

Materials Lab

HSLU, Semester 3

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Exam

10 pages individual summary, printed/written on paper (pictures allowed). Calculator, ruler, electrochemical series.

Part I

Physical metallurgy

1 Material classes, structural models, basic concepts

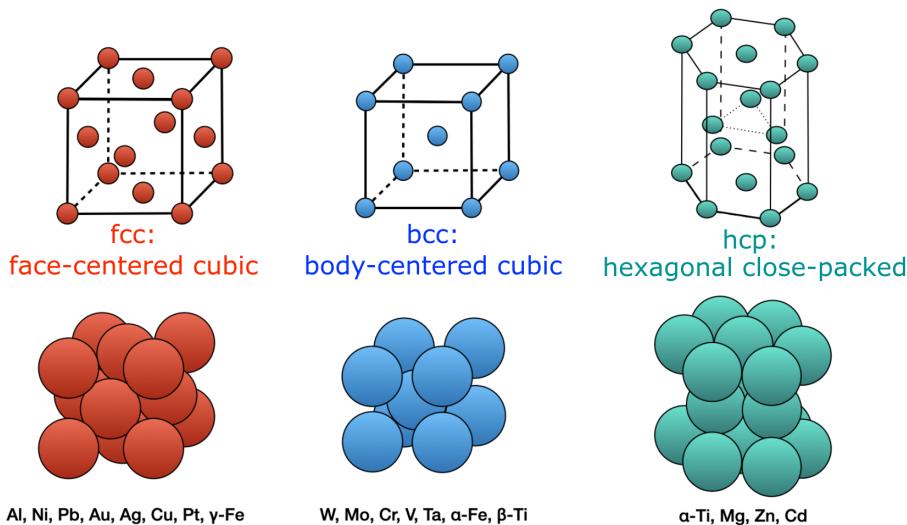
1.1 Material classes and typical properties

Class	4 Typical Properties
Metals / Alloys	1) Conductivity (electric, thermal) 2) Ductility / malleability 3) Castable 4) Shiny (reflective)
Ceramics	1) High temperature resistance 2) Compression resistance 3) Insulator (electric, thermal) 4) Wear resistance
Polymers	1) Cheap 2) Insulating (electric, thermal) 3) Longevity (corrosion resistance) 4) Moldable

1.2 Structural model of metals

In general, metals have:

- **Metallic bonding**
- Good electrical and thermal conductivity
- Simple, densely packed crystal structures (atomic distances $\sim 0.1 - 0.2$ nm)



FCC (Face-centered cubic)

BCC (Body-centered cubic)

HCP (Hexagonal close-packed)

- Packing efficiency:

$$\phi = \frac{\pi}{\sqrt{18}} \approx 74\%$$
 - Has many slip systems (12)
 - Closest packed direction
- Packing efficiency:

$$\phi = \frac{\sqrt{3}\pi}{8} \approx 68\%$$
 - Has many slip systems (6)
 - Not closest packed direction
 - Cottrell atmosphere
- Packing efficiency:

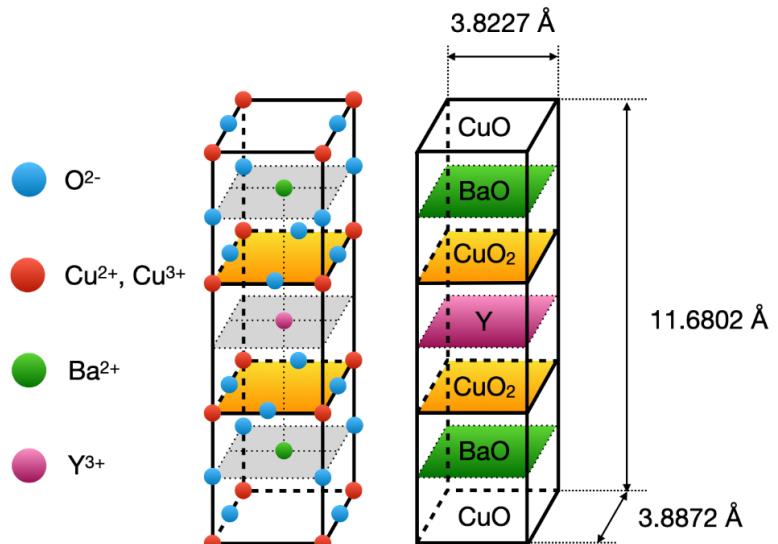
$$\phi = \frac{\pi}{\sqrt{18}} \approx 74\%$$
 - Very few slip systems (3)
 - Closest packed direction

$$\text{Packing efficiency } (\phi) = \frac{\text{Volume occupied by atoms in unit cell}}{\text{Total volume of unit cell}}$$

1.3 Structural model of ceramics

In general, ceramics have:

- Ionic bonding, complex crystal structures (ceramics), amorphous (glasses)
- Undoped: insulators (doped: semiconductors, superconductors or ionic conductors)
- Brittle, but high chemical and thermal resistance
- Wear-resistant, other special properties (e.g. ferro-/piezoelectricity)

