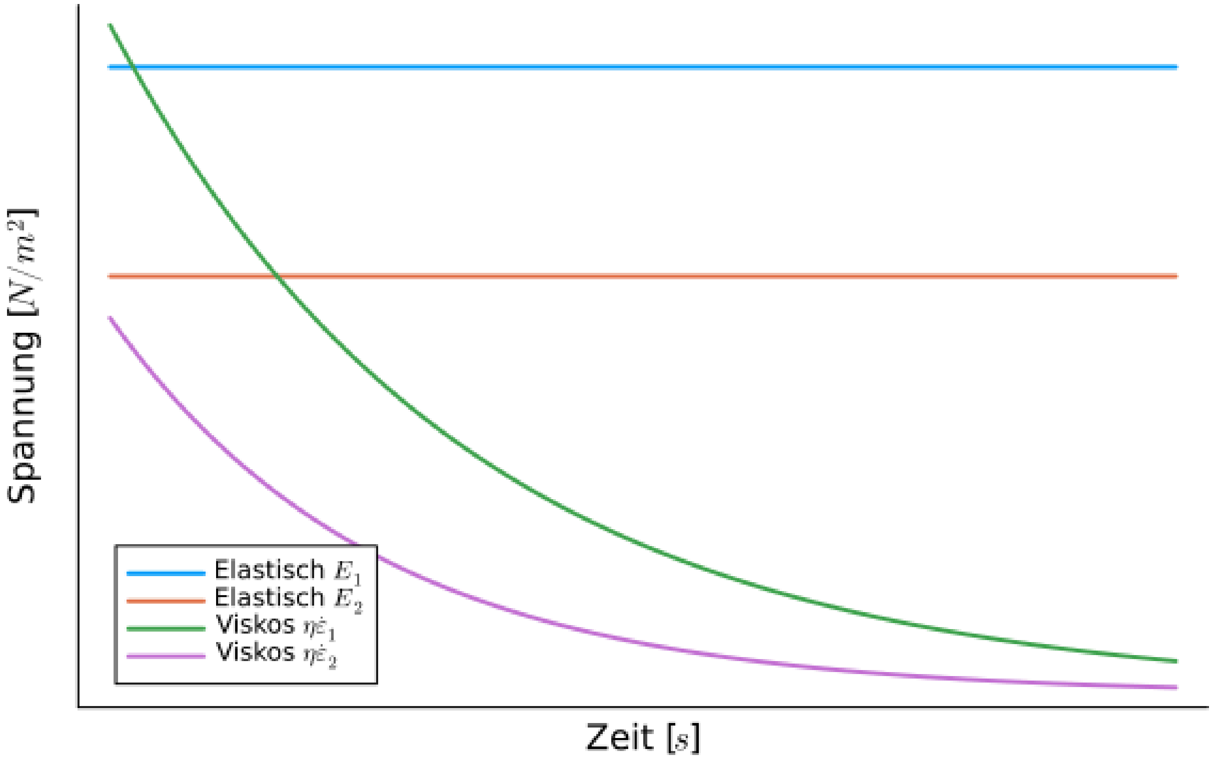
Damper $\sigma = \eta\dot{\epsilon} = \eta\frac{\partial\epsilon}{\partial t}$

