

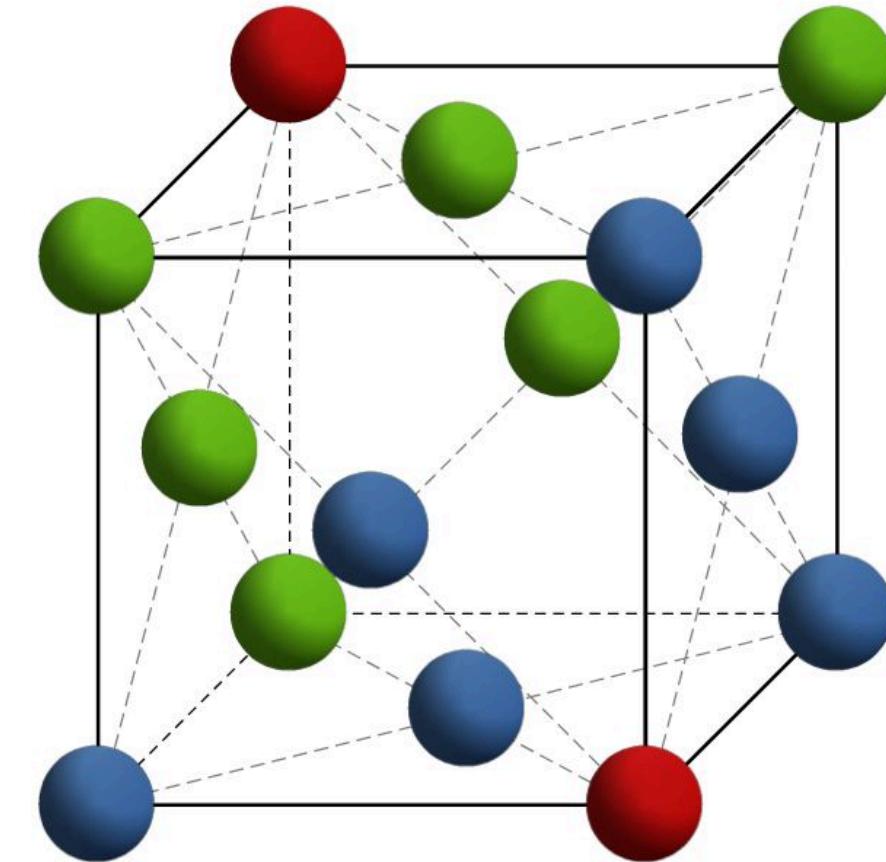
# Fine Structure

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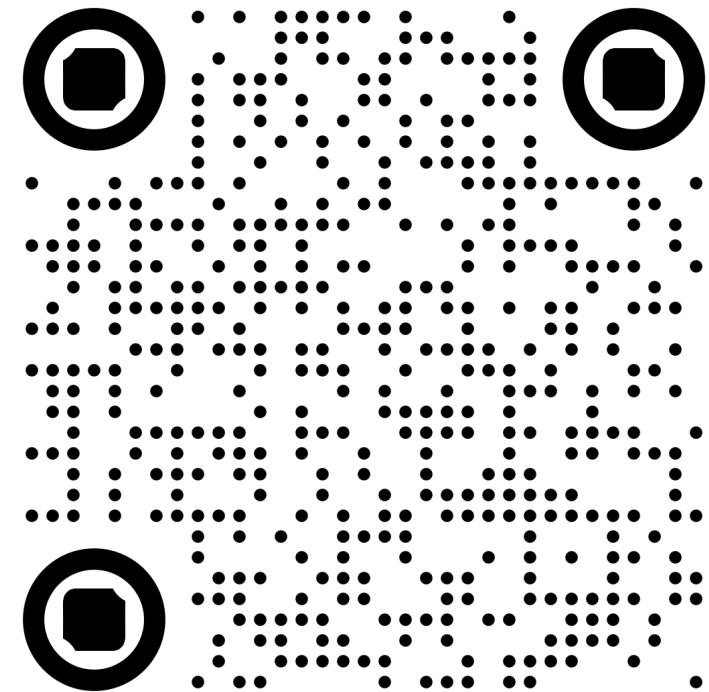
Parts of the script are taken from

Prof. Dr.-Ing. Jürgen Häberle



# Contents

- Identify and characterize crystal structures
- Understand molecular structures and their composition
- Describe real structures of crystals with their defects
- Explain relationships between structure and mechanical properties
- Plastic deformation mechanisms



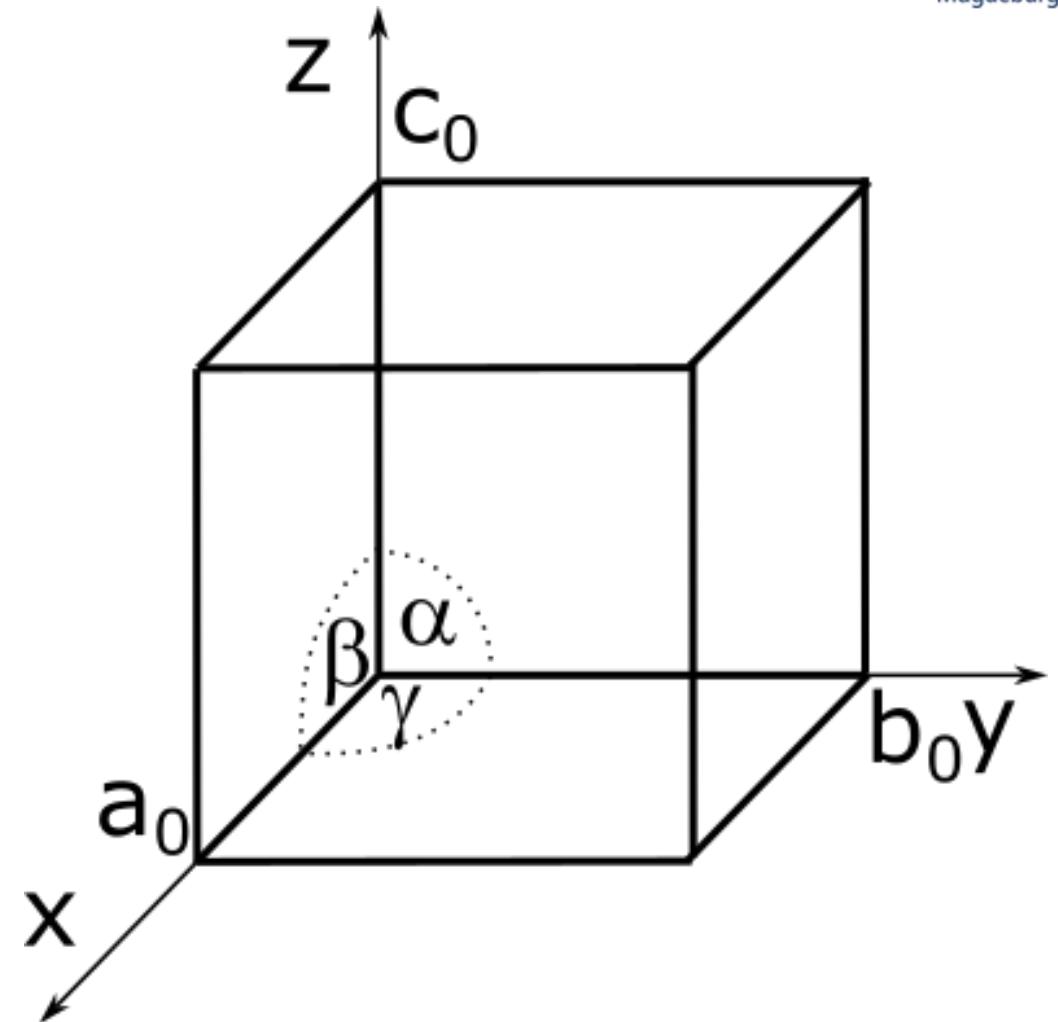
# Why is Fine Structure Important?

## Structure Determines Properties

- Mechanical properties (strength, ductility)
- Electrical conductivity
- Thermal behavior
- Optical properties
- Chemical resistance

# Space Lattice

- Created by three-dimensional periodic displacement of its building blocks
- Characterized by three spatial axes x, y, and z with angles  $\alpha$ ,  $\beta$ ,  $\gamma$  and the distances on the axes that define the respective space lattice
- $a_0$ ,  $b_0$ , and  $c_0$  (lattice constants)  
→ unit cell



Crystal System	Lattice Constants	Angles	Examples
triclinic	$a_0 \neq b_0 \neq c_0$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	Silicate minerals
monoclinic	$a_0 \neq b_0 \neq c_0$	$\alpha = \gamma = 90^\circ; \beta \neq 90^\circ$	$\text{Mo}_2\text{S}_3$ ; $\beta$ -Pu
(ortho)rhombic	$a_0 \neq b_0 \neq c_0$	$\alpha = \beta = \gamma = 90^\circ$	U, S, P, Ga, $\gamma$ -Sn
rhombohedral	$a_0 = b_0 = c_0$	$\alpha = \beta = \gamma \neq 90^\circ$	As, Hg, Sb
hexagonal	$a_0 = b_0 \neq c_0$	$\alpha = \beta = 90^\circ; \gamma = 120^\circ$	$\alpha$ -Ti, Mg, Zn
tetragonal	$a_0 = b_0 \neq c_0$	$\alpha = \beta = \gamma = 90^\circ$	B, $\text{CuTi}_3$ , Sn ( $T > 13.5^\circ$ )

## Most Common Lattice Forms in Metals

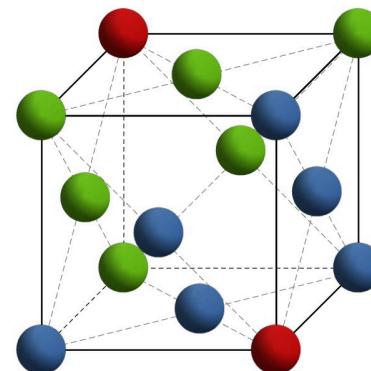
Crystal System	Lattice Constants	Angles	Examples
cubic	$a_0 = b_0 = c_0$	$\alpha = \beta = \gamma = 90^\circ$	Cu, Al, Ni, Au, Ag; $\gamma$ -iron (fcc); $\alpha$ -iron, V, Cr, W (bcc); Mn, Po (sc)

# Crystallographic Designations

**Packing Density** = Volume of atoms / Volume of unit cell

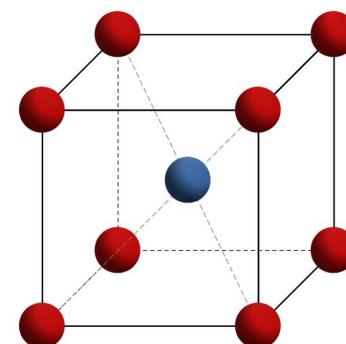
## Face-Centered Cubic (fcc)

- 4 atoms per unit cell
- Packing density: 74%
- Coordination number: 12



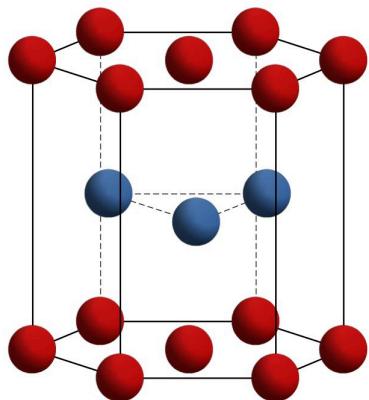
## Body-Centered Cubic (bcc)

