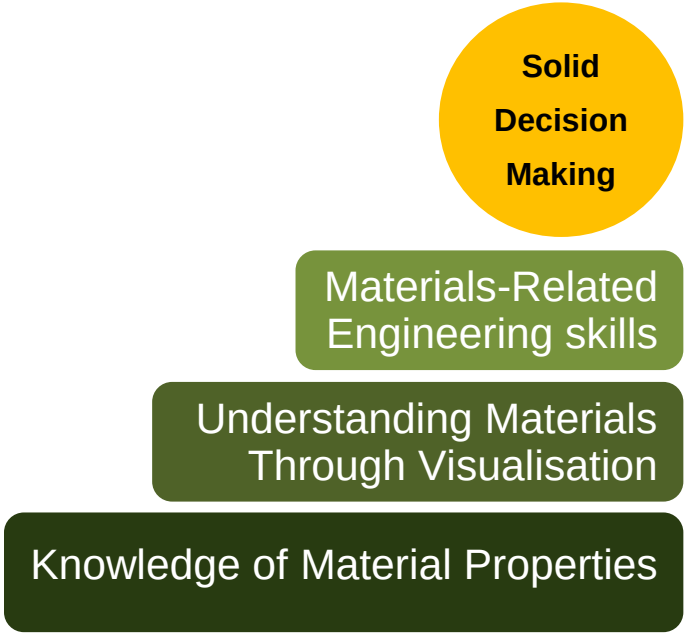
Co-funded by the Erasmus+ Programme of the European Union

Lecture 1A

Structure and properties of metals and alloys

Monday 2nd November 2020

1A. Learning Outcomes



- Ability to describe the structures of pure metals and alloys.
- Knowledge of main crystalline lattices and distortions in metal alloys
- Understanding of how to use software to explore material properties

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Study guide for lecture 1A

Minimum (mandatory) reading:

- Lecture slides 1A
- Teach yourself Crystallography, part 2-3 and exercises within

Supplementary recommended resources:

- The Elements subset within GRANTA EduPack MS&E database
- Ashby (Engineering Materials 2) Ch 1-2
- Callister (any edition): Chapters on Atomic structure, Crystallography and Crystalline solids
- Youtube links (if you have time):

The Secrets of the Super Elements BBC Documentary

https://www.youtube.com/watch?v=4LiYdbNqkwg

Recommended extra exercises:

Micro-projects 1A Structures and Properties

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Outline

- History and properties of materials
- What makes metals special
- Material structure and properties
- Crystal defects and distortion
- Materials database and software

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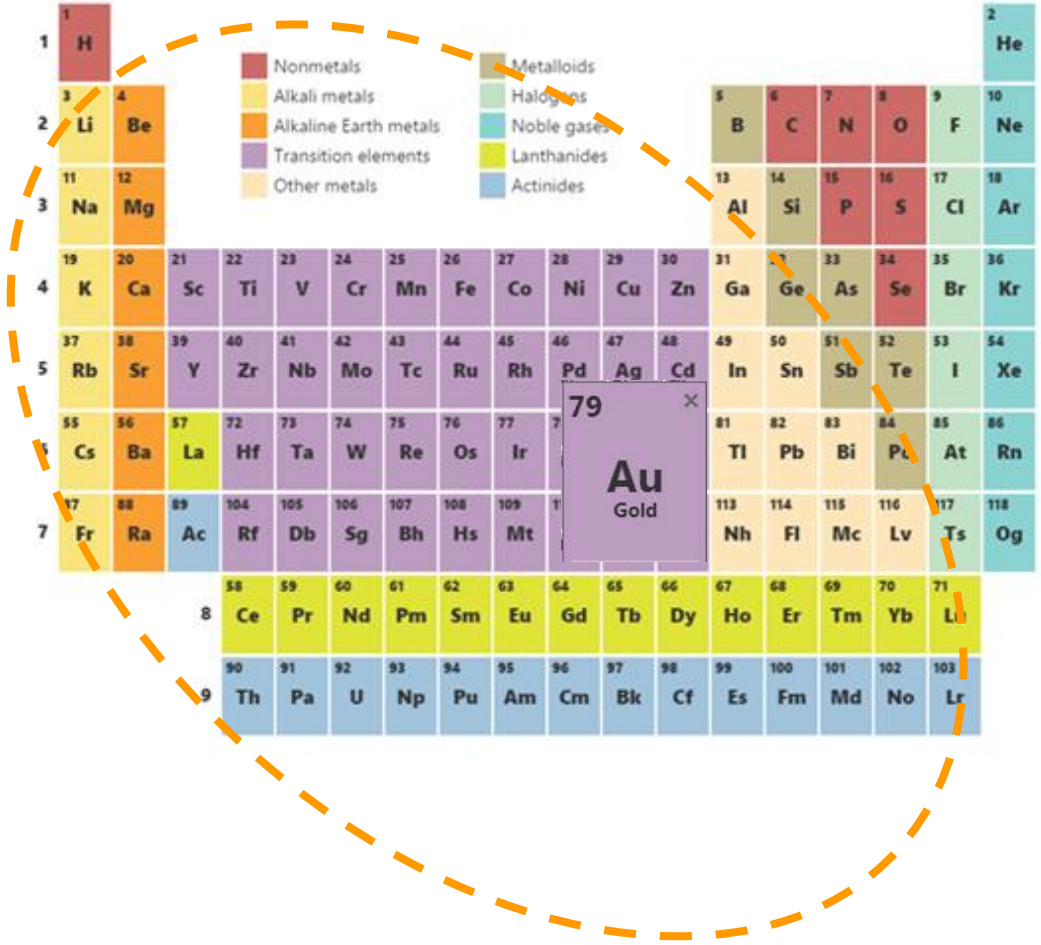
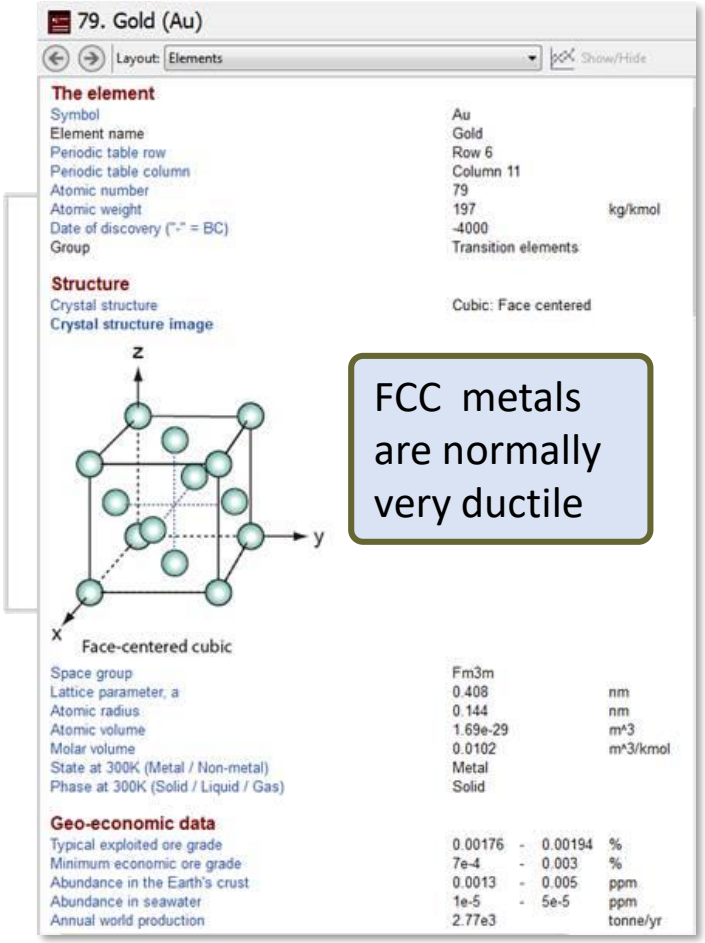
Materials are made from Elements, mostly metals…





FCC metals are normally very ductile

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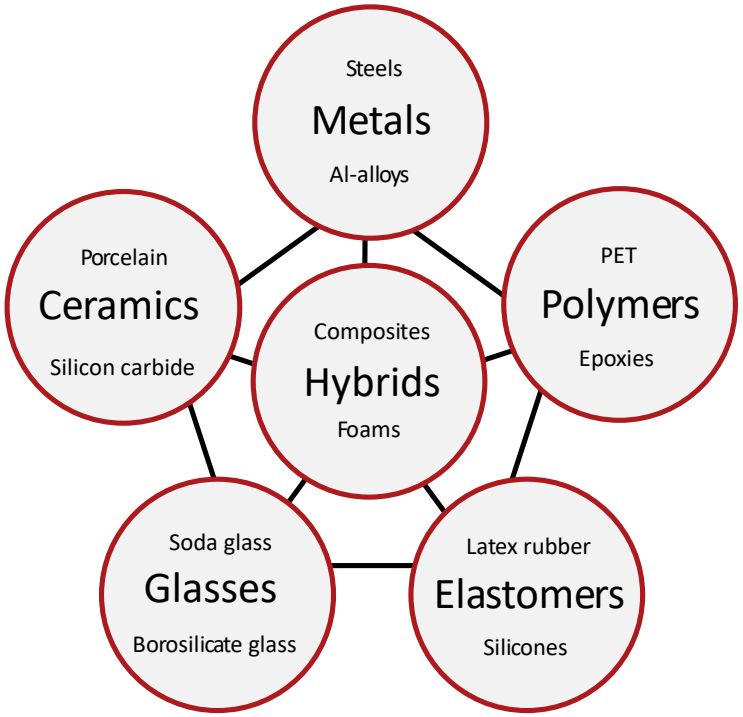
Metals are one of several “families” of Materials