- Viscous component
- Represented by damper elements

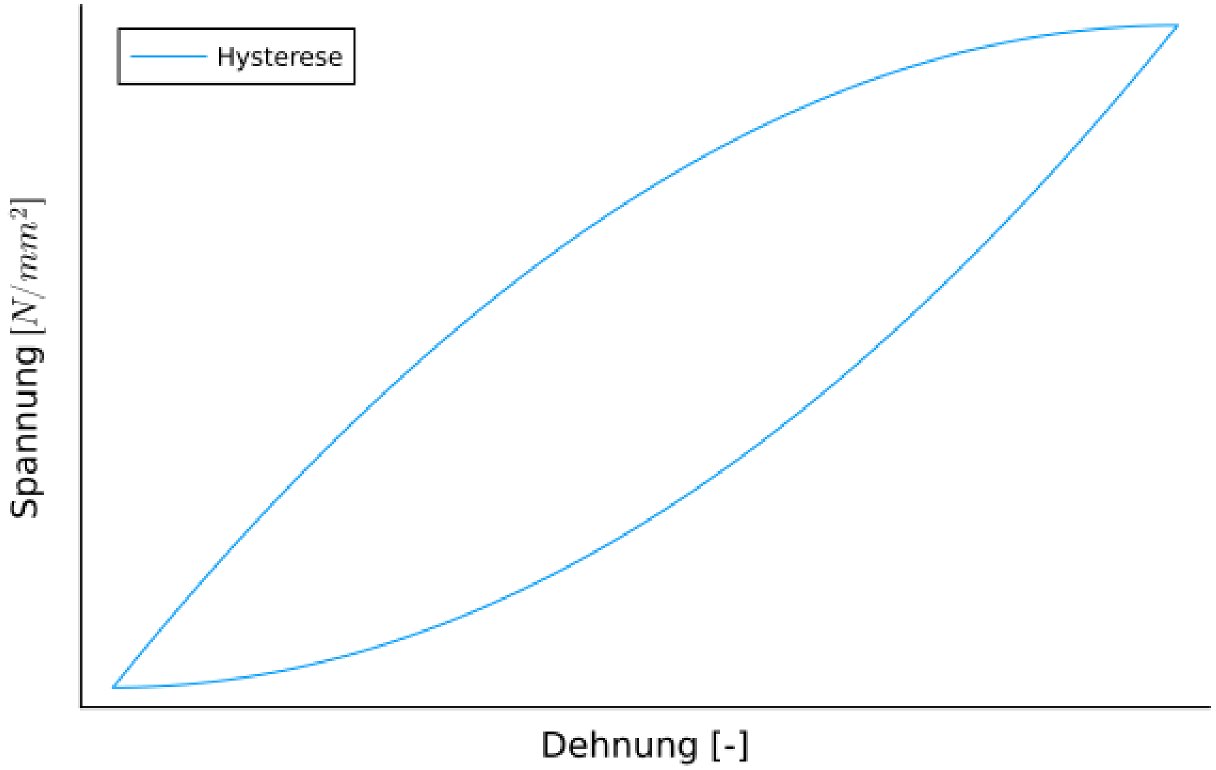



Elastisch E_1
Elastisch E_2
Viskos $\eta\dot{\varepsilon}_1$
Viskos $\eta\dot{\varepsilon}_2$
Spannung $[N/m^2]$
Dehnung [-]


Elastisch E_1
Elastisch E_2
Viskos $\eta\dot{\varepsilon}_1$
Viskos $\eta\dot{\varepsilon}_2$
Spannung $[N/m^2]$
Dehnrate $[1/s]$



Spannung $[N/m^2]$
Elastisch E_1
Elastisch E_2
Viskos $\eta\dot{\varepsilon}_1$
Viskos $\eta\dot{\varepsilon}_2$
Zeit $[s]$



Hysterese
Spannung $[N/mm^2]$
Dehnung [-]

Thermal Properties

Thermal Expansion

$$\boldsymbol{\varepsilon}_{thermal} = -\boldsymbol{\alpha}\Delta T$$

Thermal Expansion Coefficient Matrix

$$\boldsymbol{\alpha} = \begin{bmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{12} & \alpha_{22} & \alpha_{23} \\ \alpha_{13} & \alpha_{23} & \alpha_{33} \end{bmatrix}$$

1D or Isotropic

$$\varepsilon_{thermal} = -\alpha\Delta T$$

Symmetry	Model	Examples
Isotropy	$\alpha_{11} = \alpha_{22} = \alpha_{33}$ and $\alpha_{12} = \alpha_{13} = \alpha_{23} = 0$	Metals, Plastics
Transverse Isotropy	$\alpha_{22} = \alpha_{33}$ and $\alpha_{12} = \alpha_{13} = \alpha_{23} = 0$	Single-layer Fiber Composite
Orthotropy	$\alpha_{12} = \alpha_{13} = \alpha_{23} = 0$	Multilayer Fiber Composite
Anisotropy	Arbitrary α_{ij}	Homogenized view of an asymmetric multilayer composite

Thermal Properties

- Bi-metal strips
- Bridges
- Rails
- High-precision measurement devices
- Welding, soldering, etc.
- ...