- 2 atoms per unit cell
- Packing density: 68%
- Coordination number: 8



## Hexagonal Close-Packed (hcp)

- 2 atoms per unit cell
- Packing density: 74%
- Coordination number: 12



# Packing Density and Properties

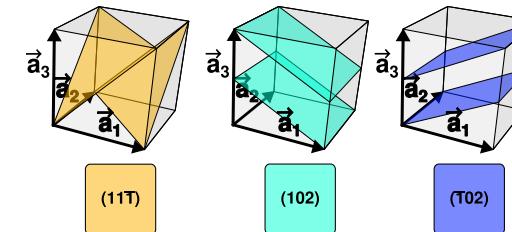
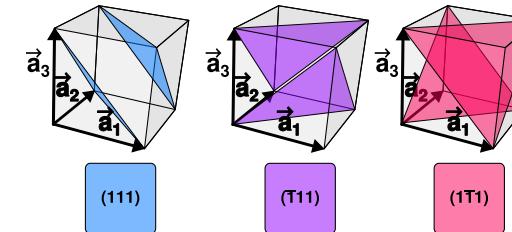
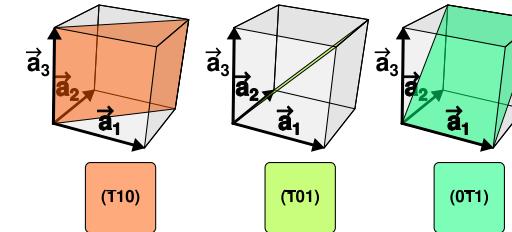
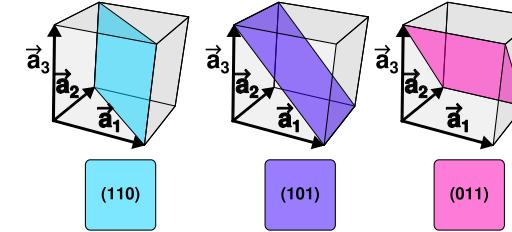
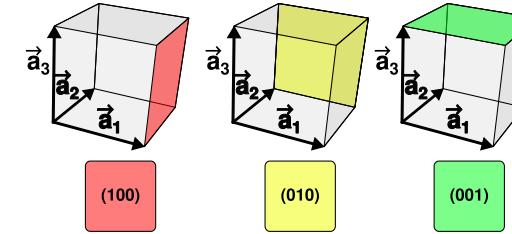
**Packing Density** = Volume of atoms / Volume of unit cell

Structure	Packing Density	Typical Properties
fcc	74%	Ductile, easily deformable
hcp	74%	Anisotropic, limited ductility
bcc	68%	Higher strength, more brittle

# Crystal planes

## Miller Indices

- Planes:  $(h k l)$
- Directions:  $[h k l]$



# Influences of Crystal Structure

- **Corrosion:** Attack by aggressive media occurs on preferred planes
- **Deformation:** Plastic deformation occurs along preferred crystallographic planes and directions → slip systems
- **Ultrasound:** Use of quartz oscillators with special crystallographic boundary surfaces
- **Conductivity:** Use of germanium or silicon wafers in  $(1\ 1\ 1)$  or  $(1\ 0\ 0)$  orientation for semiconductor elements
- **Magnetization:** Easiest magnetization of iron-silicon transformer sheets along the cube edge  $[1\ 0\ 0]$

# Anisotropy in Crystals

**Anisotropy** = Directional dependence of properties

Examples:

- Elastic modulus varies with crystal direction
- Thermal expansion is direction-dependent
- Optical properties (birefringence)

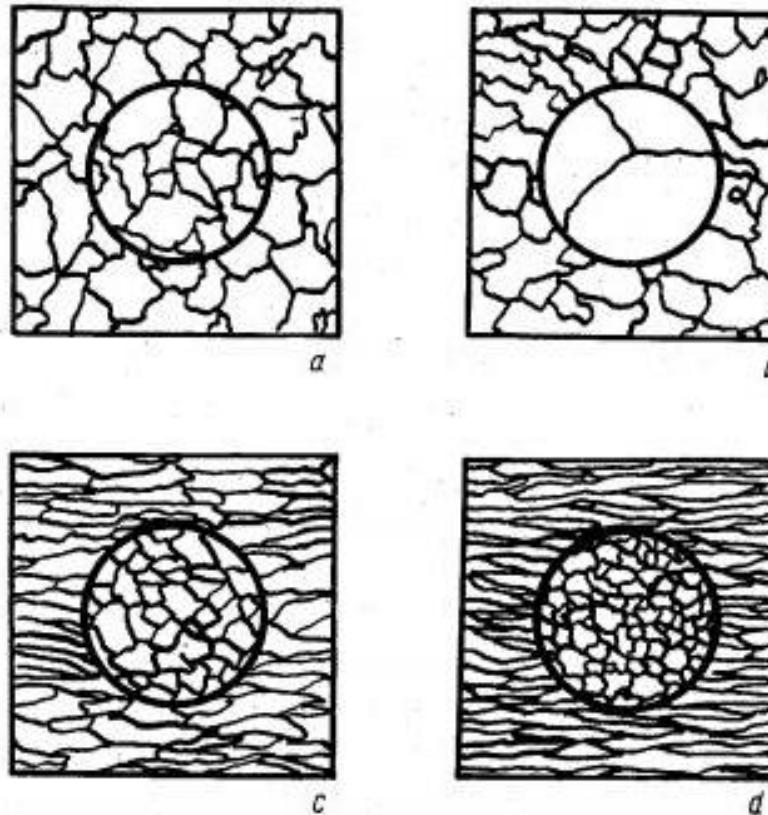


Bild 94. Veränderung des Gefüges bei plastischer Umformung (quadratische Felder) und Rekristallisationsgefüge (runde Felder) in schematischer Darstellung  
a) nicht umgeformt  
b) 10 % umgeformt  
c) 50 % umgeformt  
d) 75 % umgeformt

## Practical Significance:

- Textured materials (rolling direction)

# Polymorphism in Metals

- **Polymorphism:** Formation of different lattice structures depending on temperature
- The different lattice forms are the **allotropic modifications**

(also: Polymorphism of carbon: graphite, diamond, fullerene, graphene)

## Technical Significance:

- Heat treatment of steel
- Shape memory alloys
- Phase transformation hardening

## Example: Iron Polymorphism

Phase	Structure	Temperature	Properties
$\alpha$ -Fe	bcc	< 911°C	Ferromagnetic
$\gamma$ -Fe	fcc	911-1392°C	Paramagnetic
$\delta$ -Fe	bcc	1392-1538°C	Paramagnetic

### Volume Change During Transformation:

- $\alpha \rightarrow \gamma$ : Volume contraction (-1%)
- $\gamma \rightarrow \alpha$ : Volume expansion (+1%)

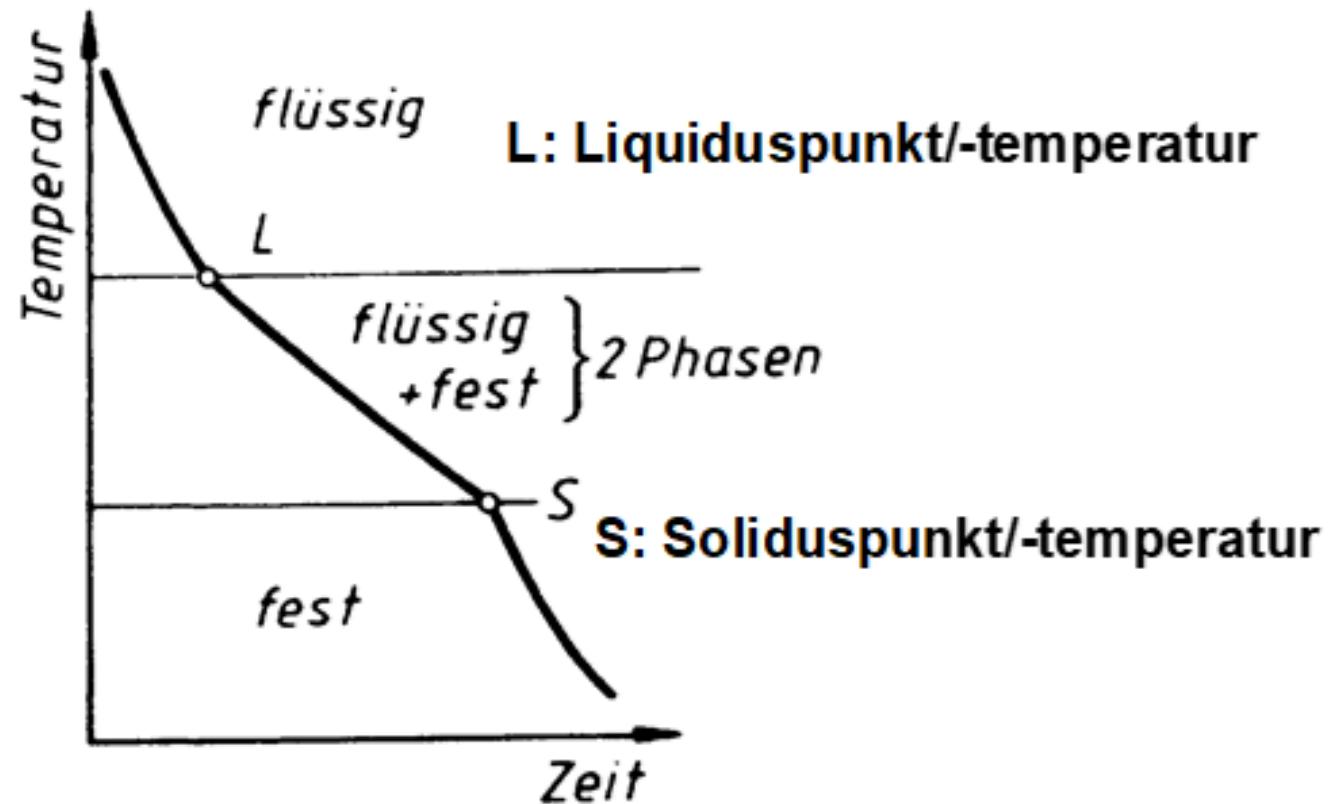
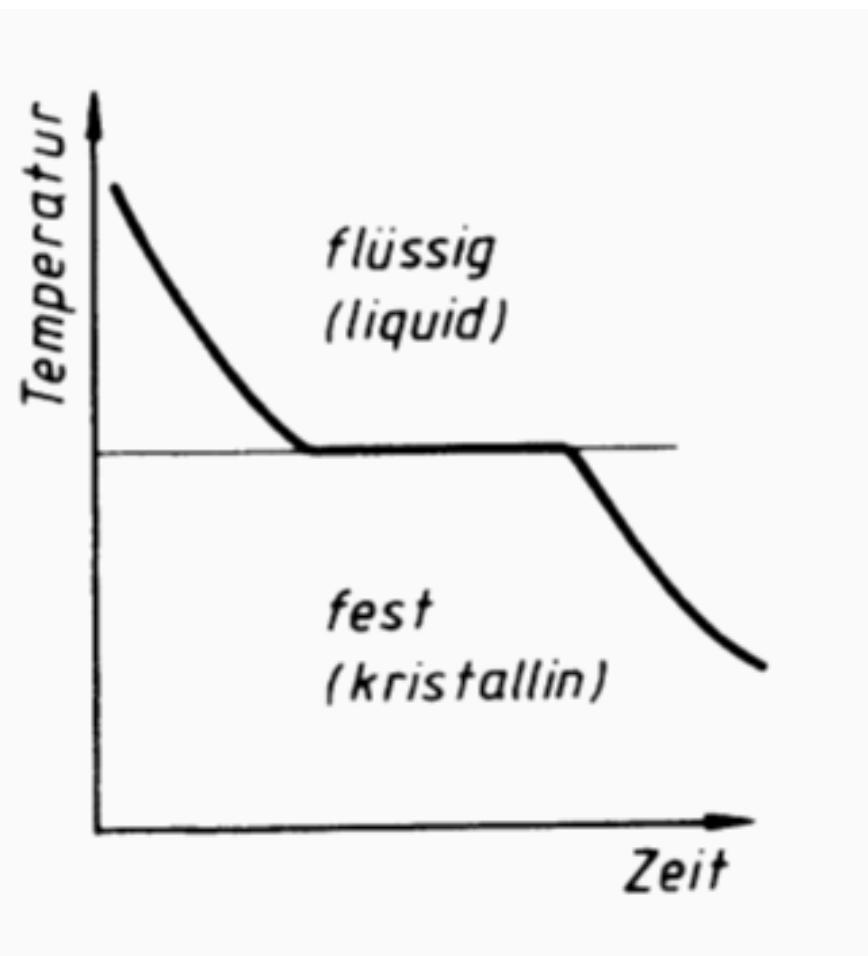
# Determination of Transformation Points

