

Materials design and selection for circular economy

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Module 1: Materials in circular economy and eco-informed material choice

Gross, Bernardo

Introduction to materials: main features (composition, structure, morphology, structure-properties relationships), main classes (metals/alloys, polymers, ceramics/glasses) their relevance in main specific sectors (plastics, building & construction, metals, apparel & textiles, energy conversion and storage) in a circular economy perspective. Eco-informed material choice. Specific topics:

Basics on circular chemistry.

Embedding sustainability in the design/manufacturing of materials. Sankey diagrams of materials flow.

How to address criticality: material design to reduce CRM content and substitution approaches.

Introduction to material properties charts: development and use. Definition of materials indices: performance of a component according to a combination of properties; selection through charts and indices. Presentation of "pure" selection case studies, with discussion of the characteristic equations and derivation of selection indices. Materials selection with conflicting objectives: trade-off analysis.

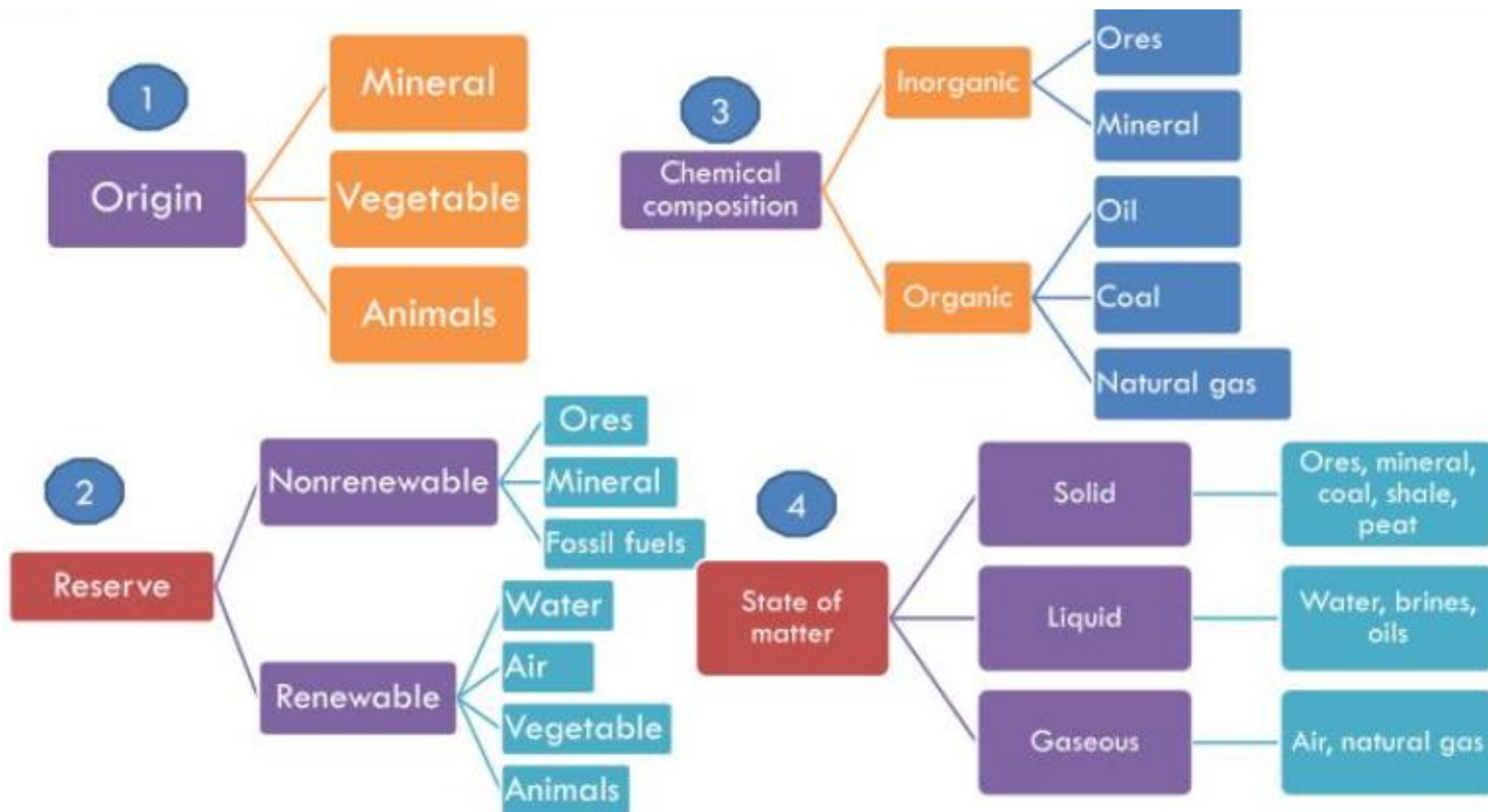
Environmental impact monitoring methods. Case studies of graphical materials selection oriented to environmental sustainability (control of energy and carbon footprint) in primary production.

Materials life cycle: definition of boundaries, introductory remarks to LCA, principles of eco-auditing. Updates on environmental sustainability from inclusion of manufacturing step. Presentation and analysis of end-of-life options. Case studies of application of eco-audits: introduction to the CES (Cambridge Engineering Selector) software, comparison between disposable and reusable constructions, material substitution

Case studies on cost/environmental sustainability trade-off

Sustainability by means of material minimization: introduction of shape factors, with case studies.

Materials: classification



Source of the picture: <https://extrudesign.com/classification-of-materials-engineering-material-classification/>

Materials, as opposed to single atoms or molecules, are solid systems deriving from more or less ordered assembly of atom/molecules/ions thought for a particular use/application.

They can be classified in:

- **natural** (bone, stone, ivory, wood, fiber, rubber, quartz, clay, mica etc.)
- **artificial** (not found in nature, prepared by humans)
- **structural**: they assolve a mechanical/structural function (e.g. stainless steel, concrete)
- **functional**: they have properties (e.g. optical, magnetic, electric/electronic) making them useful for a particular **function** (e.g. magnetic, magnetocaloric, magnetoelastic, spintronic, thermoelectric, piezoelectric, and dielectric materials)

Types of materials

- Natural materials (apatite, diatomees etc.)
- Metals and alloys
- Semiconductors, superconductors, insulators, conductors
- Non-metallic inorganic materials (oxide ceramics, not oxide ceramics)
- Glasses
- Organic polymers (also biobased: cellulose, silk etc.)
- Composite and/or hybrid materials
- Biomaterials

As a function of structure/morphology

- Porous materials (e.g. MOF, mesoporous, coordination polymer: see dedicated sections)
- Thin films
- Fibers
- Nanomaterials

