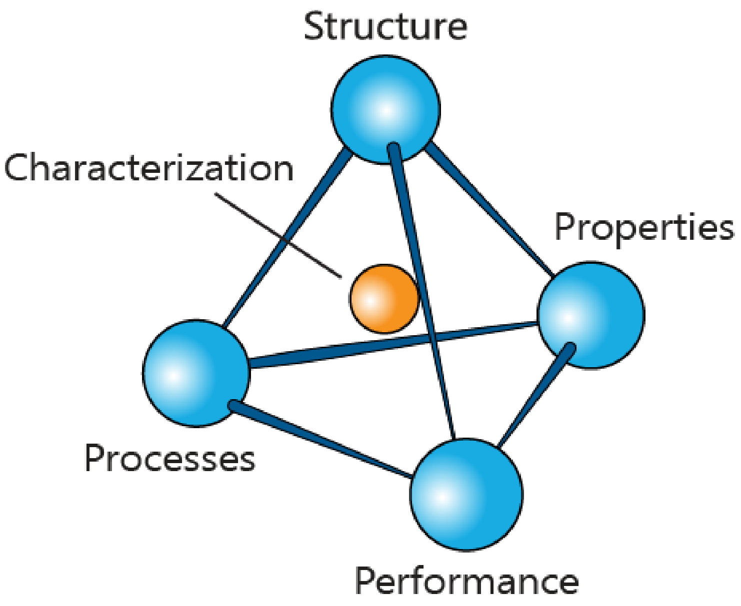
Materials Science and Engineering Database:

an overview

Mike Ashby

Department of Engineering,

University of Cambridge



Learning objectives for this lecture unit

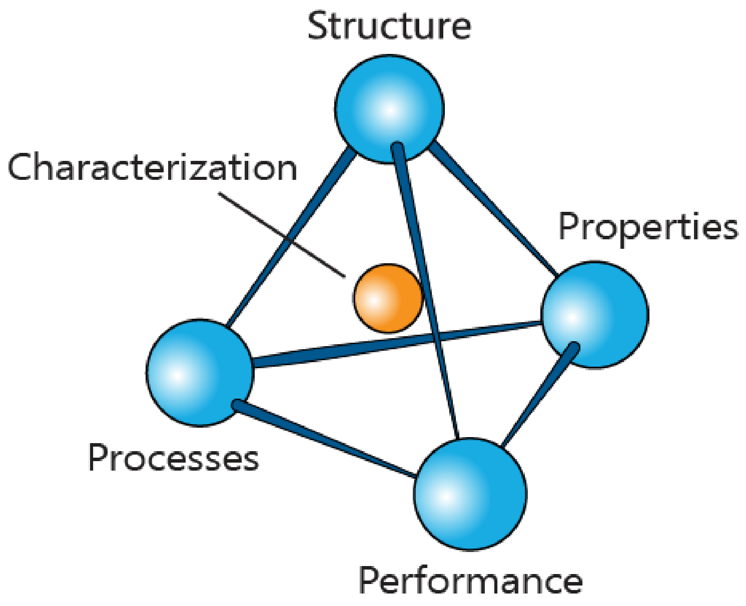
Ansys software mentioned	• Ansys Granta EduPack™, a teaching software for materials education

Intended Learning Outcomes	
Knowledge and Understanding	Understanding what is available in the MS&E database
Skills and Abilities	Ability to plot property trajectories as a function of processing
Values and Attitudes	Appreciation of the Processing, Structure, and Properties relationship

Resources

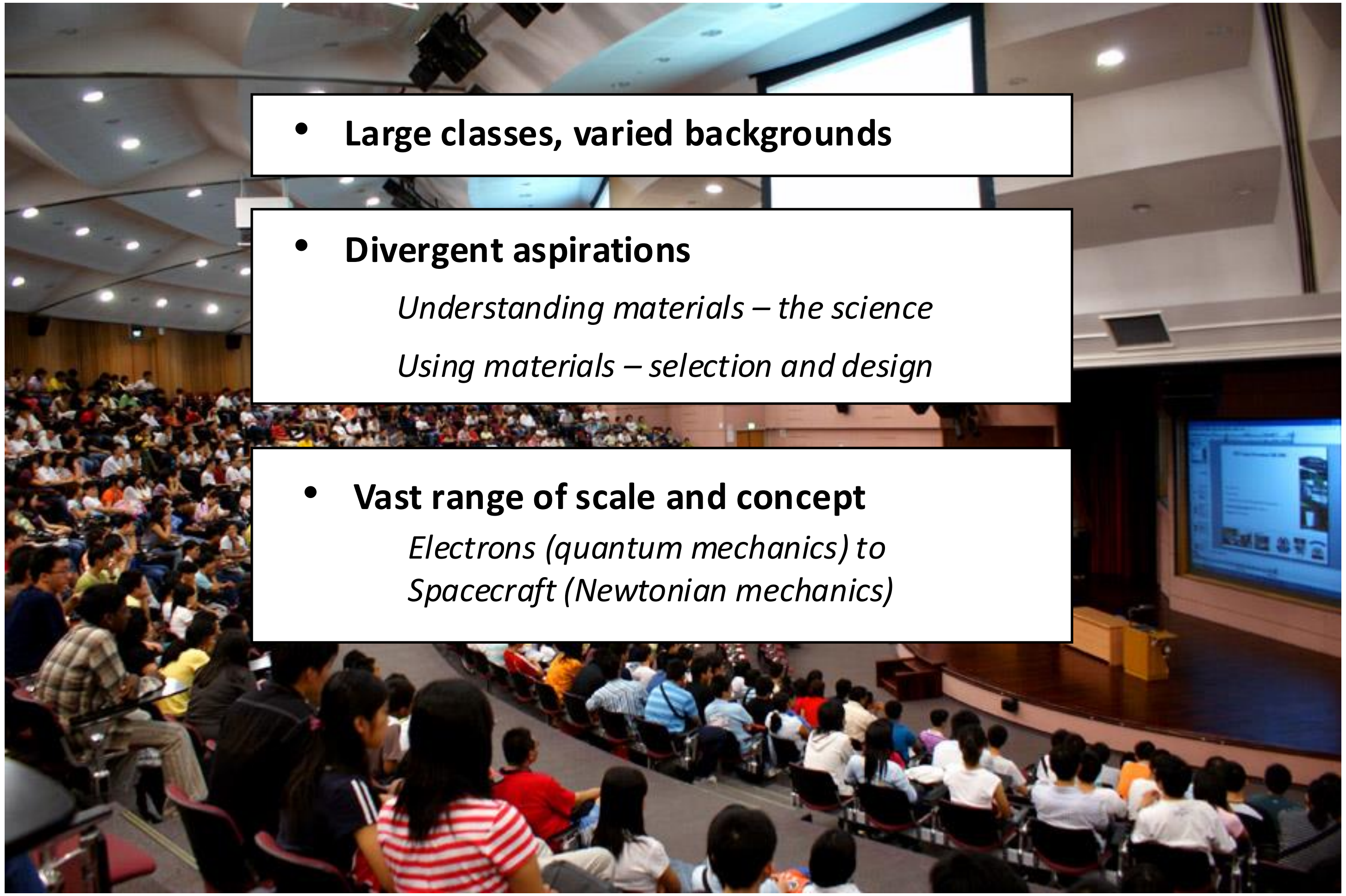
- Text: ***"Materials: engineering, science, processing and design"*** 3rd edition by M.F. Ashby, H.R. Shercliff and D. Cebon, Butterworth Heinemann, Oxford 2014, Chapter 19.
- Text: **Callister, Budinski, Askeland and others** – recommended reading in Science Notes
- ***Ansys Granta EduPack software***, The Materials Science and Engineering database
- White Paper: *The Granta EduPack Materials Science and Engineering Package*

Lecture unit outline



- Teaching Materials Science and Engineering
- The MS&E Package and homepage
- Elements data-table
- Material records in MS&E
- Process records in MS&E
- Phase Diagram Tool
- Process-Property Profiles
- Characterization techniques data-table

Challenges to 1st year materials-teaching



- **Large classes, varied backgrounds**

- **Divergent aspirations**

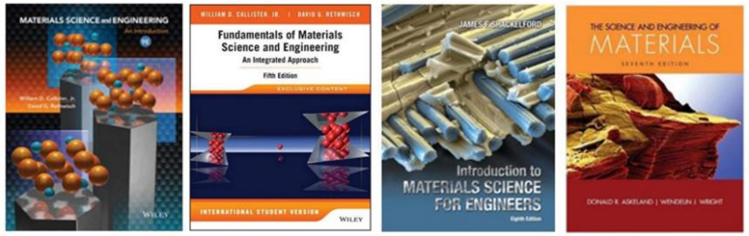
  Understanding materials – the science

  Using materials – selection and design

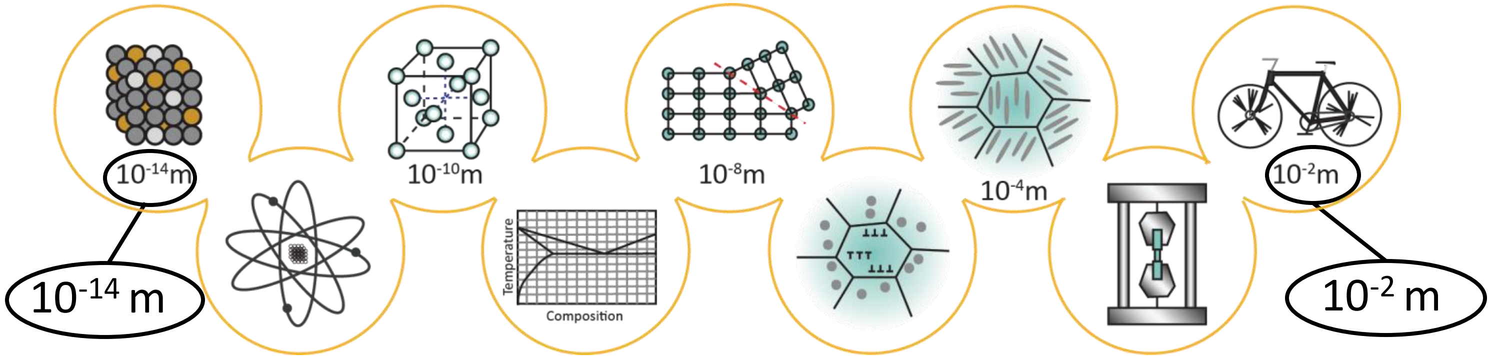
- **Vast range of scale and concept**

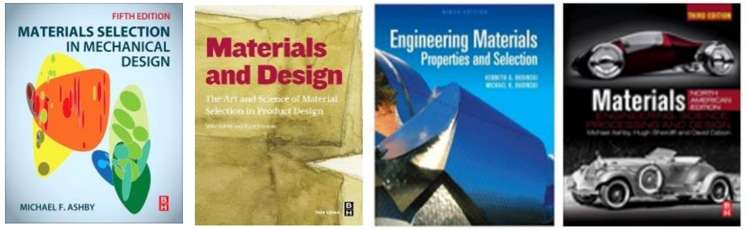
  Electrons (quantum mechanics) to
  Spacecraft (Newtonian mechanics)

Materials Science and Engineering: approaches



Science-driven approach

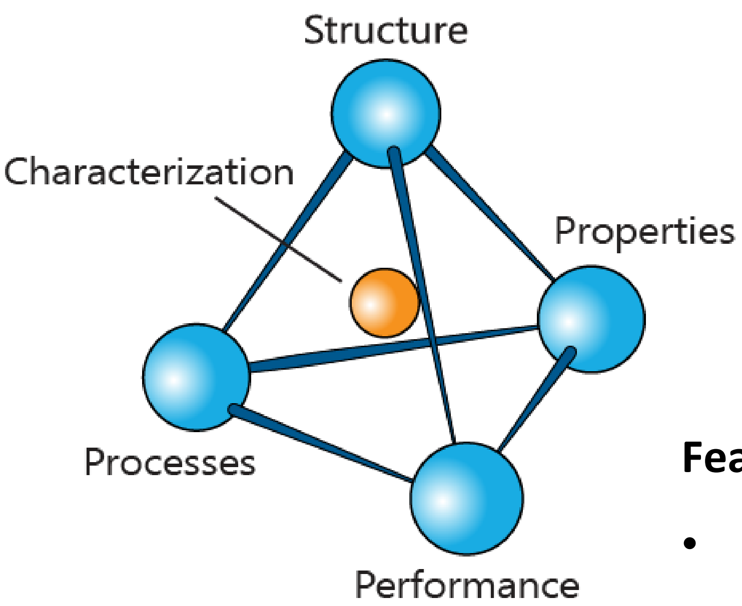




Design-driven approach

Ansys Granta EduPack software MS&E Package: a set of resources to support both approaches