## *Dilatometry*

- Measurement of length change due to lattice transformation
- Precision:  $\pm 0.1 \mu\text{m}$
- Application: Determination of critical temperatures

## *Thermal Analysis (DTA/DSC)*

- Recording of temperature profile
- Lattice transformations (phase changes) require or release thermal energy
- Arrest or inflection points in heating or cooling curves
- Arrest points: for pure metals
- Inflection points: for alloys

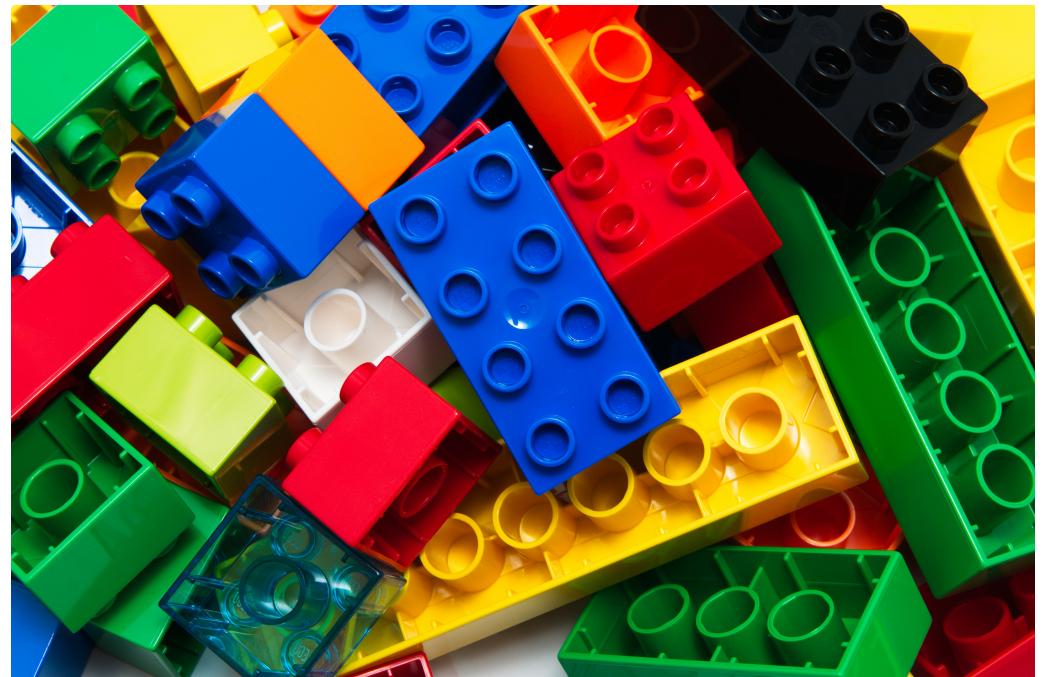


# Molecular Structures - Introduction

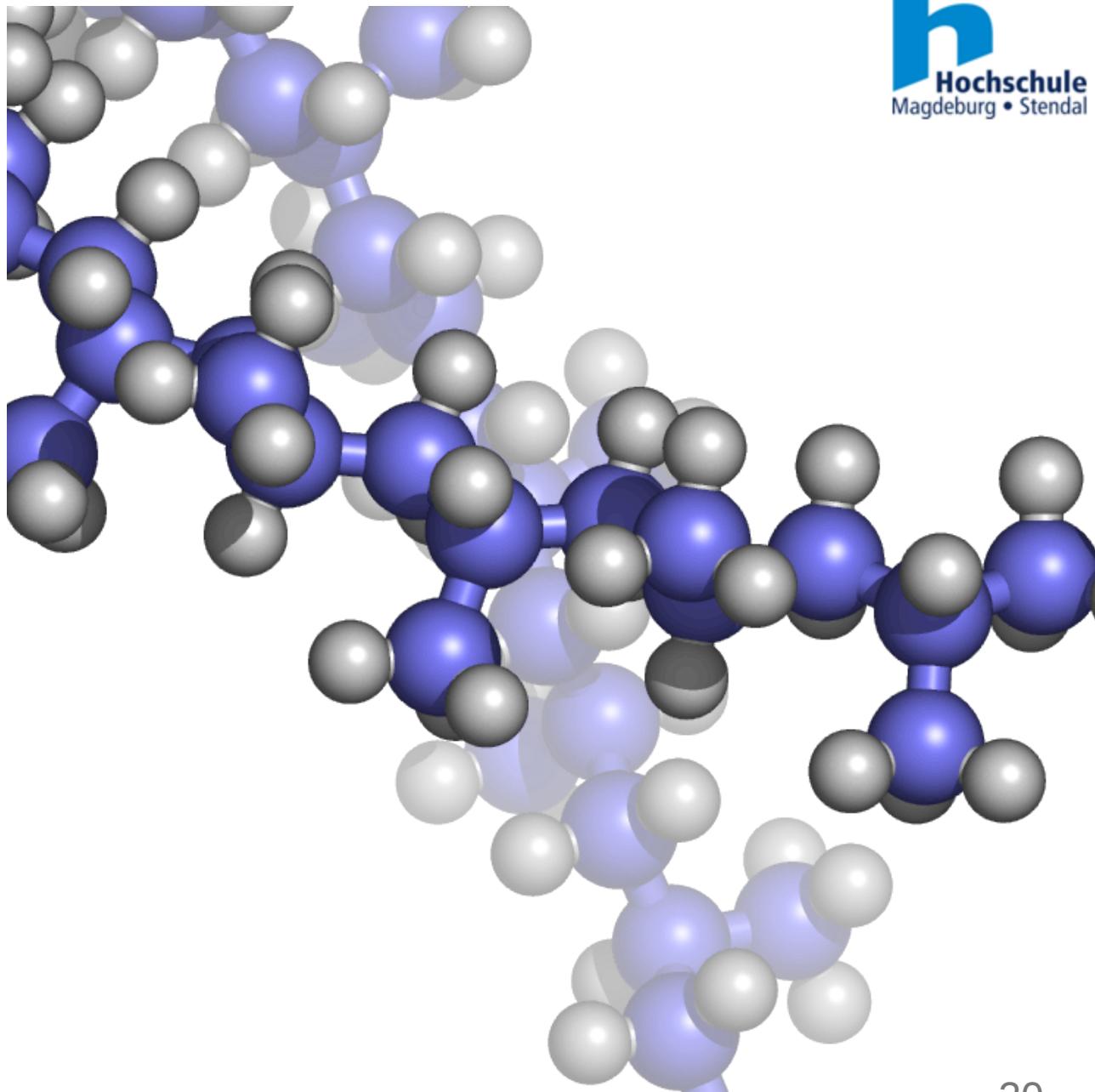
- Typical for non-metallic organic materials
  - Natural materials: wood, rubber, leather, fibers, etc.
  - Synthetic plastics: PMMA, epoxy, etc.

## Difference from Metals:

- Covalent and Van der Waals bonds
- Chain molecules instead of crystal lattice
- Temperature-dependent behavior

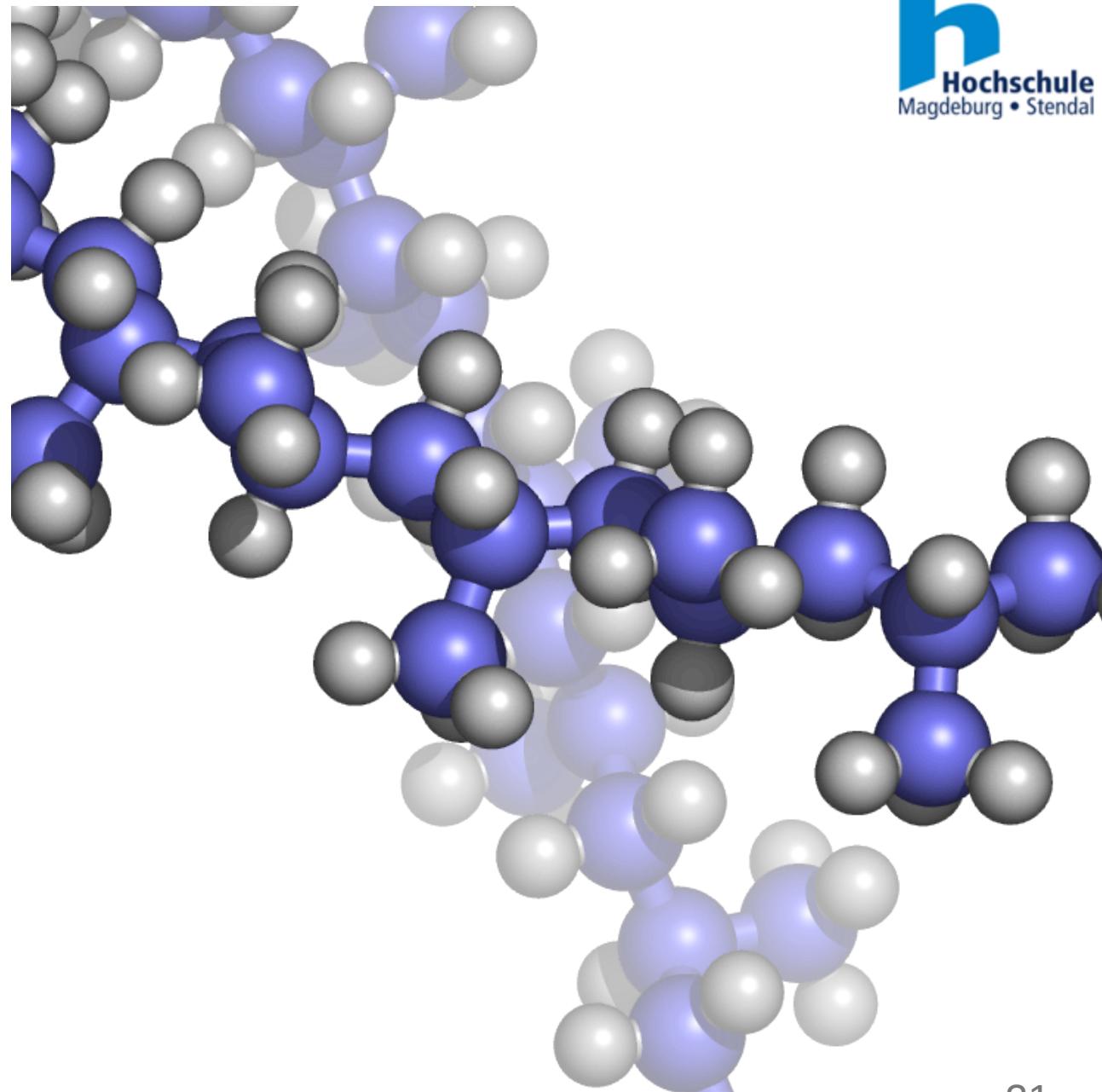


- Created by assembly reactions of monomeric building blocks into chain molecules
- Atomic bonds occur within the chains
- Secondary valence bonds and molecular entanglements exist between chains