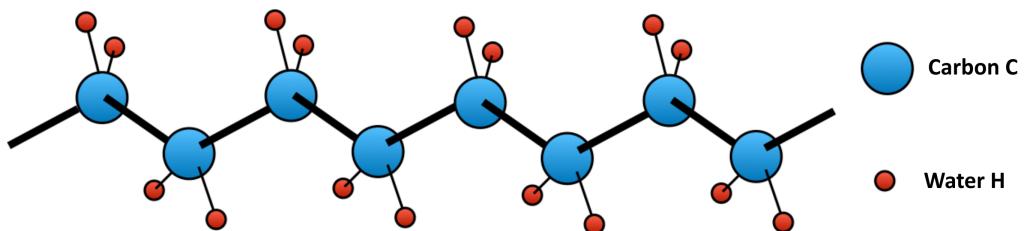


YBCO superconducting ceramic with layered perovskite-like structure

1.4 Structural model of polymers

In general, polymers have:

- Macromolecules (10^3 to 10^5 C atoms)
- Weaker intermolecular bonds (strong atomic bond in molecular chain)
- Electrically and thermally insulating (without special modifications)
- Cheap, moldable, massive waste problem (e.g. ocean pollution)
- Matrix for many composite materials (recycling problem)



Polymeric hydrocarbon chain

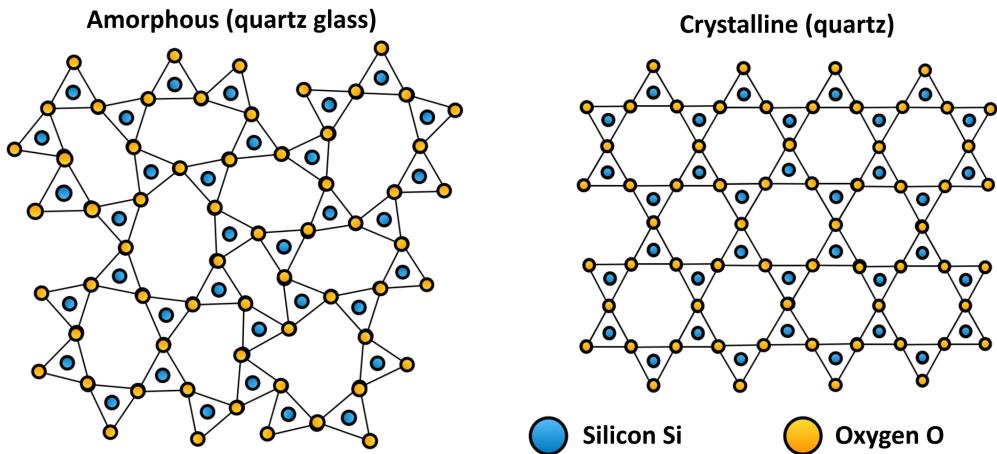
1.5 Amorphous and crystalline materials

Amorphous materials

- No crystal lattice (e.g. quartz glass, polymers)
- Atomic distances defined by chemical bonds
- Bond angles are variable

Crystalline materials

- Crystal lattice (e.g. metals, ceramics, quartz)
- Atomic distances and bonding angles are defined



1.5.1 Polycrystalline materials

Most metal components are polycrystalline (made of many grains/crystals), i.e. they consist of countless microscopic crystals (crystallites, “grains”).

1.5.2 Monocrystalline materials

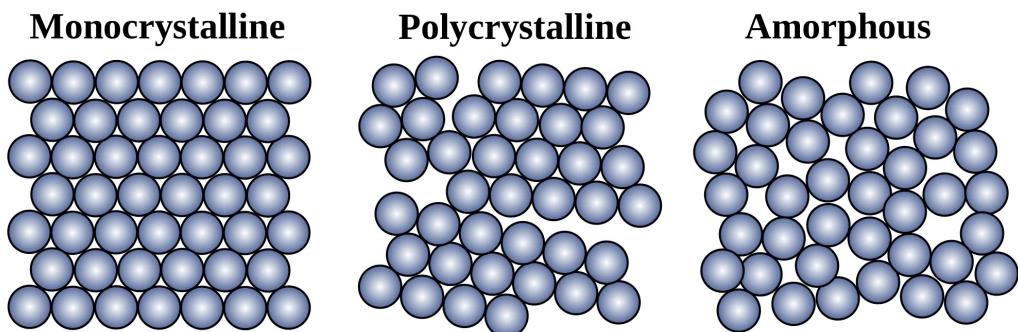
Only for special applications, expensive

- Single-crystal turbine blades ($T > 1000^{\circ}\text{C}$, creep-resistant)
- Semiconductors, MEMS components made of silicon (e.g. gyroscopes in smartphones, accelerometers)
- Optical elements (e.g. laser crystals, $\lambda/4$ plates, crystals for frequency doubling of lasers)

1.5.3 Amorphous materials

- Inorganic glasses (also Gorilla glass of smartphones)
- Metallic glasses (ferrous transformer sheet metal)
- Amorphous plastics (e.g. PMMA - plexiglass, COC, ...)