The Materials Science and Engineering package



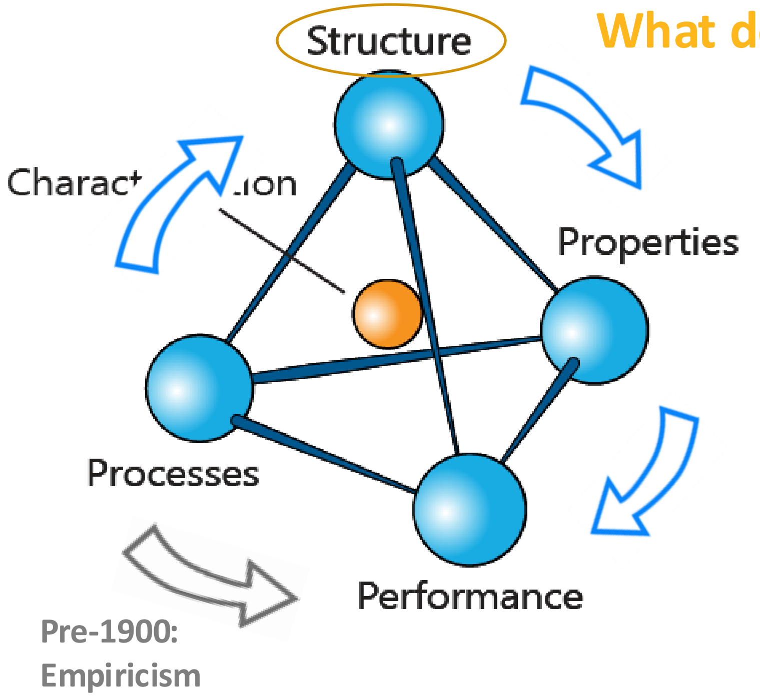
A linked set of resources to support many approaches to teaching

Features

- Learning by discovery
- Intuitive interface to comprehensive Materials Science database
- "Teach Yourself" units for *Phase Diagrams* and *Crystallography*
- MicroProjects to stimulate self-motivated discovery
- Lecture unit and exercises with solutions
- Teaching package: for instructor and student

Basic insight of materials science

The basic insight of Materials Science:
The Process – Structure – Properties – Performance tetrahedron



What do we mean by structure?

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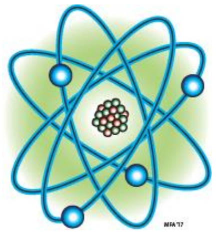
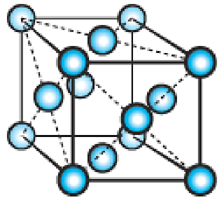
What we mean by “structure”

Structure at electronic and atomistic levels

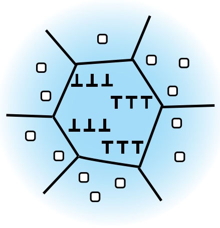


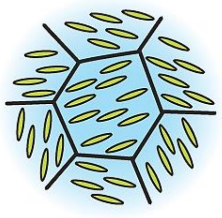


Nucleus and Bonding-sensitive properties

Density
Modulus
Specific heat
Expansion coefficient
Saturation magnetization

Structure at the lattice and phase levels





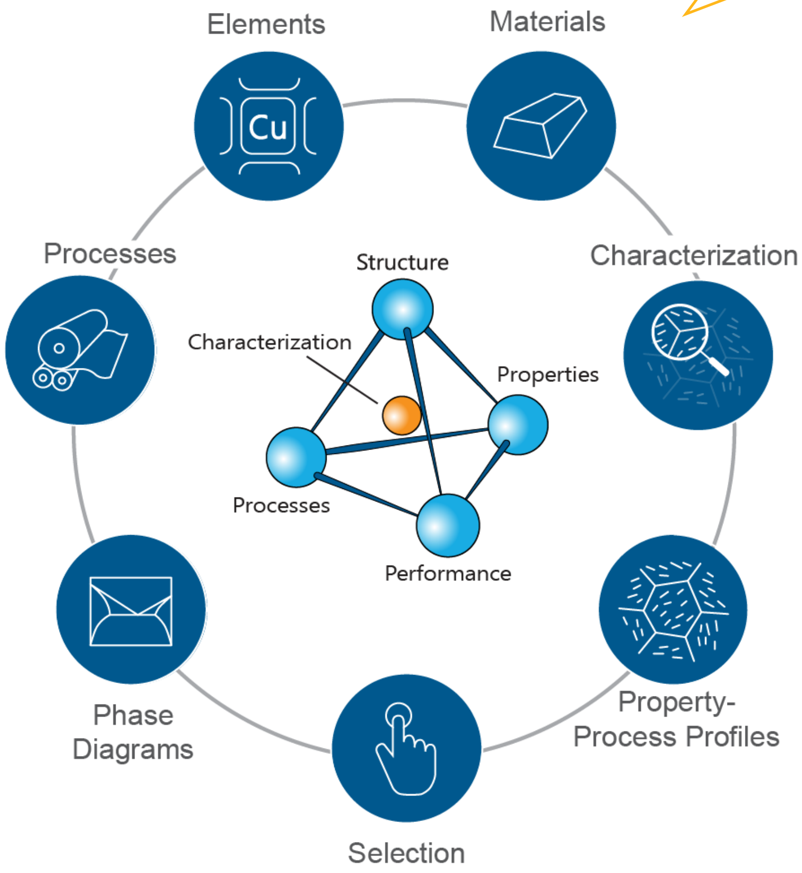
Microstructure-sensitive properties

Strength
Toughness
Elongation
Electrical, thermal conductivities
Coercive field, Energy product

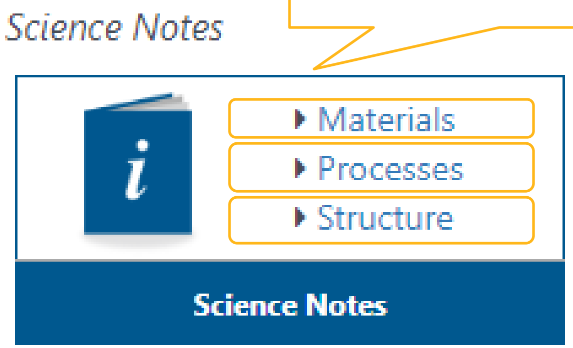
The MS&E main homepage

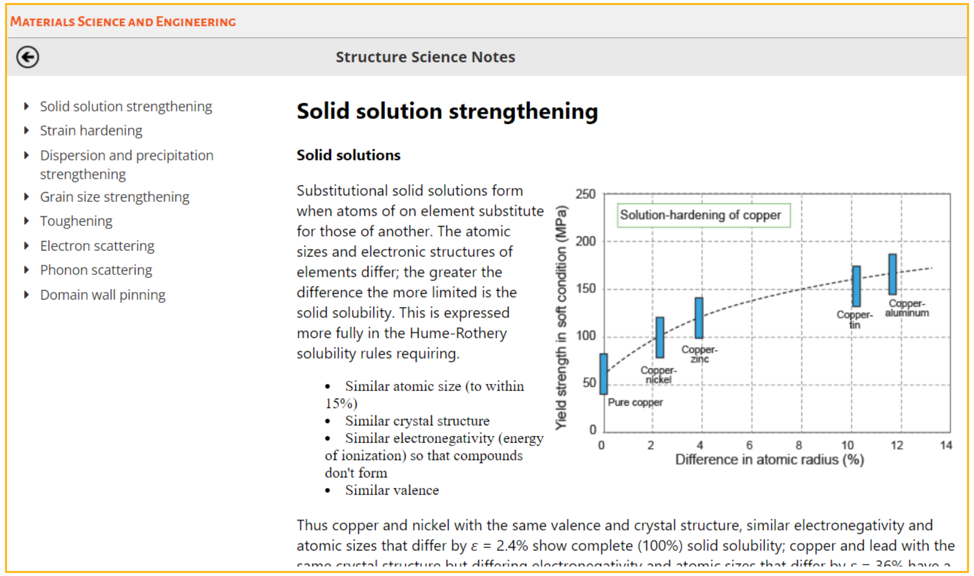
All-in-one homepage

Unique interaction point for the user



Directly accessible from the homepage





MATERIALS SCIENCE AND ENGINEERING

Structure Science Notes

- Solid solution strengthening
- Strain hardening
- Dispersion and precipitation strengthening
- Grain size strengthening
- Toughening
- Electron scattering
- Phonon scattering
- Domain wall pinning

Solid solution strengthening

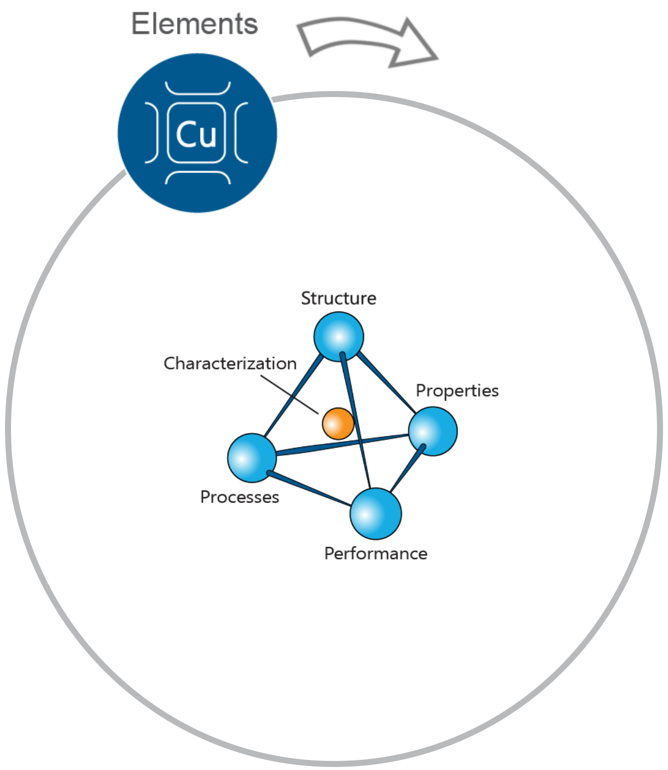
Solid solutions

Substitutional solid solutions form when atoms of on element substitute for those of another. The atomic sizes and electronic structures of elements differ; the greater the difference the more limited is the solid solubility. This is expressed more fully in the Hume-Rothery solubility rules requiring.

- Similar atomic size (to within 15%)
- Similar crystal structure
- Similar electronegativity (energy of ionization) so that compounds don't form
- Similar valence

Thus copper and nickel with the same valence and crystal structure, similar electronegativity and atomic sizes that differ by ε = 2.4% show complete (100%) solid solubility; copper and lead with the

The Elements data-table



Explore

Nucleus and Bonding-sensitive

properties

Iron, alpha (Fe)

Datasheet view: Elements | Show/Hide | Find Similar

The Periodic Table > I, K, L, M >

The element

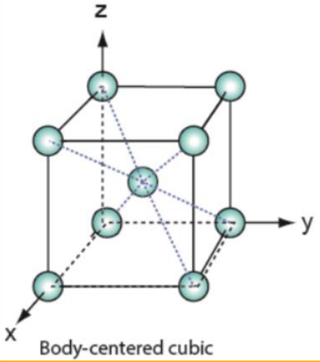
Symbol	ⓘ	Fe	
Element name	ⓘ	Iron	
Periodic table row	ⓘ	Row 4	
Periodic table column	ⓘ	Column 8	
Atomic number	ⓘ	26	
Atomic weight	ⓘ	55.8	kg/kmol
Date of discovery ("-" = BCE)	ⓘ	-1400	
Group	ⓘ	Transition elements	

Electronic structure

Electronic structure	ⓘ	[Ar] 3d6 4s2	
Valence	ⓘ	3	
First ionization energy	ⓘ	7.9	eV
Second ionization energy	ⓘ	16.2	eV
Electronegativity (Pauling)	ⓘ	1.83	