# Structure of Polymers

- Created by assembly reactions of monomeric building blocks into chain molecules
- **Within the chains:** strong atomic bonds (covalent)
- **Between the chains:** weak secondary valence bonds and molecular entanglements (Van der Waals and hydrogen bonding)



# Polymer Classification

## By Structure:

1. Linear: Thermoplastics (PE, PP, PS)
2. Branched: Thermoplastics with reduced crystallinity
3. Cross-linked: Thermosets (epoxy), Elastomers (rubber)

## By Behavior:

- Thermoplastics: meltable
- Thermosets: non-meltable
- Elastomers: rubber-elastic

# Assembly Reaction (Polymerization)

- Free bonds must be created in the monomers
- The monomers "need" new partners to reach the energy minimum again

## Degree of Polymerization (n):

- Number of monomer units
- Molar mass  $M = n \times M_0$
- Typical:  $n = 1,000 - 100,000$
- e.g. Polyethylene (PE):  $n \text{ CH}_2=\text{CH}_2 \rightarrow (-\text{CH}_2-\text{CH}_2-)_n$

## Properties change with n:

- Strength ↑
- Melting temperature ↑
- Solubility ↓

# Crystallinity in Polymers

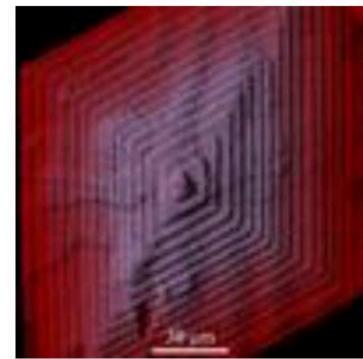
## Semi-crystalline:

- Ordered (crystalline) and disordered (amorphous) regions
- Crystallinity: 30-80%
- Examples: PE, PP, PA

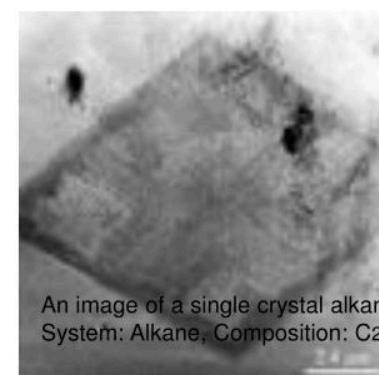
## Amorphous:

- No order
- Typical for branched and cross-linked polymers
- Examples: PS, PMMA, epoxy

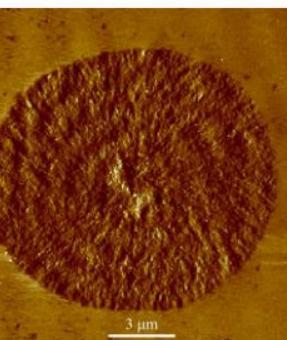
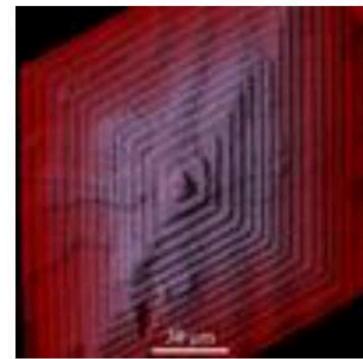
## Crystallinity in Polymers



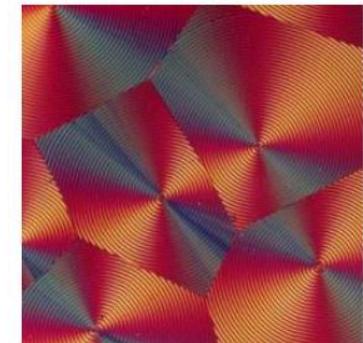
An image of an alkane crystal taken by AFM  
 System: Alkane, Composition: C<sub>36</sub>H<sub>74</sub>



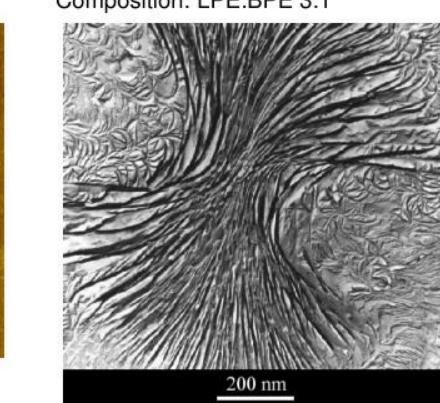
An image of a single crystal alkane  
 System: Alkane, Composition: C<sub>29</sub>H<sub>59</sub>O



Single PE spherulite AFM



Maltese cross spherulites



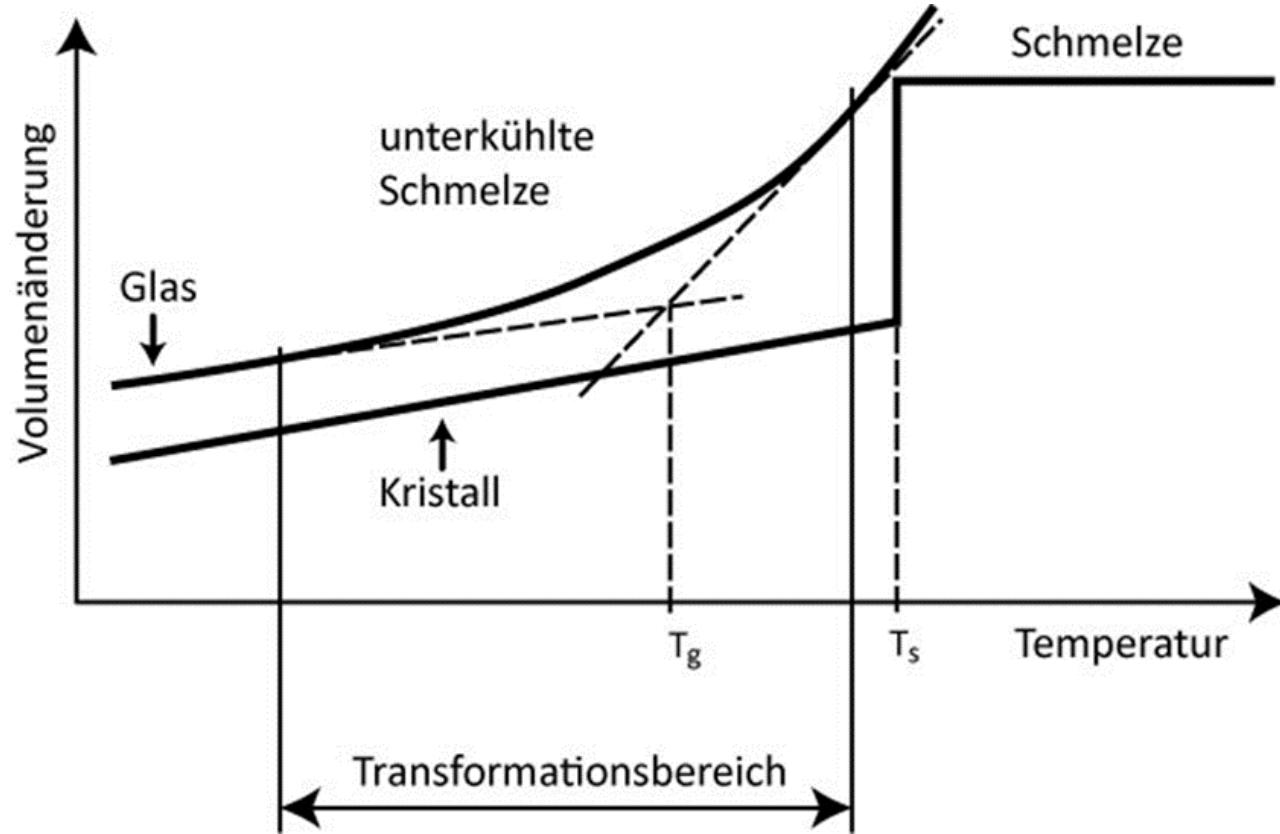
Sheaf-like arrangement of lamellae  
 in a blend of polyethylenes  
 System: Polyethylene (PE),  
 Composition: LPE:BPE 3:1

## Influence on Properties:

- Higher crystallinity → higher strength, stiffness
- Lower crystallinity → better transparency, flexibility

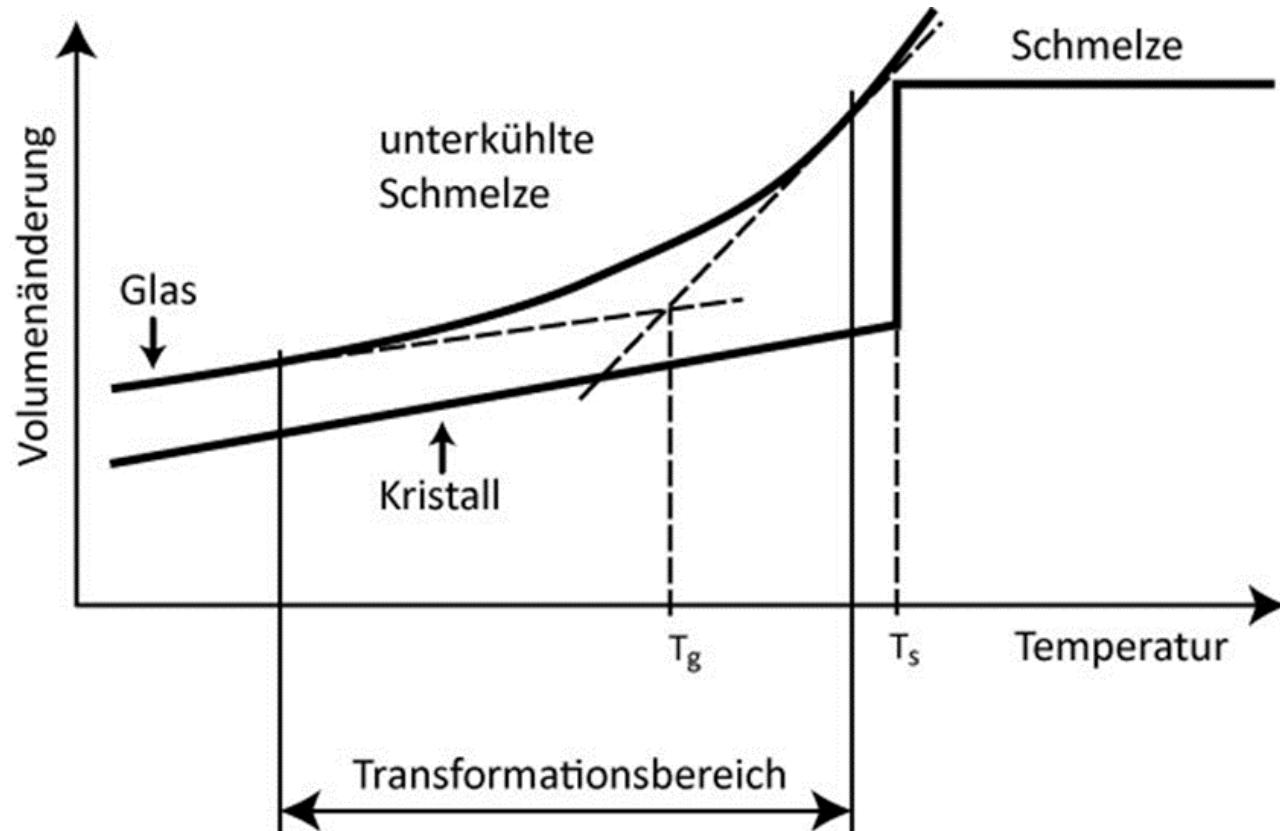
# Glassy-Amorphous Structures

- Glasses are a non-metallic inorganic, preferably silicate melt product
- **Non-crystalline, i.e., amorphous state**
- With glass, the melt is first supercooled and then "frozen" below the transformation temperature  $T_g$