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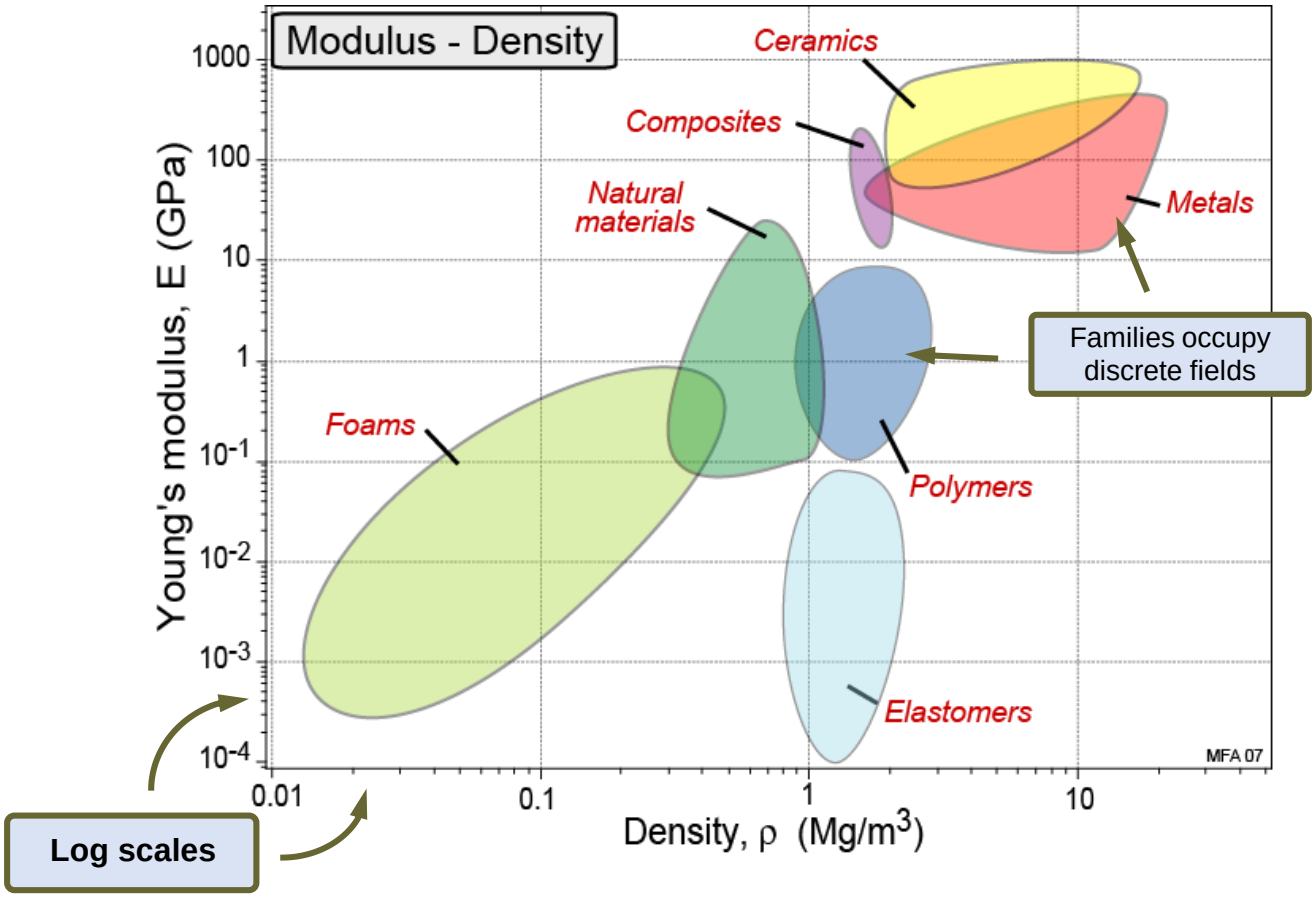
Property Charts, or Bubble Charts (Ashby Charts)



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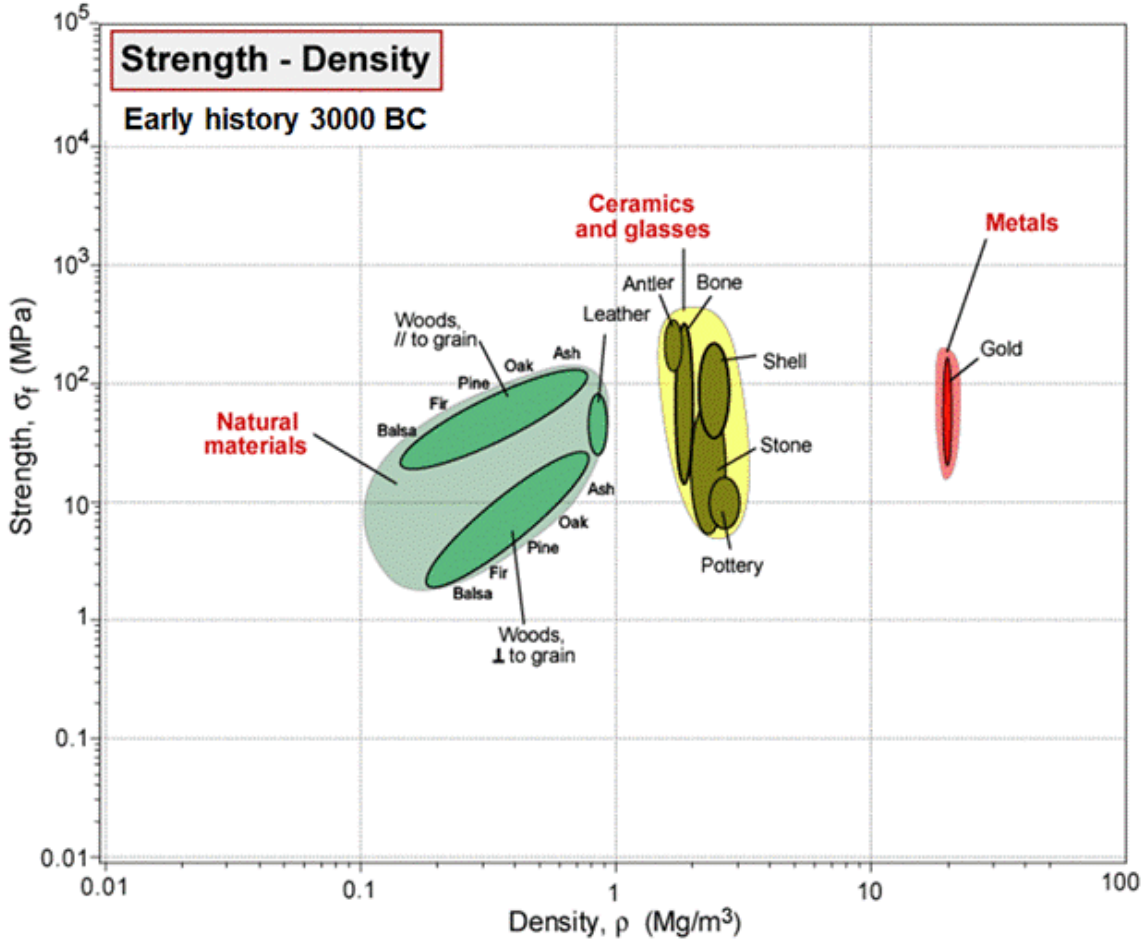
Evolution of Metals and alloys through history