Structure

Crystal structure	ⓘ	Cubic: Body centered
Crystal structure image	ⓘ	



Body-centered cubic

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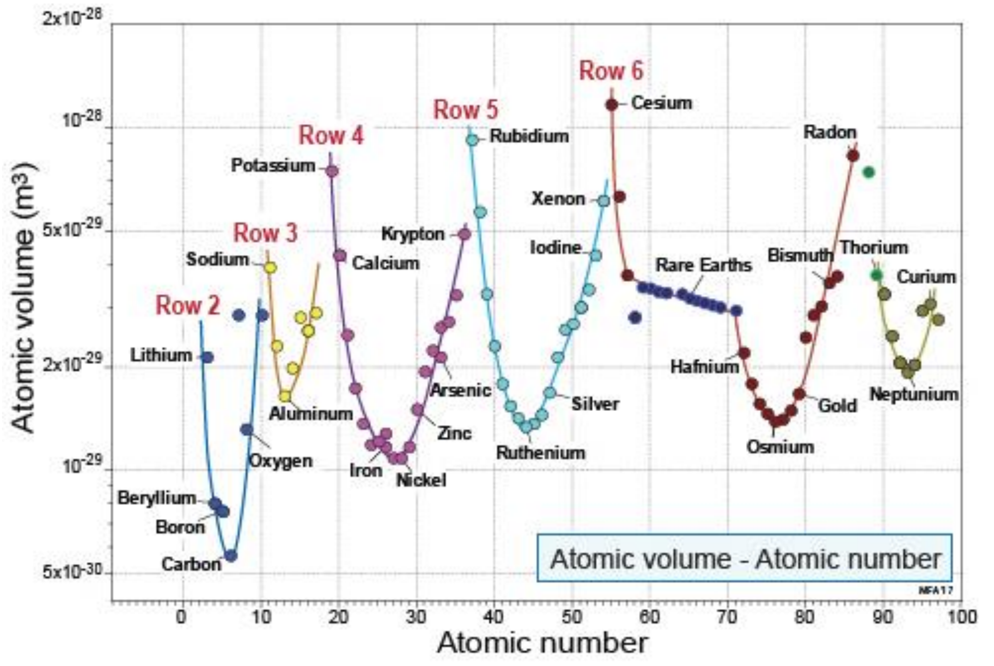
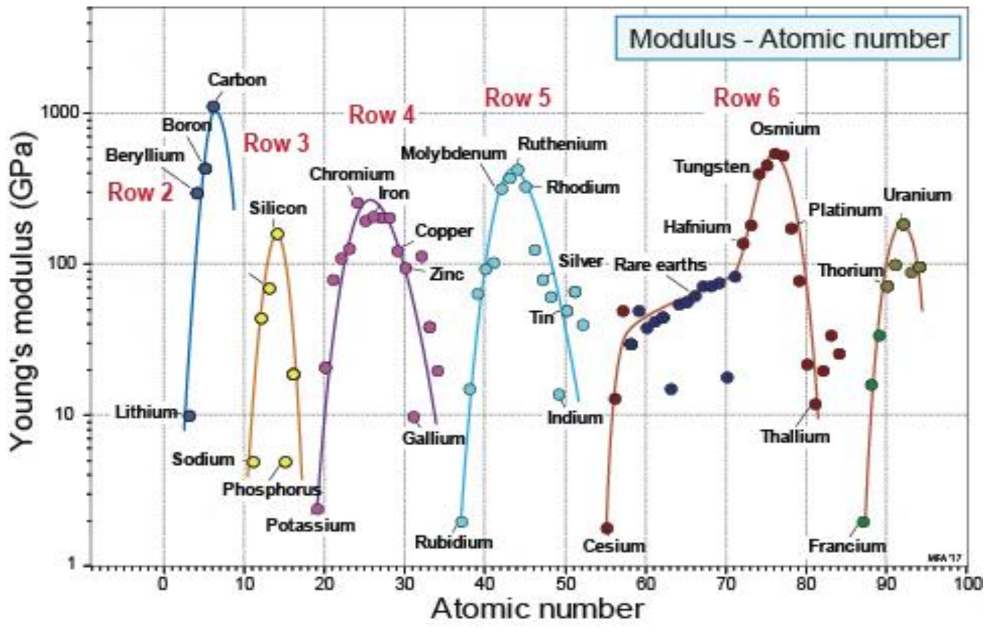
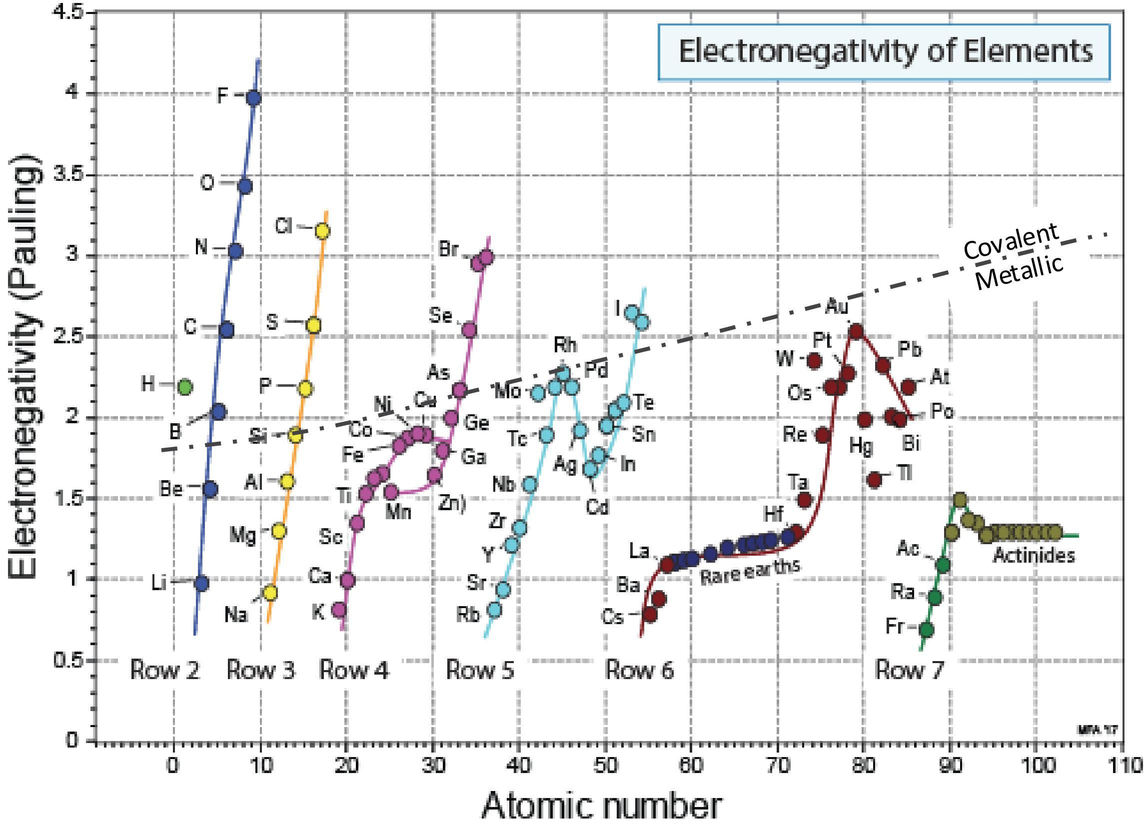
Variation of properties across the Periodic Table



Bonding-packing sensitive properties
10^{-9} m



Electronegativity and bonding



Low electronegativity :
Metallic bonding

Alloys

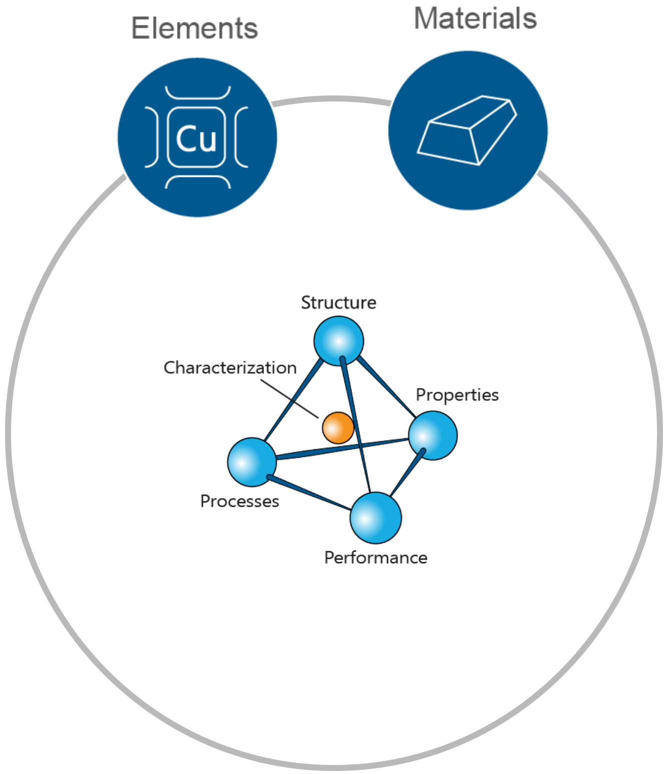
Difference in electronegativity > 1.7
Ionic bonding

Difference in electronegativity < 1.7
Covalent bonding

Hume-Rothery rules for solid solutions:

- Atoms size difference less than 15%
- Similar electronegativity
- Valence is similar

Materials data-table



Cast iron, ductile (nodular)

Datasheet view: All properties | Show/Hide | Find Similar

Metals and alloys > Ferrous >

Description

Image

Caption

Ductile or malleable cast irons are used for heavily loaded parts such as gears and automotive suspension components.

The material

The foundations of modern industrial society are set, so to speak, in cast iron: it is the material that made the industrial revolution possible. Today it holds a second honor: that of being the cheapest of all engineering metals. Cast iron contains at least 2% carbon -- most have 3 to 4% -- and from 1-3% silicon. The carbon makes the iron very fluid when molten, allowing it to be cast to intricate shapes. There are five classes of cast iron: gray, white, ductile (or nodular), malleable and alloy; details are given under Design Guidelines, below. The two that are most used are gray and ductile. This record is for ductile cast iron.

Composition (summary)

Fe/3.2-4.1%C/1.8-2.8%Si/<0.8%Mn/<0.1%P/<0.03%S

General properties

Density	7.05e3	-	7.15e3	kg/m^3
Price	* 0.396	-	0.575	USD/kg
Date first used	1948			

Mechanical properties

Young's modulus	170	-	180	GPa
Shear modulus	64	-	71	GPa
Bulk modulus	120	-	140	GPa
Poisson's ratio	0.27	-	0.28	
Yield strength (elastic limit)	246	-	630	MPa
Tensile strength	400	-	900	MPa
Compressive strength	* 273	-	639	MPa
Elongation	2	-	26	% strain

Materials records

Cast iron, ductile (nodular)

Datasheet view: All properties | Show/Hide | Find Similar

95 Engineering materials

Image

Caption

Ductile or malleable cast irons are used for heavily loaded parts such as gears and automotive suspension components.

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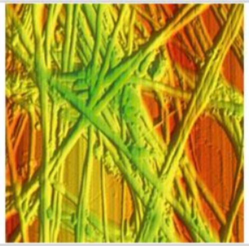
Collagen

Datasheet view: All properties | Show/Hide | Find Similar

88 Biological materials

Image



Caption

Collagen strands imaged by atomic force microscopy. (Image generated with an Asylum Research MFP-3D Atomic Force Microscope, image courtesy of Asylum Research UK)

The material

Collagens form a family of closely-related fibrous proteins. They are found throughout the animal kingdom and in virtually every tissue, ranging from shock-absorbing cartilage to light-transmitting corneas, and from tendons and muscle to blood vessels and skin. Collagens provide the stiffness and strength of soft tissues and also play a major role determining properties of mineralized tissues like bone.
There are at least 20 different sub-types of collagen. A collagen has a triple-helix structure formed by the assembly of three protein chains. There are at least 20 different sub-types of collagen, depending on the amino-acid sequence in the protein chains. Type I collagen as two chains with the same sequence (called alpha-1) entwined with one of a different sequence (called alpha-2). In type II collagen three chains are the same (alpha-1).

Composition (summary)

Collagen is a protein: a long-chain polymer of amino-acids. The basic motif in the amino acid sequence of collagens is Gly-X-Y where X or Y are commonly proline or hydroxyproline; a common motif is Gly-Pro-Hyp. The tiny glycine molecule as every third residue assists in triple helix formation. Individual 300 nm long tropocollagen triple helices self-assemble into a quarter-staggered array with a 67 nm characteristic spacing visible on TEM.

General properties

Density	1.3e3	-	1.45e3	kg/m^3

Mechanical properties

Young's modulus	0.2	-	0.8	GPa
Shear modulus	0.06	-	0.2	GPa
Bulk modulus	* 4	-	5	GPa
Poisson's ratio	* 0.45	-	0.46	
Yield strength (elastic limit)	44	-	70	MPa

Silicon, device grade

Datasheet view: All properties | Show/Hide | Find Similar

46 Functional materials

Image

Caption

Device grade silicon boules and wafers. (Image courtesy of http://www.chipsetc.com/silicon-wafers.html.)

The material

Silicon is the second most abundant element, exceeded only by oxygen and making up 26% of the earth's crust by weight. It is found largely as silicon oxides such as sand (silica), quartz, rock crystal, amethyst, agate, flint, jasper and opal, and as silicates asbestos, feldspar, clay and mica. It is a reactive element, important as an alloying element in steels, cast irons, and certain copper and aluminum alloys where it gives both corrosion resistance and strength. Silicon is transparent to infrared and is used a windows and lenses for IR lasers. Its most important application, of course, is as a semiconductor, the mainstay of the electronics industry. Silicon is present in the sun and stars and is a principal component of a class of meteorites known as aerolites. Silicon is important in plant and animal life. Diatoms in both fresh and salt water extract silica from the water to use as a component of their cell walls. Silicon is an important ingredient in steel. Silicon carbide is one of the most important abrasives. Workers in environments where silica-containing dust is breathed may develop a serious lung disease known as silicosis. Hydrolysis and condensation of substituted chlorosilanes can be used to produce a very great number of polymeric products, or silicones. These range from liquids to hard, glasslike solids with many useful properties. Elemental silicon transmits more than 95% of all wavelengths of infrared and has been used in lasers to produce coherent light at 456 nm.