## Glass Transition Temperature $T_g$ :

- Below: brittle, hard
- Above: low hardness, deformable



# Glass Formation

## Conditions for Glass Formation:

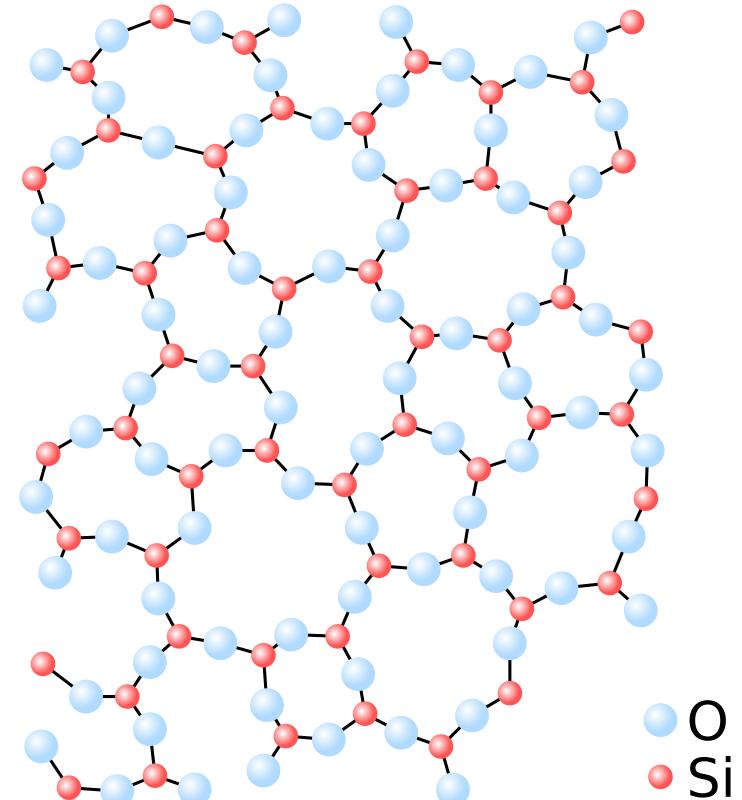
1. Rapid cooling (supercooling)
2. High viscosity of melt
3. Complex molecular structures

## Technical Glasses:

- Soda-lime glass (windows)
- Borosilicate glass (laboratory glass)
- Quartz glass (optics)
- Metallic glasses (amorphous metals)

## Properties:

- Isotropic
- Transparent (often)
- Brittle at room temperature



# Metallic Glasses

## Production:

- Extremely rapid cooling ( $10^6$  K/s)
- Prevents crystallization

## Properties:

- Very high strength
- No dislocations
- Corrosion resistant
- Soft magnetic

# Real Structure of Crystals

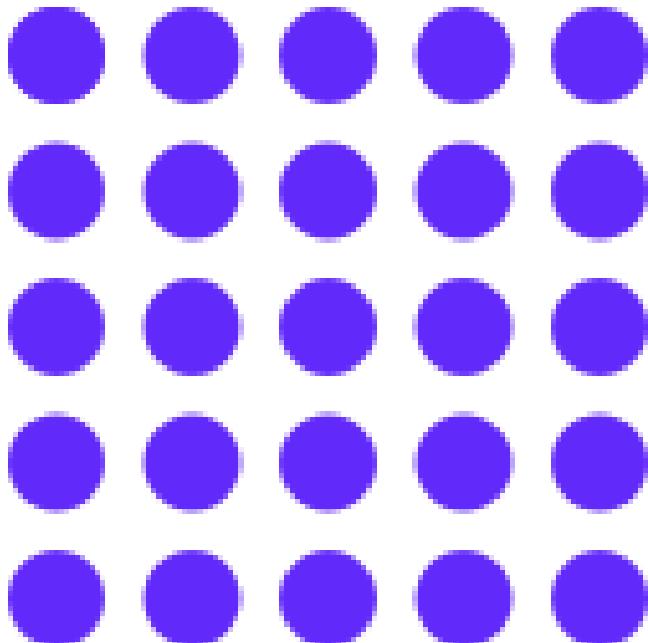
# Lattice Defects

- **Zero-dimensional defects** (point defects): vacancies, interstitial atom, interstitial foreign atoms, substitutional foreign atom
- **One-dimensional defects** (line defects): dislocations
- **Two-dimensional defects** (planar defects): stacking faults, grain boundaries, subgrain boundaries, phase boundaries
- **Three-dimensional defects**: pores, inclusions, cracks

# Zero-Dimensional Defects

## Types:

- Vacancies
- Interstitial atoms
- Substitutional foreign atom
- Interstitial foreign atom
- Frenkel defect (vacancy + interstitial atom)
- Schottky defect (vacancy pair)



# Vacancies

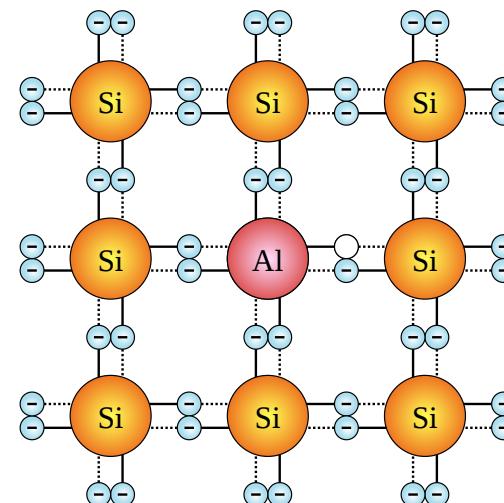
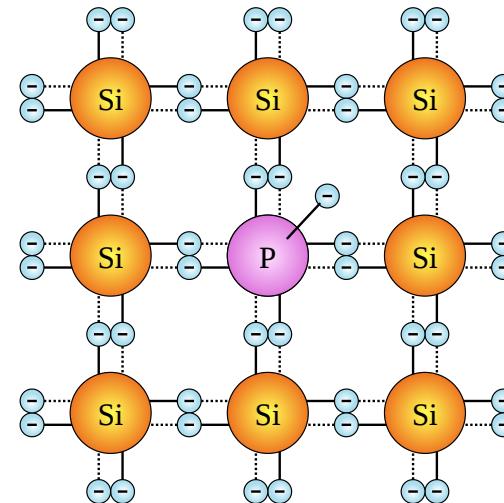
## Effects:

- Enable diffusion
- Reduce strength
- Vacancy migration

# Foreign Atoms

## Benefits:

- Doping in semiconductors
  - Targeted manipulation of electrical conductivity by introducing additional atoms



- Interstitial and substitutional foreign atoms
  - Increase in strength through natural "crack stopper" or locally easier displacement and local reduction of stresses
  - Size and chemical similarity define substitution or interstitial position

### Solid Solution Strengthening:

- Atomic size difference creates lattice distortions
- Hindrance of dislocation movement
- Strength increase proportional to square root of concentration

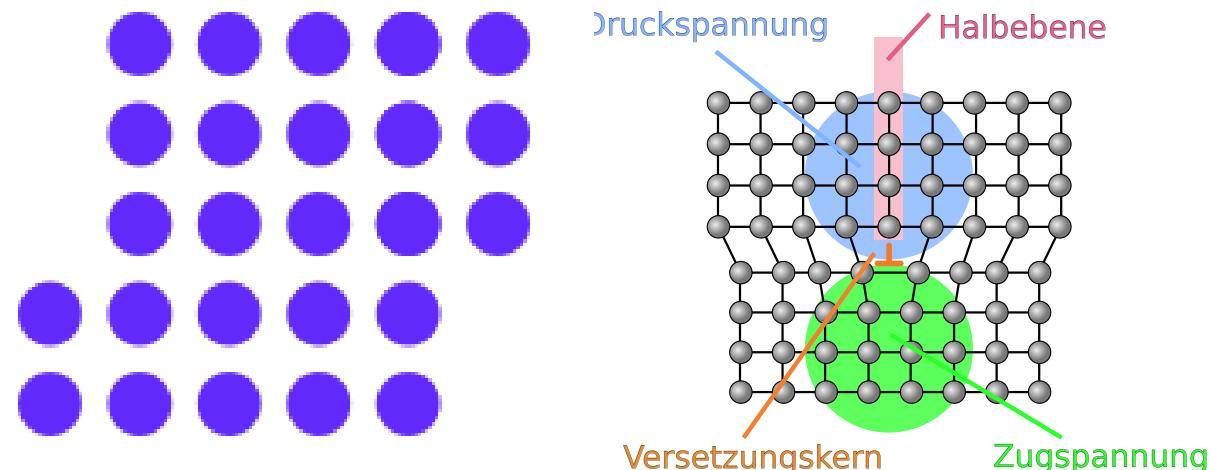
# Dislocations

Dislocations arise

- During crystal growth
- Due to internal stresses
- Through plastic deformation

Dislocation Density:

- Annealed crystal:  $10^6 - 10^8 \text{ cm}^{-2}$
- Deformed crystal:  $10^{10} - 10^{12} \text{ cm}^{-2}$



# Types of Dislocations

## Burgers Vector

### Definition:

- Vector describing the lattice displacement
- Magnitude: usually one lattice constant
- Direction: slip direction

### Significance:

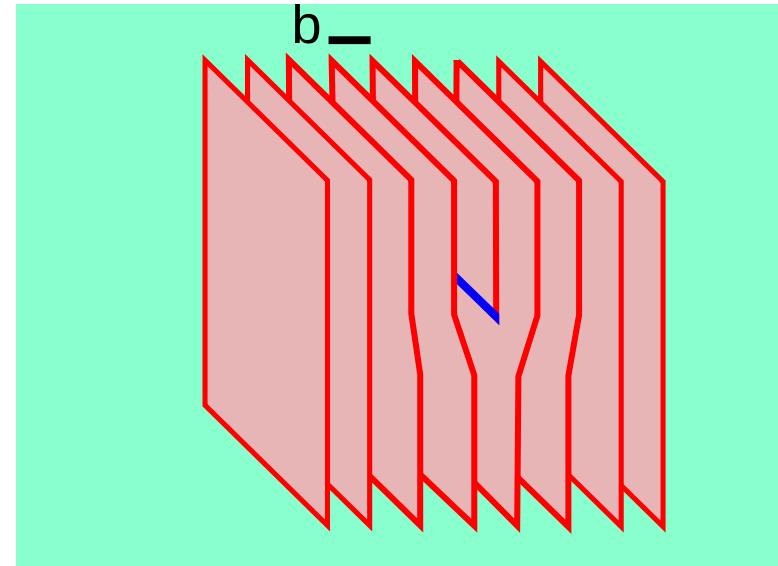
- Characterizes the dislocation
- Remains constant along the dislocation line
- Mixes edge and screw character

## Determination:

- Burgers circuit in crystal
- Closure failure = Burgers vector

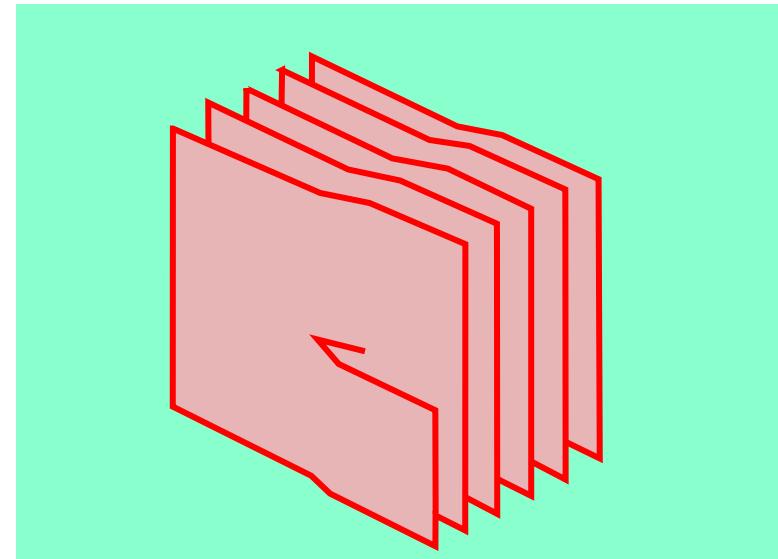
## Edge Dislocation

- Extra half-plane in crystal
- Energy:  $E \approx \frac{3}{4}Gb^2$
- Burgers vector  $\perp$  dislocation line