Old Kingdom, Egypt

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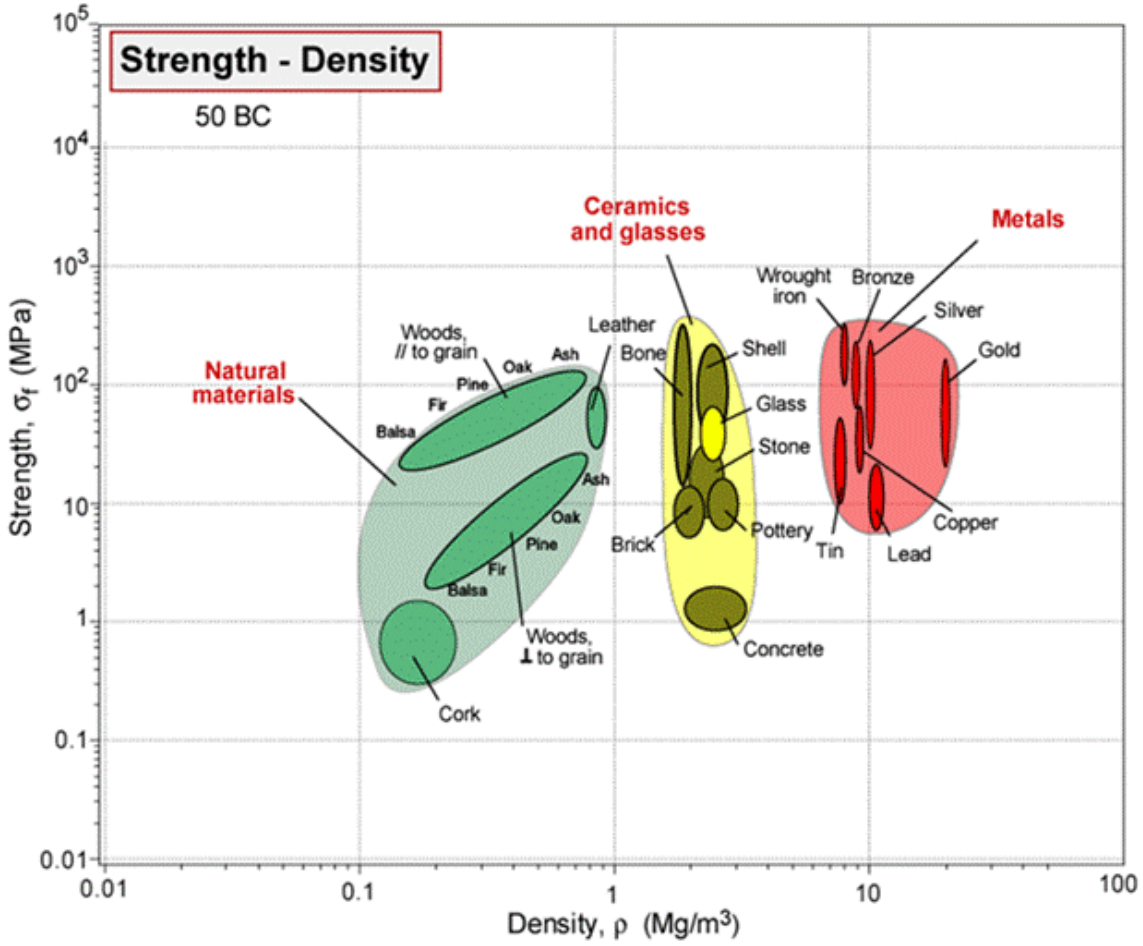
Evolution of Metals and alloys through history



Empire of Rome

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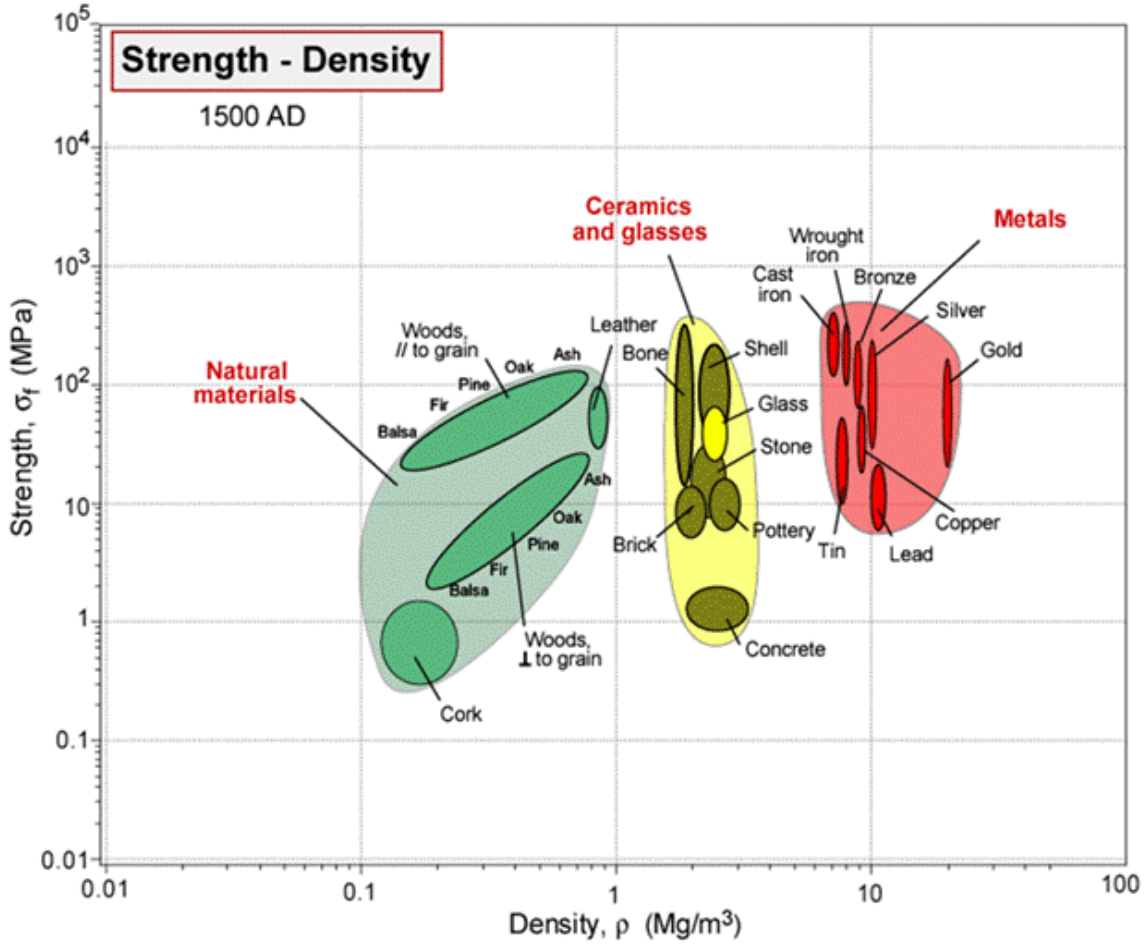
Evolution of Metals and alloys through history



Medieval, south India

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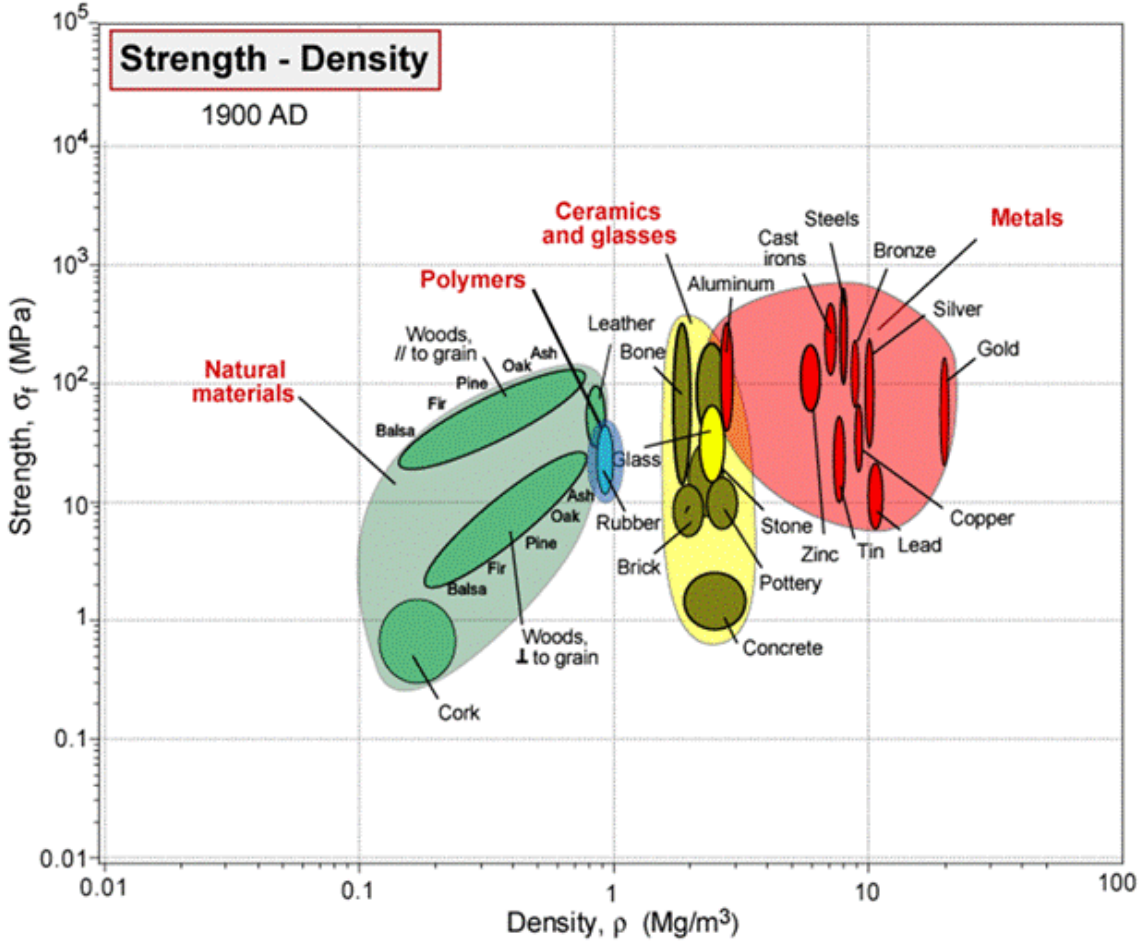
Evolution of Metals and alloys through history