May lead to thermal residual stresses, distortion, etc.

Example: Thermal Stresses 1D

$$\sigma = E\varepsilon = E(\varepsilon_{mechanical} + \varepsilon_{thermal}) = E(\varepsilon_{mechanical} - \alpha\Delta T)$$

> Pre-stretching can reduce the load on a component.

Example: Thermal Length Change 1D

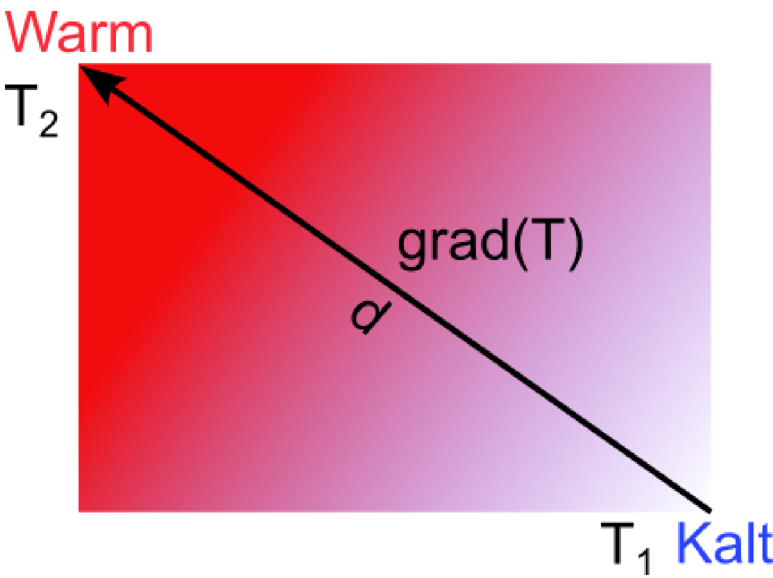
$$\Delta l = l_0\varepsilon_{mechanical}$$

> For free expansion, i.e., no stresses are acting.

$$0 = E\varepsilon = E(\varepsilon_{mechanical} + \varepsilon_{thermal}) = E(\varepsilon_{mechanical} - \alpha\Delta T)$$
$$\varepsilon_{mechanical} = \alpha\Delta T$$
$$\Delta l = l_0\varepsilon_{thermal} = l_0\alpha\Delta T$$

Heat Conduction

- Also conduction and heat diffusion
- $T_{high} \rightarrow T_{low}$ (2nd Law of Thermodynamics)
- No heat is lost due to energy conservation (1st Law of Thermodynamics)



Heat Flux $[W]$

$$\dot{\mathbf{q}} = -\boldsymbol{\lambda}\mathrm{grad}(T)$$

- $\mathrm{grad}(T)$ is the gradient of temperature change $\frac{\partial T}{\partial dx_i}$;
- In the linear case $\mathrm{grad}(T) = \Delta T/d = \frac{T_2 - T_1}{d}$

$$\dot{\mathbf{q}} = -\boldsymbol{\lambda}\mathrm{grad}(T)$$

$$\dot{\mathbf{q}} = \frac{\partial \mathbf{q}}{\partial t}$$

- Indicates that something changes -> dt

$$\boldsymbol{\lambda} = \begin{bmatrix} \lambda_{11} & 0 & 0 \\ 0 & \lambda_{22} & 0 \\ 0 & 0 & \lambda_{33} \end{bmatrix}$$

is the matrix of thermal conductivity.

Special Cases

- When $T_1 = T_2$, there is no conduction.
- When $\boldsymbol{\lambda} = 0$, perfect insulation, no heat conduction.

Symmetry	Model	Examples
Isotropy	$\lambda_{11} = \lambda_{22} = \lambda_{33}$	Metals, Plastics
Transverse Isotropy	$\lambda_{22} = \lambda_{33}$	Single-layer Fiber Composite
Anisotropy	Arbitrary λ_{ij}	Multilayer Fiber Composite

> Example -> Paraview

Heat Transfer

Transfer of heat from a solid body to a fluid or gas.

> Important when machines need to be cooled or heated.