Materials main features

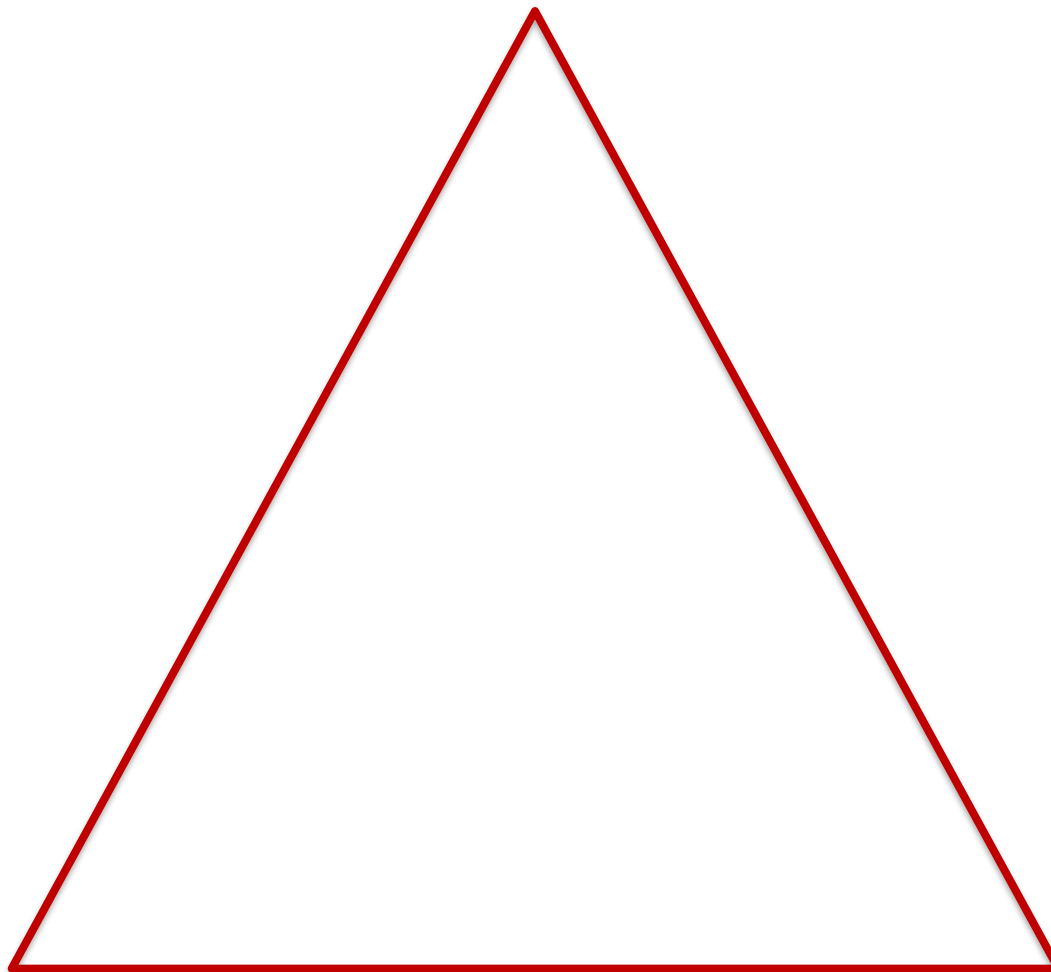
- **Composition:** it refers to the kind (**qualitative**) and to the relative atomic ratio or absolute number (**quantitative**) of atoms/ions or molecules present in a given material.
- **Structure:** it refers to the 3D (typically periodic) arrangement of atoms/ions/molecule constituting a solid material. Crystalline & amorphous materials.
- **Morphology:** it refers to shape, optical appearance, or form of phase domains in substances, such as high polymers, polymer blends, composites, and crystals. For a polymer blend or composite, the morphology describes the structures and shapes observed, often by microscopy or scattering techniques, of the different phase domains present within the mixture.

IUPAC. Compendium of Chemical Terminology, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). Online version (2019-) created by S. J. Chalk. ISBN 0-9678550-9-8. <https://doi.org/10.1351/goldbook>.

SEE LECTURE PROF. PAOLO DOLCET ON THEIR STUDY/ DETERMINATION

The triangle of materials

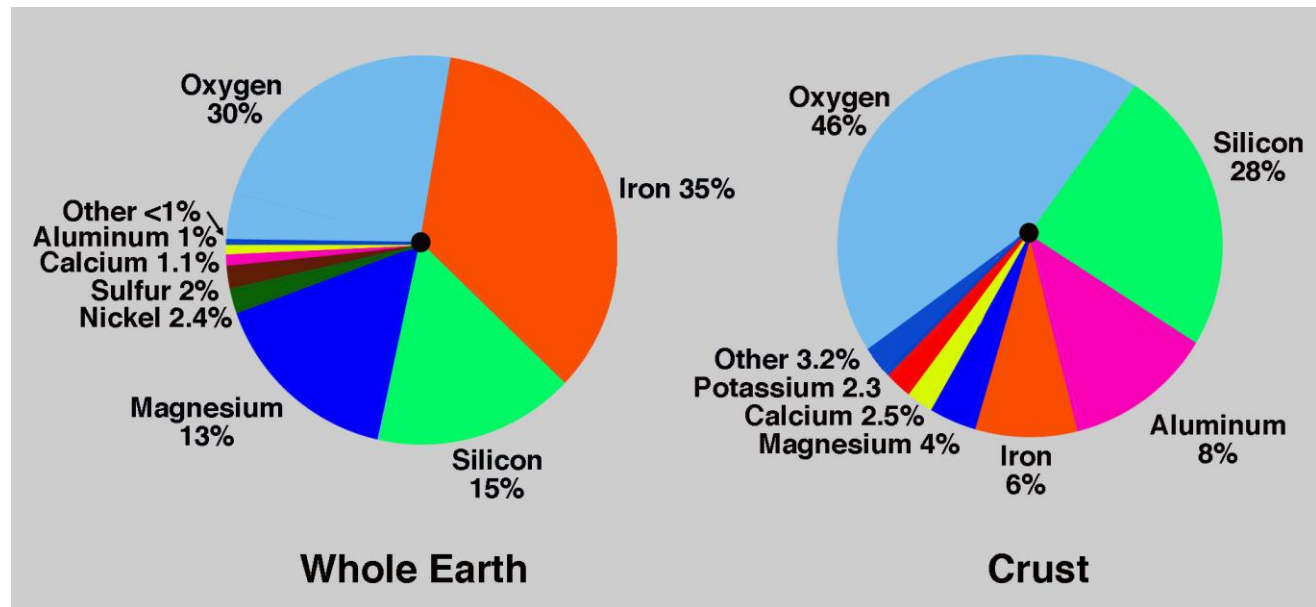
Synthesis & Processing



Composition & Structure

Properties & Performances

Materials features: composition



Composition:

Chemical composition refers to the nature of elements, bonding, amount and ratio of atoms in molecules of chemical substances. Chemical composition varies when chemicals are added or subtracted from a substance, when the ratio of substances changes, or when other chemical changes occur in chemicals.

It can be:

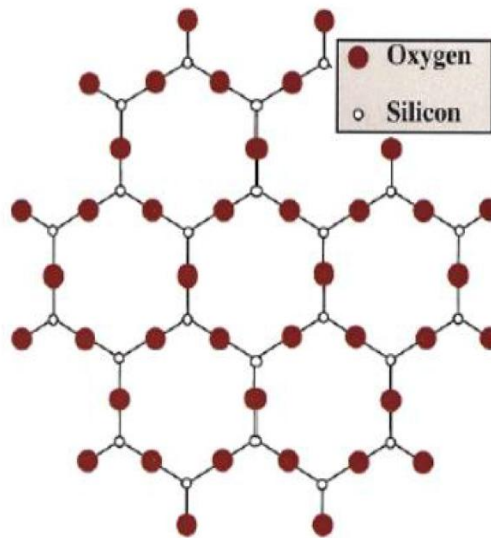
- Qualitative: types of atoms and their arrangement (bonds, chemical environment, oxidation state)
- Quantitative: atomic ratios, weight percent, weight ratio, volume ratio...

SEE LECTURE PROF. PAOLO DOLCET ON COMPOSITION DETERMINATION

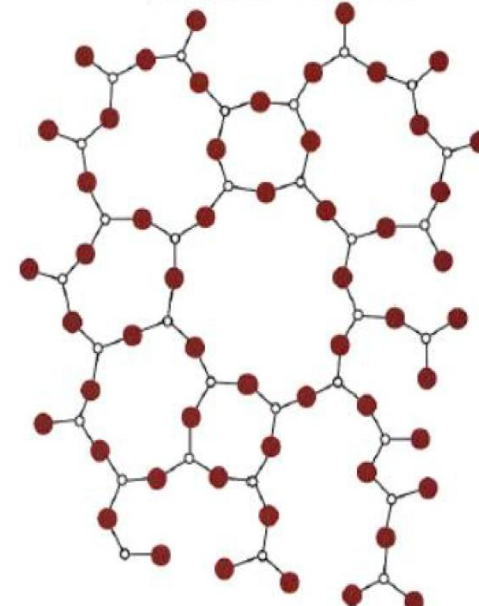
Materials features: structure

- **Crystalline** materials have long-range order, with components composed of many individually oriented grains.
- **Glassy (amorphous) materials** possess short-range order, and generally do not form individual grains.
- The distinction is made based on x-ray diffraction characteristics (see lecture Dr. Lorandi in the II semester or 8 h Prof. Gross course Inorganic Chemistry III).
- Most of the mineral/inorganic materials are crystalline.