Fin de siècle

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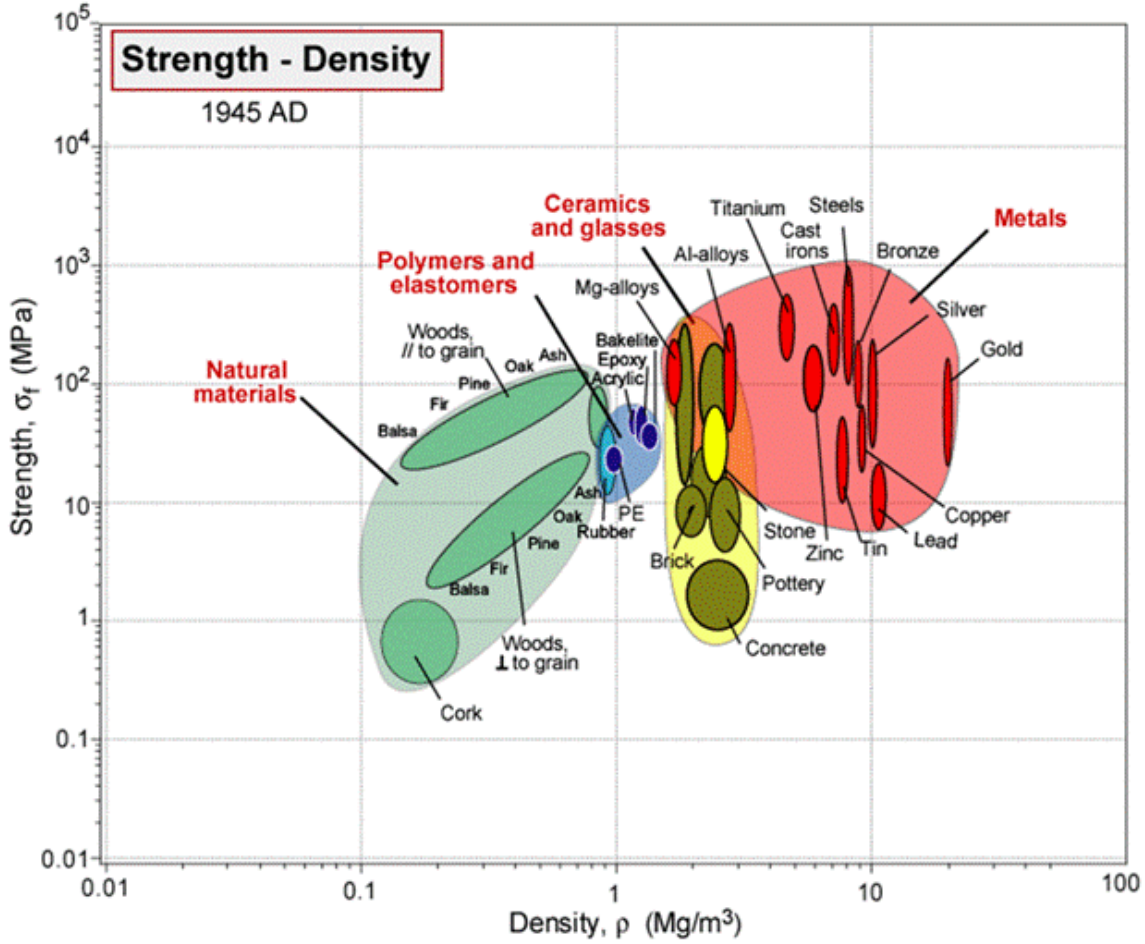
Evolution of Metals and alloys through history



Mid-20th century

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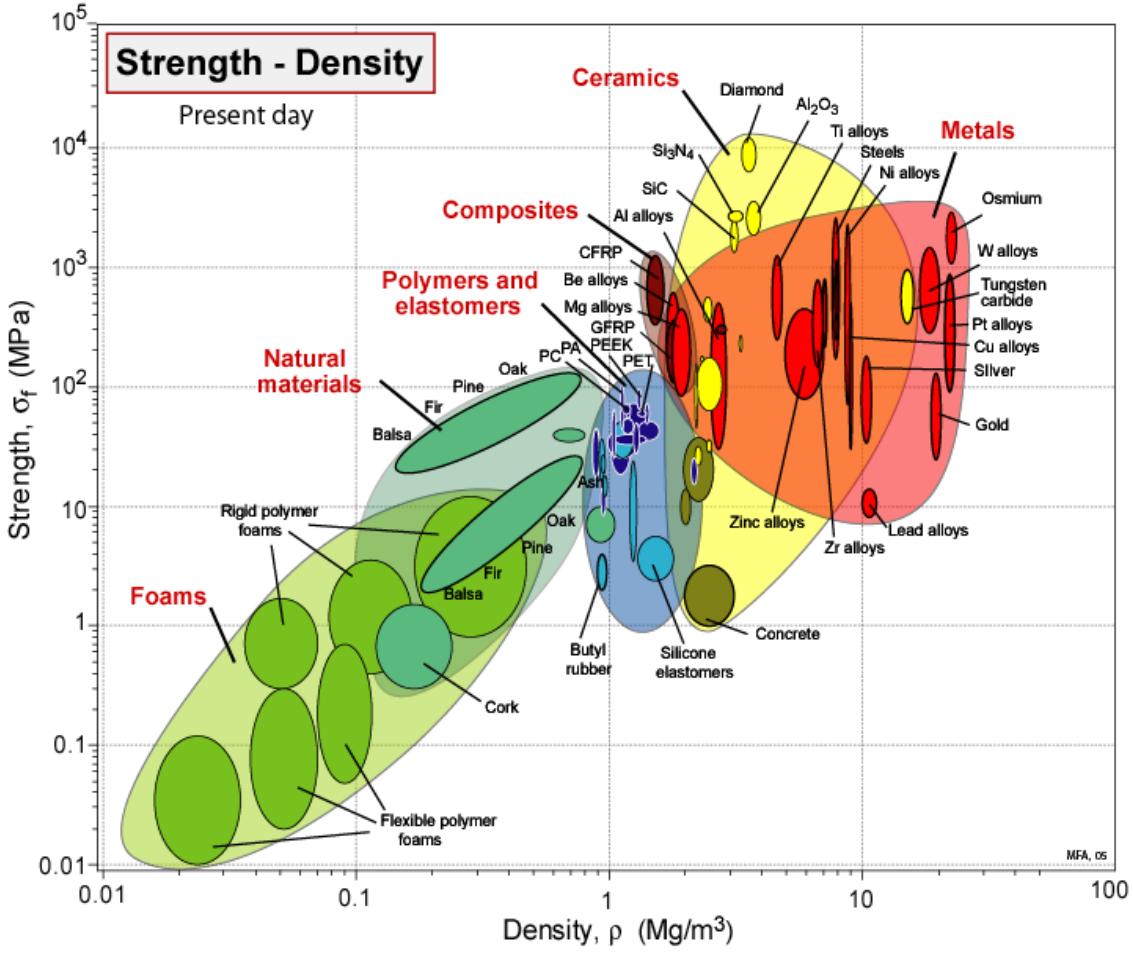
Evolution of Metals and alloys through history



21st century

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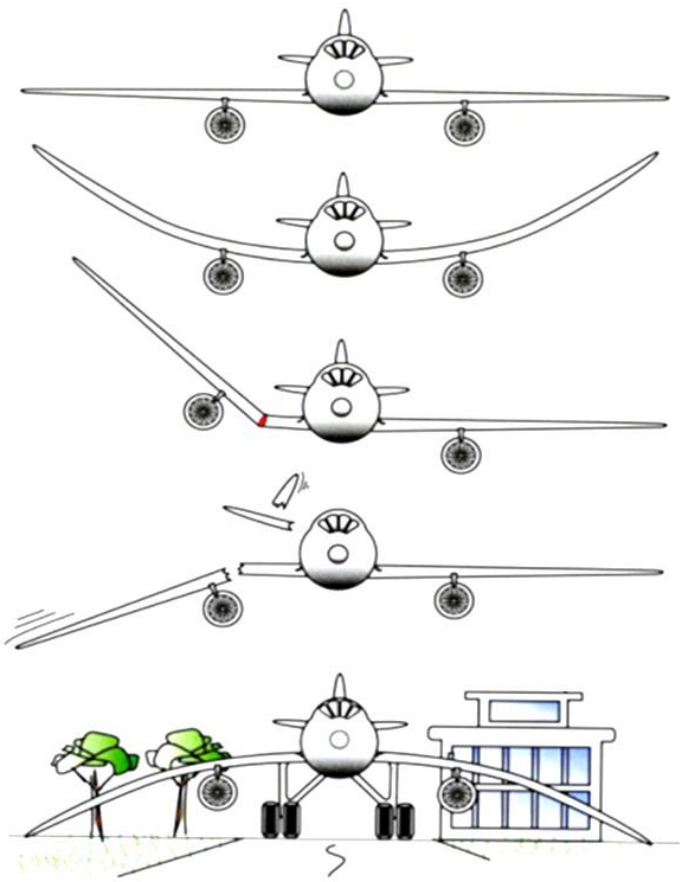
Material properties are important for performance



← Stiff, Strong, Tough, Light } All OK !

