Institute Core Course for BTech Program

IC250: Materials Chemistry II

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Overview

Course Content:

- Introduction of material sciences, classification and selection of materials, different structures of materials and structural defects
- Organic/Inorganic Hybrid Materials: synthesis and characterization, properties, applications in gas adsorption, molecular recognition and catalysis
- Cluster Compounds: synthesis and applications
- Organometallic Materials: Classification and application
- Materials for energy storage systems and fuel cells
- Materials for batteries

Overview

Books:

1) William D. Callister, Jr, *Materials Science and Engineering – An introduction*, sixth edition, John Wiley & Sons, Inc. 2004.
2) M. F. Ashby and D. R. H. Jones, *Engineering Materials 1, An introduction to Their Properties and Applications*, second edition, Butterworth-Heinemann, Woburn, UK, 1996.
3) L. R. MacGillivray, C. M. Lukehart *Metal-Organic Framework Materials*, first edition, John Wiley & Sons, Inc. 2014.

Evolution Methodology

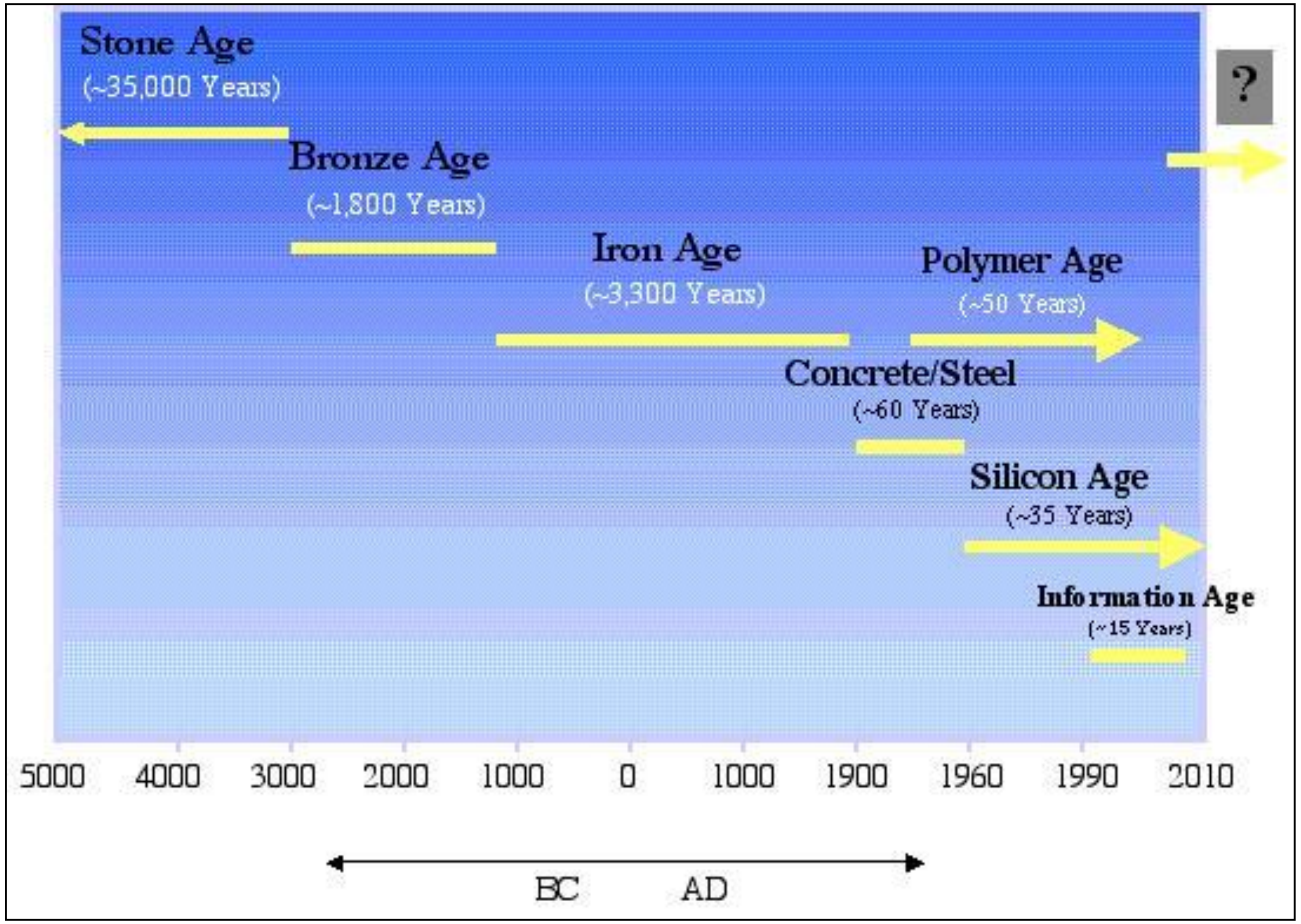
- The tentative proposal is the following which is subject to be change as per the situation.