Quartz: (Crystalline)
Both Short and Long Range Order

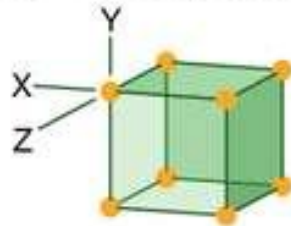


Glass: (Amorphous)
Short Range Order Only



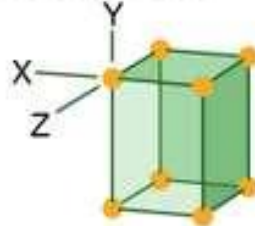
Crystal structures and crystal systems

The seven primitive crystal systems



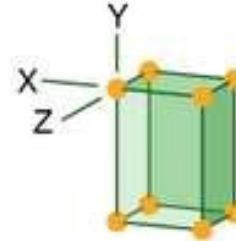
Isometric (or cubic)

All three axes are equal in length, and all are perpendicular to one another.



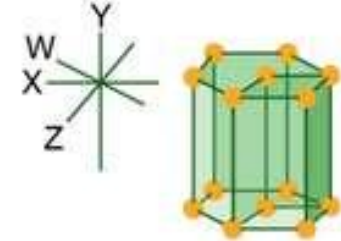
Tetragonal

Two of the three axes are equal in length, and all three axes are perpendicular to one another.



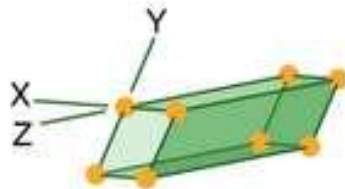
Orthorhombic

All three axes are unequal in length, and all are perpendicular to one another.



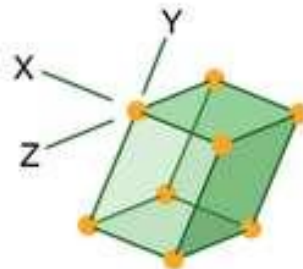
Hexagonal

Of four axes, three are of equal length, are separated by equal angles, and lie in the same plane. The fourth axis is perpendicular to the plane of the other three axes. Hexagonal cells have lattice points in each of the two six-sided faces.



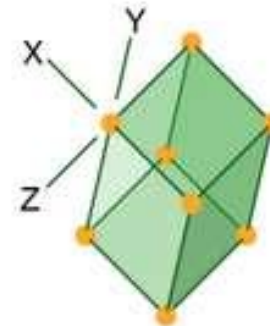
Triclinic

All three axes are unequal in length, and none is perpendicular to another.



Monoclinic

All three axes are unequal in length, and two axes are perpendicular to each other.



Rhombohedral (or trigonal)*

All three axes are of equal length, and none of the axes is perpendicular to another, but the crystal faces all have the same size and shape.

Allotrope

Different structural modifications of an **element**.

<http://goldbook.iupac.org/terms/view/A00243>

Polymorph

a structural modification of a given **compound**

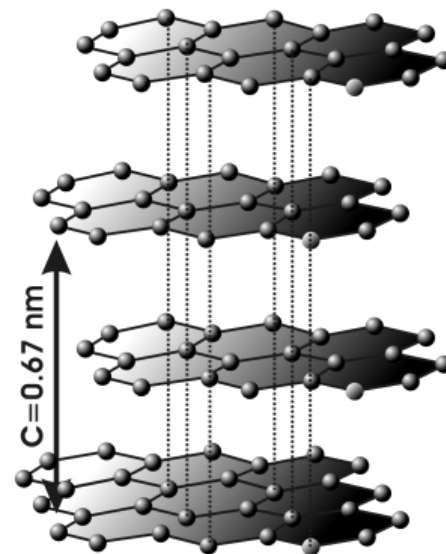
Polymorphic transition

A reversible transition of a solid crystalline phase at a certain temperature and pressure (the inversion point) to another phase **of the same chemical composition with a different crystal structure**. Example:

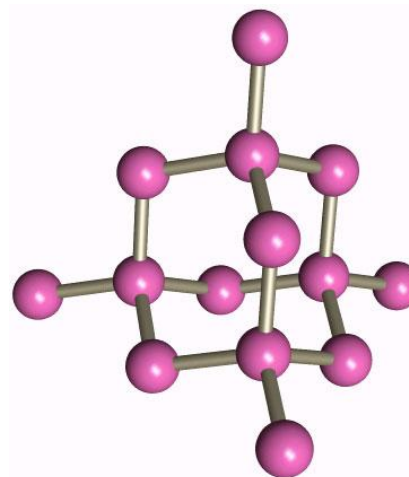
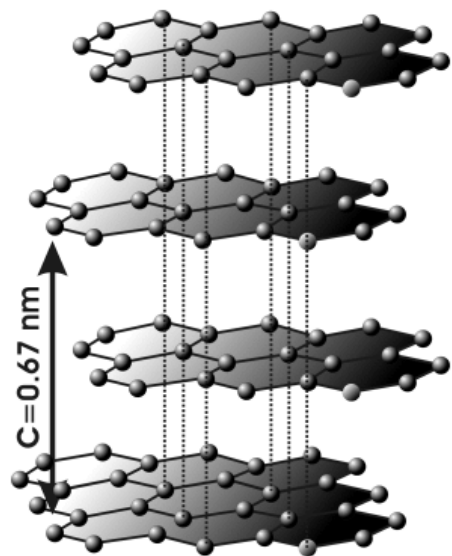
1. transitions of SiO_2 (quartz-type) at 1143 K to SiO_2 (tridymite-type), and at 1743 K to SiO_2 (cristobalite-type).

<https://goldbook.iupac.org/terms/view/P04748>

Examples of allotropes

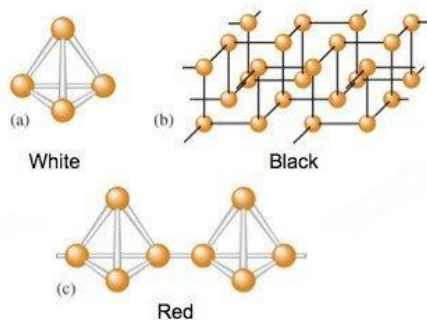
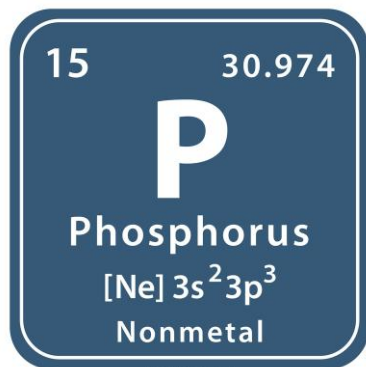