← Not stiff enough (need bigger E)

← Not strong enough (need bigger σ_y)

← Not tough enough (need bigger K_{ic})

← Too heavy (need lower ρ)

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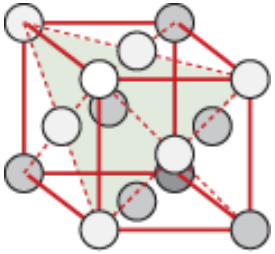
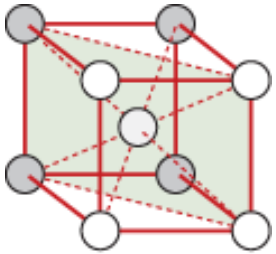
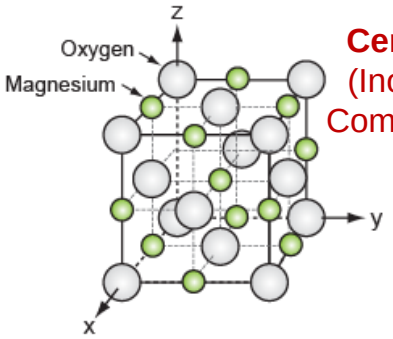
Structures of the materials influence properties

Metals
(most Elements)



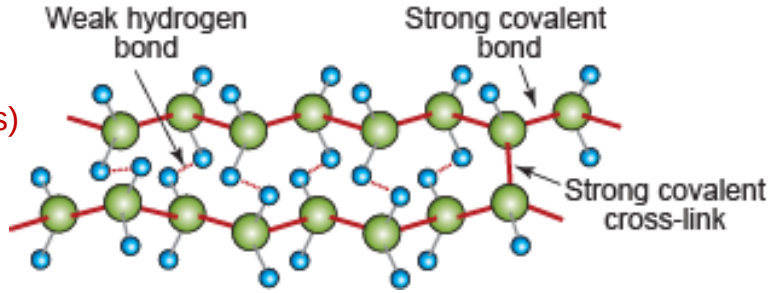
Crystalline packing, metallic bonding

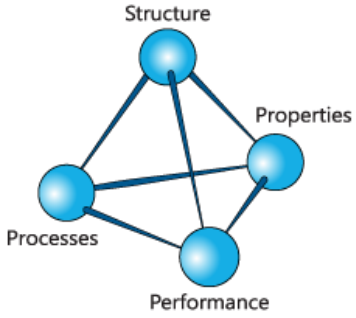




Ceramics
(Inorganic Compounds)

Polymers
(Organic Compounds)





Processing → Structure → Properties → Performance

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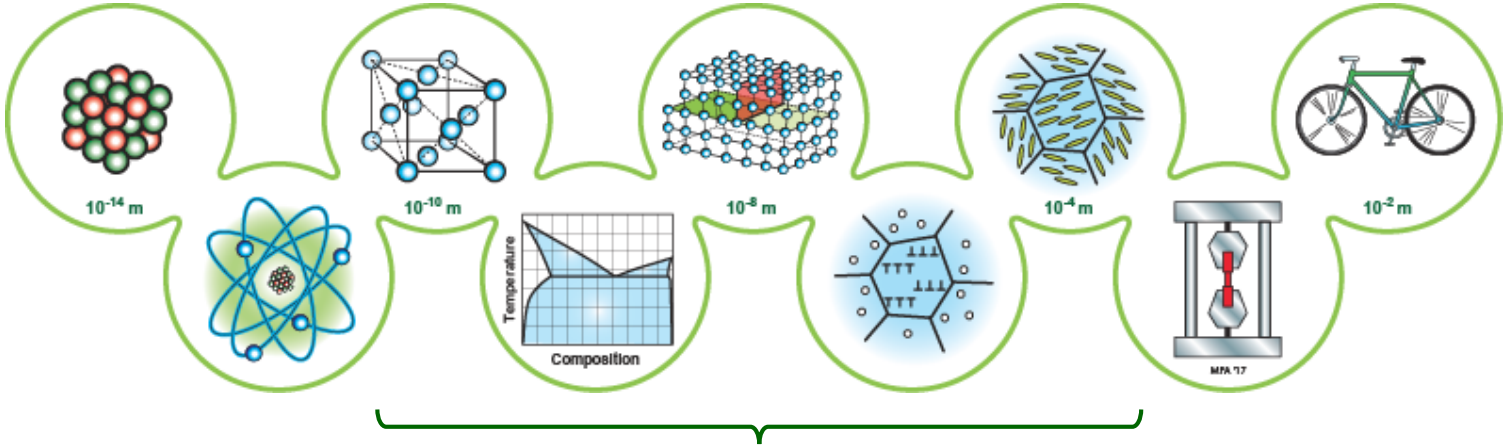
Some Structural Definitions

Most (but not all) solids are *crystalline*. The common engineering metals and ceramics are made up of many small crystals, or *grains.*
These are stuck together at *grain boundaries* to make *polycrystalline aggregates*.
The properties of the material - its strength, stiffness, toughness, conductivity and so forth - are strongly influenced by the underlying crystallinity.
Disordered, or non-crystalline, solids are called *amorphous*



Microstructure

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Impacts of microstructure

Fused Silica Glass

Quartz

How can these compositions be identical when the products and uses are so different?

- Highly resistant to temperature and thermal shock
- Piezoelectric
- Helps keep time in watches

- Chemical composition: SiO_2
- Chemical composition: SiO_2

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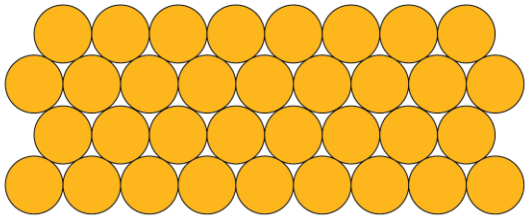
Crystalline vs. Amorphous

Crystalline Materials:

- A solid material characterized by a periodic, repeating, 3D arrangement of atoms, ions, or molecules
- Often opaque

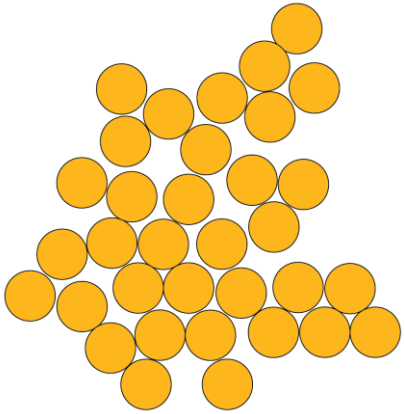
Example: Quartz, salt, aluminum



Amorphous Materials:

- A solid material that lacks a long-range crystalline order
- Often transparent

Example: Glass, some polymers



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More Structural Definitions

- **DEF.** A *crystal* is a regularly-repeating pattern of atoms (our spheres) in 2 or 3 dimensions which can be extended, without change of pattern, indefinitely.
- **DEF.** The *unit cell* of a crystal structure is the unit of the structure, chosen so that it packs to fill space, and which, translated regularly, builds up the entire structure. The *primitive unit cell* is the smallest such cell.
- **DEF.** The *interstitial space* is the unit of space between packed atoms or molecules.
- **DEF.** We describe all crystals in terms of a periodic *lattice*, with an identical group of atoms attached to each lattice point.

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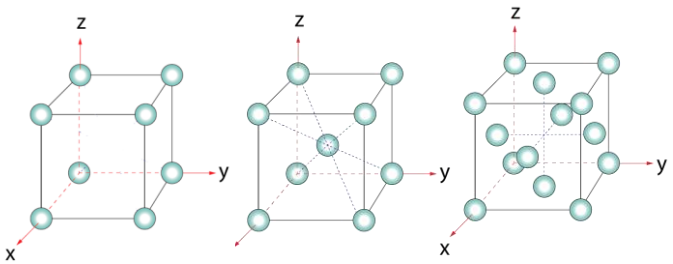
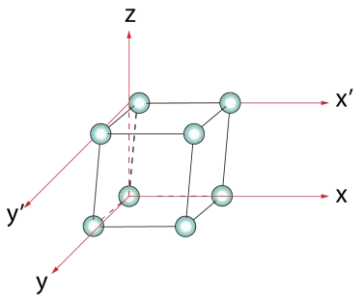
Unit Cells: the Basics of Crystals

There are seven crystal systems:

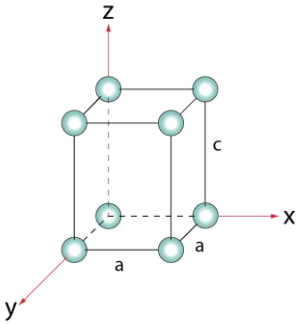
Cubic



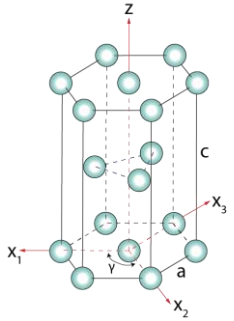
Rhombohedral



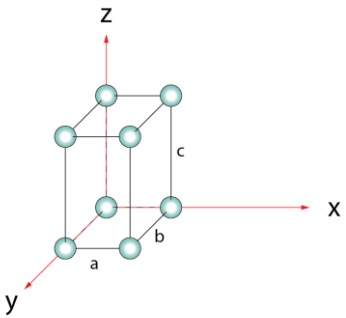
Tetragonal



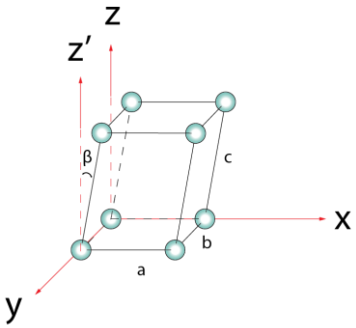
Hexagonal Close-Packed



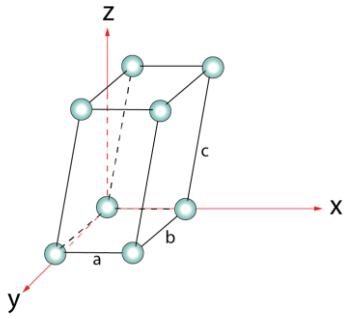
Orthorhombic



Monoclinic



Triclinic



The smallest repeating unit within a crystal

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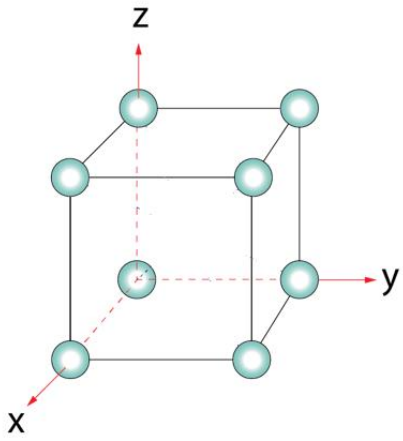
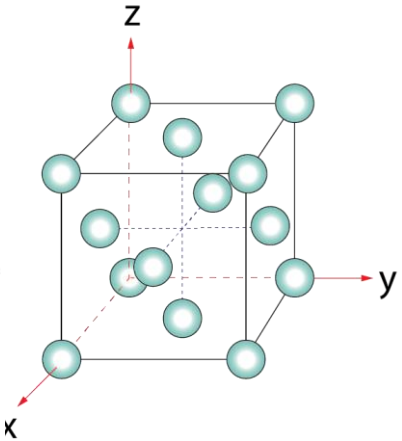
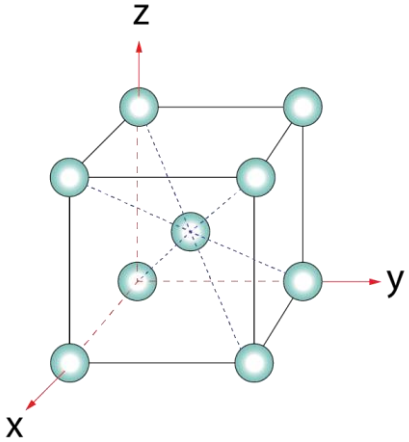
Important Unit Cells of Metals



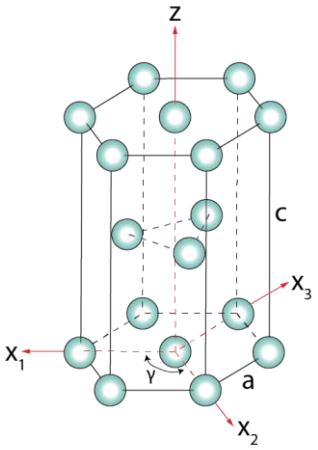
Simple Cubic (SC)



Face-Centered Cubic (FCC)



Body-Centered Cubic (BCC)



Hexagonal Close Packed (HCP)

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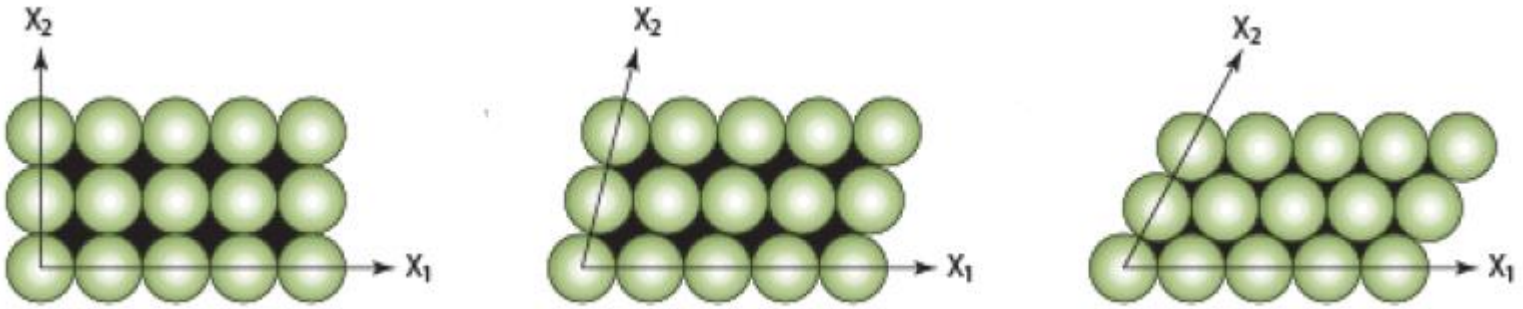
The Close Packed Concept

Hexagonal arrangement of atoms in a plane is more efficient than Cubic – smaller interstitial holes



Close packed planes of atoms are important in deformation

In 2 dimensions:

- Provides good conditions for “slipping”

In 3 dimensions:

- Provides good directions for slipping – slip planes

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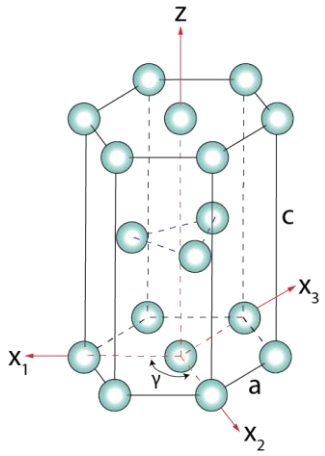
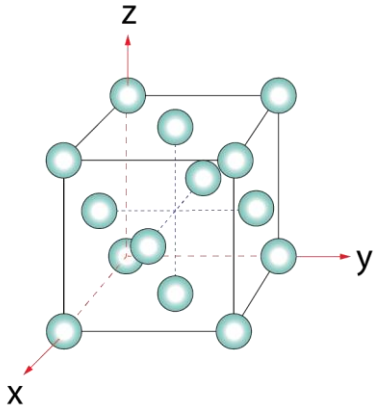
Close Packed Crystal Structures and Crystal Planes

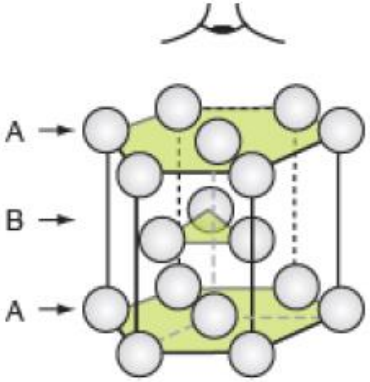


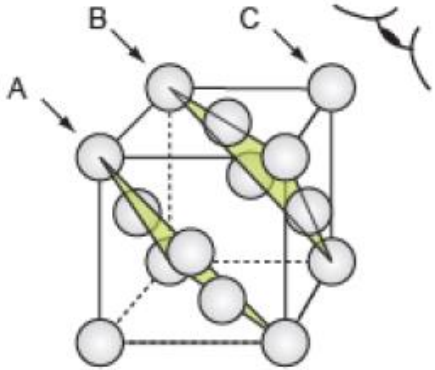
Hexagonal Close Packed (HCP)
Packing density: 74%