Described by the heat transfer coefficient $\alpha_{transfer}$. It depends, among other things, on the specific heat capacity, density, and thermal conductivity of both the heat-removing and heat-delivering medium.

$$\dot{q} = \alpha_{transfer} A \Delta T$$

> Example: Heat pump and underfloor heating.

Specific Heat Capacity

Indicates how much energy in the form of heat needs to be stored in a material to increase its temperature.

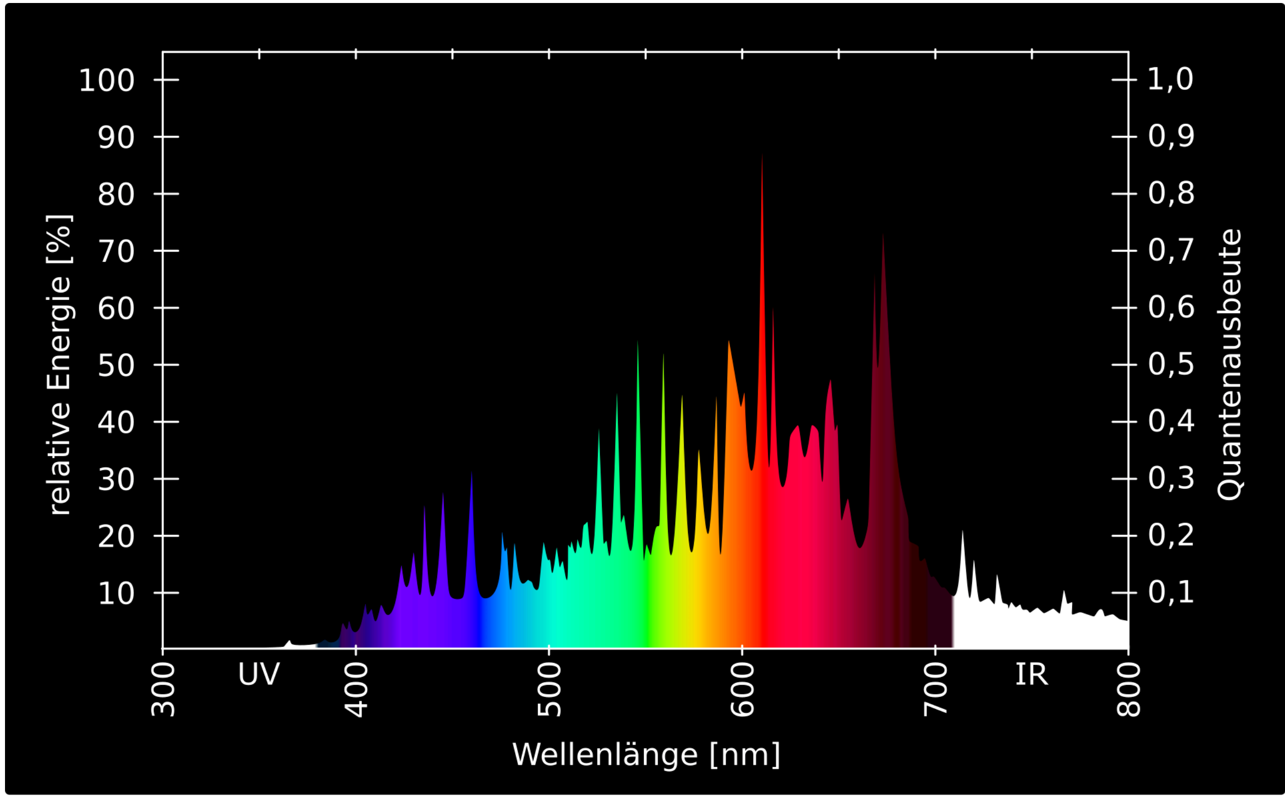
$$C_p = \frac{\Delta q}{m \Delta T}$$

Thermal Radiation

$$\dot{q} = \epsilon_{emissivity} \sigma_{Stefan-Boltzmann} A T^4$$

The emissivity $\epsilon_{emissivity}$ ranges from 0 (perfect mirror) to 1 (ideal black body) and is partially material-dependent.

> Useful for spectral analysis to determine the composition of materials.



Special Temperatures

Phase Transition Temperature

The temperature where a phase transition in a crystal structure occurs (see Phase Diagrams). Significantly influenced by added substances (see Alloys).