Composition (summary)

100% Si

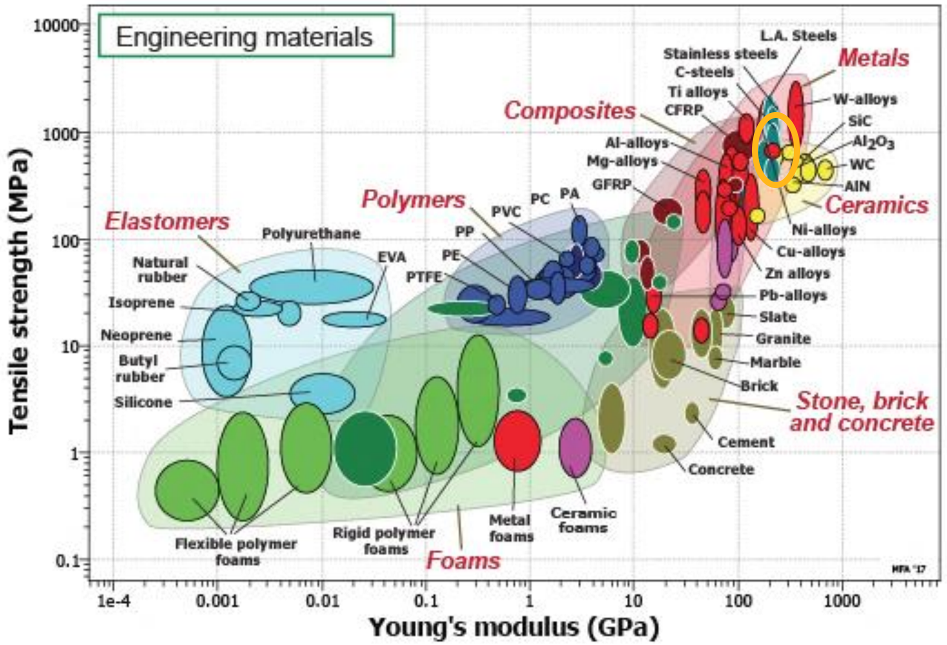
General properties

Density	2.3e3	-	2.35e3	kg/m^3
Price	* 40	-	200	USD/kg
Date first used	1952			

Mechanical properties

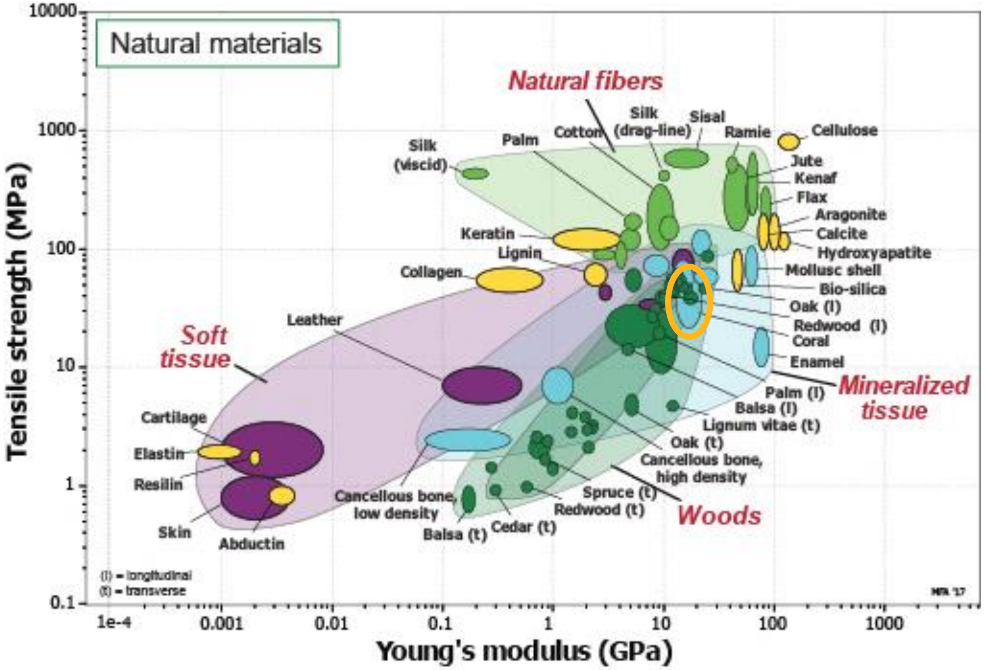
Young's modulus	140	-	155	GPa
Shear modulus	62	-	65	GPa
Bulk modulus	95	-	105	GPa
Poisson's ratio	0.21	-	0.22	

Engineering and natural materials



Coral

Carbon steel



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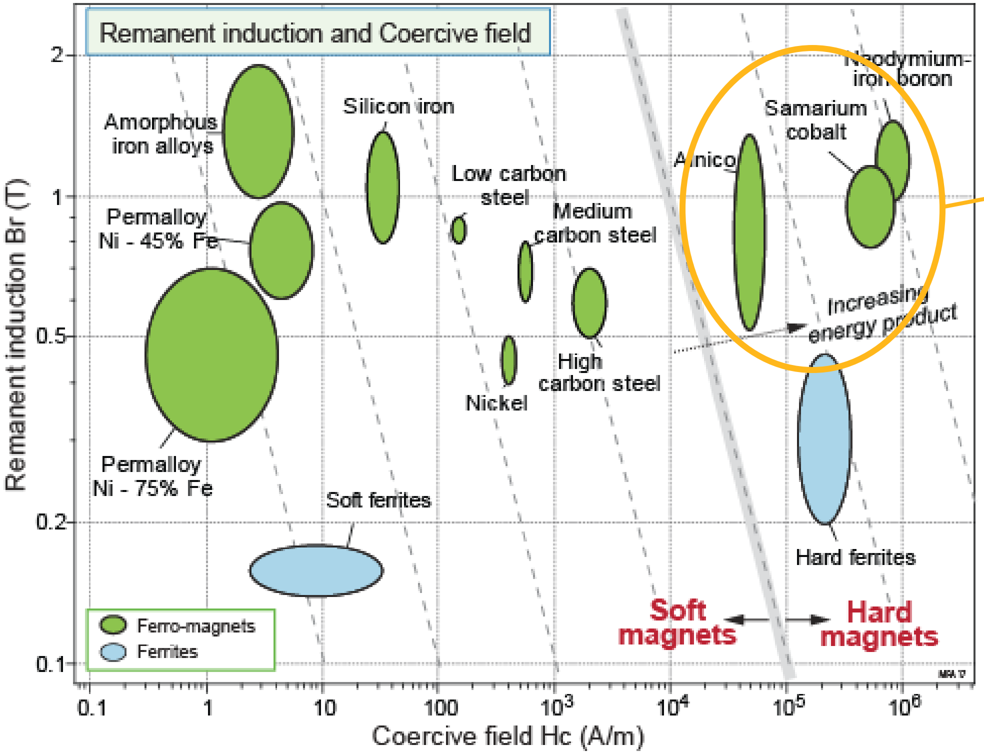
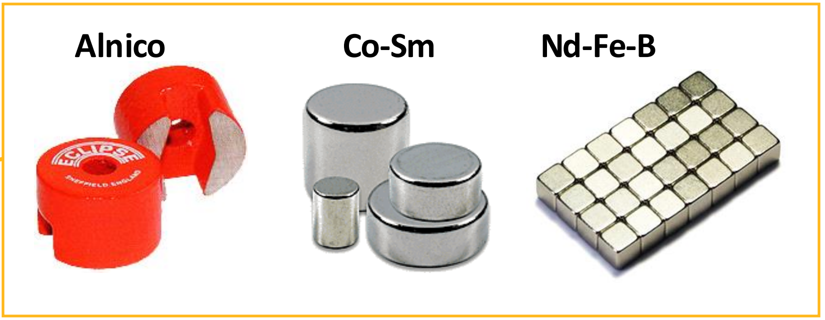
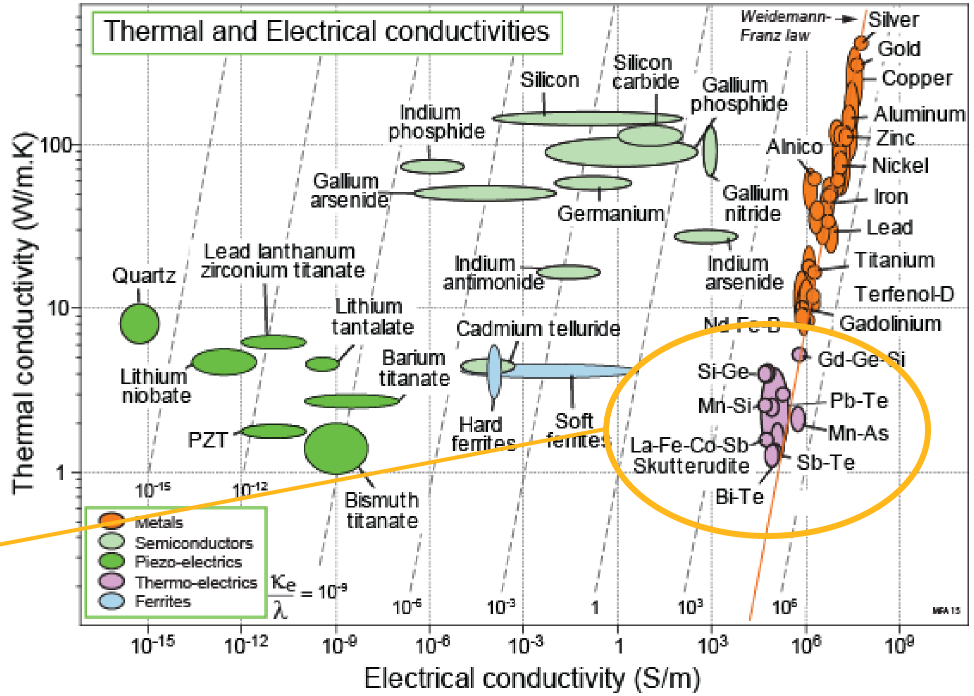
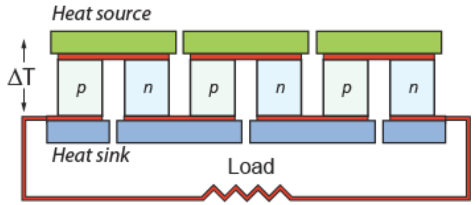
Magnetic and thermoelectric materials



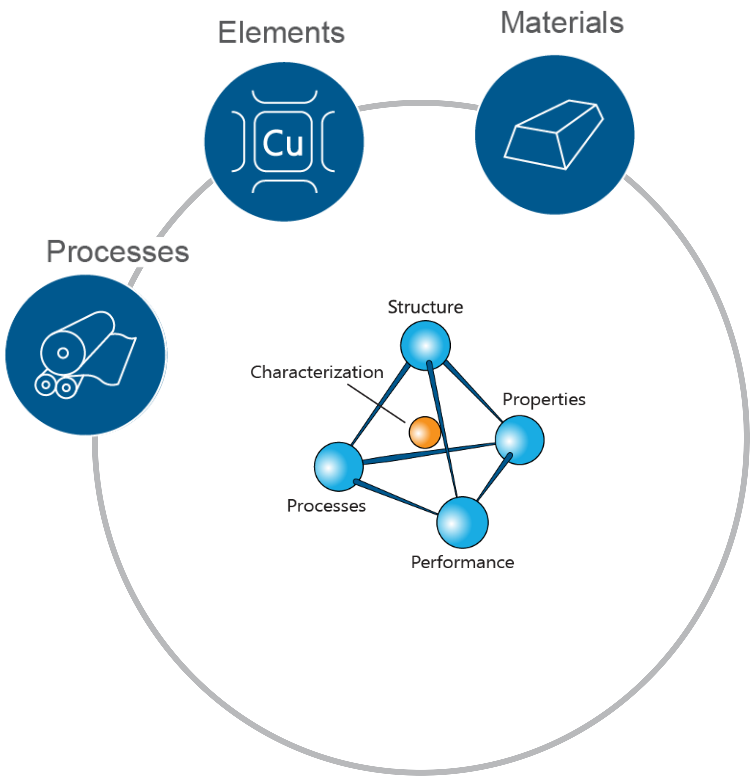




Thermo-electric energy harvester



Processes data-table



Forging

Datasheet view: All processes | Show/Hide | Find Similar

Shaping > Deformation > Bulk deformation processes >

Description

Image

Image caption

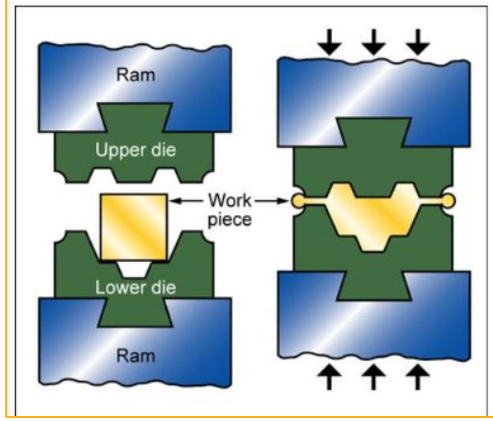
(1) Manual forging © TiBine at Pixalbay [Public domain] (2) Flashless forged 2-cylinder crankshaft © IPH Hannover at Wikimedia Commons (CC BY 2.0) (3) Forged ornament of a castle gateway © Mh-grafik at Pixalbay [Public domain]