1.5.4 Structure difference



1.6 Directional dependence of the properties of materials

1.6.1 Anisotropy and Isotropy

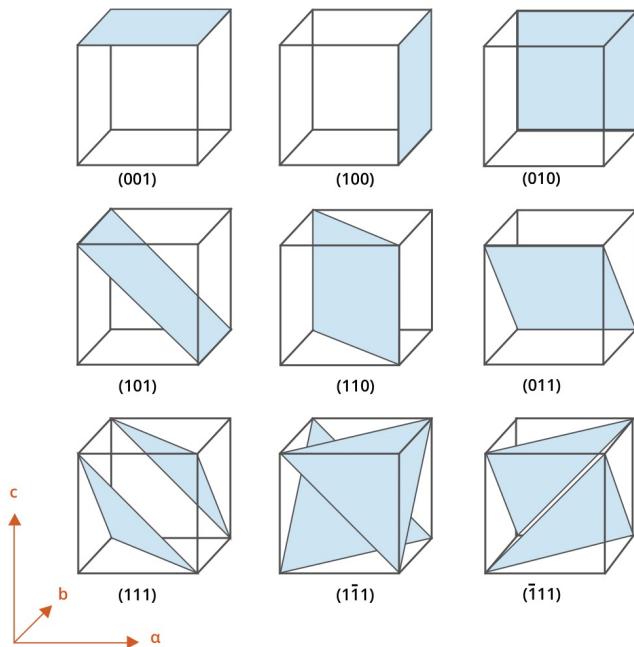
- Anisotropic: Properties depend on direction (e.g. single crystals, wood, composites)
- Isotropic: Properties do not depend on direction (e.g. polycrystalline metals, amorphous materials)

1.6.2 Anisotropy of the Young's Modulus E in most cubic crystals

In most cases, the E is the largest in the direction of the closest packed atomic planes, in direction of the space diagonal $\langle 111 \rangle$.

1.6.3 Miller indices for crystal directions

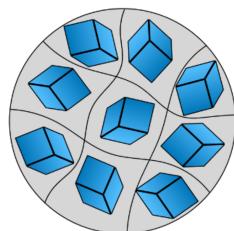
In short, the Miller indices are the reciprocals of the fractional intercepts that the plane makes with the crystallographic axes:



1.7 Directional dependence of properties in polycrystalline materials

1.7.1 Polycrystalline materials without texture

The polycrystalline materials without texture are considered **quasi-isotropic**, because the grains are randomly oriented.

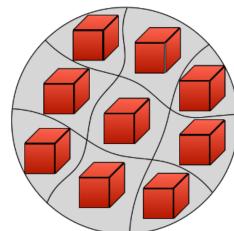


Polycrystalline material without texture

Notice: each crystal is anisotropic. but the material is quasi-isotropic to the outside, directional dependence “averages out”

1.7.2 Polycrystalline materials with texture

The polycrystalline materials with texture are considered **anisotropic**, because the grains are preferentially oriented.



Polycrystalline material with texture

1.8 Material properties wrap-up

1.8.1 Single crystal materials

- Anisotropic
- Properties depend on direction
- Not uniform = anisotropic

1.8.2 Polycrystalline materials without texture

- Quasi-isotropic
- Each crystal: anisotropic
- Uniform properties in all directions: isotropic → quasi-isotropic

1.8.3 Polycrystalline materials with texture

- Anisotropic
- Preferential orientation of the crystallites: texture → anisotropic
- Examples: rolled and recrystallized electrical sheets with Goss texture

1.8.4 Amorphous materials

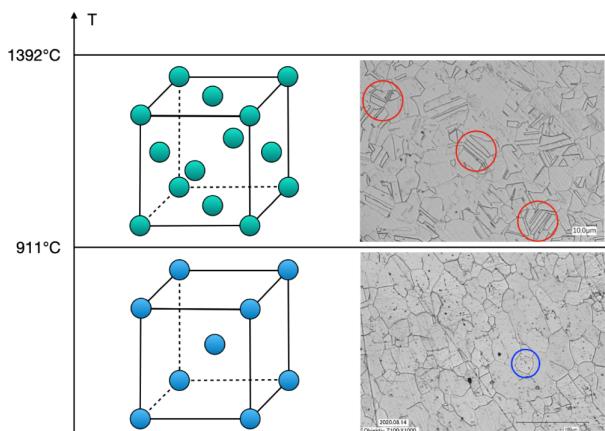
- Isotropic (e.g. glass or amorphous metals)

1.9 Polymorphism (Allotropy)

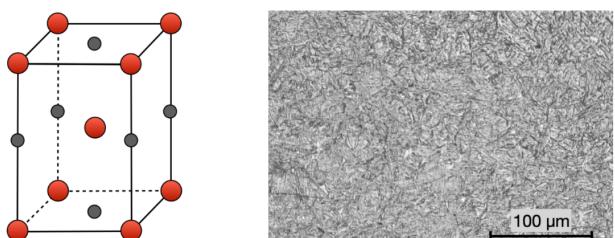
Some materials may exhibit more than one crystal structure:

- Iron $\begin{cases} \alpha\text{-Fe (ferrite, BCC)} & \text{below } 911^\circ\text{C} \\ \gamma\text{-Fe (austenite, FCC)} & 911^\circ\text{C to } 1392^\circ\text{C} \\ \delta\text{-Fe (ferrite, BCC)} & 1392^\circ\text{C to } 1536^\circ\text{C} \end{cases}$
- Titanium $\begin{cases} \text{HCP} & \text{below } 880^\circ\text{C} \\ \text{BCC} & \text{above } 880^\circ\text{C} \end{cases}$
- Shape memory alloys (e.g. NiTi)
- Carbon (graphite, diamond, graphene, fullerene, CNT, ...)
- Zirconia (high crack resistance due to phase transformation toughening)
- Ferro- and piezoelectric materials (e.g. PZT, quartz, ...)