## Screw Dislocations

- Spiral lattice distortion
- Energy:  $E \approx \frac{1}{2}Gb^2$
- Burgers vector  $\parallel$  dislocation line



# Dislocation Movement

## Glide:

- Dislocation moves in glide plane
- Low required shear stress
- Main mechanism of plastic deformation

## Climb:

- Dislocation leaves glide plane
- Requires diffusion of vacancies
- Only at high temperatures
- Important in creep

## Cross-slip:

- Screw dislocation changes glide plane
- Enables three-dimensional deformation

# Dislocation Interactions

## Dislocation Pileup:

- Dislocations pile up at obstacles
- Stress concentration
- Can lead to crack formation

## Dislocation Entanglement:

- Dislocations block each other
- Strengthening mechanism
- "Forests" of dislocations

## Dislocation Reactions:

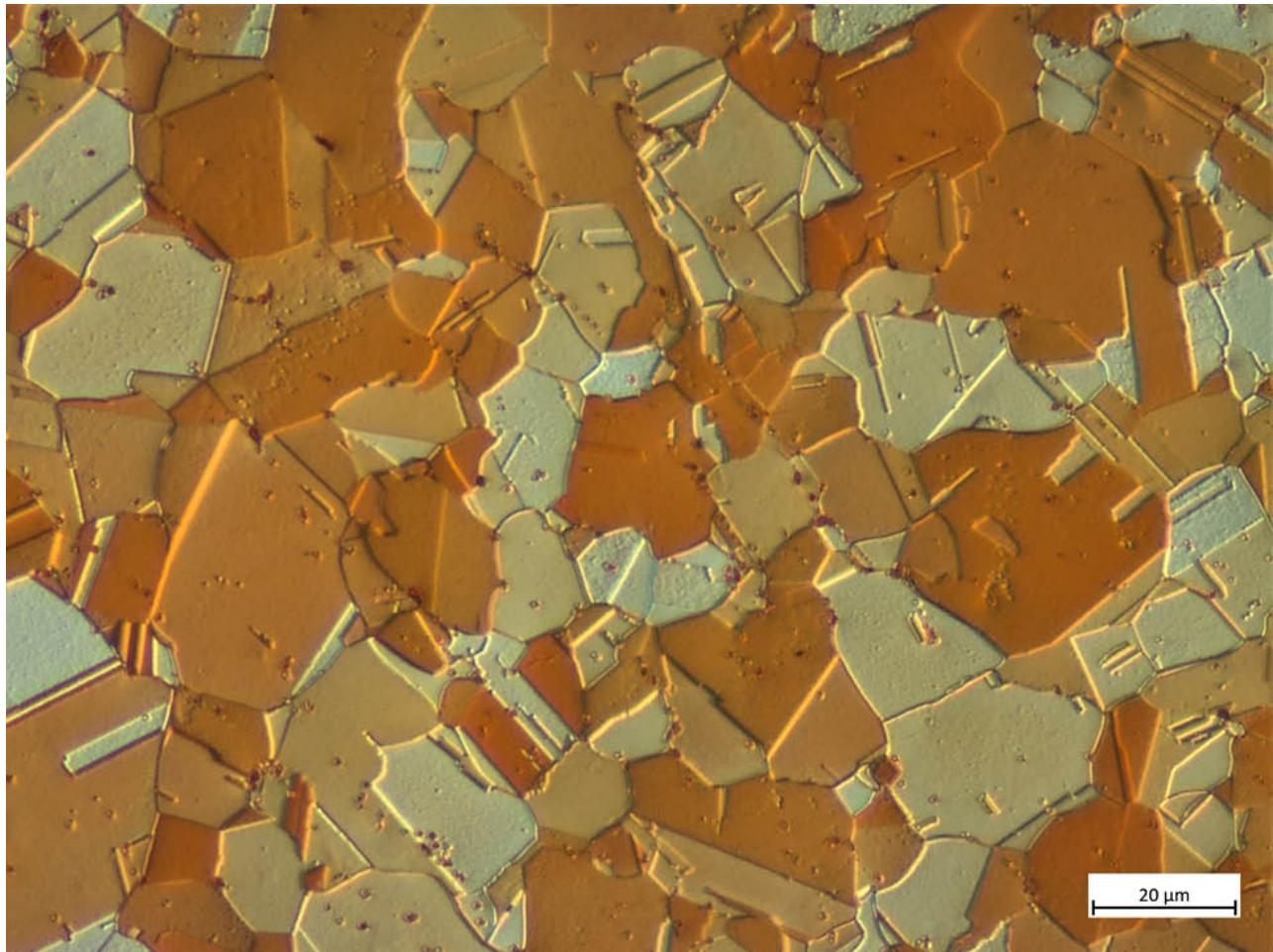
- Two dislocations can merge
- New dislocation with different Burgers vector
- Frank-Read source: dislocation multiplication

# Defect Overview

## Two-Dimensional Defects - Grain Boundaries

- Grain boundaries
- Phase boundaries
- Subgrain boundaries

Script



## Grain Boundaries:

- High-angle grain boundaries ( $\theta > 15^\circ$ )
- Low-angle grain boundaries ( $\theta < 15^\circ$ )
- Special grain boundaries (twin boundaries)

## Phase Boundaries:

- Coherent boundaries (epitaxial)
- Semi-coherent boundaries (with dislocations)
- Incoherent boundaries (disordered)

## Subgrain Boundaries:

- Arrangement of dislocations
- Formed during recovery

# Grain Boundary Properties

## Structural Features:

- Higher energy than crystal interior
- Reduced atomic density
- Increased chemical activity

## Influence on Properties:

- Diffusion along grain boundaries faster
- Preferred corrosion attack sites
- Hindrance of dislocation movement (Hall-Petch)
- Starting point for recrystallization

# Large Grains (Coarse Microstructure)

- **Lower Strength**
  - Fewer grain boundaries as dislocation barriers
  - Long free paths for dislocations
- **Higher Ductility**
  - More space for dislocation movement
  - Better formability

## High Temperature Behavior

- **Better Creep Resistance**
  - Less grain boundary diffusion
  - More stable at elevated temperatures

## Applications

- Turbine blades (high temperature)
- When ductility is more important than strength
- Single crystals for special applications

## Small Grains (Fine Microstructure)

- **Higher Strength**
  - Many grain boundaries = many barriers
- **Higher Hardness**
  - Resistance to local deformation
- **Good Toughness**
  - Crack arrest at grain boundaries

## Deformation Behavior

- **More Homogeneous Deformation**
  - Many small regions active
- **Slightly Reduced Ductility**
  - But often acceptable

## Applications

- High-strength steels (automotive)
- Structural components
- Wherever strength + toughness is required

# Plasticity

Good or Bad



# Examples

## High Plasticity:

- Modeling clay
- Wet clay
- Metals and metal alloys with suitable atomic lattice:
  - Glowing steel during forging
  - Cold forming of sheet metal

## Low Plasticity:

- Rubber
- Ceramics
- Fiber-reinforced composites (epoxy-glass fiber or epoxy-carbon fiber)

## Advantages of Plasticity:

- Formability (manufacturing)
- Energy absorption (crash)
- Toughness (no spontaneous crack propagation)
- Stress relief

## Disadvantages of Plasticity:

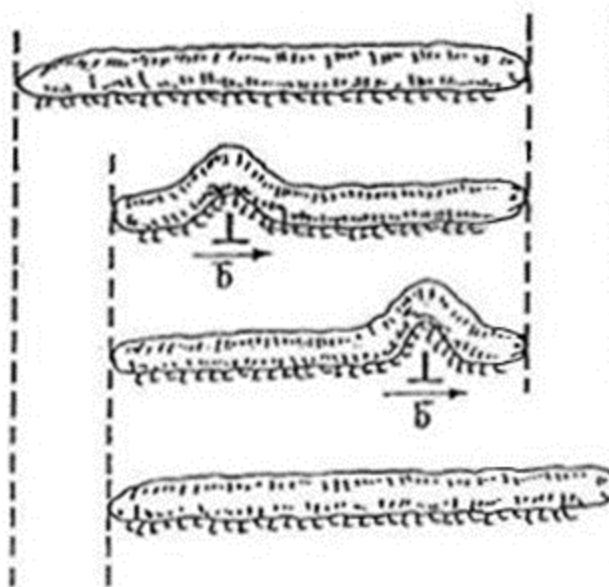
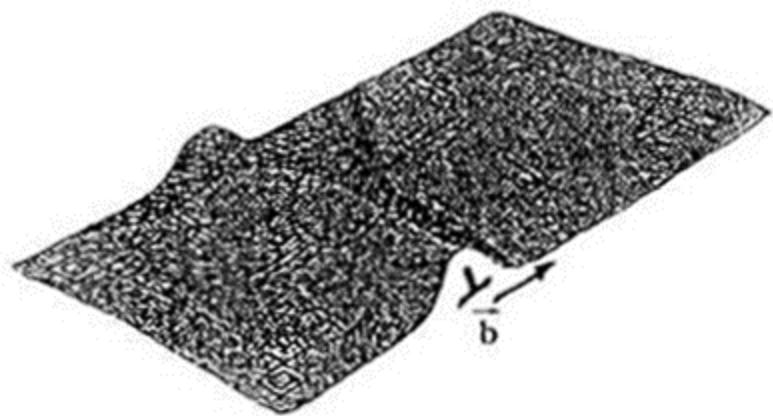
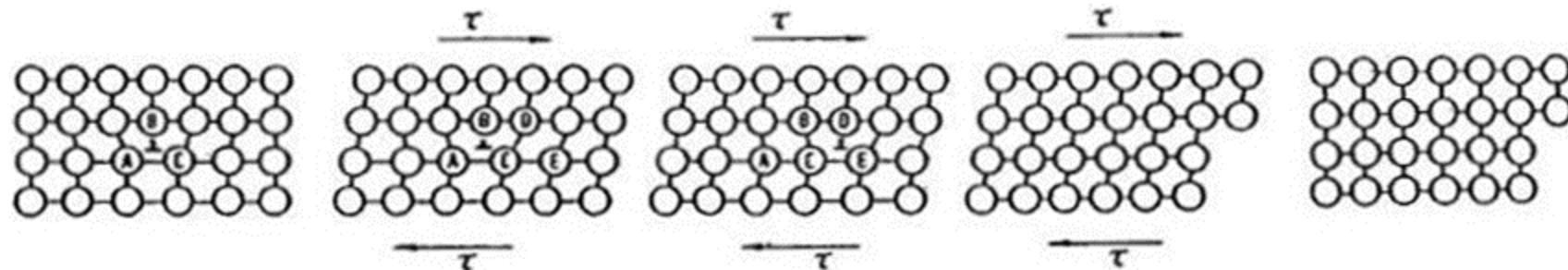
- Dimensional change
- Creep deformation
- Component failure under overload
- Fatigue

## Plasticity - Single Crystal

The plastic deformation of a crystal occurs essentially through sliding of atomic planes along certain crystallographic planes and directions under the action of shear stresses.