The process

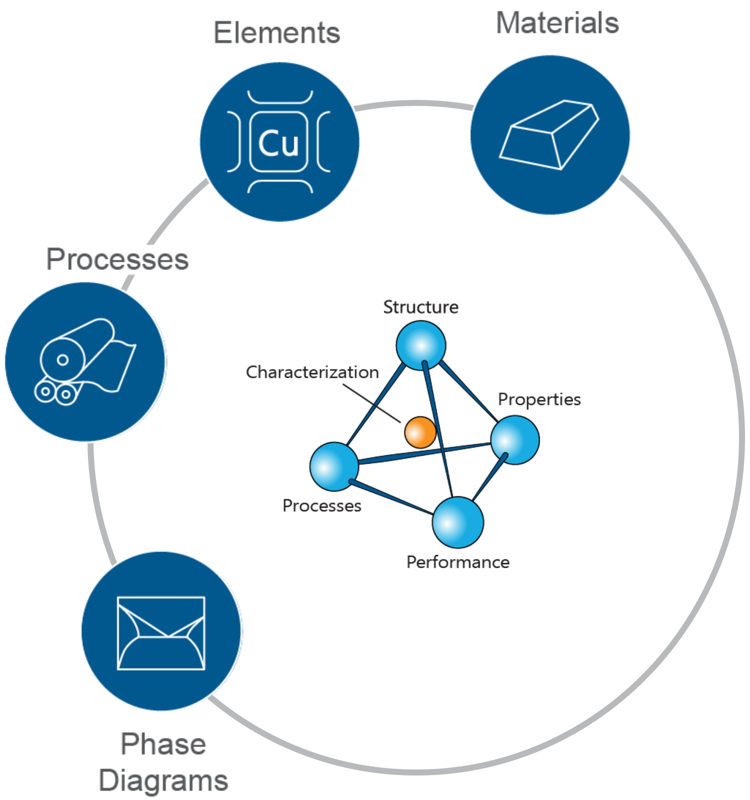
In forging a metal ingot is squeezed to shape by dies that subject it to large plastic deformation. Nearly 90% of all steel products are either forged or rolled. In hot die forging a heated blank is formed between open or closed dies in a single compressive stroke. Often a succession of dies is used to create the final shape. In cold rolling and forging the metal blank is initially cold, although deformation causes some heating.

The greatest precision and shape complexity is given by closed-die forging, illustrated below, but the size of component is limited to about 20 kg. Open-die forging is less precise, but can be applied to much larger components (up to 5000 kg).

Process schematic



Phase diagrams



Phase Diagrams

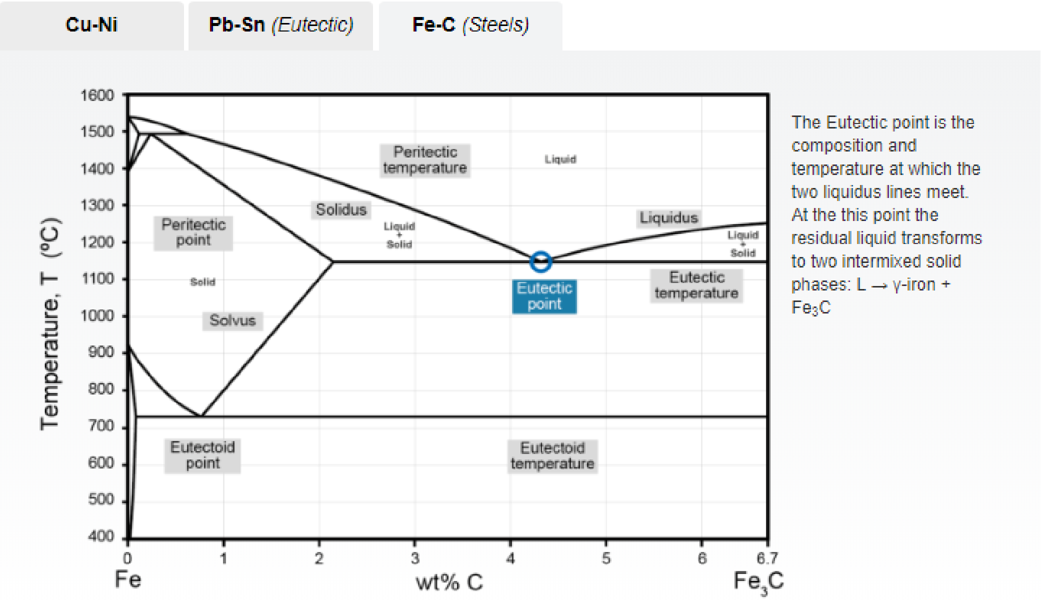
Phase Diagram glossary

Lever Rule

Phases

Cooling paths

Phase diagram datatable

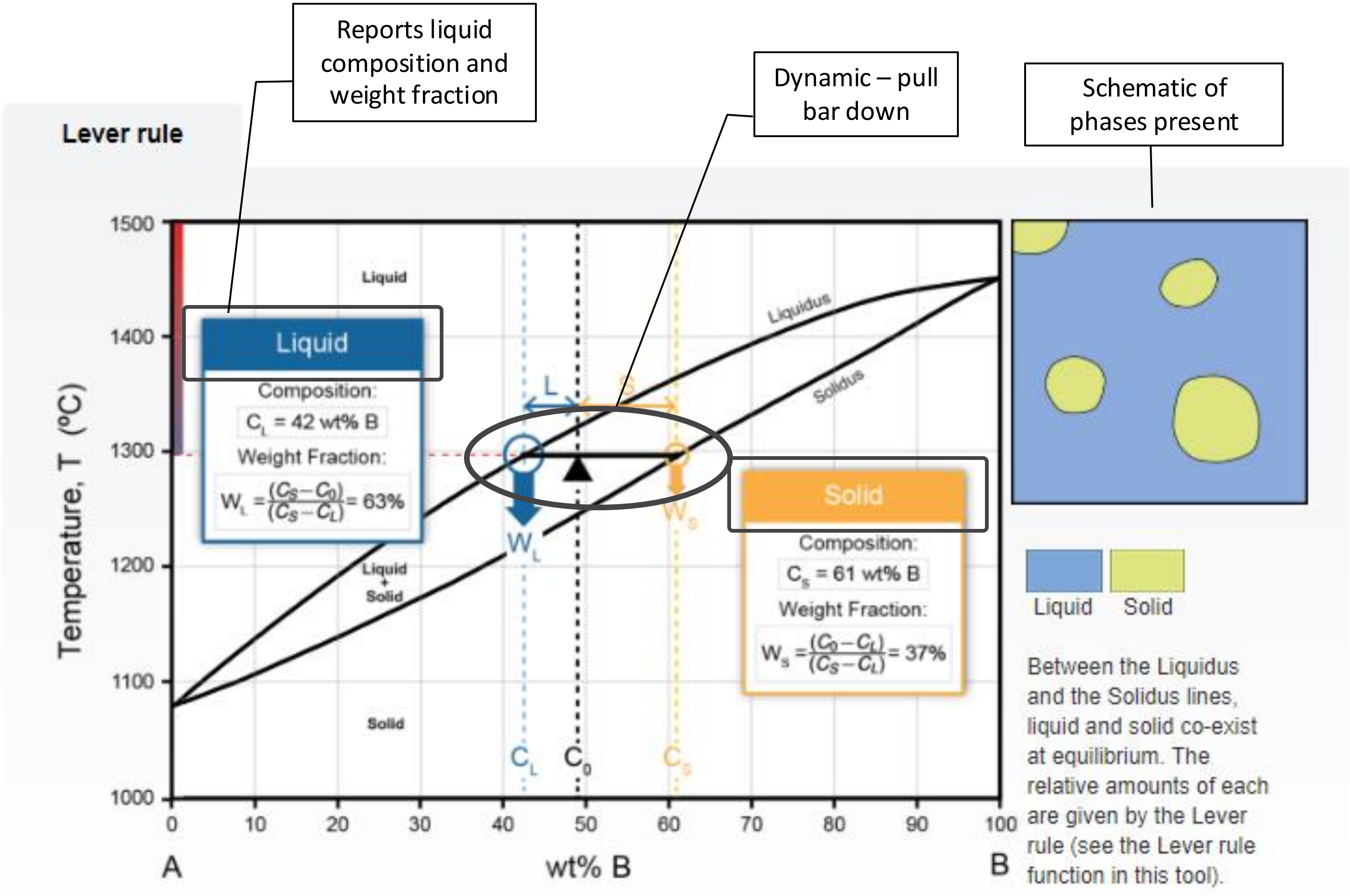


GRANTA EDUPACK

Lever rule

Phase Diagrams

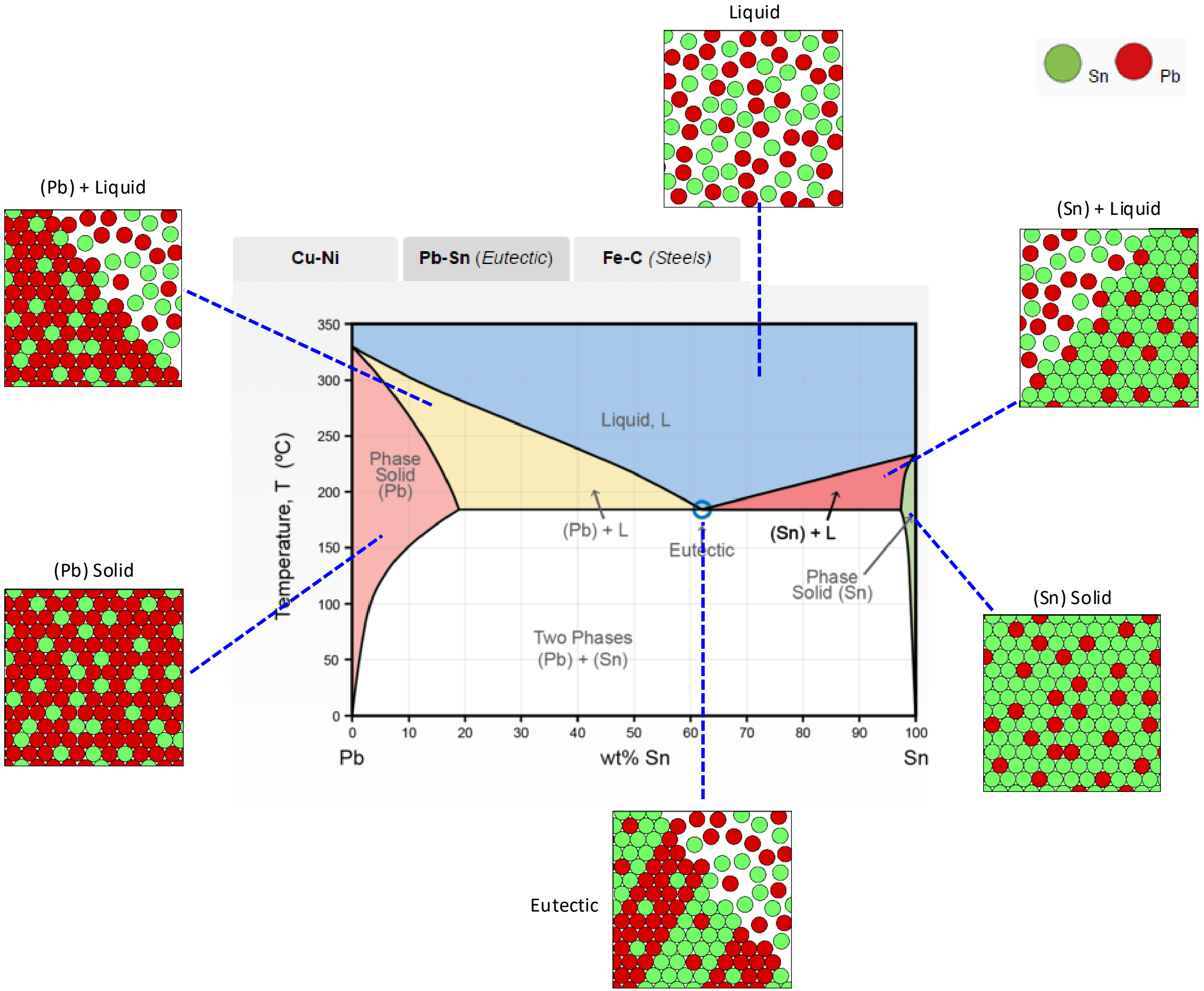
- Phase Diagram glossary
- Lever Rule
- Phases
- Cooling paths
- Phase diagram datatable