1.9.1 Polymorphism of Iron (Fe)

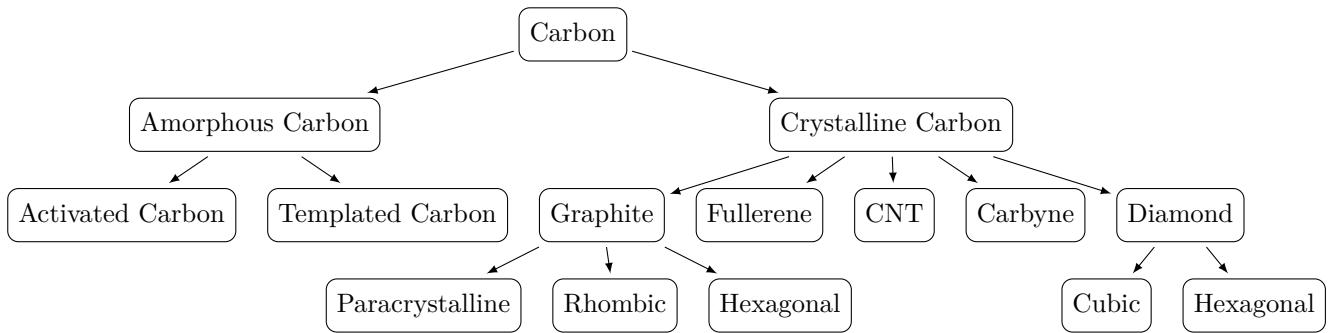


Slow Austenite transformation in steel: Ferrite



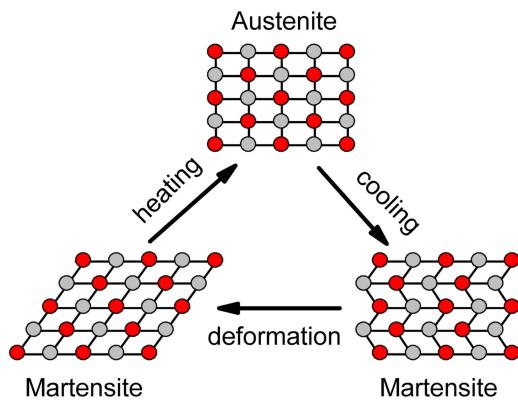
Fast Austenite transformation: Martensite

1.9.2 Polymorphism of Carbon (C)



1.9.3 Polymorphism of Nitinol (NiTi)

NiTi is a shape memory alloy (SMA), used for screen lock of tablet notebooks, medtech, and spectacle frames.



1.10 Microstructure and Phases

Phases are **homogeneous** subsections of a material with uniform physical and chemical properties:

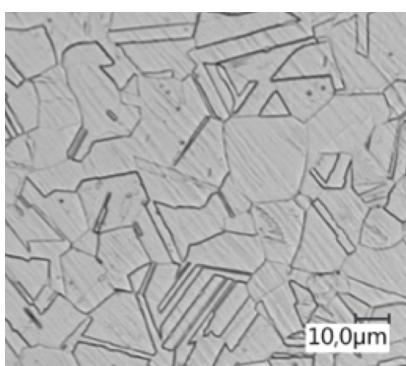
- A phase can be crystalline or amorphous
- At the phase boundaries, a sudden change in structure, properties and chemical composition occurs

Polycrystalline materials can consist of:

- One phase (homogeneous microstructure, e.g. only iron crystals)
- Different phases (heterogeneous microstructure, e.g. graphite and iron)

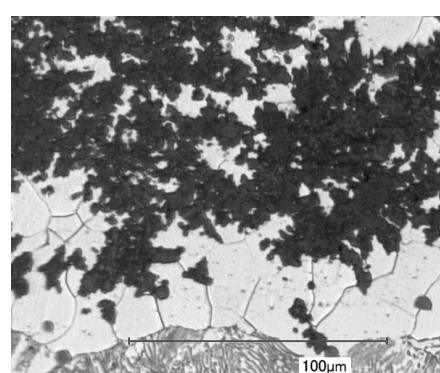
1.10.1 Homogeneous microstructure

They have only one phase and crystal structure:



1.10.2 Heterogeneous microstructure

They have multiple phases and many types of crystal structures:



1.11 Alloys

1.11.1 Definition of an alloy

An alloy is a metallic material of at least 2 types of atoms:

- Metal + Metal (iron-nickel, gold-silver, tin-lead, aluminum-copper, ...)
- Metal + Non-metal (iron-carbon (steel), nickel-phosphorus, ...)