- Slip system consists of slip plane and slip direction
- Critical shear stress ( $\tau_{K_r} \approx G/10$  - estimation or theoretical shear strength)
- Reality lower by factor ~100 due to dislocations

# Image



# Plastic Deformation of Polycrystalline Materials

- Micro- and Macroplasticity
  - Plastic deformation begins at "unfavorable" orientations
- Grain Boundaries
  - Barrier for dislocation movement
  - At high temperatures grain boundaries can slide (creep)
  - Targeted manufacturing can increase toughness through grain boundaries
- Heterogeneity
  - Multiphase nature
  - Inhomogeneous distribution of stresses and strains
- Anisotropy

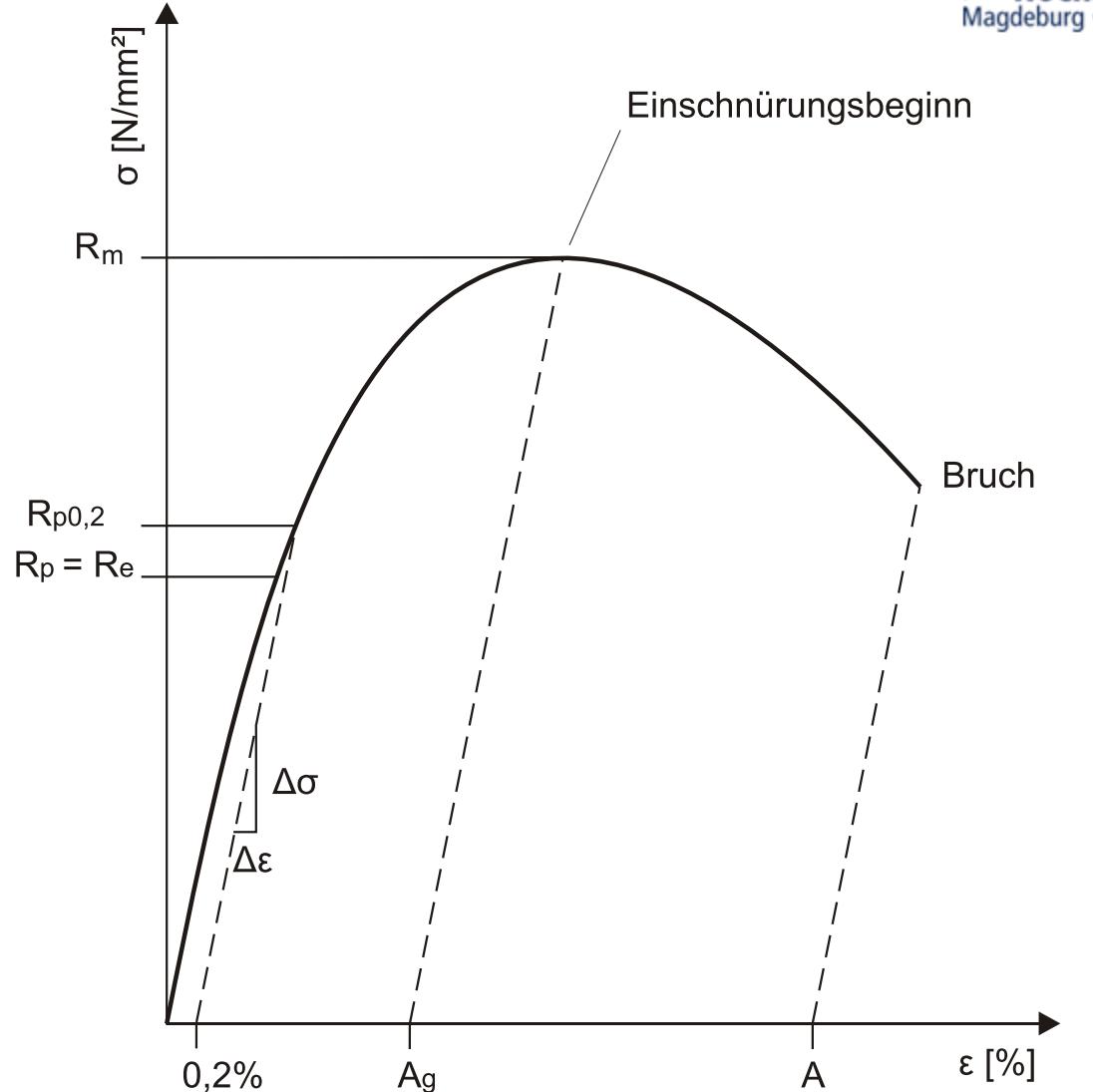
# Polycrystal Plasticity

Example from a simulation

# Yield Strength

## Characteristic Points:

- $R_m$  - Tensile strength (maximum)
- $R_e$  - Yield strength (elastic limit at linear curve)
- $R_{p0,2}$  - Proof stress (0.2% permanent strain)
- $A$  - Elongation at fracture (in %)
- $Z$  - Reduction of area (in %)



[Example video](#)

# **Yield Strength and Proof Stress**

## **Yield Strength Re:**

- For materials with pronounced yield point
- Characteristic for low-alloy steel
- Marks transition elastic → plastic

## **Proof Stress Rp0.2:**

- Substitute yield strength for materials without pronounced yield point
- Loading up to 0.2% permanent strain, then unloading
- Standard for aluminum alloys, high-alloy steels

[Steel datasheet](#)

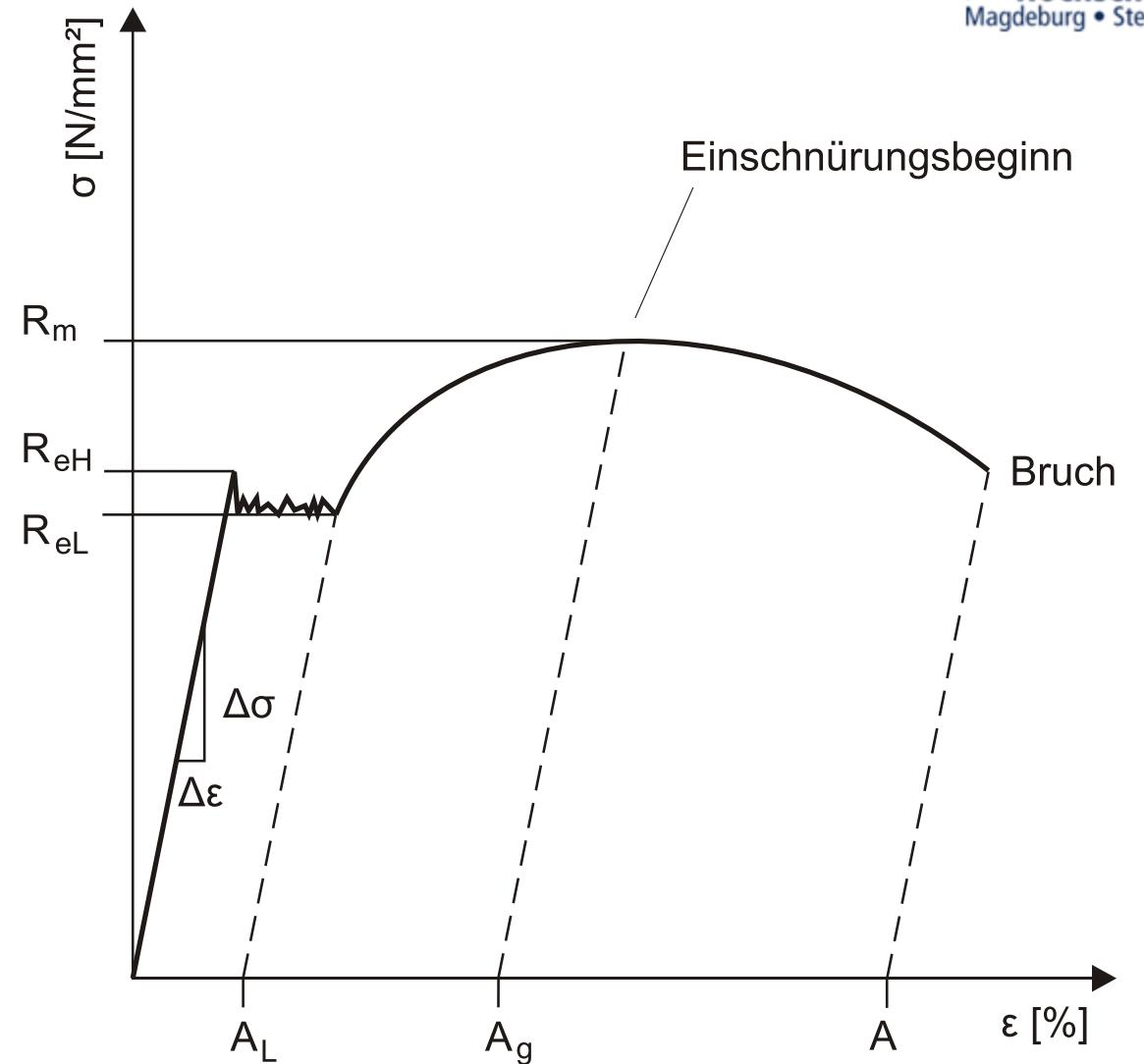
# Yield Point Phenomenon

## Upper and Lower Yield Point:

- $R_{eH}$  - Upper yield point (maximum)
- $R_{eL}$  - Lower yield point (plateau)

## Lüders Region:

- Serrated region after yield point
- Lüders bands migrate through specimen
- Precipitates block dislocations
- After breaking free: dislocations move freely



# Plasticity - Forming

## Bulk Forming:

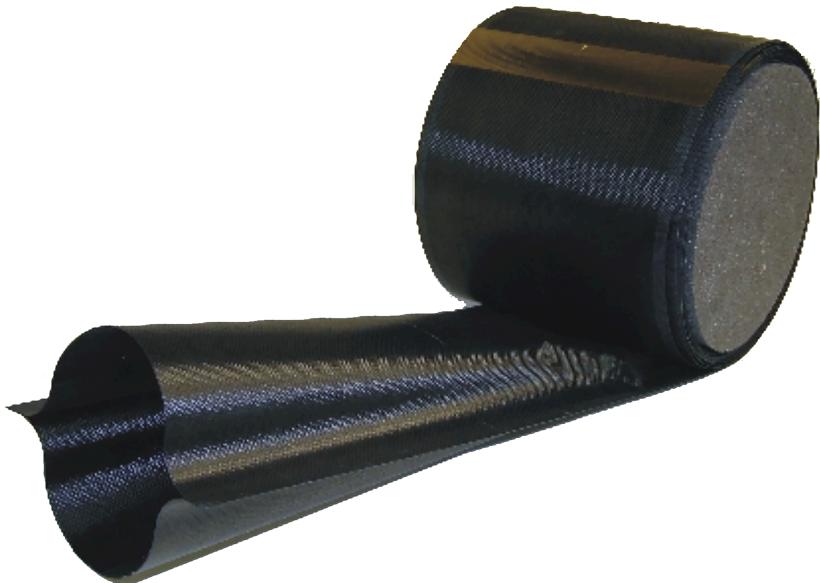
- Forging, pressing, rolling, **deep drawing principle**
- Large shape changes
- Grain refinement