Phases

Phase Diagrams

- Phase Diagram glossary
- Lever Rule
- Phases
- Cooling paths
- Phase diagram datatable



Cooling paths

Phase Diagrams

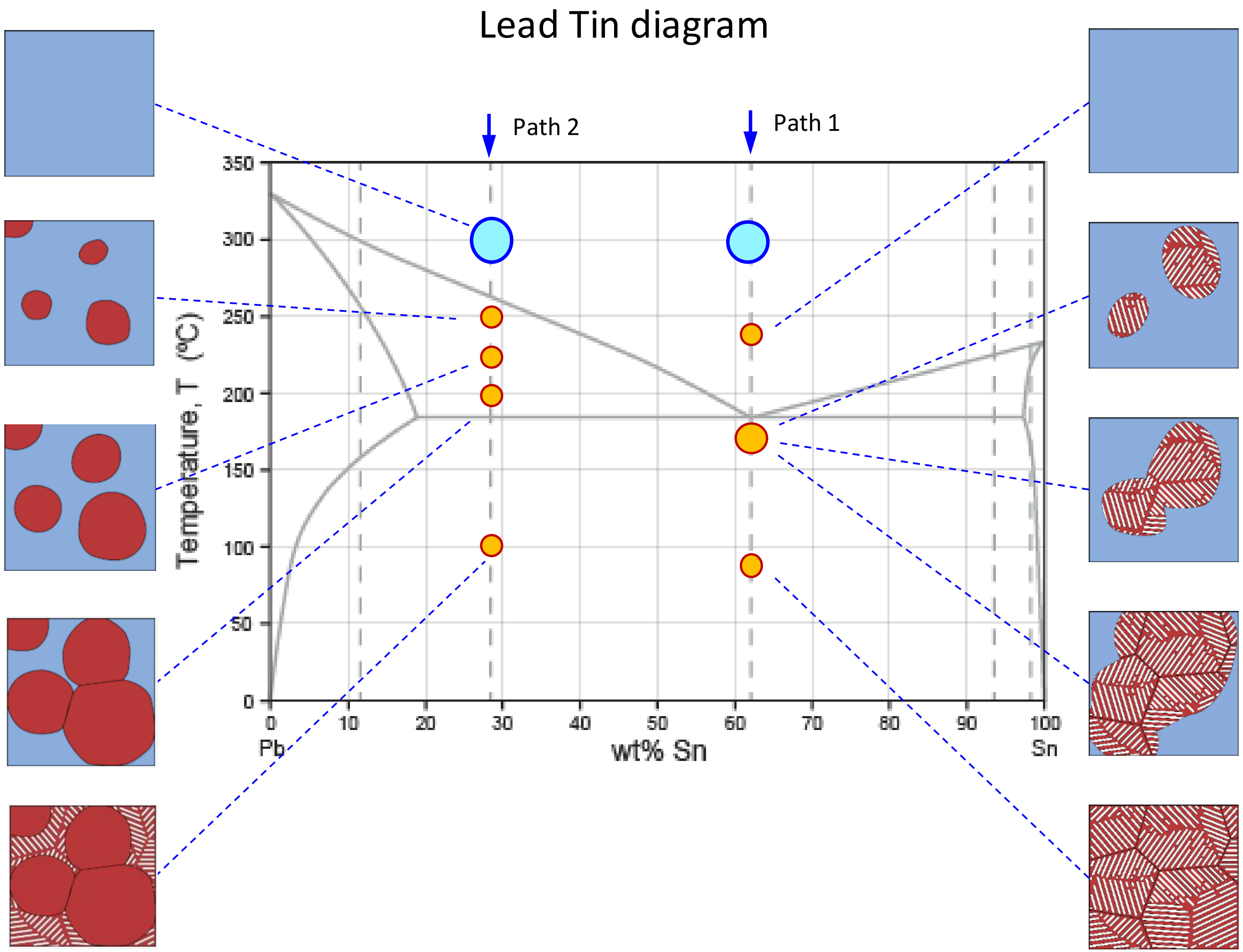
Phase Diagram glossary

Lever Rule

Phases

Cooling paths

Phase diagram datatable



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Phase diagram data-table

Phase Diagrams

- Phase Diagram glossary
- Lever Rule
- Phases
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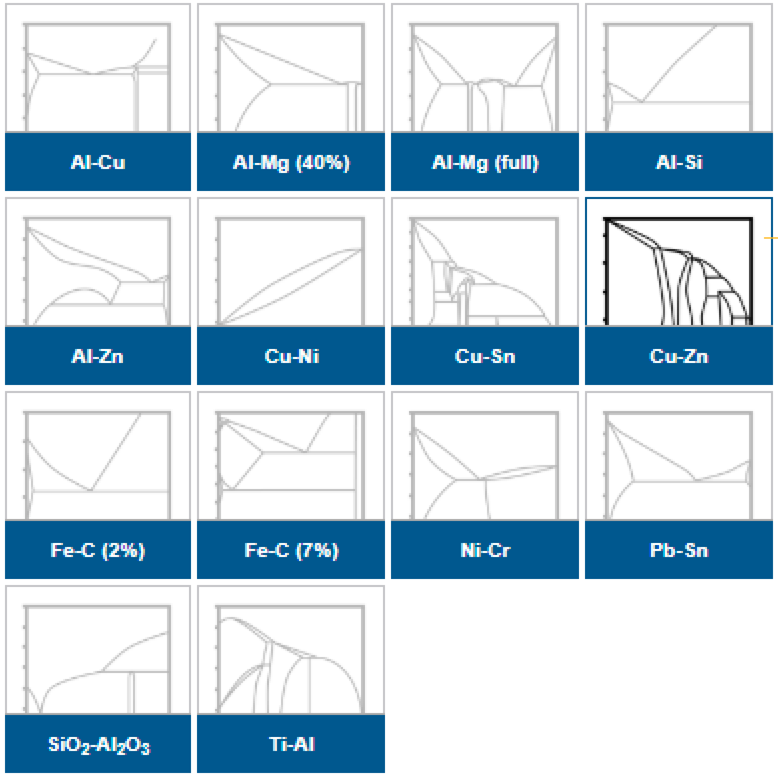
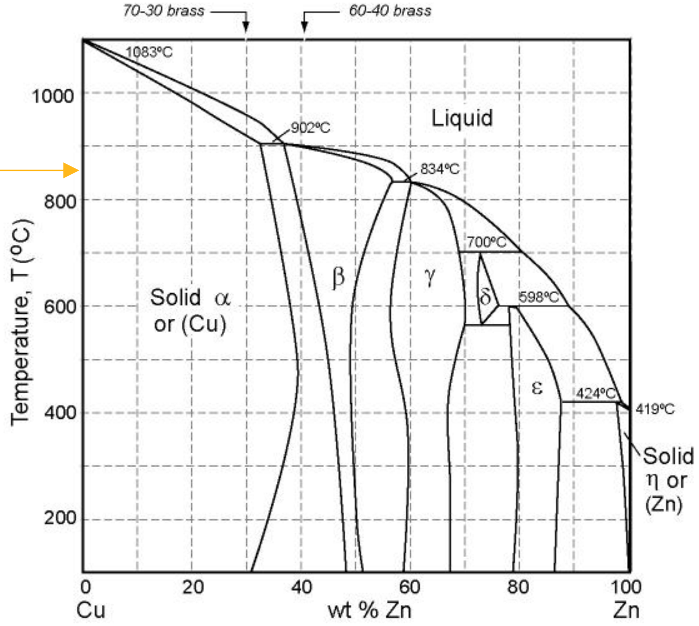




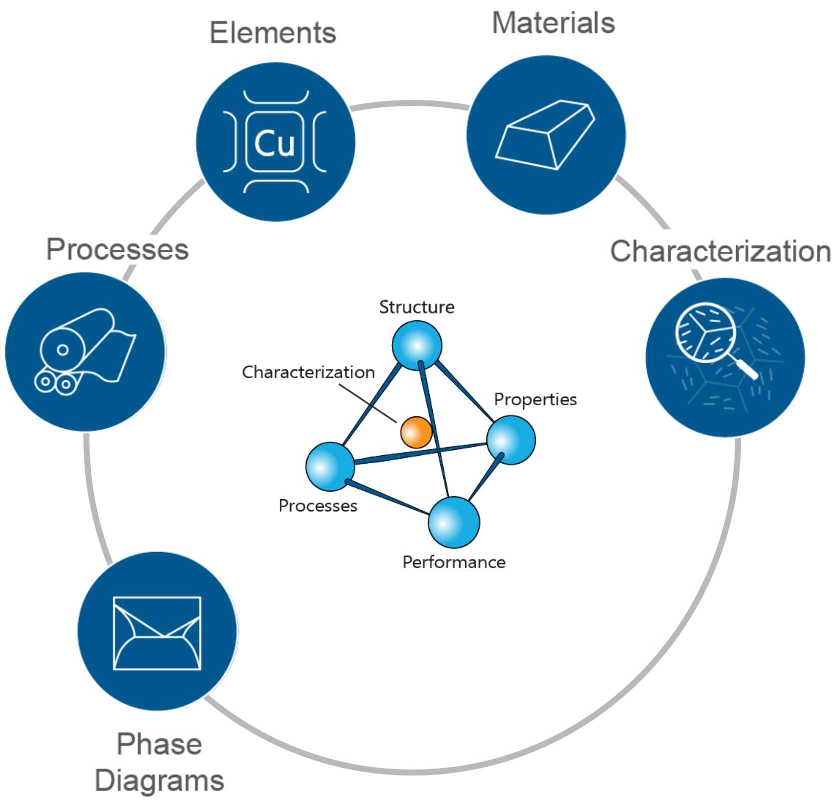
Description

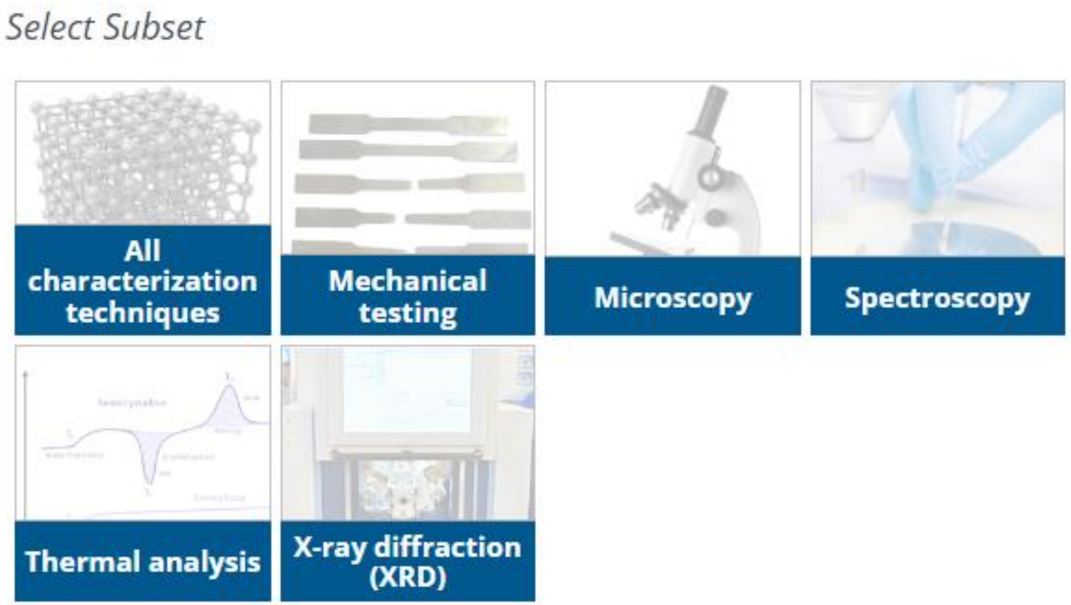
Brasses, alloys of copper with 5-40% zinc, combine high formability with good corrosion resistance. The two most widely used compositions, 70%Cu-30%Zn and 60%Cu-40%Zn, are shown above the diagram. The major phases in brass are the fcc alpha phase and the bcc beta phase. Alpha brasses are malleable and easier to work, whereas beta brasses are harder and stronger.

Links

- Elements
- MaterialUniverse
- Property-Process Profiles

Characterization data-table





Datasheet example

Charpy impact

Datasheet view: All characterization techniques | Show/Hide | Find Similar

Mechanical testing >

Description

Image

Image caption

Two images of Charpy impact test specimens after testing is complete. Images used under license from Adobe Stock.