COMPONENT	WEIGHTAGE
Exam (Number of Exam)	50% (1st Tierce Exam)
Assignment	20% (?)
Quiz	20% (1 Quiz)
Presentation	10%
Total	**100%**

Materials Chemistry II : Basic Introduction

Historical Perspective

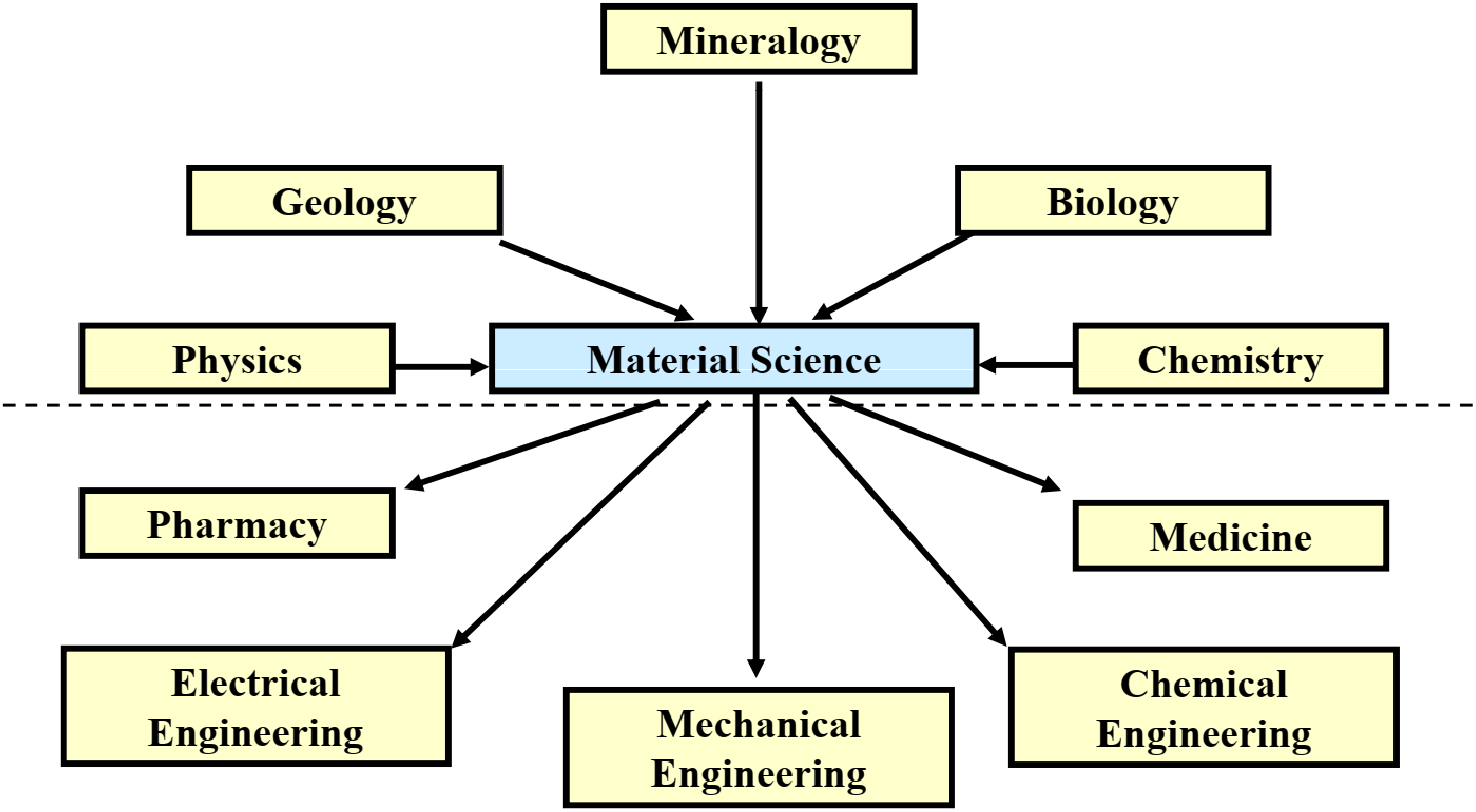
- Materials are very important in development of human civilization.
- In respect, their names are associated in history, e.g. Stone Age, Bronze Age, Iron Age, etc.
- The development and advancement of societies are dependent on the available materials and their use.