1.11.2 Microstructure of alloys

- **Homogeneous**, single-phase, only one type of cristal: SOLID SOLUTION CRYSTAL
- **Heterogeneous**, multi-phase, MIX OF DIFFERENT CRYSTAL TYPES:
 - Crystals of pure metals without impurity atoms (no solid solution crystals)
 - Solid solution crystals with impurity atoms,
 - Crystals of intermetallic or intermediate phases (chem compounds crystals with their own distinguished crystal structure e.g. Ni₃Ti, Fe₃C, ...)
 - (Impurity particles, e.g. added ceramic particles or slag residues)

2 Most important metal structures and crystal lattice defects

2.1 Lattice defects

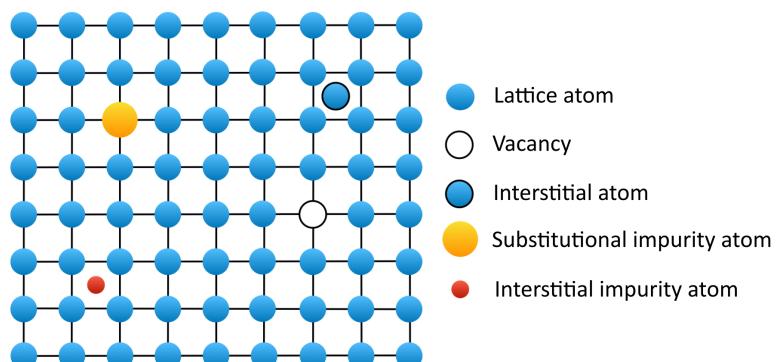
Lattice defects are irregularities in the crystal structure:

- **0-dimensional defects** (point defects)
- **1-dimensional defects** (line defects)
- **2-dimensional defects** (surface defects)
- **3-dimensional defects** (volume defects)

2.1.1 0-dimensional defect

0-dimensional defects include vacancies (missing atoms) and impurity atoms (foreign atoms in the lattice).

The approximate atomic size is 0.1nm.

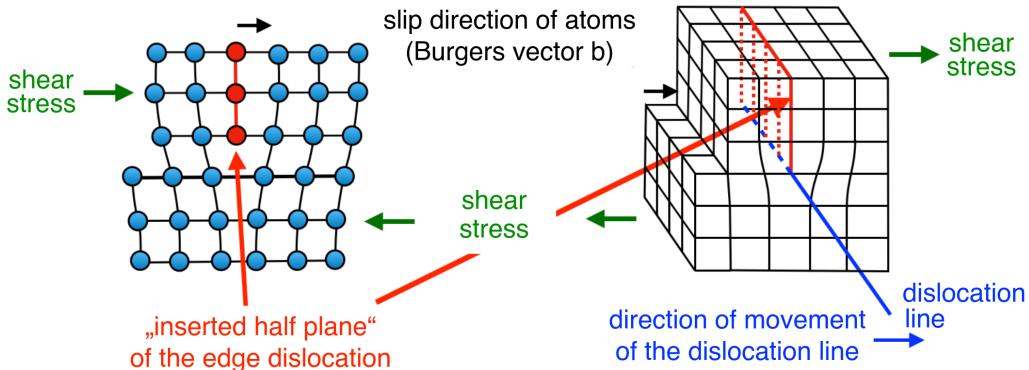


Point defects: vacancy, interstitial atom, substitutional atom

2.1.2 1-dimensional defect

1-dimensional defects are dislocations (line defects) in the crystal structure.

Edge dislocations insert an extra half-plane of atoms in the crystal, distorting the nearby planes of atoms.



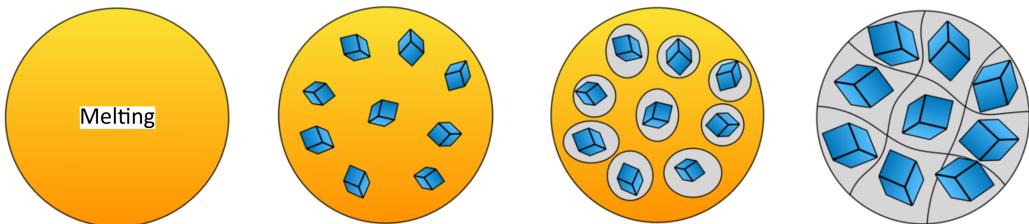
Line defects: edge dislocation, screw dislocation

2.1.3 2-dimensional defect

2-dimensional defects are grain boundaries (surface defects) in polycrystalline materials:

- Crystal growth starts at multiple locations within the molten metal.
- Finally, the growing grains merge to form the microstructure of the solid metal.

The approximate atomic size is 10 to 100 μm .