Schematic

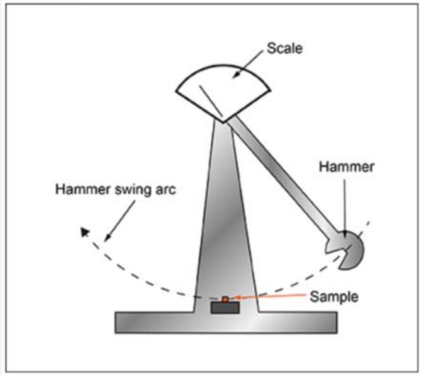


Figure caption

Charpy impact tests utilize a large lever arm with a heavy "hammer" at the end to strike the sample (shape noted in the schematic).

Description

Fracture toughness is an important consideration for designers and engineers, especially with brittle materials like cast iron or high carbon steel. The fracture toughness of a material is typically measured using a Charpy impact test. In this test, a specimen with a notch is placed on two fixtures such that its 2 edges are supported, but the center, where the notch is present, is suspended in air. A pendulum is raised to a prescribed height, and then dropped in a trajectory where the pendulum hits the specimen on the side opposite to the notch. The pendulum breaks the specimen and climbs to a specific height on the other side. The difference between the final and initial height is measured, and using the principle of energy conservation, the impact energy of the material is measured. The test can be run at different temperatures, but is repeated a few times at each temperature to ensure the accuracy of the results.
Instron and ZwickRoell are common instrument producers for measuring charpy impact properties of materials.

Sample preparation characteristics

The specimen should be a uniform rectangular cuboid with dimensions adhering to the relevant standard (ASTM A370). Using a prescribed V-notch cutter, a V-notch must be cut in the middle of the specimen.

Standards

ASTM A370, ASTM E23, ASTM D6110, ISO 179

Physical and quality attributes

Technique family	Mechanical testing
Is specific sample geometry needed?	✓
Is specific sample preparation needed?	✗
Is non-destructive test?	✗

Material compatibility

Ceramics	✓
Foams	✗
Glasses	✗
Metals - ferrous	✓
Metals - non-ferrous	✓
Natural materials	✓
Polymer composites	✓
Polymers - thermoplastics	✓
Polymers - thermosets	✓

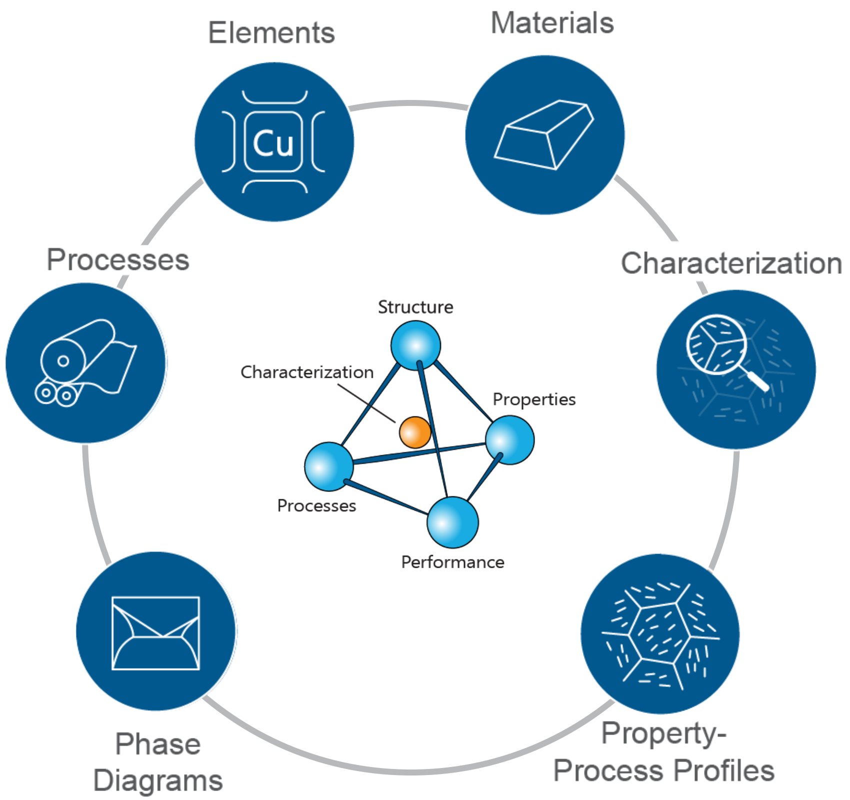
Measured properties

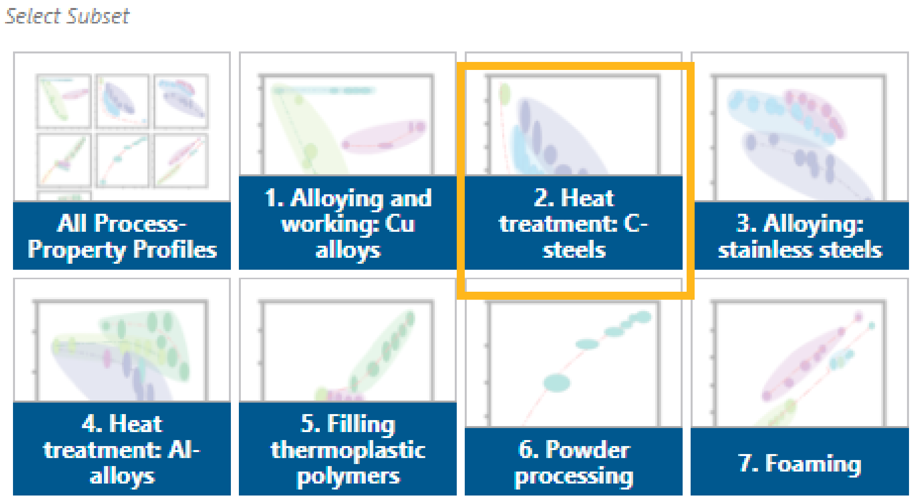
Fracture toughness	✓

Economic compatibility

Tool price	2.5e4 - 2.1e5 USD

Process-Property Profiles data-table





Subset selected

2. Heat treatment: C-steels

The properties of carbon steels are controlled by heat treatment. The steel is austenitized at 850 C to dissolve the carbon, quenched to convert the austenite to martensite and tempered at a controlled temperature and time achieve the desired property profile. Heat treatment has a profound effect on structure-dependent mechanical properties (strength, fatigue resistance, elongation, toughness, mechanical damping). These dependencies can all be explored using this data set for two grades of medium carbon steel: a 0.35% C carbon steel and a 0.4% C low alloy steel.

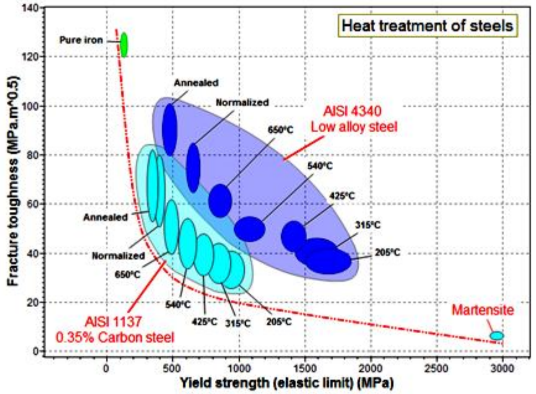
Process-Property Profiles data-table

2. Heat treatment: carbon and low alloy

Datasheet view: Process-Property Profiles | Show/Hide

Description

Image



Process-property set

The set

The properties of carbon steels are controlled by heat treatment. The steel is austenitized at 850 C to dissolve the carbon, quenched to convert the austenite to martensite and tempered at a controlled temperature and time achieve the desired property profile. Heat treatment has a profound effect on structure-dependent mechanical properties (strength, fatigue resistance, elongation, toughness, mechanical damping). These dependencies can all be explored using this data set for two grades of medium carbon steel: a 0.35% C carbon steel and a 0.4% C low alloy steel.

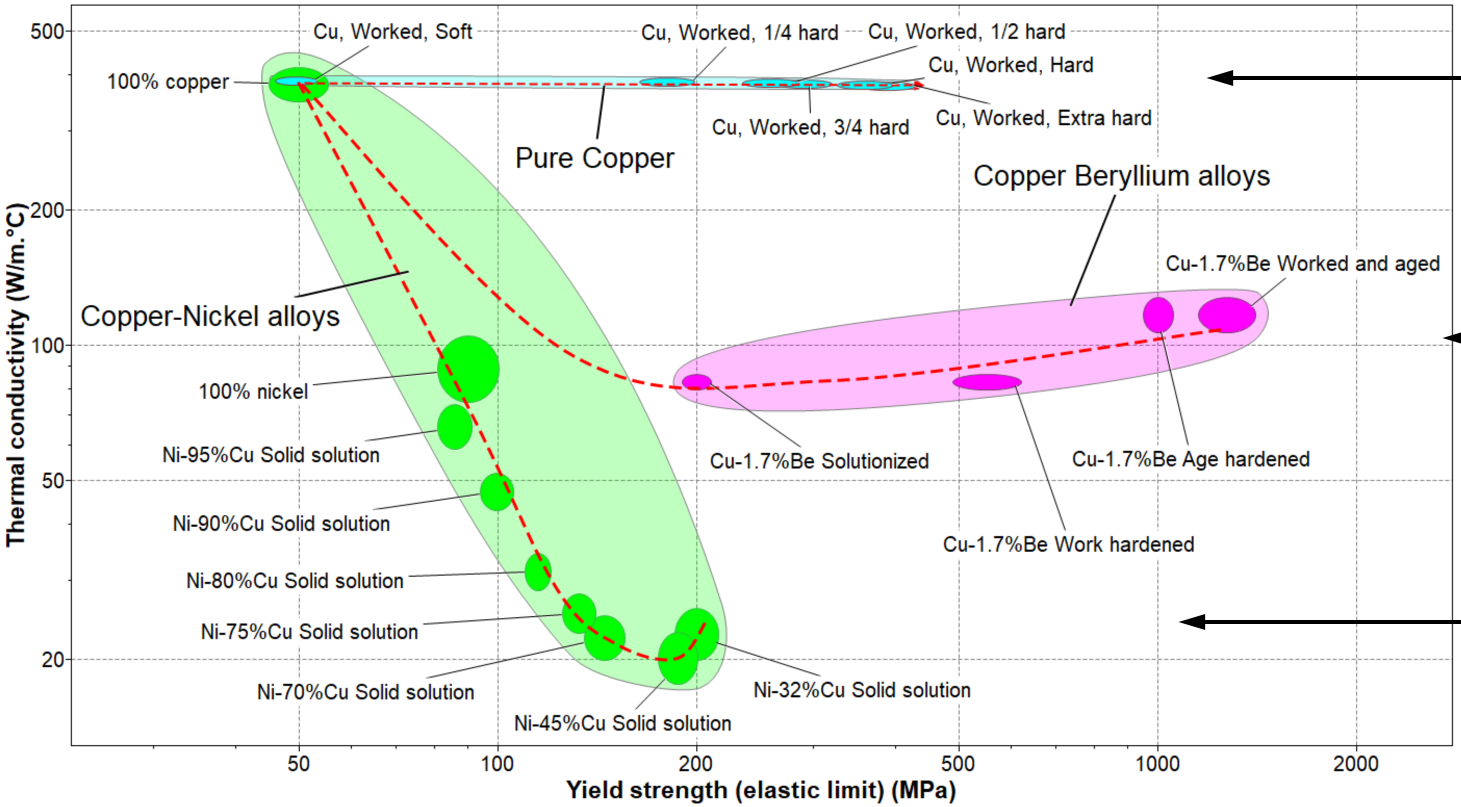
What's in it?

The folder contains 16 records for
- Pure iron
- Martensite
- Iron 0.35% C, 1.5% Mn steel (AISI1137) in seven states of heat treatment (tempered at the indicated temperature followed by an oil quench)
- A low alloy steel (AISI 4340), 0.4% C, in seven states of heat treatment (tempered at the indicated temperature followed by and oil quench).

What can you do with it?

The chart of below shows the trade-off between two key mechanical properties – Fracture Toughness and Yield strength – as the heat treatment schedule is changed. The bubbles are labeled with the tempering temperature. "Annealed" refers to steel heated into the austenite region and the furnace-cooled slowly to room temperature. "Normalized" refers to steel heated to austenite then air cooled more rapidly to room temperature.