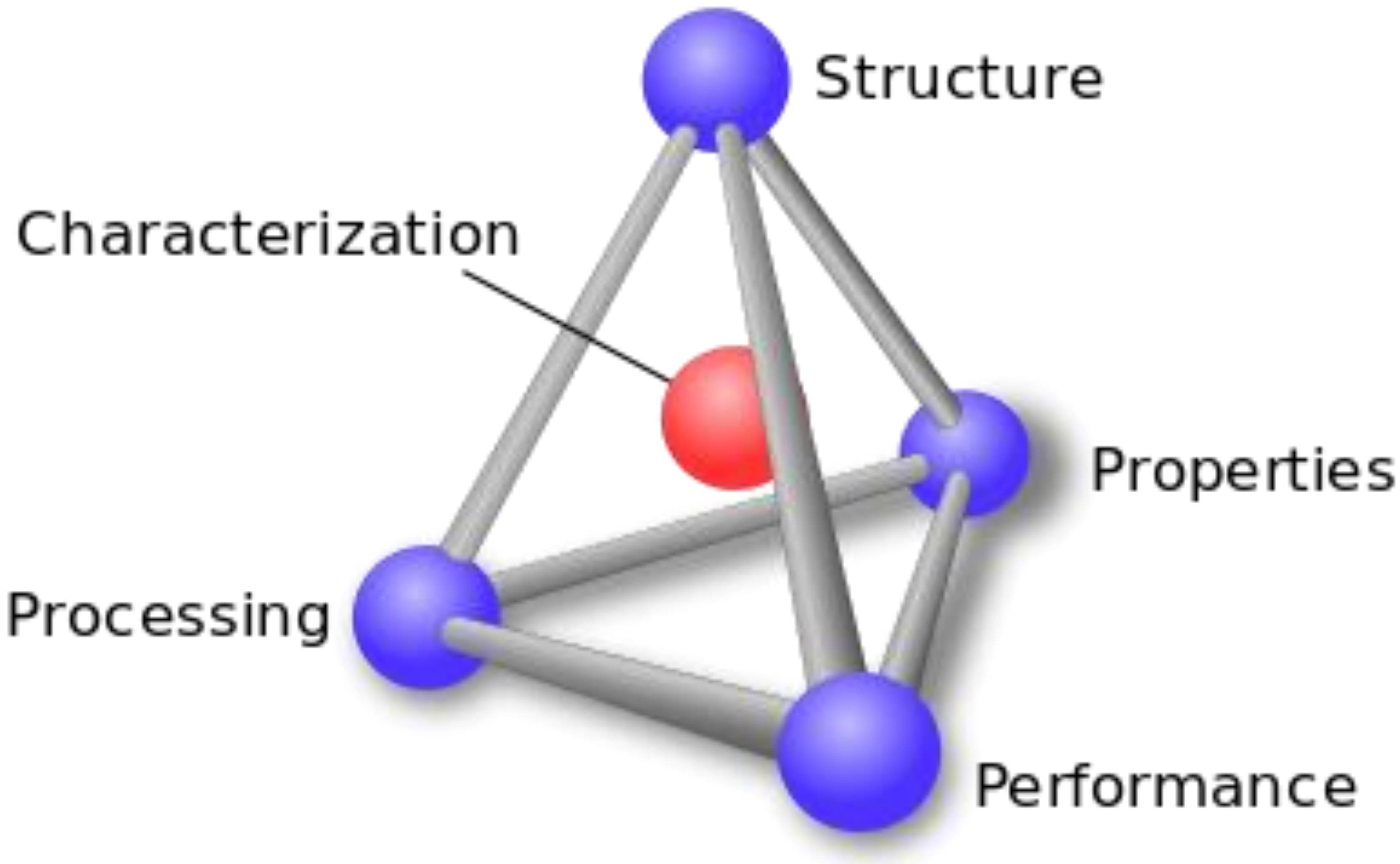
Materials Science And Engineering

- The discipline of *materials science* involves investigating the relationships that exist between the structures and properties of materials.
- In contrast, *materials engineering* is, on the basis of these structure–property correlations, designing or engineering the structure of a material to produce a predetermined set of properties.
- The relationships between material properties and structural elements will be discussed further.