Melting Temperature

The temperature at which a material transitions from a solid to a liquid state.

Boiling Temperature

The temperature at which the phase transition from liquid to gas occurs. Relevant for lubricants, for example.

Curie Temperature

Named after Pierre Curie. Refers to the temperature at which ferromagnetic or ferroelectric properties of a material completely disappear, so that above it, they are only paramagnetic or paraelectric.

Residual Stresses

- Thermal
- Deformation
- Microstructural Transformation
- Chemical

Electrical and Magnetic Properties

Electrical and magnetic properties are generally closely related and influence each other.

Permittivity

Describes the relationship between electric flux density and the electric field.

ε_0 is the permittivity in a vacuum.

$$\mathbf{D} = \varepsilon_0 \, \boldsymbol{\varepsilon}_{permittivity} \, \mathbf{E}$$

$$\boldsymbol{\varepsilon}_{permittivity} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{bmatrix}$$

Depending on the crystal structure, permittivity may be direction-dependent.

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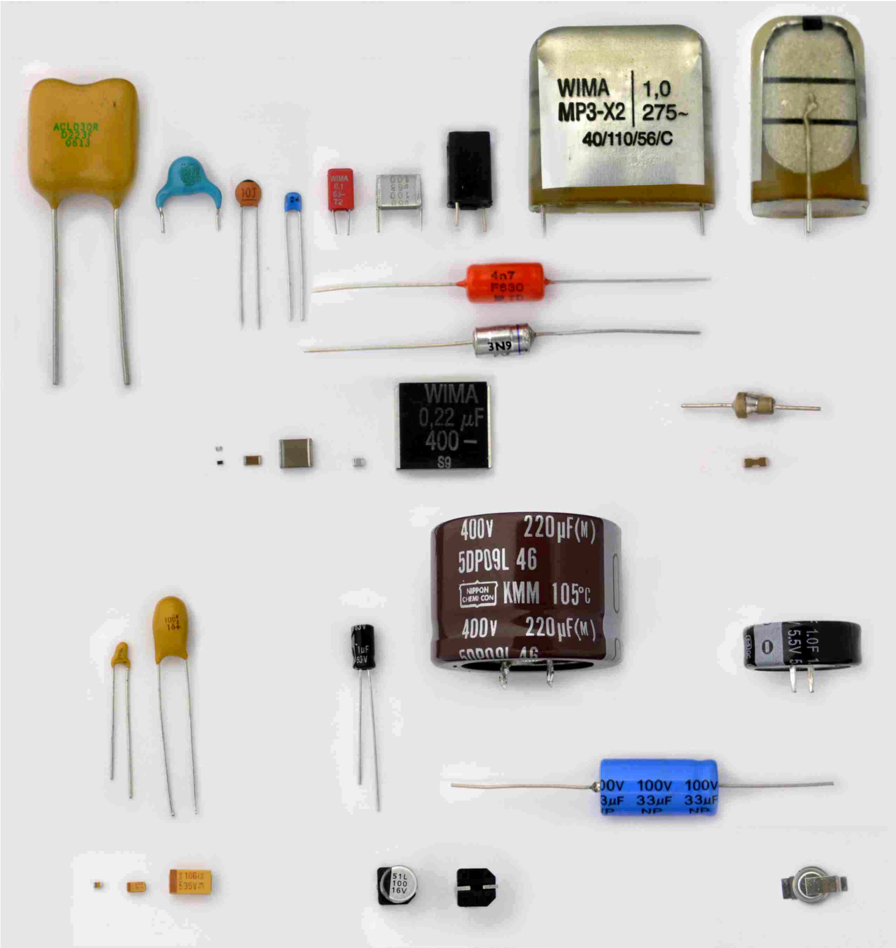
Often specified as relative permittivity

$$\varepsilon_r = \frac{\varepsilon_{permittivity}}{\varepsilon_0}$$

- Capacitance of a plate capacitor

$$C = \varepsilon_0 \, \varepsilon_r \, \frac{A}{d}$$

- High permittivity allows stronger capacitors.



Electrical Conductivity

- The conductivity of a substance or mixture depends on the availability and density of mobile charge carriers.
- In metals, these are loosely bound in the form of electrons. All materials have some level of conductivity.