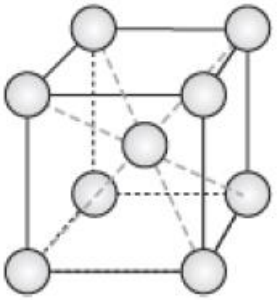


Face-Centered Cubic (FCC)
Packing density: 74%

(No Close Packing in BCC)
Packing density: 68%







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Quiz question

1. Which are the two common metallic crystal structures that contain close-packed planes?

a) BCC and FCC

b) HCP and SC

c) FCC and HCP

d) BCC and HCP

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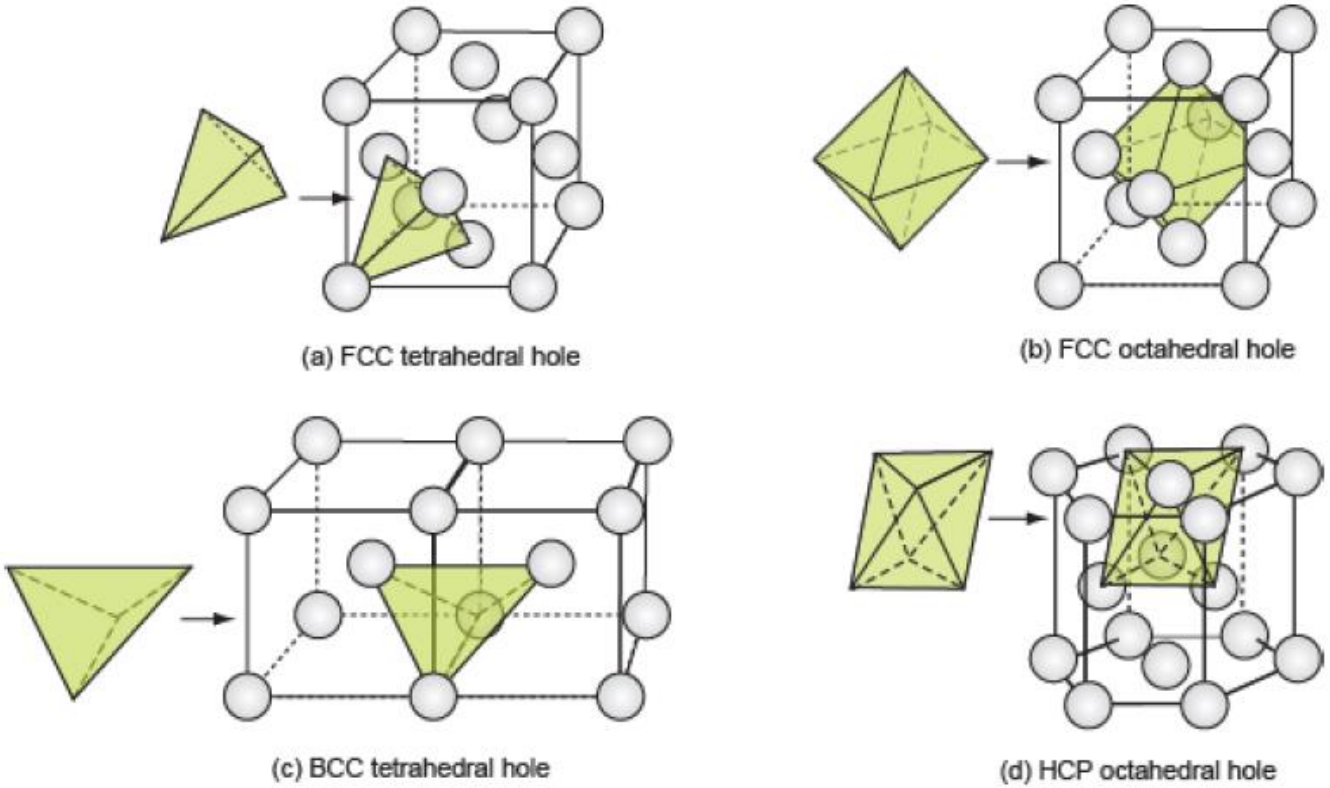
Interstitial holes



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Quiz question

2. Which statement is true about unit cells and interstitial holes, relevant for impurity defects?

a) The tetrahedral holes in BCC and FCC have the same size

b) The octahedral hole of FCC is larger than the tetrahedral hole of BCC

c) The octahedral hole of HCP is larger than the octahedral hole of FCC

d) Octahedral and tetrahedral holes all have the same size in BCC, FCC and HCP structures.

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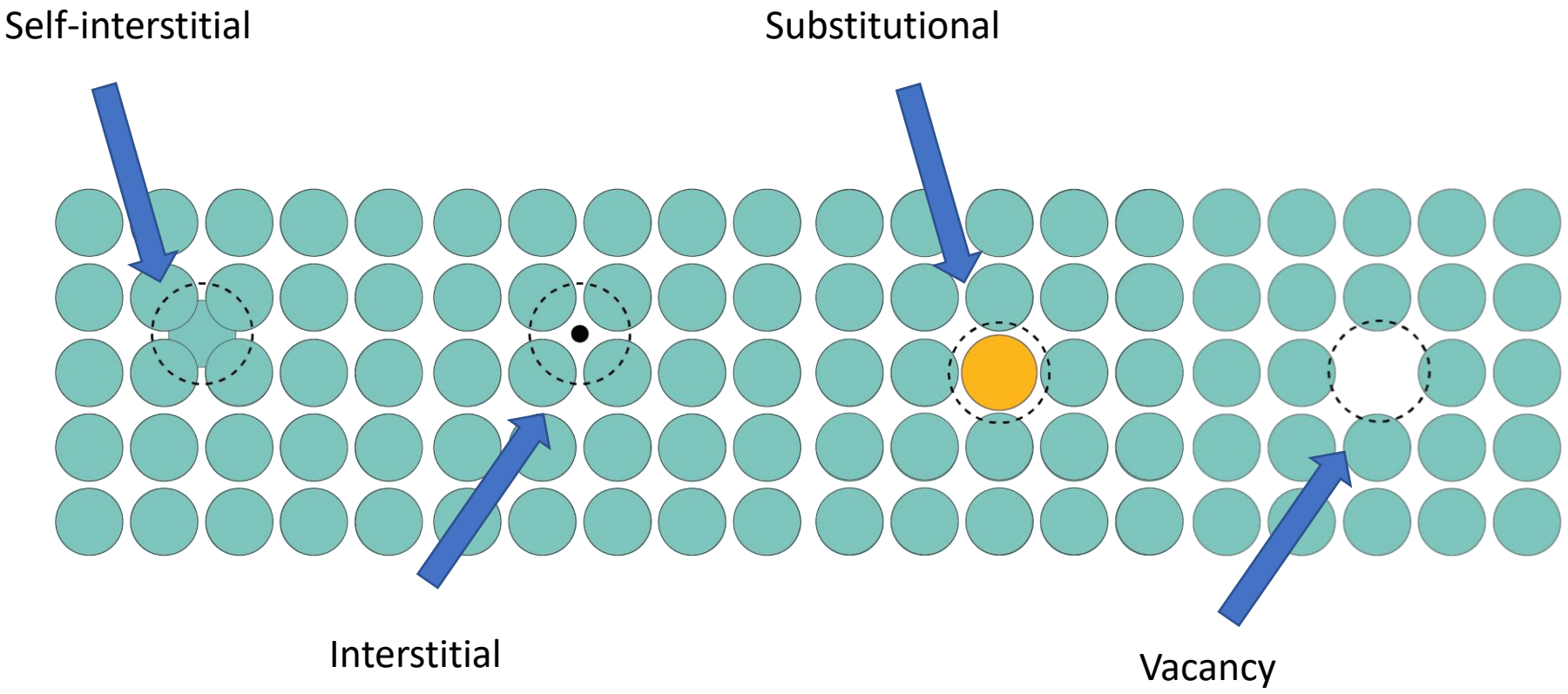
Point Defects



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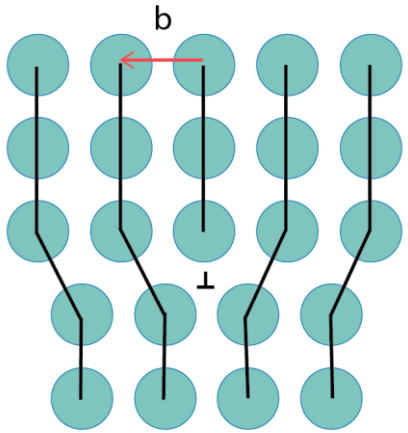
Linear Defects: Dislocations

Type of dislocation is defined by the orientation and magnitude of the lattice distortion or the so-called Burger's Vector, b