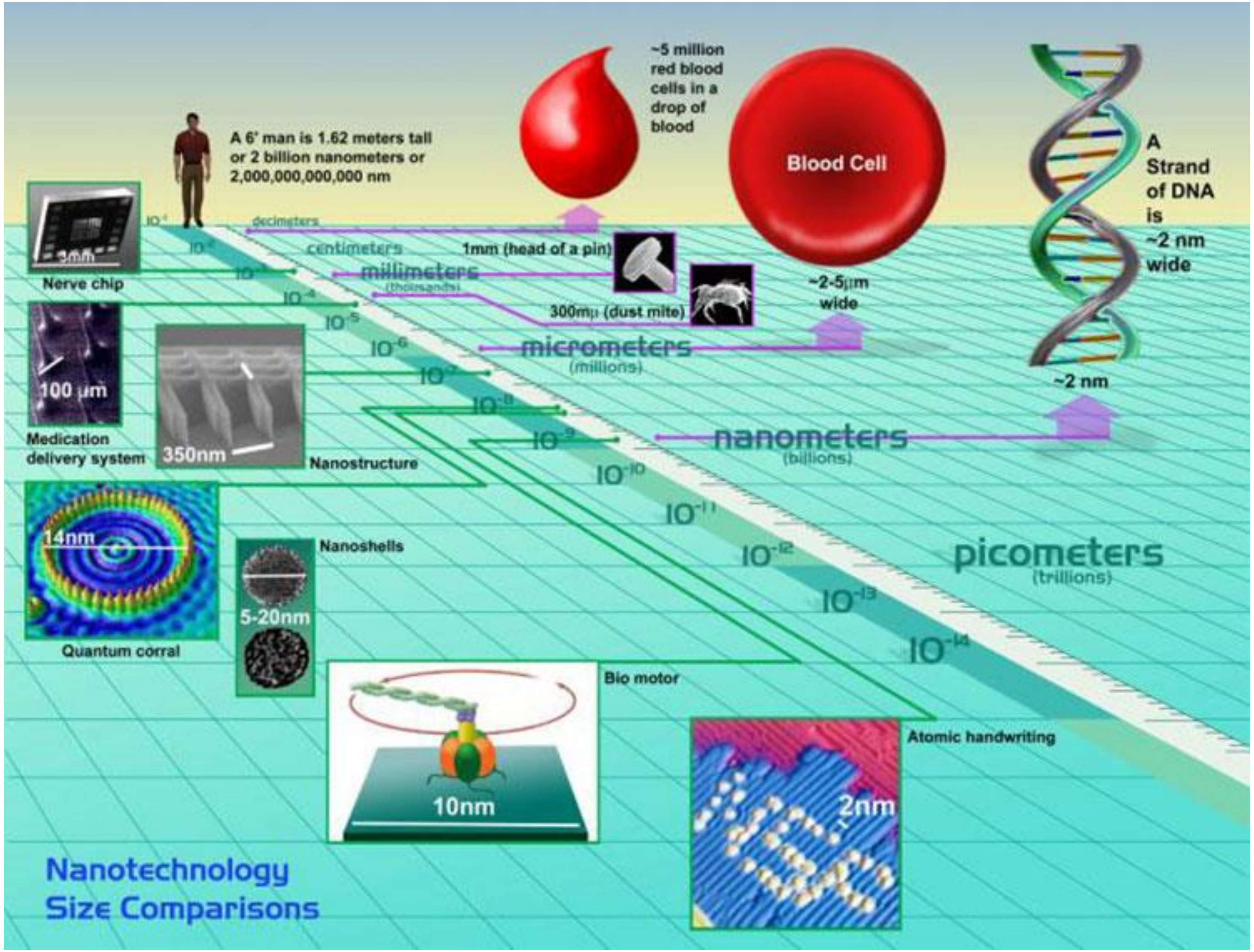
Materials Science And Engineering



Materials Science And Engineering



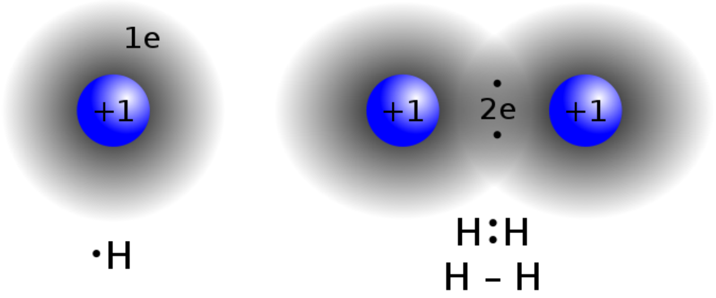
Structure of Materials

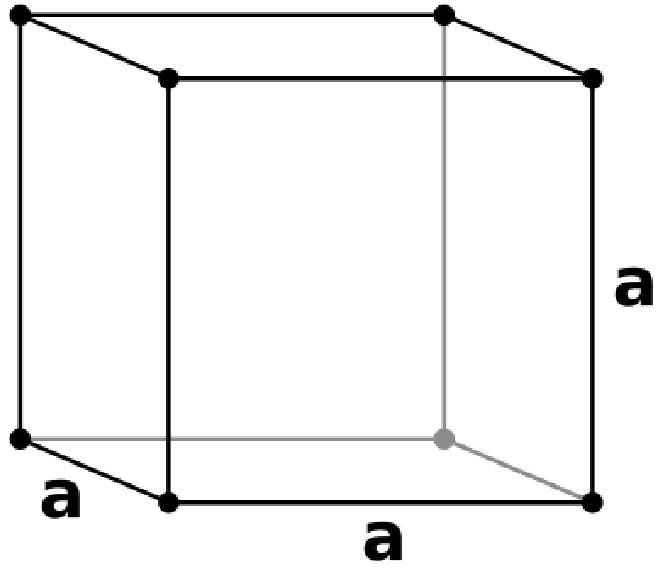


- Atomic: < 10^{-10} m
- Nano: 10^{-9} m
- Micro: 10^{-6} m
- Macro: > 10^{-3} m

Atomic Structure of Materials

- Pertains to atom electron structure and atomic arrangement.
- Includes electron structure – atomic bonding
  - Ionic
  - Covalent
  - Metallic
  - London dispersion forces (Van der Waals)
- Atomic ordering – long range (metals), short range (glass)
- 7 lattices – cubic, hexagonal among most prevalent for engineering metals and ceramics
- Different packed structures: Gives total of 14 different crystalline arrangements (Bravais Lattices).
- Primitive, body-centered, face-centered