graphite

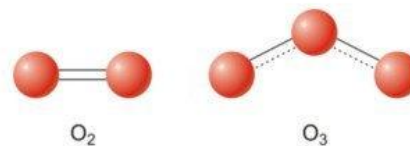


diamond

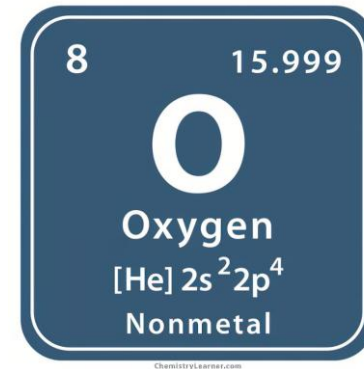
Examples of allotropes



Allotropes of phosphorus

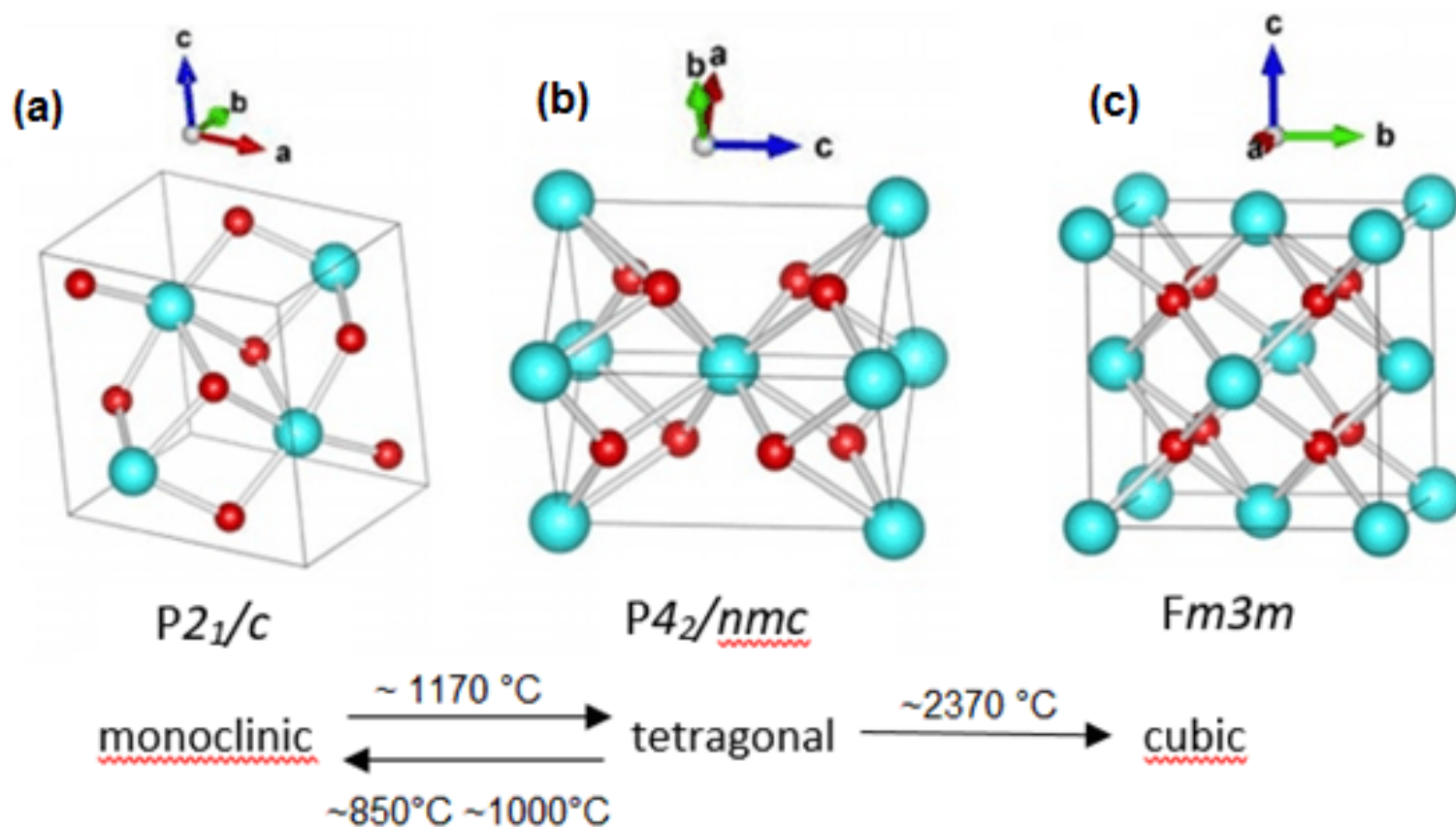


Allotropes of oxygen

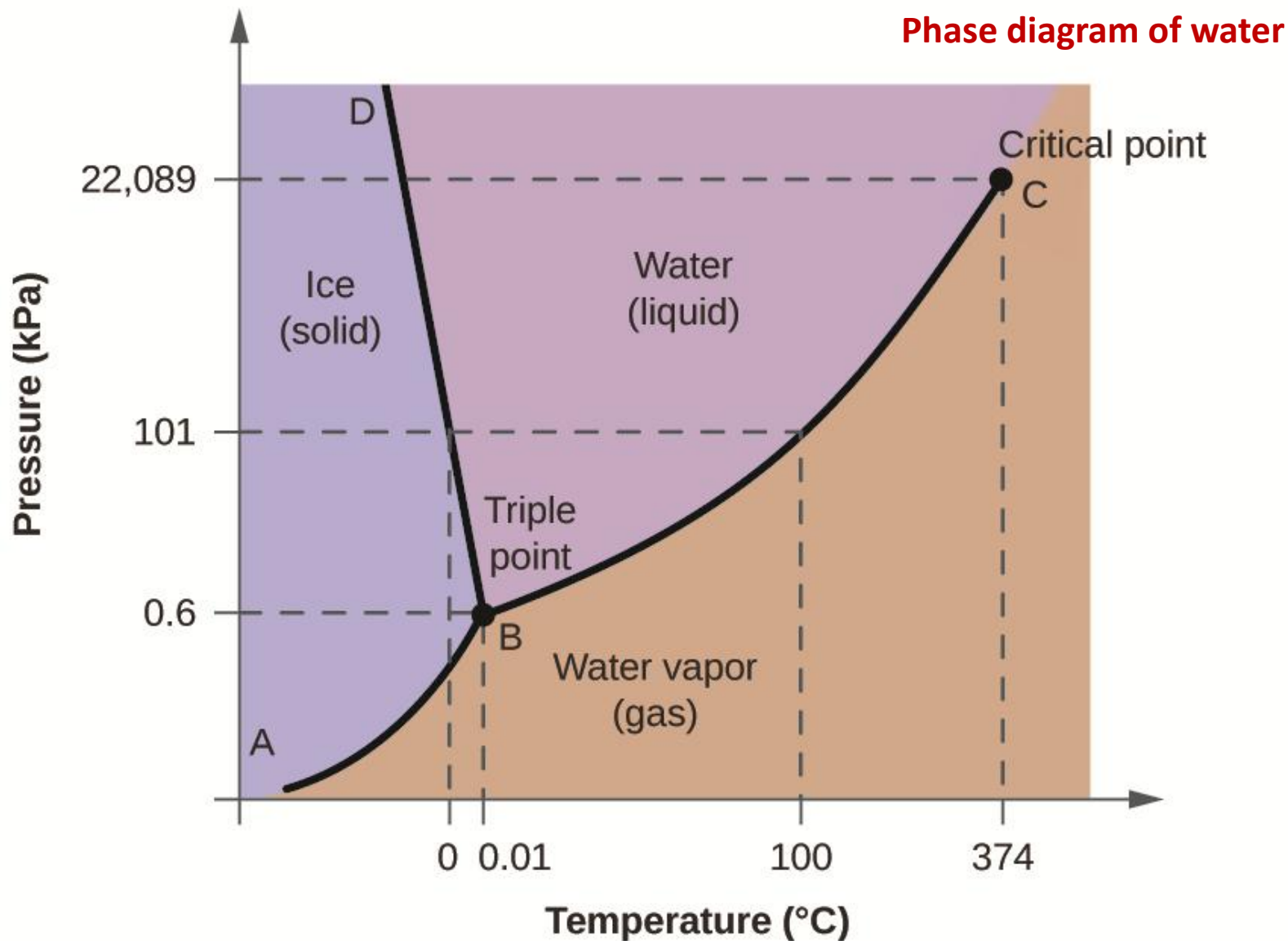


Zirconium oxide (ZrO_2) = zirconia

Zirconia has several characteristics that are superior, such as refractory properties, hardness, absence of toxicity.