## Sheet Metal Forming:

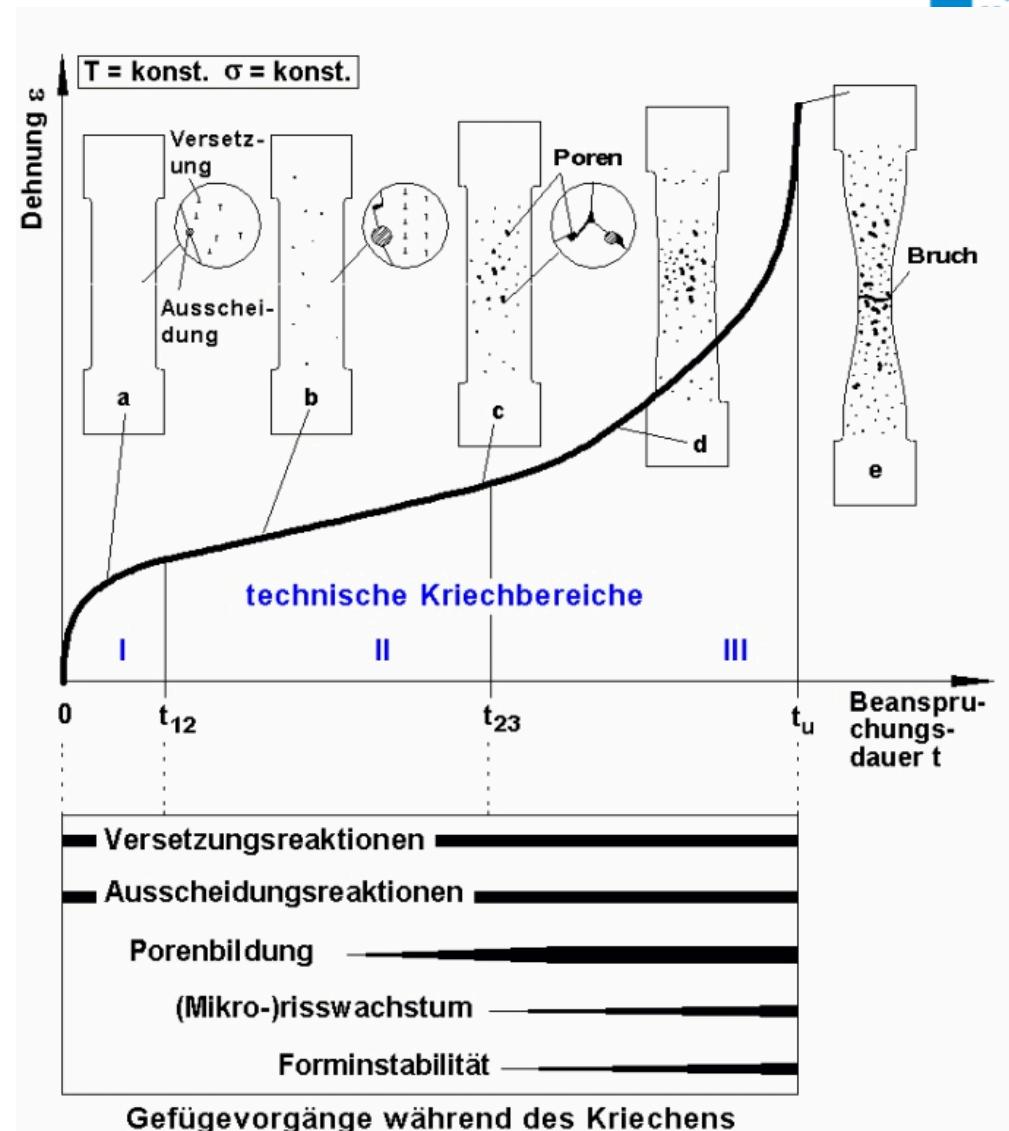
- Bending, stretch forming, **deep drawing**
- Limited shape change
- Anisotropy important

## Creep

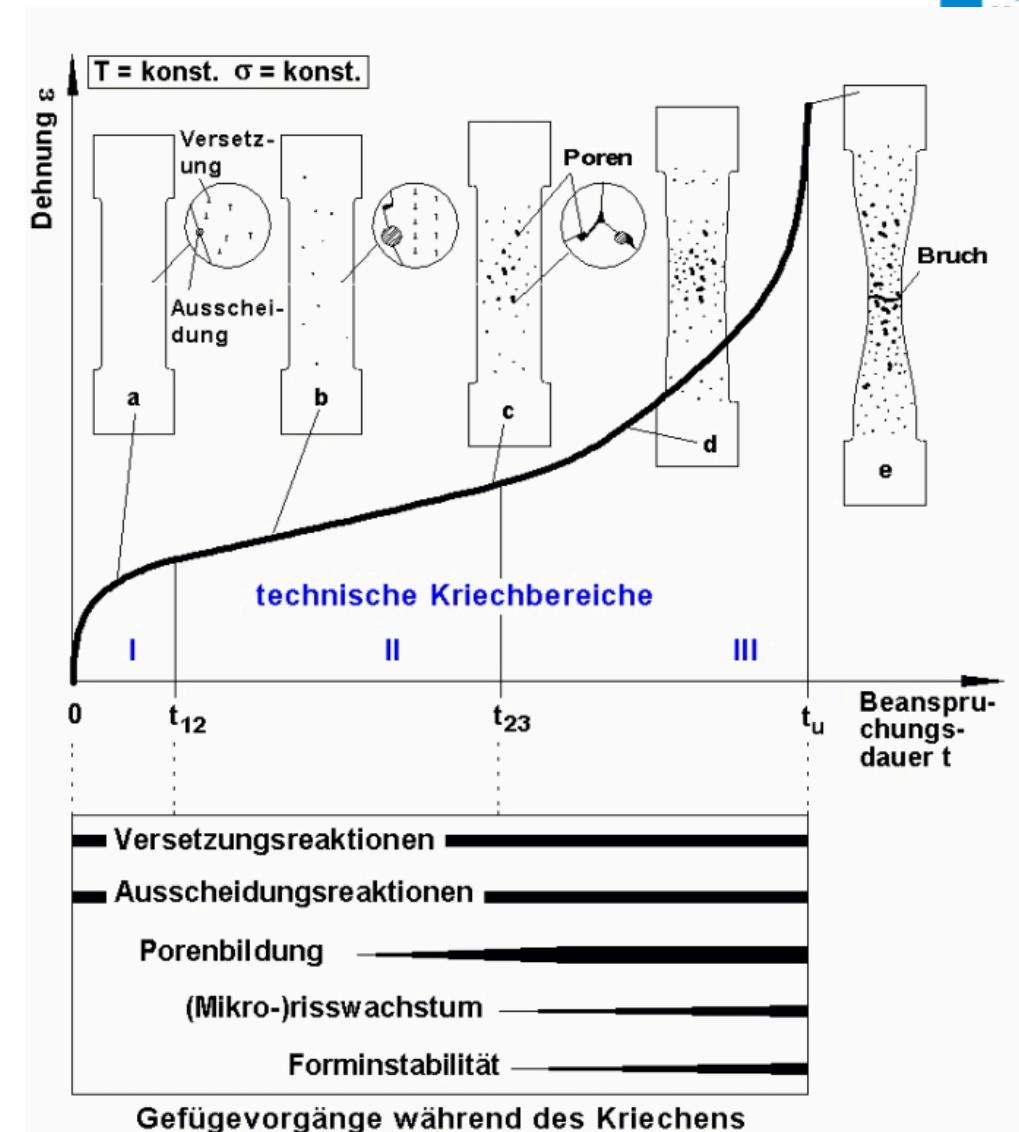
- Time-dependent deformation under constant load
- Example [deployable space structures](#)



- Occurs in metals above a transition temperature ( $0.3 - 0.4 \cdot T_S$ )
- Even at low mechanical stresses below the yield strength  $R_e$ , irreversible plastic deformation occurs, progressing slowly but steadily



- Temperature-, stress-, time- and material-dependent
- **Cause:** Dislocation movements, vacancy diffusion, grain boundary sliding, grain boundary diffusion



## 1. Primary Creep:

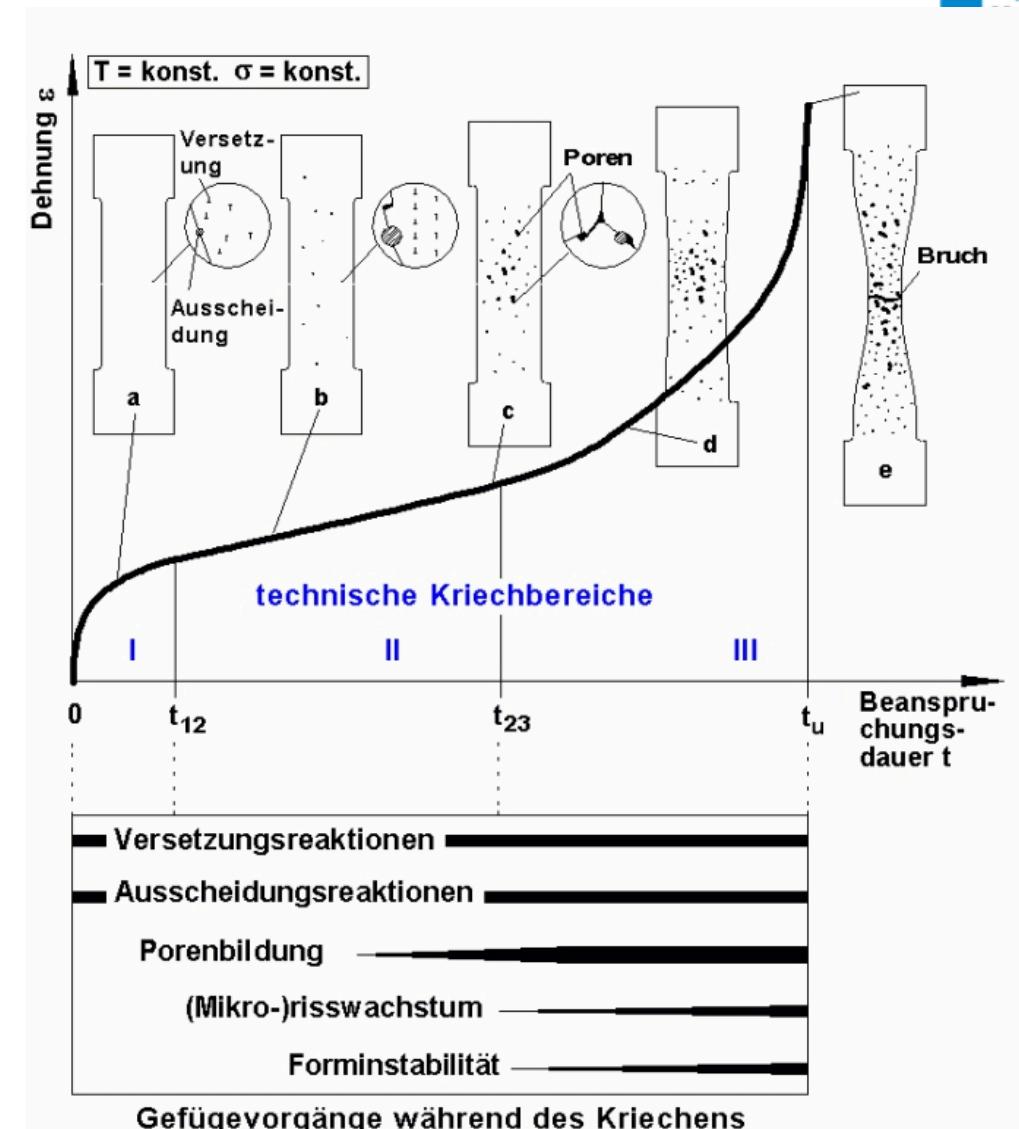
- Decreasing creep rate
- Hardening dominates

## 2. Secondary Creep:

- Constant creep rate (steady-state)
- Equilibrium: hardening - recovery

## 3. Tertiary Creep:

- Increasing creep rate
- Damage (holes, cracks)
- Leads to fracture



# Creep in Polymers

- Consist of molecular chains
- These slide or uncoil under external load
- Secondary bonds between macromolecules are reformed and deformation remains

# Summary

## Key Points:

1. Crystal structures determine fundamental properties
2. Real structures always contain defects
3. Defects enable plastic deformation
4. Dislocations are carriers of plasticity
5. Grain size influences strength (Hall-Petch)
6. Temperature activates additional mechanisms (creep)
7. Structure-property relationships are fundamental