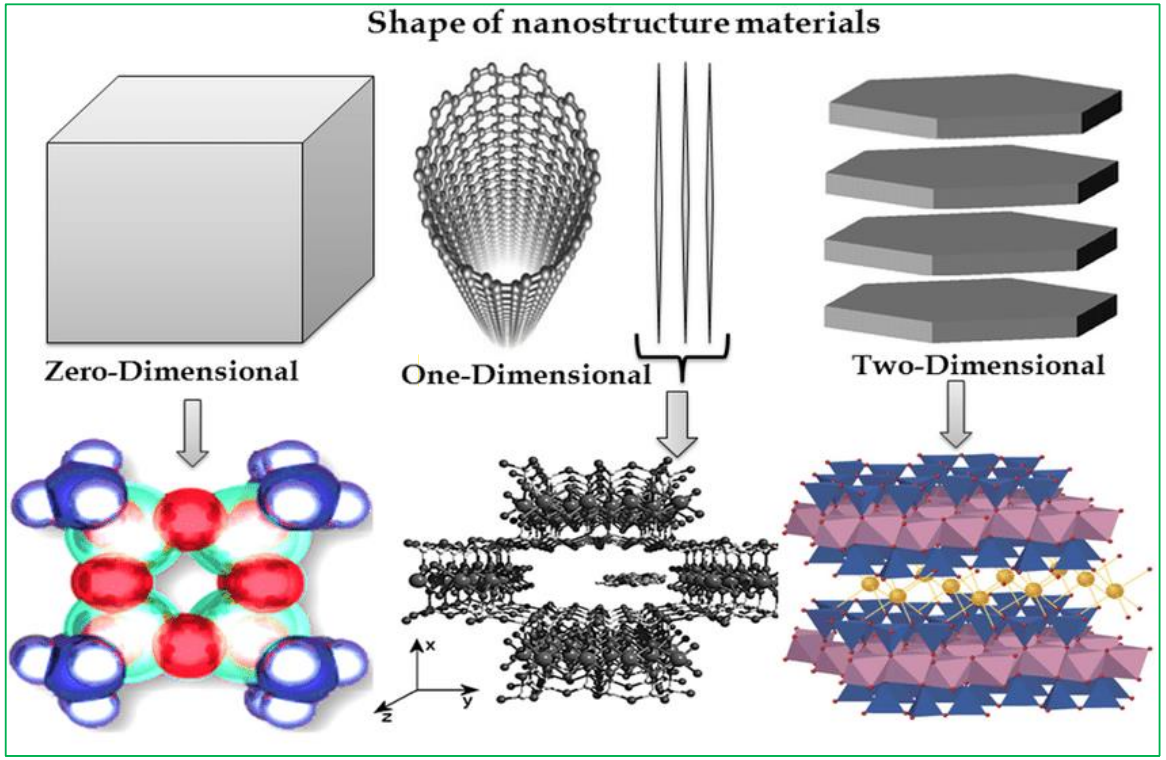
Nanostructure of Materials

- Length scale that pertains to clusters of atoms that make up small particles or material features.

- Show interesting properties because increase surface area to volume ratio

a) More atoms on surface compared to bulk atoms

b) Optical, magnetic, mechanical and electrical properties change



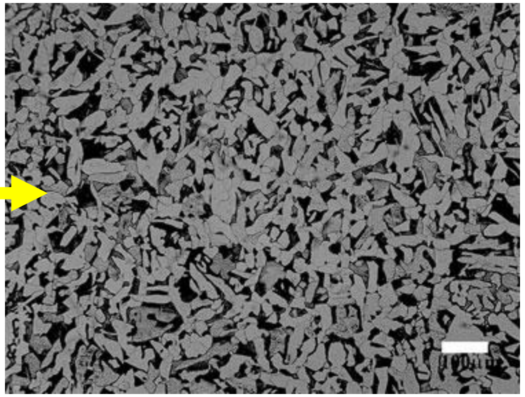
1-100 nm range

Microstructure of Materials

- Larger features composed of either nanostructured materials or periodic arrangements of atoms known as crystals.

100 nm to a few mm range

- Features are visible with high magnification in light microscope.
  - Grains, inclusions other micro-features that make up material
  - These features are traditionally altered to improve material performance



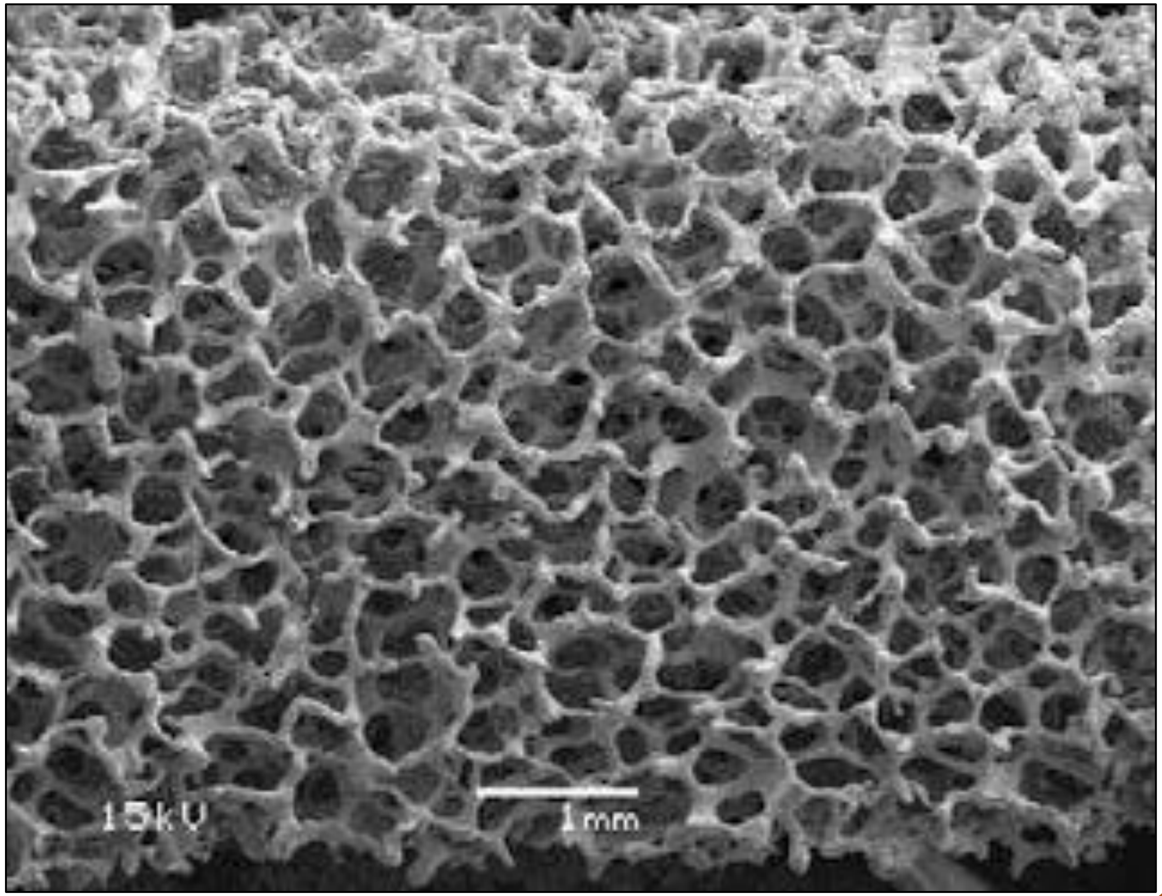
Microstructure of materials can strongly influence physical properties, such as strength, toughness, ductility, hardness, corrosion resistance etc.