Unit $\left[\frac{S}{m}, \frac{\Omega}{m}\right]$

$$\mathbf{J} = \sigma_{electrical\ conductivity}\,\mathbf{E}$$

- Superconductors possess infinite conductivity.

Electrical Resistance

- In the case of constant electrical conductivity, this corresponds to Ohm's law.

Ohm's Law

$$R = \frac{U}{I} = \rho_{specific} \frac{l}{A}$$

- The specific resistance $\rho_{specific}$ is a material constant. It is temperature-dependent.
- Used for thermocouples.

Conductors - metals (copper, silver, etc.), graphite

$$\rho_{specific} < 100 \, \frac{\Omega \, mm^2}{m}$$

Semiconductors - silicon, boron, selenium, ...

$$100 < \rho_{specific} < 10^{12} \, \frac{\Omega \, mm^2}{m}$$

Insulators - aluminum oxide ceramics, epoxy resins

$$\rho_{specific} > 10^{12} \, \frac{\Omega \, mm^2}{m}$$

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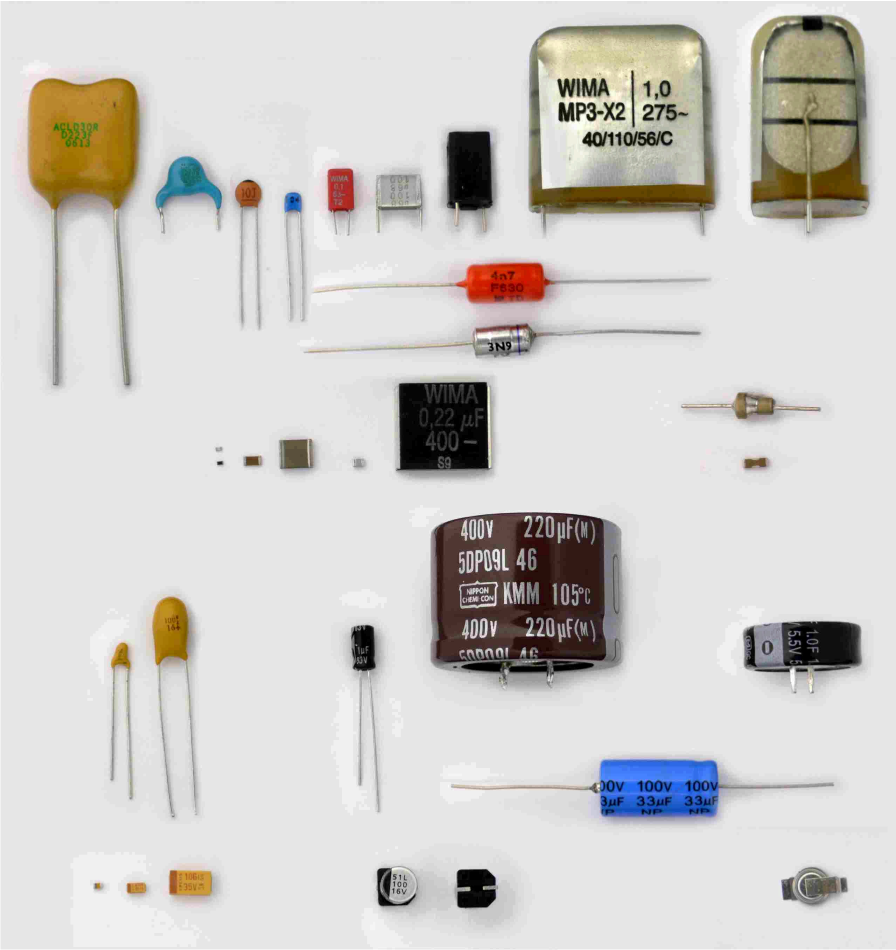

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Doping

- The conductivity of semiconductors can be significantly influenced by doping, often by several orders of magnitude.
- High-purity material is required.

n-doping - Addition of electron donors (extra electrons)
p-doping - Addition of electron acceptors

- p-doping creates electron deficiencies, also known as holes or defect electrons.
- These enable the conduction of electric current.
- Conductivity occurs because the holes or electrons are mobile, though not as mobile as electrons in metals.