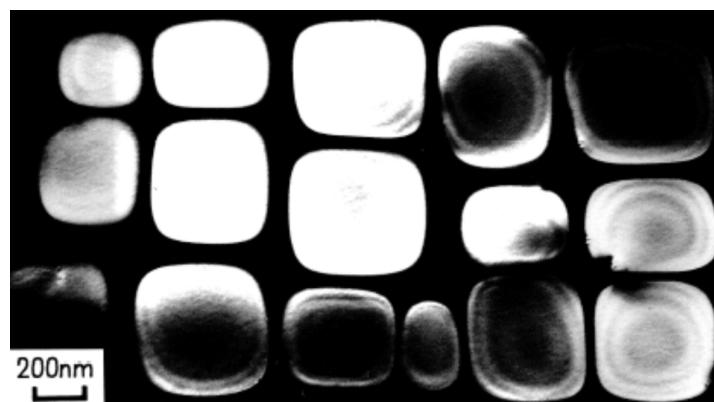
Crystallization from a melt:

(1) homogeneous melt, (2) nucleation of crystals, (3) crystal growth surrounded by residual melt, (4) fully solidified polycrystalline structure with grain boundaries

2.1.4 3-dimensional defect

3-dimensional defects are precipitates, inclusions, voids, cracks (volume defects) in the crystal structure.

The size is very small (nanometers)



Coherent Ni_3Al precipitates (white) in a Ni solid solution crystal (black)

3 Elastic and plastic deformation

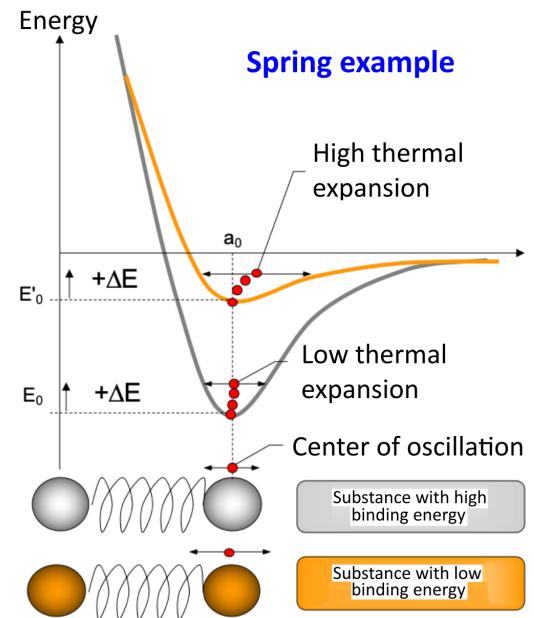
3.1 Elastic deformation

3.1.1 Atomic energy-distance model

The atomic energy-distance model describes the interaction between two atoms.

The coefficient of thermal expansion α is inversely proportional to:

- Young's modulus E (in case of springs, the force)
- Bonding energy
- Melting temperature



3.2 Elastic constants of isotropic materials

3.2.1 Elastic stress, strain, and Young's modulus

Letting the load be unidirectional and in x-direction, then:

$$\varepsilon_x = \frac{1}{E} \cdot \sigma_x \iff \sigma_x = E \cdot \varepsilon_x$$

3.2.2 Poisson's ratio ν

When a material is stretched in one direction (x-direction), it tends to contract in the other two directions (y- and z-directions).

The ratio of the transverse strain to the axial strain is called Poisson's ratio:

$$\nu = -\frac{\varepsilon_y}{\varepsilon_x} = -\frac{\varepsilon_z}{\varepsilon_x}$$

3.2.3 Relationship between the 3 isotropic elastic constants G

For isotropic materials, the following relationships hold:

$$G = \frac{E}{2(1+\nu)} = \frac{\sigma_x}{2\varepsilon_x(1+\nu)}$$

3.3 Plastic deformation in metals

The plastic deformation has as characteristics to be permanent and non-reversible.

3.3.1 At room temperature

- Dislocations move on densely packed slip planes in densely packed directions
- Smaller slip distances require less external force or energy

Note: There are exceptions. For example, metals with relatively low stacking fault energy show:

- Twin formation (e.g. nitinol)
- Partial dislocations pairs with stacking faults in between (e.g. Ni, Cu)

3.3.2 At high temperatures

The metal creeps, leading to diffusion of atoms, especially at grain boundaries.

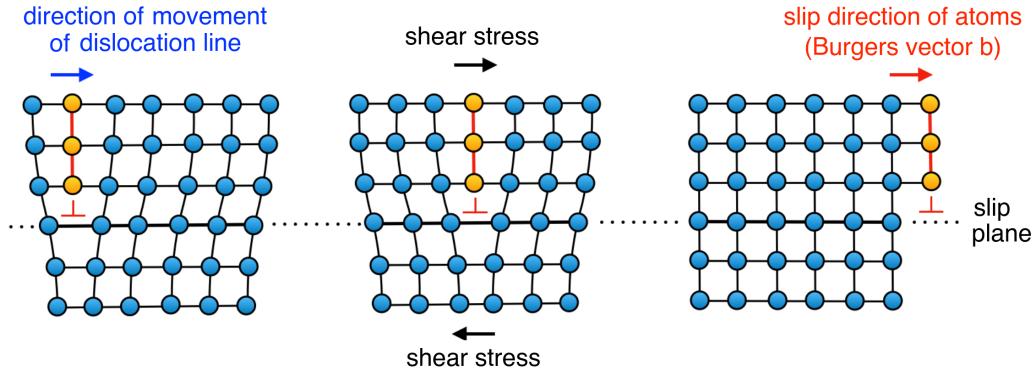
3.4 Dislocation Slip Model

The dislocation slip model describes the plastic deformation of metals by dislocation motion.