Macrostructure of Materials

- Macrostructure pertains to collective features on microstructure level.

- Grain flow, cracks, porosity are all examples of macrostructure features.

mm to m range

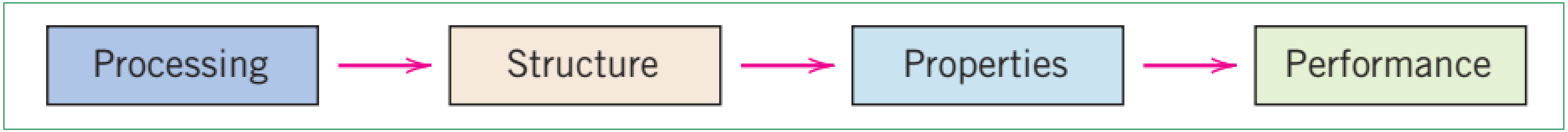


Properties of Materials

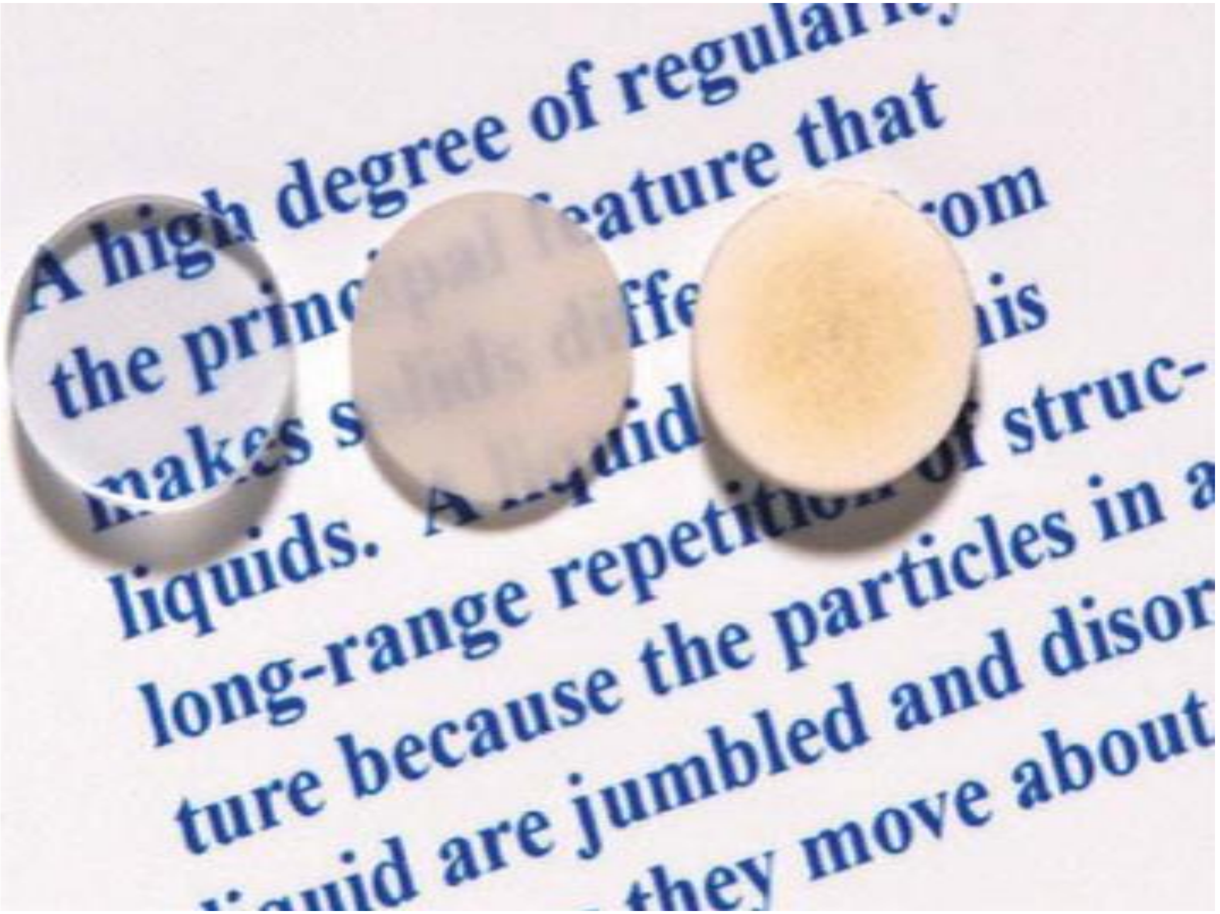
- All solid engineering materials are characterized for their properties.
- Engineering use of a material is reflection of its properties under conditions of use.
- All important properties can be grouped into six categories: **Mechanical, Electrical, Thermal, Magnetic, Optical, and Deteriorative**.
- Each material possess a structure, relevant properties, which dependent on processing and determines the performance.