Magnetism

Types of Magnetism

Diamagnetism

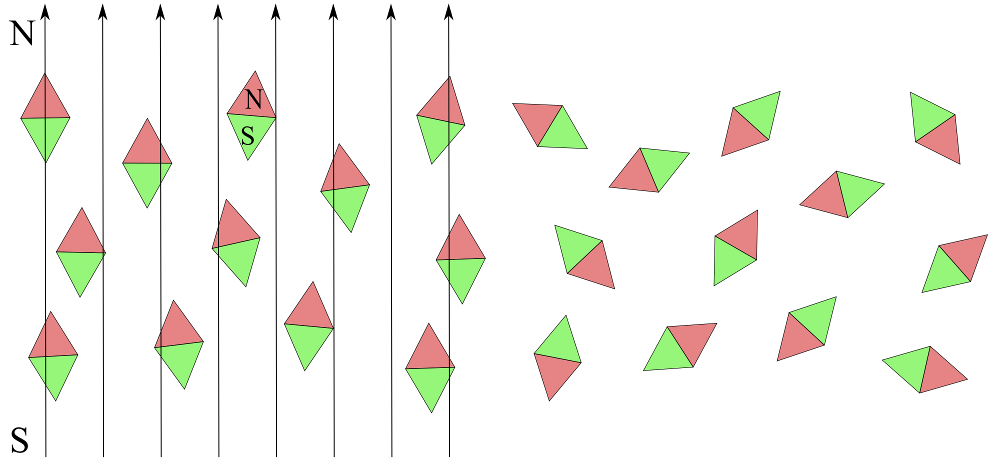
Leads to a weakening of the magnetic field due to the Lenz's law effect in the atomic shell (locally induced magnetic field opposes the external field).

Examples: All materials

Paramagnetism

- Atoms, ions, or molecules have a magnetic moment that aligns with the external magnetic field, strengthening the field.
- Higher temperatures reduce the effect as atoms, ions, or molecules move more freely.

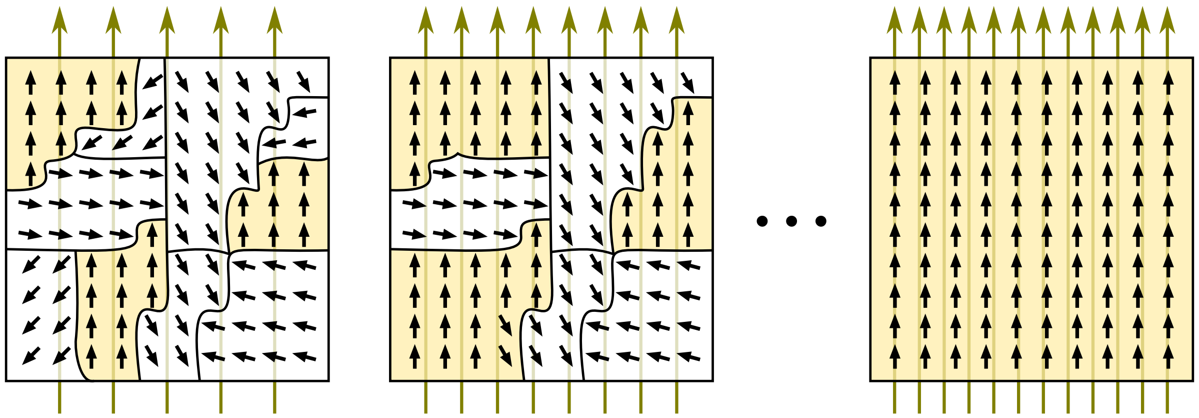
Examples: Lithium, sodium, rare earth metals (scandium, neodymium, holmium)



Ferromagnetism

- The magnetic moments align spontaneously in parallel.
- The smallest crystalline unit is called a **Weiss domain**.
- The effect can be destroyed by the Curie temperature.