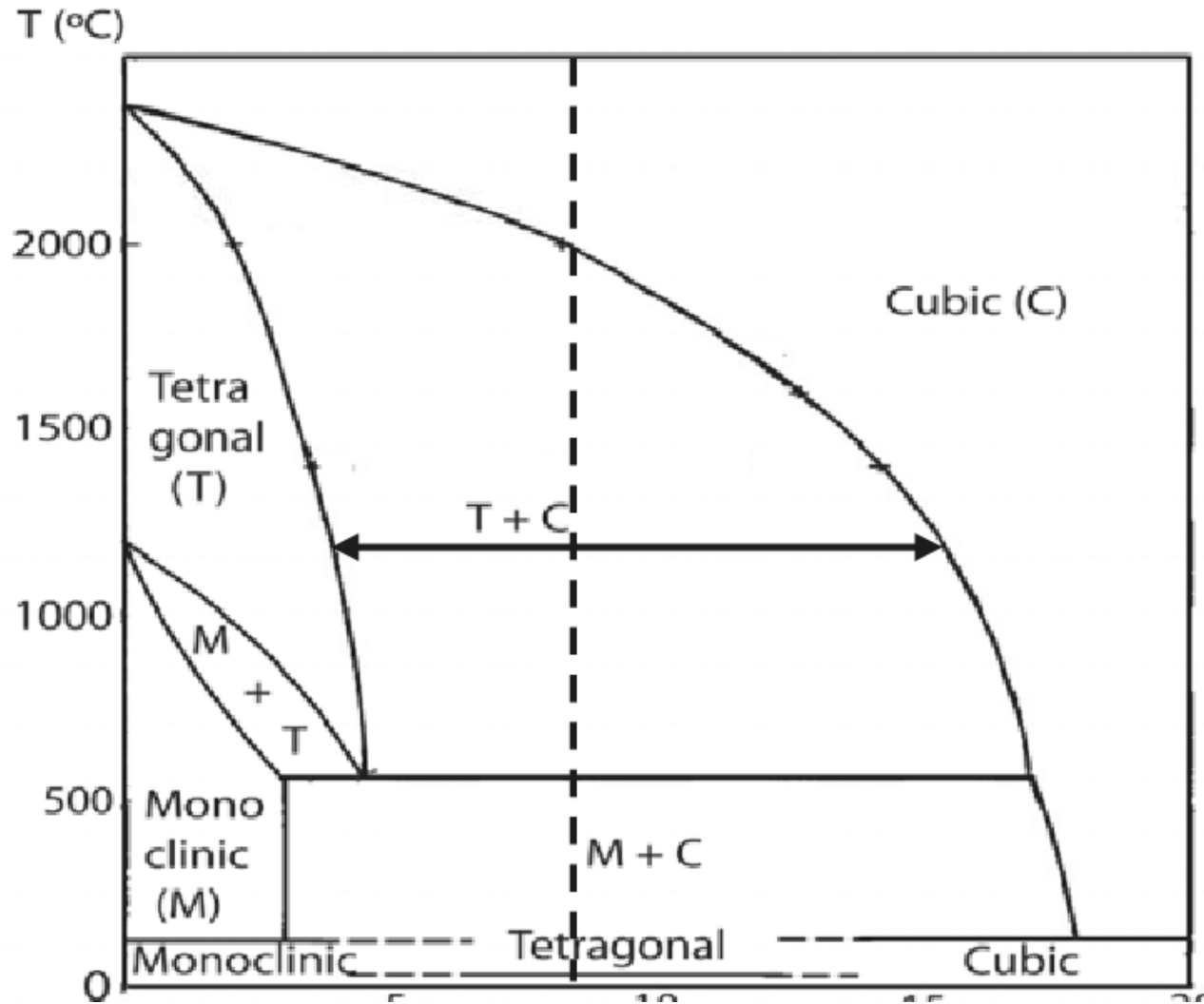


Understanding phase diagrams



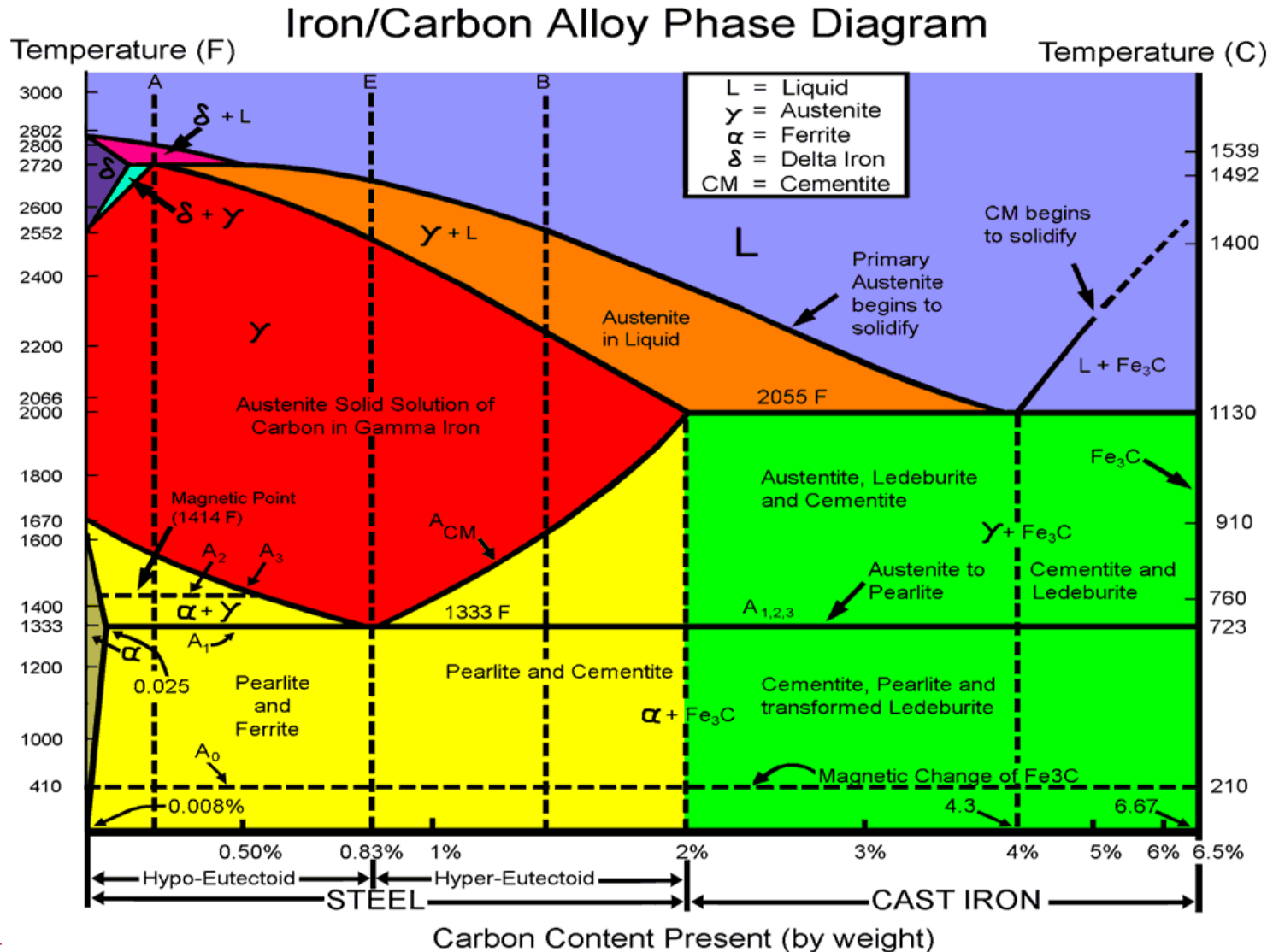
Understanding phase diagrams

Phase diagram of zirconia (ZrO_2)