Solution hardening, work hardening, ppt hardening

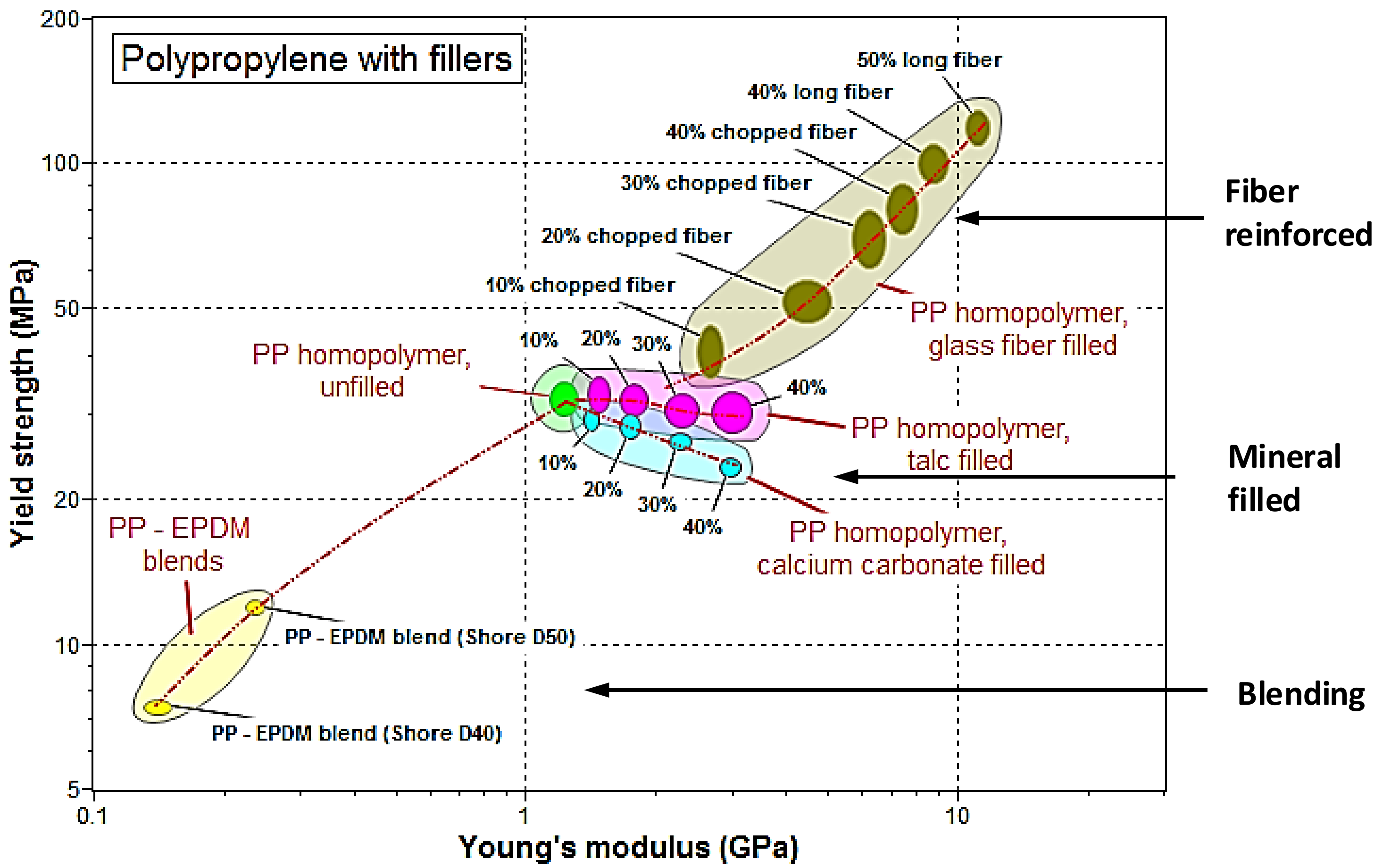


Work hardening

Precipitation hardening

Solid solution hardening

Filling, blending, reinforcement (composition)



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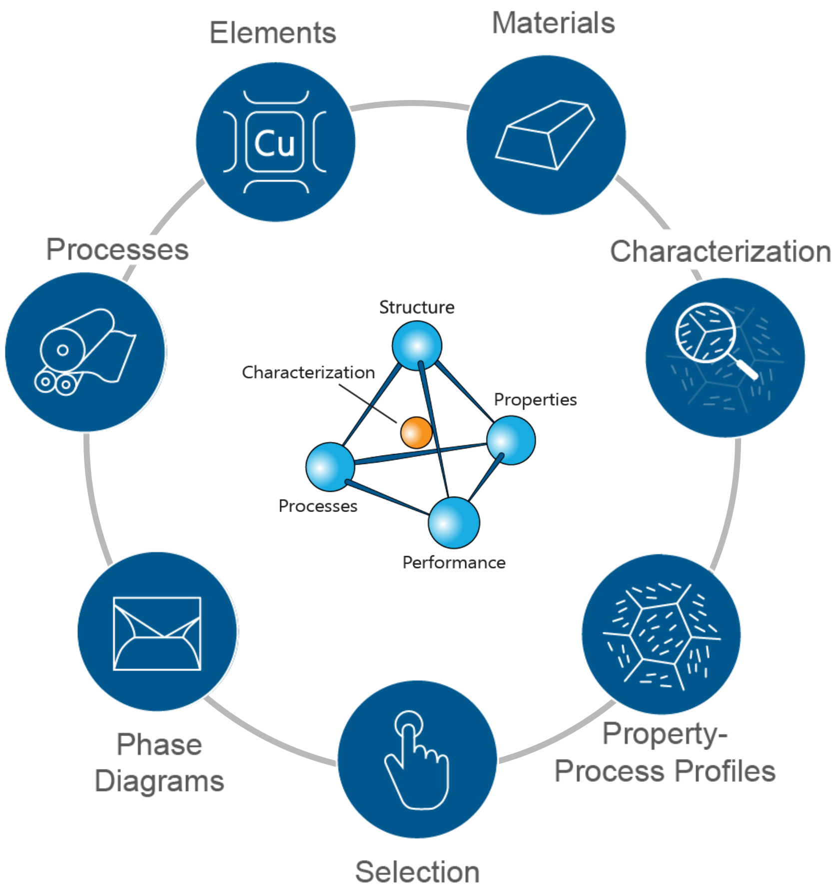
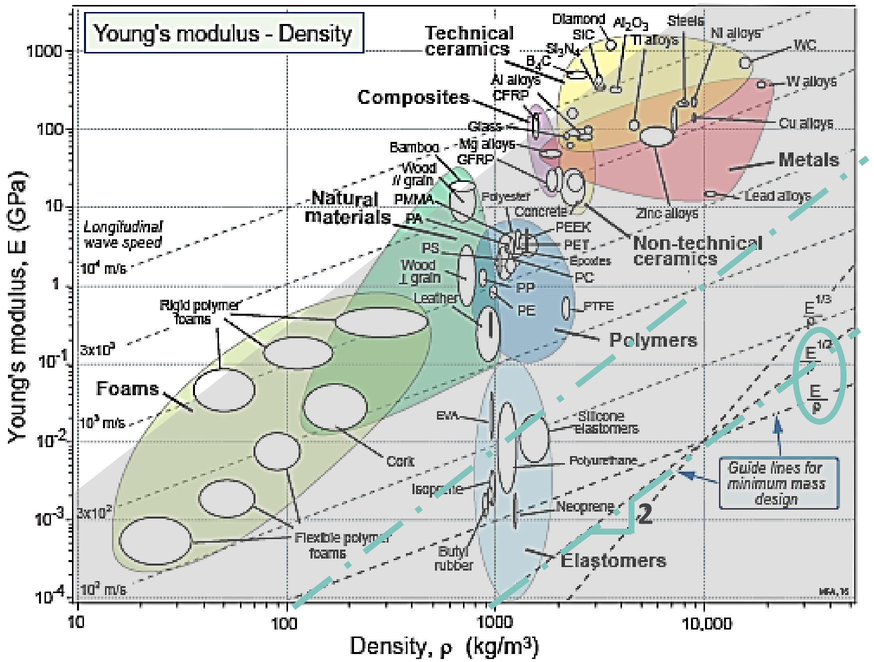
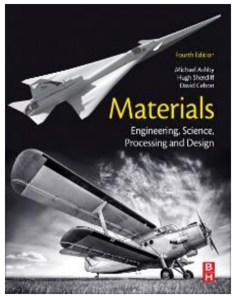
Systematic selection for performance, environment

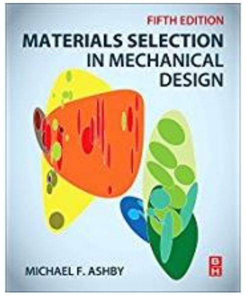


2. Selection Stages

Chart/Index | Limit | Tree







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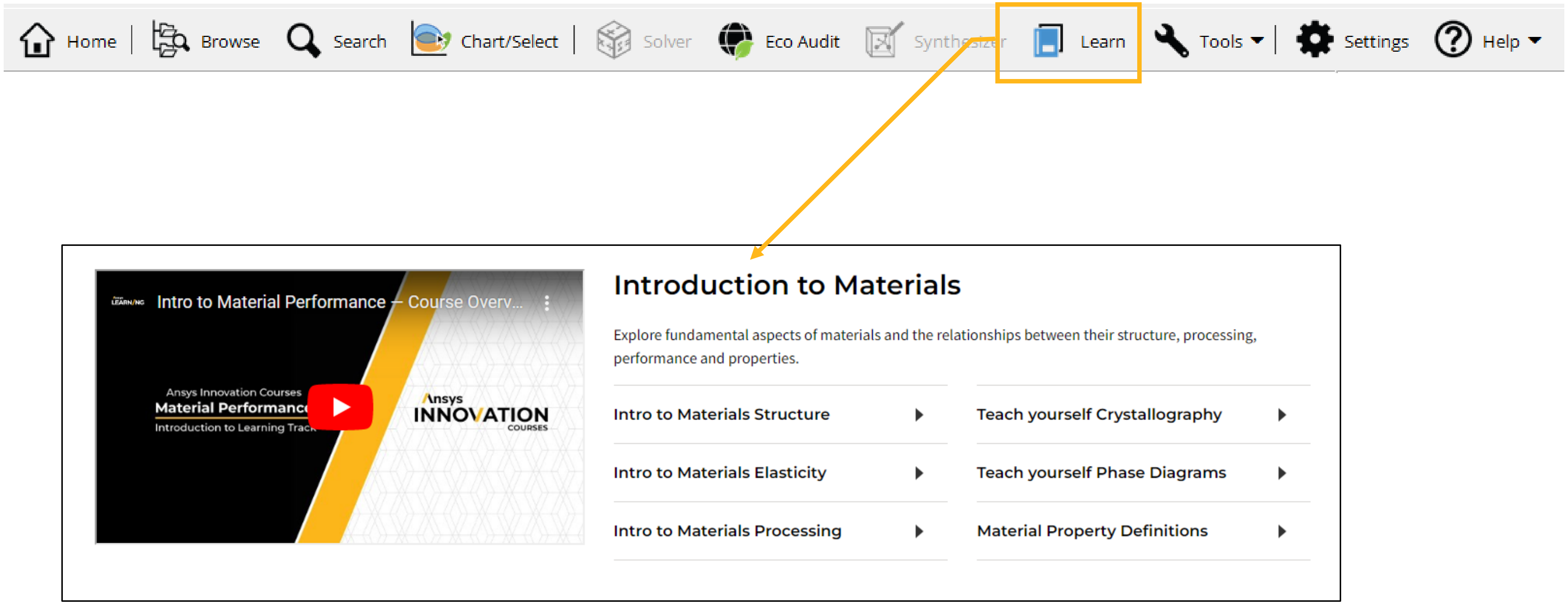
Learning resources



MS&E-related resources on the Ansys Education Resources Page

White Papers

Granta EduPack White Paper

The Granta EduPack Materials Science and Engineering Package

Mike Ashby[1], Hannah Melia[2], Madga Figuerola[2], Lee Philips[2], Stéphane Gorse[3]

[1]Department of Engineering, University of Cambridge
[2]Ansys Materials Education Division
[3]Bordeaux INP & Institut de Chimie de la Matière Condensée de Bordeaux, France.

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This version: July 2021

Exercises with Solutions

Granta EduPack Exercises with solutions: Materials Science and Engineering

-To accompany Lecture Unit 6

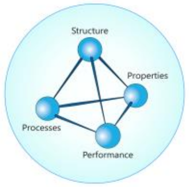
Mike Ashby

Department of Engineering, University of Cambridge

Lecture Units

Unit 6.
Materials Science and Engineering Package:
an overview

Mike Ashby
Department of Engineering,
University of Cambridge



Micro-projects

Granta EduPack MicroProjects + Solutions

Materials Science and Engineering

Mike Ashby

Department of Engineering, University of Cambridge

First published: July 2018
Current edition: October 2021

Teach Yourself...

Teach Yourself Crystallography

Mike Ashby

Department of Engineering, University of Cambridge

6th edition, October 2021

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// 5. Filling and reinforcement: polymers

:::: Which filler gives higher strength and stiffness to polypropylene
given the same degree of filling?
{=long glass-fiber ~chopped glass-fiber ~talc ~calcium carbonate}

:::: In metals, increased hardness often comes at the cost of reduced
toughness. Is this true in filled polypropylene?
{=no ~yes}

:::: The failure elongation percentage of polypropylene decreases with
increased degree of filling.
{T}

:::: A greater stiffness of filled polymer leads to a greater mechanical
loss coefficient.
{F}

:::: Which filler gives the greatest increase in thermal conductivity for
polypropylene?
{=long glass-fiber ~chopped glass-fiber ~talc ~calcium carbonate}
```

GIFT format for Moodle

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