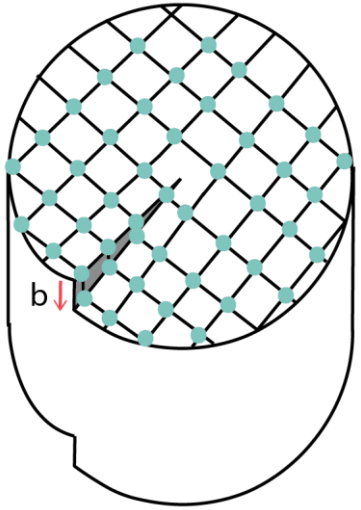
Edge Dislocation

b ⊥ to the dislocation line



Screw Dislocation

b // to the dislocation line



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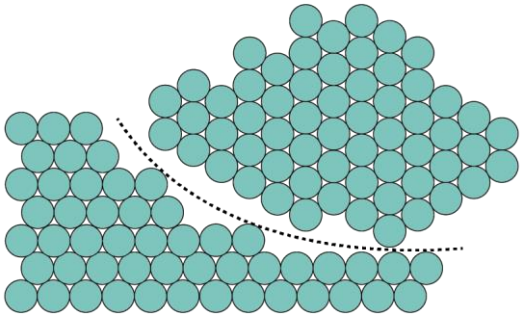
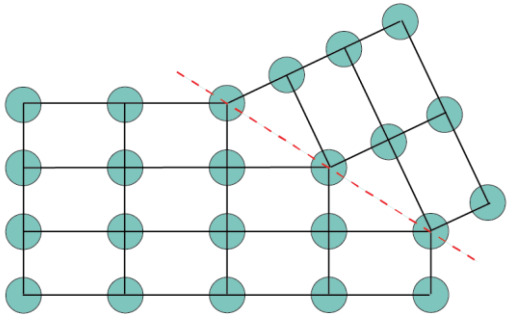
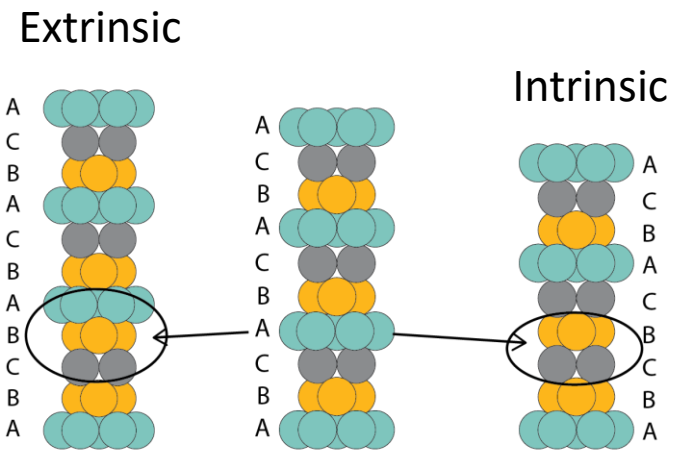
Planar Defects



Grain Boundaries



Twin Boundaries



Stacking Faults

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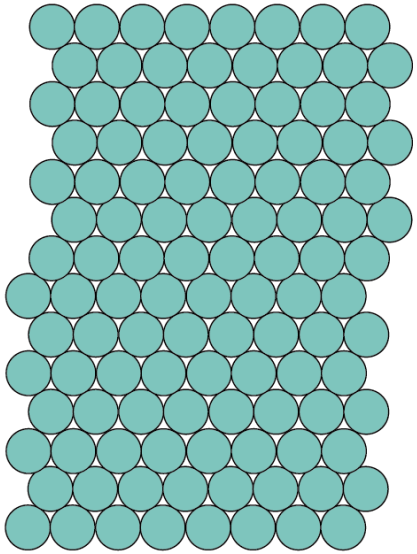
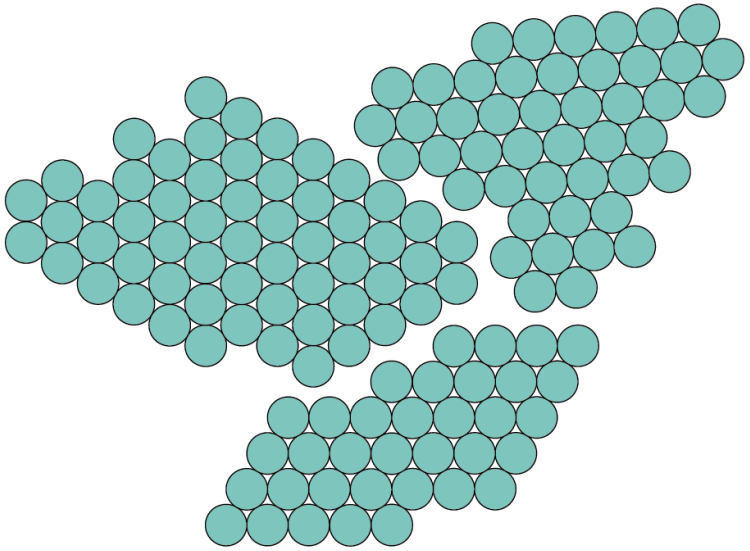
Single vs. Polycrystalline



Uniform crystal orientations throughout the whole material



Segments of different crystal orientations throughout the whole material

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Why do we care about single crystal?

Jet engine turbine blades are grown as single crystals for improved mechanical properties at extreme high temperatures

Otherwise, the blades would droop!

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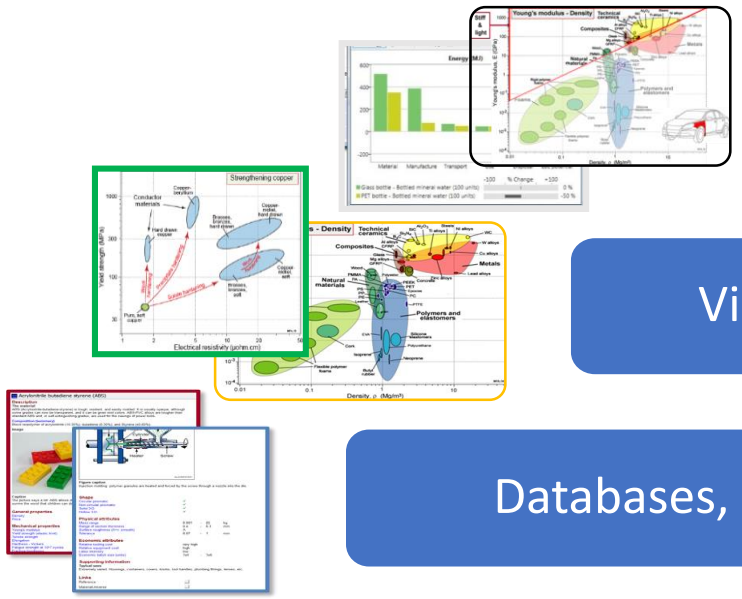
A brief introduction to GRANTA EduPack 2020



Tools, Links

Visualization, Charts

Databases, Data Tables, Data

- Life-cycle and circularity aspects through the ***Eco Audit tool***
- Create hybrids and estimate properties with the ***Synthesizer tool***

Licensing questions: Alex Cazacu <Alex.Cazacu@ansys.com>

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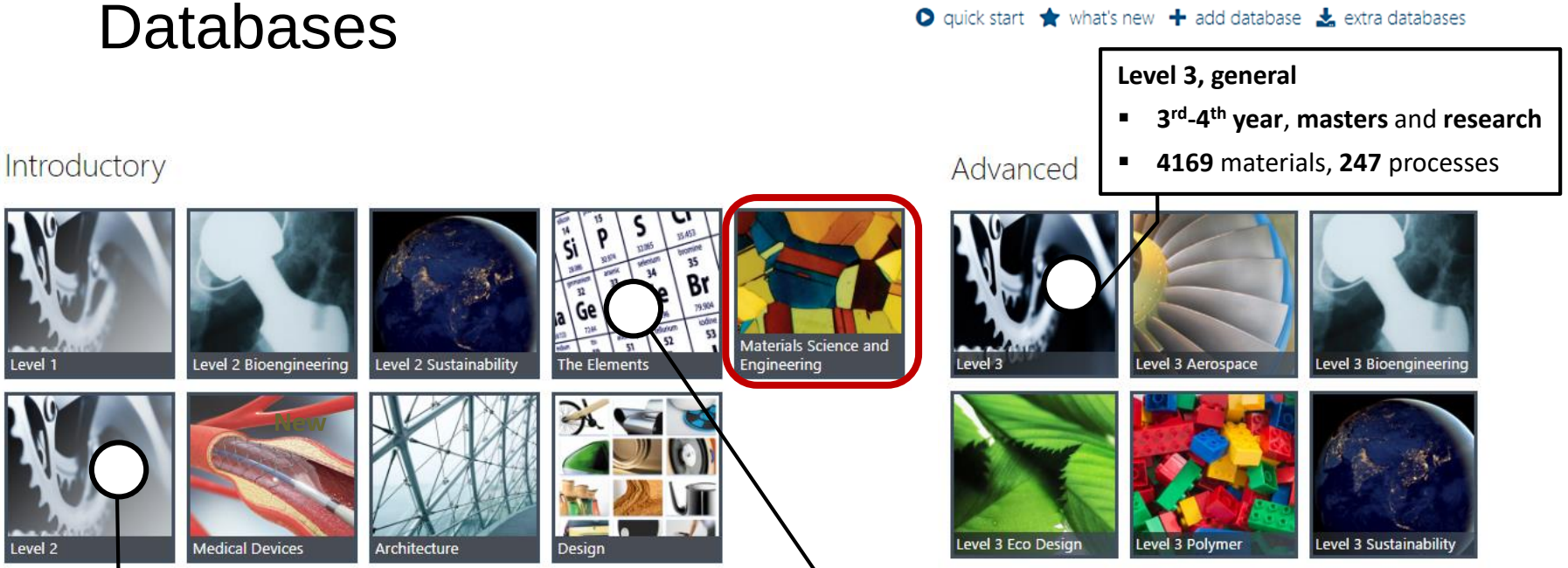
GRANTA EduPack 2020

Databases



Level 3, general

- **3rd-4th year**, **masters** and **research**
- **4169** materials, **247** processes

Level 2, general

- **1st-3rd year** students of Engineering, Materials Science and Design
- **100** materials, **116** processes

The Elements Database

- Schools-University students
- **149** records, periodic table

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Any Questions ???

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