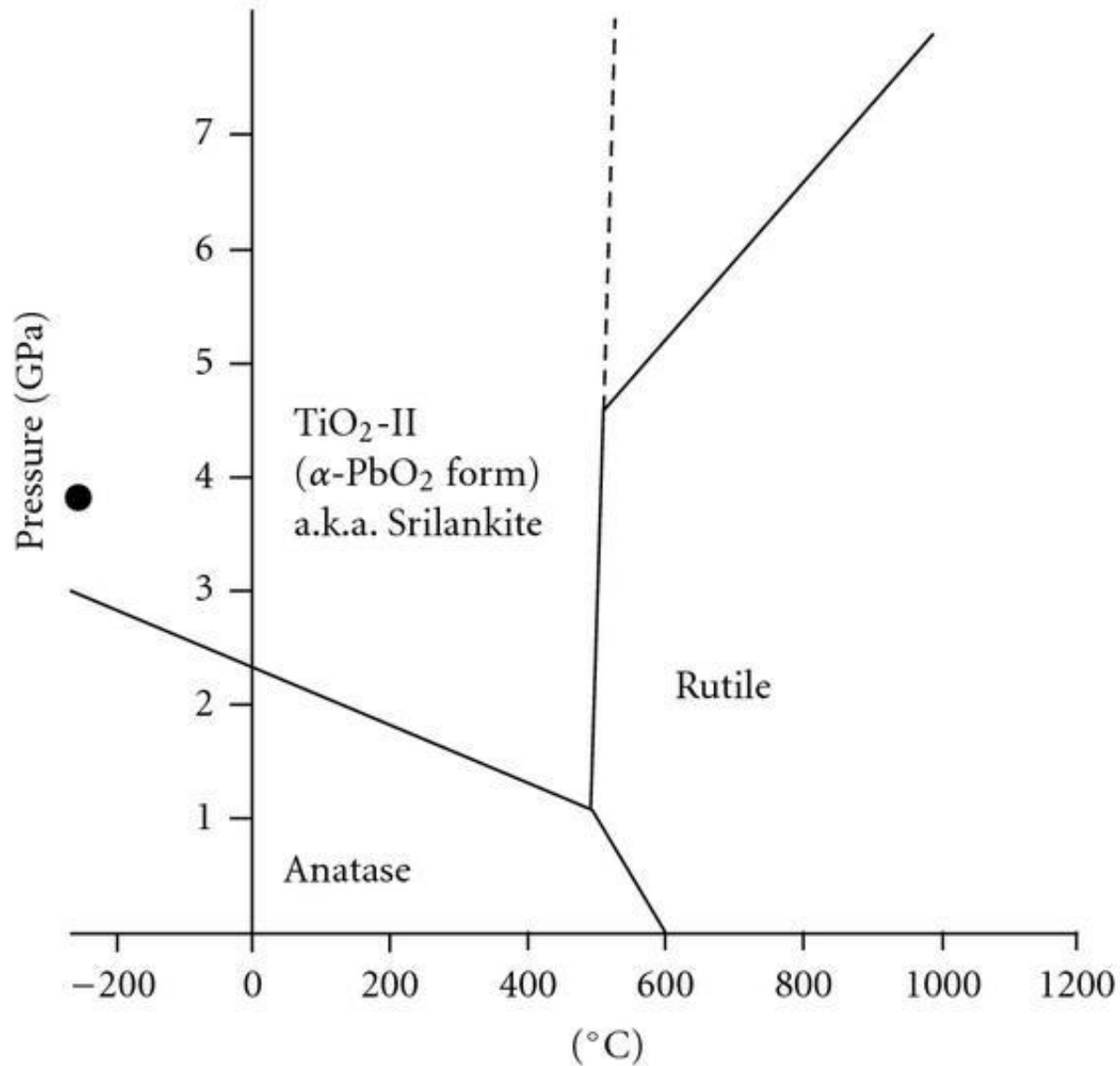
Understanding phase diagrams

Phase diagram of the system Fe/C (see lectures Prof. Dabalà)

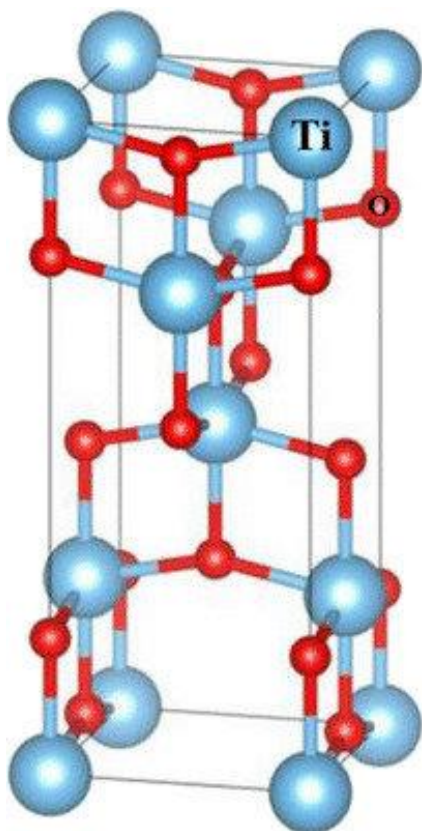


Properties depend upon polymorph

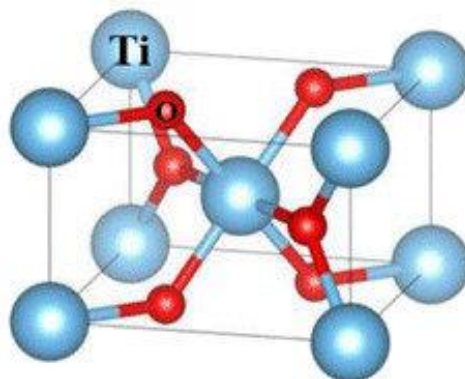
Phase diagram of titania (TiO_2)



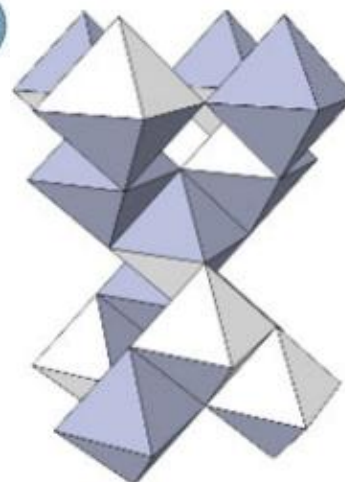
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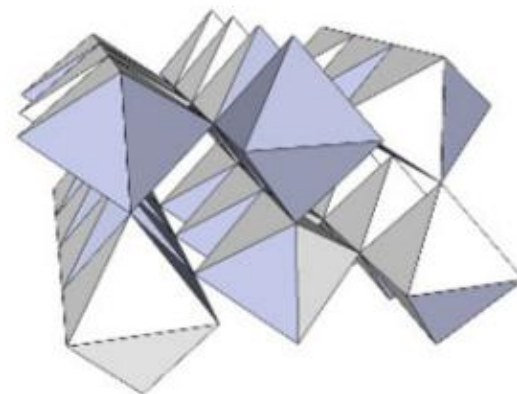
(a)



(b)



Anatase

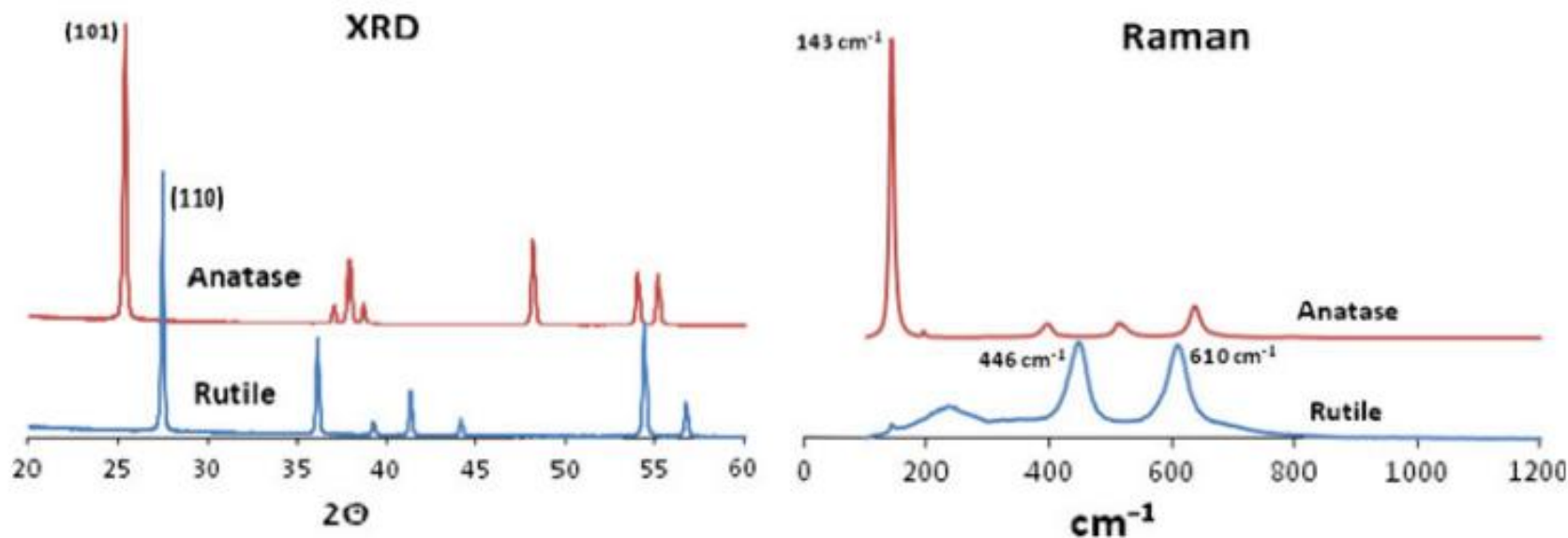


Rutile

Unit cells of anatase TiO_2 (a) and rutile TiO_2 (b). Large light-blue and small red spheres are Ti^{4+} and O^{2-} ions, respectively. Source: Nanoscale Research Letters. 11. 10.1186/s11671-016-1531-5.