Material Chemistry

- In addition to structure and properties, two other important components are involved in the science and engineering of materials, such as **Processing and Performance**.
- The structure of a material will depend on how it is processed.
- Material's performance will be a function of its properties.



Aluminum Oxide (Al_2O_3)



Single-crystal (transparent)	Polycrystalline, fully dense (translucent)	Polycrystalline, 5% porosity (opaque)

Why Do We Need to Study Properties of Materials?

Aluminum

Glass

Plastic

Why Do We Need to Study Properties of Materials?

- Since there are thousands of materials available it is almost impossible to select a material for a specific task unless otherwise its properties are known.
- There are several criteria on which the final decision is based on.
- There are less chances of material possessing optimal or idle combination of properties.
- A need to trade off between number of factors!

Why Do We Need to Study Properties of Materials?

- First, the in-service conditions must be characterized.
- The classic example involves strength and ductility:
  - Normally material possessing strength have limited ductility. In such cases a reasonable comprise between two or more properties are important.
- A second selection consideration is any deterioration of material properties that may occur during service operation.
- Finally, probably the overriding consideration is economics.

Factors Affecting Selection of Materials

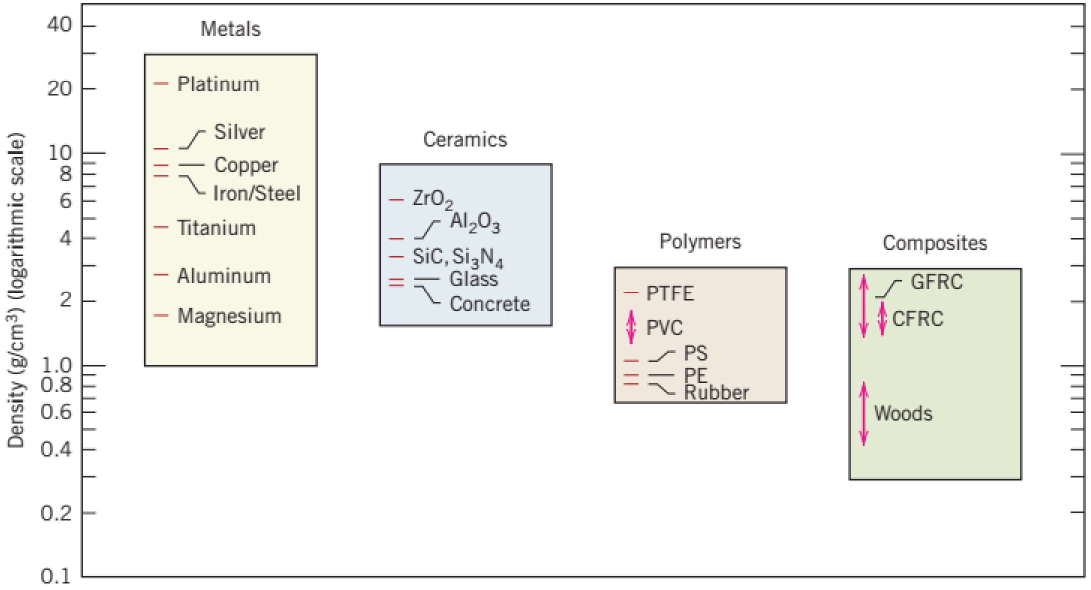
(i) *Manufacturing processes*	*(ii)* *Functional requirements*	*(iii)* *Cost considerations*	*(iv)* *Operating parameters*
• Plasticity	• Strength	• Raw material	• Pressure
• Malleability	• Hardness	• Processing	• Temperature
• Ductility	• Rigidity	• Storage	• Flow
• Machinability	• Toughness	• Manpower	• Type of material
• Casting properties	• Thermal conductivity	• Special treatment	• Corrosion requirements
• Weldability	• Fatigue	• Inspection	• Environment
• Heat	• Electrical treatment	• Packaging properties	• Protection from fire
• Tooling	• Creep	• Inventory	• Weathering
• Surface finish	• Aesthetic look	• Taxes and custom duty	• Biological effects

Classification of Materials

- Three basic groups of solid engineering materials based on atomic bonds and structures:
  1) **Metals**
  2) **Ceramics**
  3) **Polymers**
- Classification can also be done based on either properties (mechanical, electrical, optical), areas of applications (structures, machines, devices). Further we can subdivide these groups. According to the present engineering needs:
  1) **Composites**
  2) **Semiconductors**
  3) **Biomatrials**