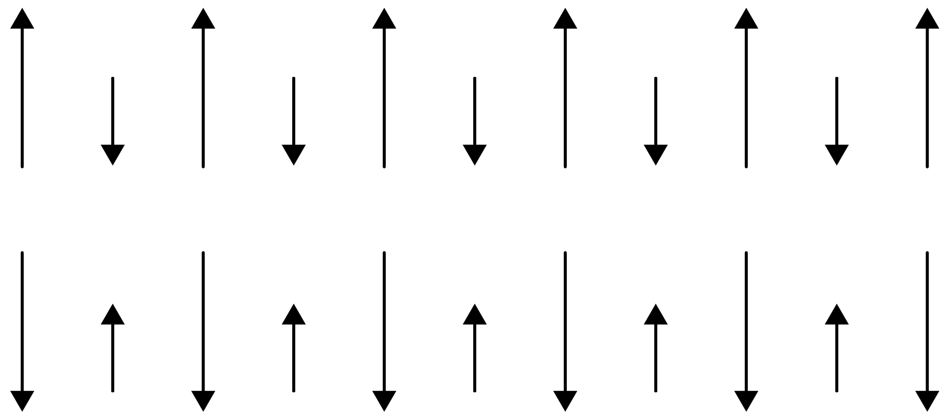
Examples: Iron, nickel, alnico (alloys of iron, aluminum, nickel, cobalt, copper)



Ferrimagnetism

- The magnetic moments of atoms are aligned in alternating antiparallel directions and do not completely cancel each other out.
- Appears as a weaker form of ferromagnetism.

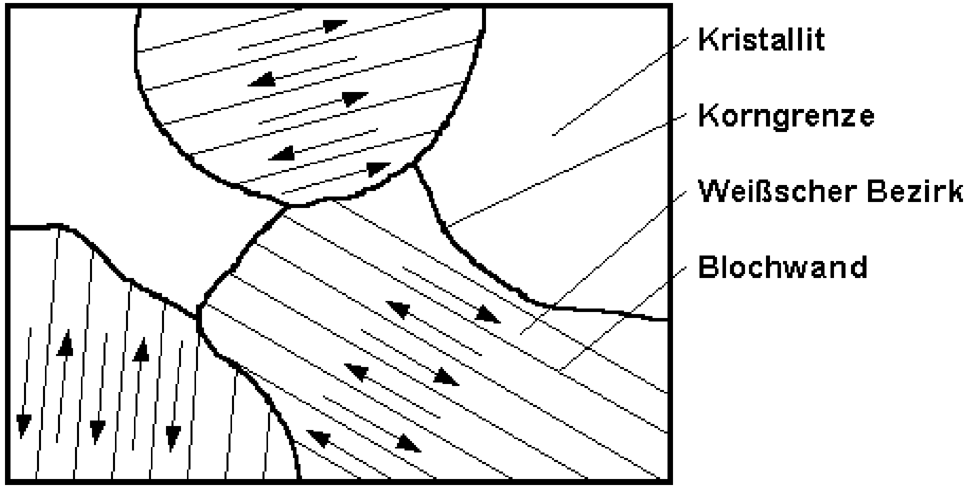
Examples: Nickel, copper, magnesium



Antiferromagnetism

- Similar to ferrimagnetism, but the antiparallel magnetic poles completely cancel each other out.
- An ideal antiferromagnet shows no external magnetic behavior.
- When heated above the Néel temperature, the material becomes paramagnetic.

Examples: Some nickel compounds, chromium



antiferromagnetischer Werkstoff

Permeability

The ratio between magnetic flux density and magnetic field strength.

$$\mathbf{B} = \mu_0 \, \boldsymbol{\mu} \, \mathbf{H}$$

Similar to permittivity. Here, too, there is a constant, the magnetic field constant μ_0, which describes permeability in a vacuum.

In general:

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_{11} & \mu_{12} & \mu_{13} \\ \mu_{12} & \mu_{22} & \mu_{23} \\ \mu_{13} & \mu_{23} & \mu_{33} \end{bmatrix}$$

Relative permeability:

$$\mu_r = \frac{\mu}{\mu_0}$$

Diamagnetic materials $0 \leq \mu_r < 1$

Paramagnetic materials $\mu_r > 1$

Superparamagnetic materials $\mu_r \gg 1$

Ferrimagnetic materials $ 20 \lessapprox \mu_{r} \lessapprox 15000$

Ferromagnetic materials $\mu_r \gg 1; 40 \lessapprox \mu_r \lessapprox 10^6$

Type 1 superconductors $\mu_r = 0$.