Properties depend upon polymorph

Property	Rutile	Anatase
Colour	Dark red	White
Crystal structure	Tetragonal	Tetragonal
Density	4259 kg/m ³	3894 kg/m ³
Band gap	3.0 eV	3.2 eV
Thermodynamic stability	more stable	less stable
Solubility in HF	insoluble	soluble
Hardness (Mohs)	6.0-6.5	5.5-6.0



XRD pattern and Raman spectra of the two polymorphs

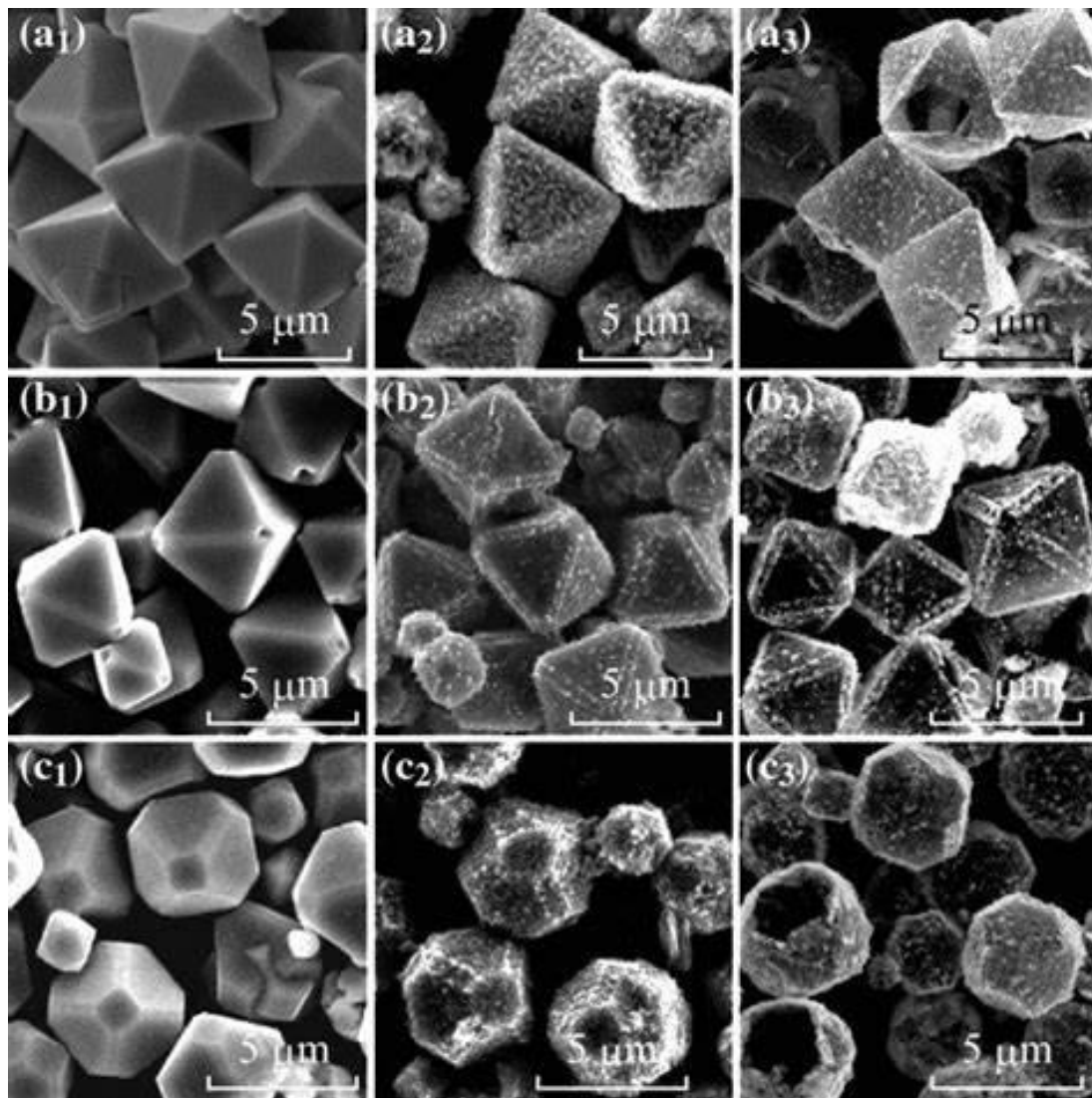
J Mater Sci (2011) 46:855–874
DOI 10.1007/s10853-010-5113-0

REVIEW

Review of the anatase to rutile phase transformation

Dorian A. H. Hanaor · Charles C. Sorrell

Materials features: morphology



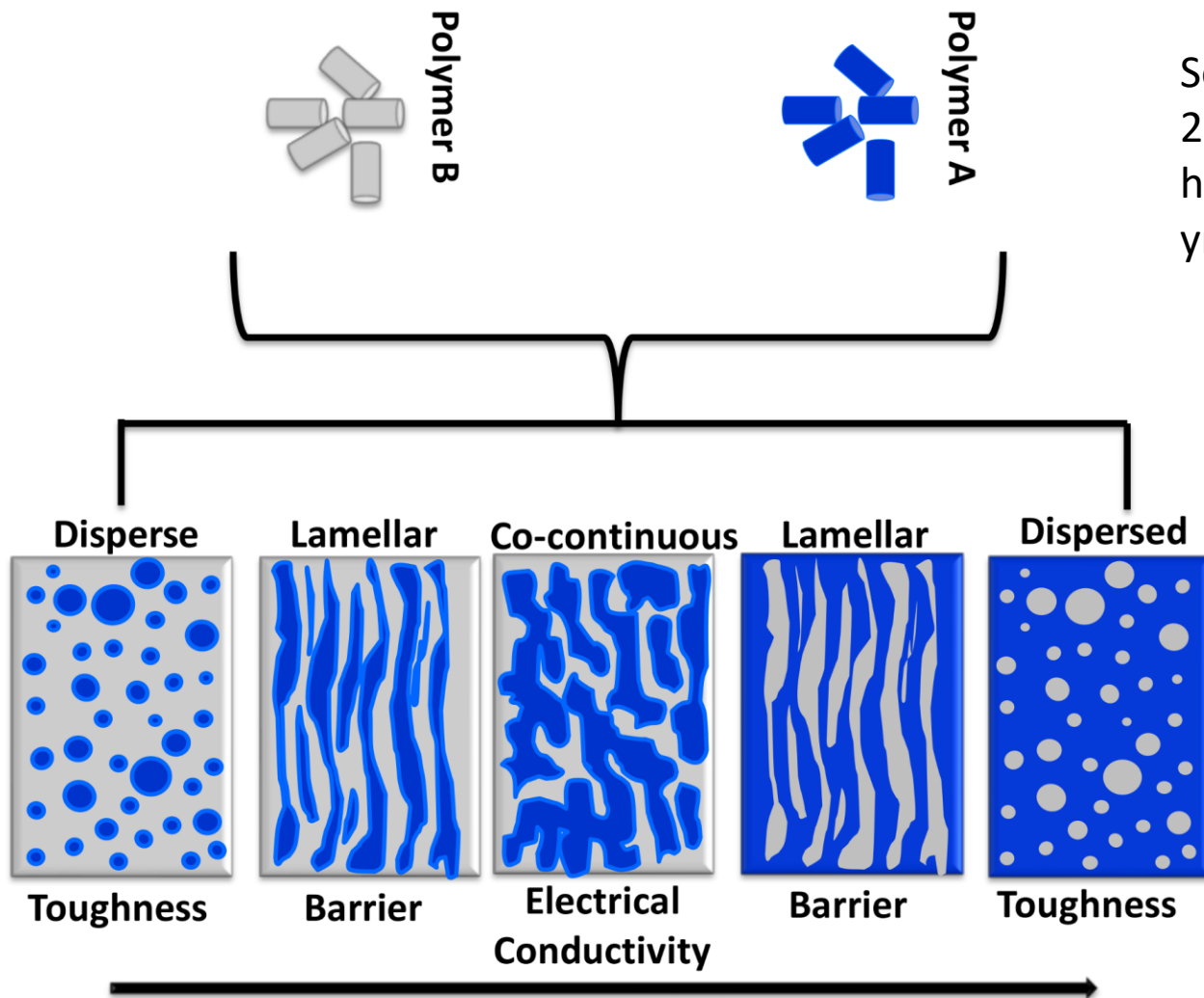
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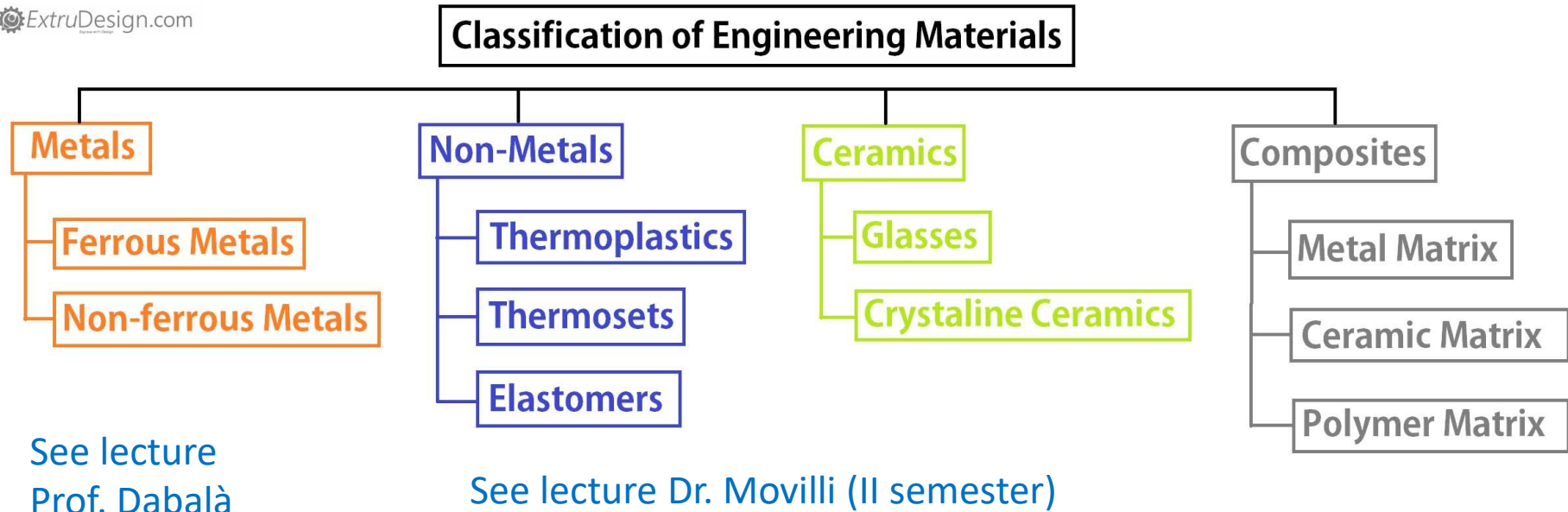
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Materials features: morphology