3.4.1 Simplified model

The simplified dislocation slip model is sufficient for practical understanding of plastic deformation:

- Inserted half-plane, the end of which forms the dislocation line
- Dislocation moves on densely packed slip planes

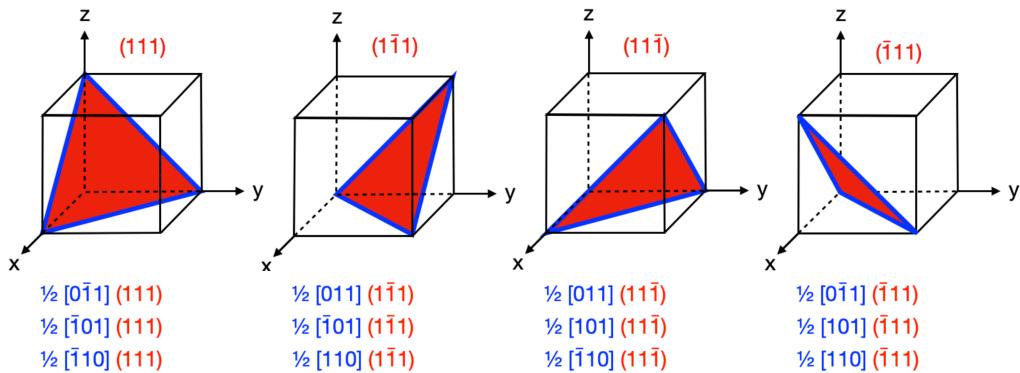


Edge dislocation motion under shear stress

3.5 Slip systems

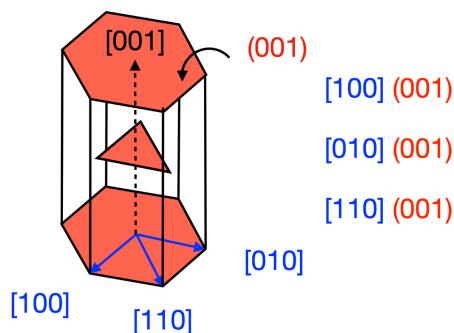
3.5.1 Slip systems in FCC metals (Miller indices)

FCC metals have 12 close-packed slip systems, making them soft and highly ductile (e.g. Au, Ag, Cu, Al, α -Fe)



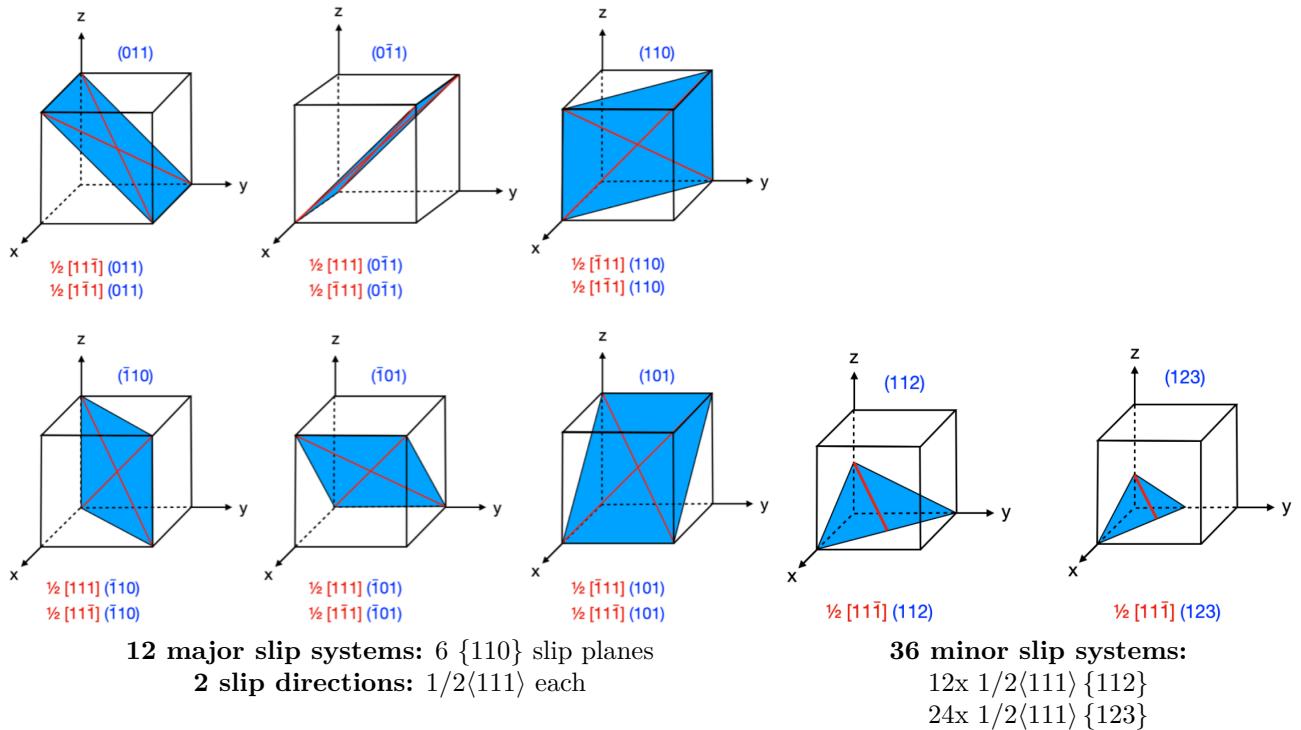
3.5.2 Slip systems in HCP metals (Miller indices)

HCP metals are closely packed but deform on only one slip plane with 3 slip systems, resulting in limited ductility (e.g. Ti, Zn, Mg).



3.5.3 Slip systems in BCC metals (Miller indices)

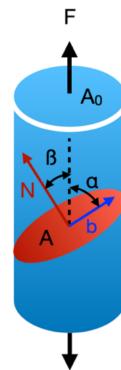
BCC metals have 48 slip systems but are less closely packed, leading to higher strength and lower ductility (e.g. α -Fe, Cr, W, Mo, Ta, Nb)



3.6 Schmid's law of critical resolved shear stress

The Schmid's law states that slip begins in a crystalline material when the resolved shear stress on a slip system reaches a critical value.

- Plastic deformation occurs only on closely packed slip planes where the applied shear stress exceeds a critical value
- Under uniaxial loading, the maximum shear stress acts on slip planes inclined at 45° to the load axis



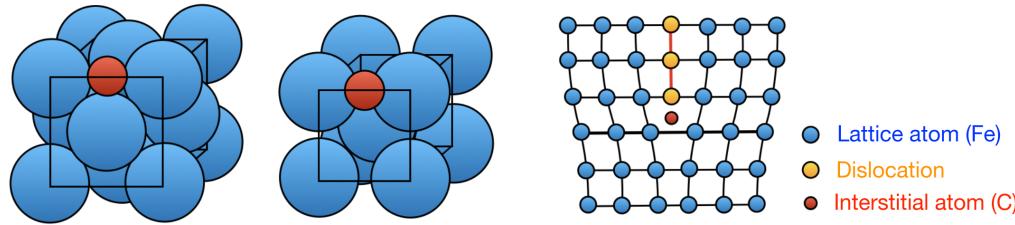
3.7 Correlation between metals crystal structure and ductility

Metal	Ductility	Packing structure	Slip systems	Slip system orientation
FCC	Highest ductility among metals	Closest-packed (74%)	4 slip planes \rightarrow 12 slip systems	Very high probability of favorable orientation (Schmid's law)
BCC	Lower ductility than FCC, but still generally good	Less closely packed (68%)	Many slip planes and slip systems	Strength often higher than FCC metals
HCP	Limited ductility under normal conditions	Closest-packed (74%)	Only 1 slip plane \rightarrow 3 slip systems	Low probability of favorable orientation (-45° to load axis)

3.8 Particularities in BCC metals

3.8.1 Cottrell atmospheres and Dislocation pinning

- In α -iron with a BCC structure (ferrite), the octahedral sites for interstitial atoms such as carbon or nitrogen are much smaller than in γ -iron with an FCC structure (austenite)
- As a result, carbon atoms in ferrite preferentially diffuse into the distortion fields near dislocation lines, where more space is available, forming so-called **Cottrell atmospheres**
- These atmospheres are responsible for the pronounced upper yield point (R_{eH}) observed in tensile tests of many BCC metals, as well as for the brittle fracture behavior at low temperature in impact tests
- During plastic deformation, dislocations must first break free from the Cottrell atmosphere. This process is especially difficult at low temperatures or high strain rates, leading to strong dislocation pinning



Carbon atoms occupy small octahedral sites (left), preferentially diffuse to dislocation regions (center), which forms Cottrell atmospheres that pin dislocations (right)

4 Strengthening mechanisms

A Glossary

Alloy A mixture of two or more elements, where at least one element is a metal.

Amorphous Non-crystalline material with no long-range order.

Anisotropy Direction-dependent properties of a material ([Monocrystalline and polycrystalline with texture](#))

Crystalline Material with atoms arranged in a highly ordered microscopic structure, forming a crystal lattice that extends in all directions.

Dislocation A linear defect in the crystal structure where there is an irregularity in the arrangement of atoms.

Heterogeneous Non-uniform composition and properties throughout the material.

Homogeneous Uniform composition and properties throughout the material.

Isotropy Direction-independent properties of a material ([Amorphous](#))

Monocrystalline Material consisting of a single crystal or a continuous crystal lattice with no grain boundaries.

Polycrystalline Material composed of many crystallites of varying size and orientation.

Polymorphism / Allotropy Ability of a material to exist in more than one form or crystal structure.

Quasi-isotropy Approximate isotropy in polycrystalline materials with random grain orientation ([Polycrystalline without texture](#))

Slip Large displacement of one part of a crystal relative to another part along crystallographic planes and directions.

Vacancy A point defect in a crystal lattice where an atom is missing from its regular lattice site.