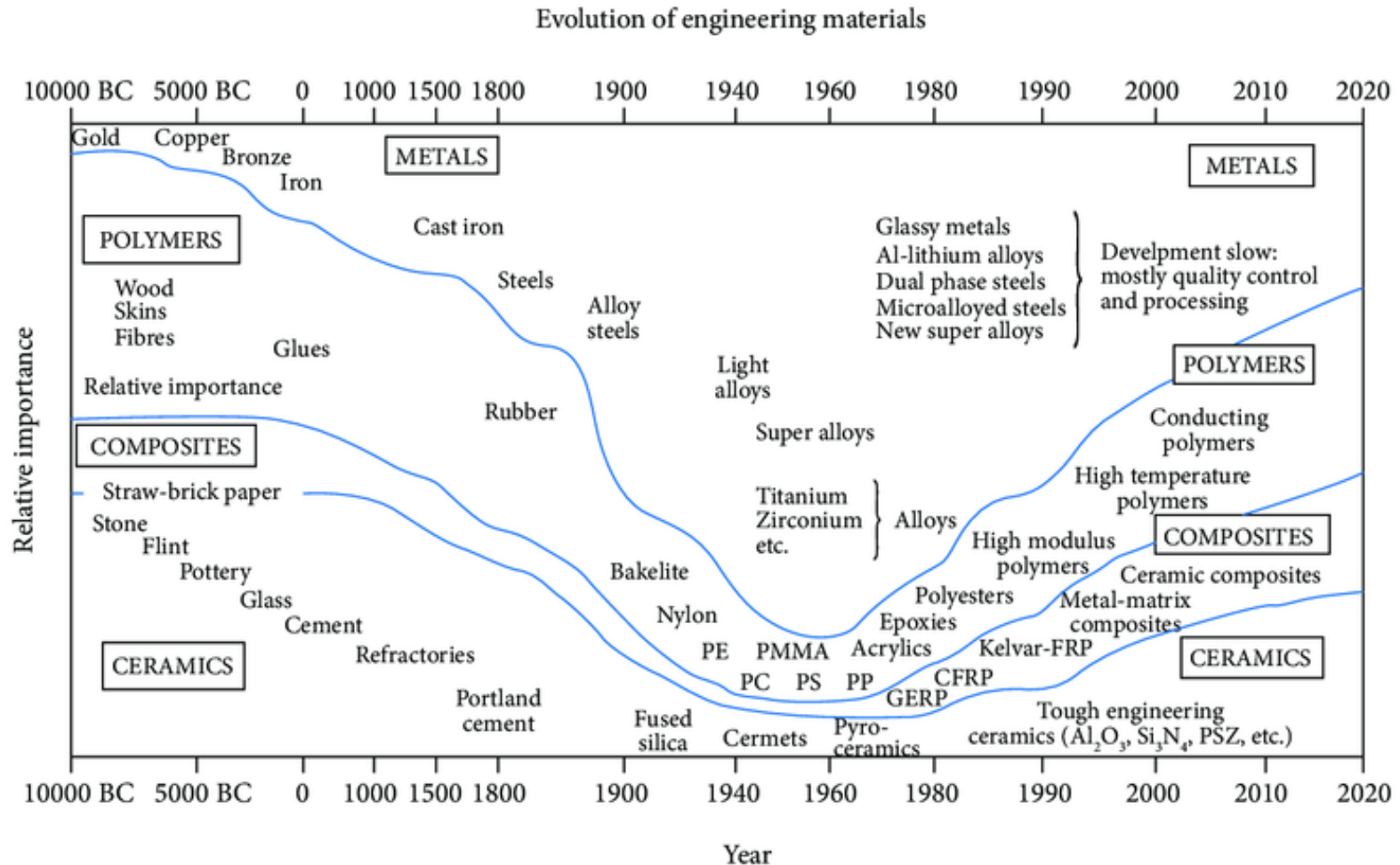
Source of figure: Polymers
2021, 13(2), 230;
<https://doi.org/10.3390/polym13020230>

Classification of materials



Source of the picture: <https://extrudesign.com/classification-of-materials-engineering-material-classification/>

Classification of materials



Source of the picture: Alemour, Belal & Badran, Omar & Hassan, Mohd. (2019). A Review of Using Conductive Composite Materials in Solving Lightning Strike and Ice Accumulation Problems in Aviation. Journal of Aerospace Technology and Management. 11. 10.5028/jatm.v11.1022.

Main features and uses of materials

<i>Group</i>	<i>Important Characteristics</i>	<i>Common Examples of Engineering use</i>
<i>Metals and Alloys</i>	Lusture, Hardness, Resistance to Corrosion, Thermal and Electrical Conductivity, Malleability, Stiffness and Property of Magnetism.	Iron and Steels, Aluminium, Copper, Zinc, Magnesium, Brass, Bronze, Invar, Super Alloys, Super-conductors, etc.
<i>Ceramics</i>	Thermal Resistance, Brittleness, Opaqueness to Light, Electrical Insulation, High-temperature Strength, abrasiveness, Resistance to Corrosion.	Silica, Glass, Cement, Concrete, Refractories, Silicon Carbide, Boron Nitride abrasives, Ferrites, Insulators, Garnets, etc.
<i>Organic Polymers</i>	Soft, Light in weight, Dimensionally unstable, Poor Conductors of Heat and Electricity, Ductile, Combustible, Low-thermal Resistance.	Plastics – Poly Vinyl Chloride, Poly Tetra Fluoroethylene, Polycarbonates. Natural and Synthetic Fibers – Nylon, Terylene, Leather, etc. Other uses – Explosives, Refrigerants, Insulators, Lubricants, Detergents, Fuels, Vitamins, Medicines, adhesives, etc.

Metals and alloys: see lecture Prof. Dabalà

Polymers: see lectures Dr. Movilli, II semester

Ceramics, composites: explained in this lecture

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