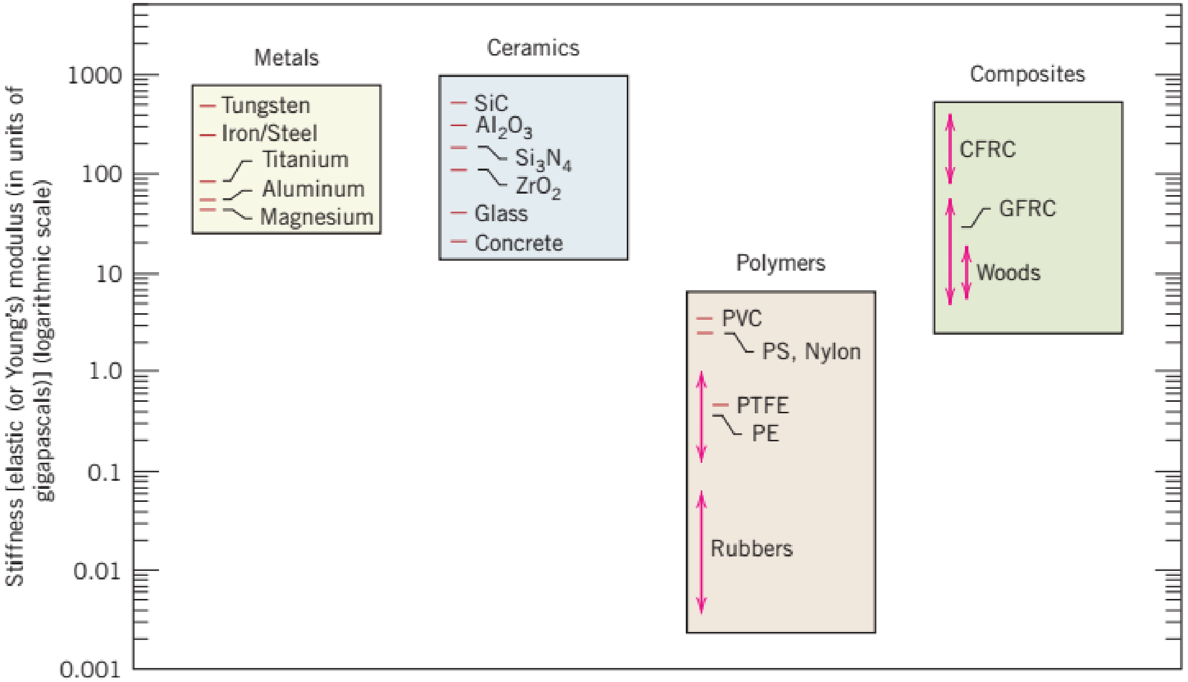
Metals

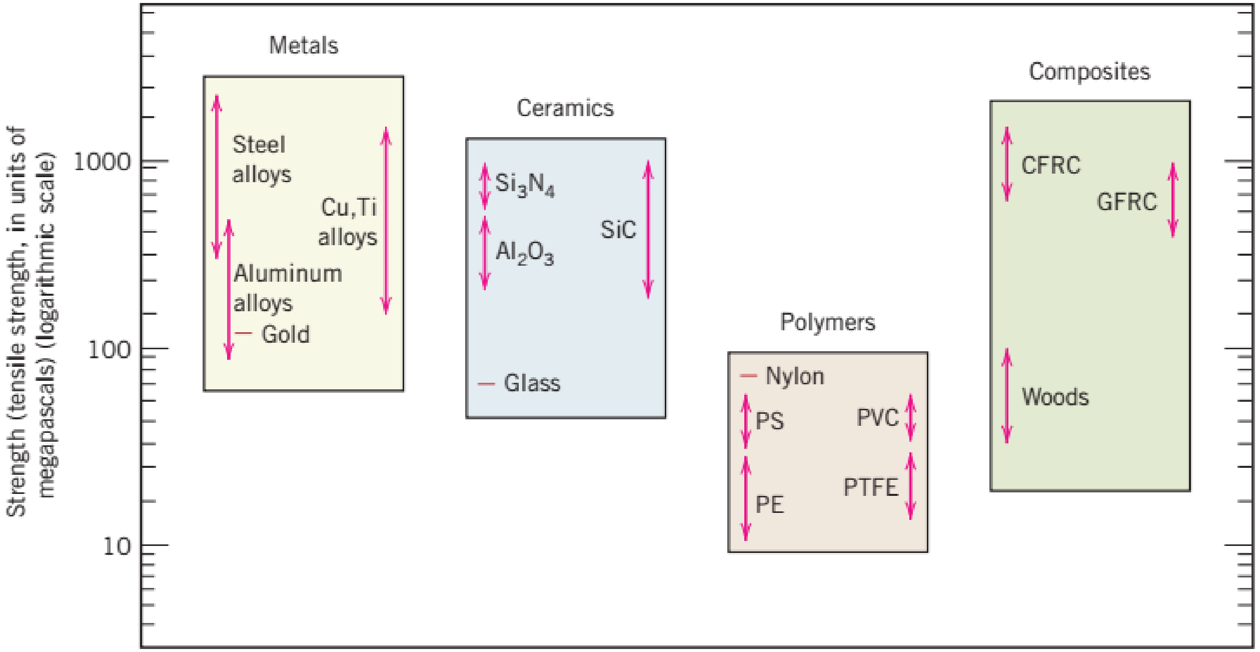
- Metals are composed of one or more metallic elements (e.g., iron, aluminum, copper, titanium, gold, nickel), and often also nonmetallic elements (e.g., carbon, nitrogen, oxygen) in relatively small amounts.
- Atoms in metals and their alloys are arranged in a very orderly manner and are relatively dense in comparison to the ceramics and polymers.



Metals

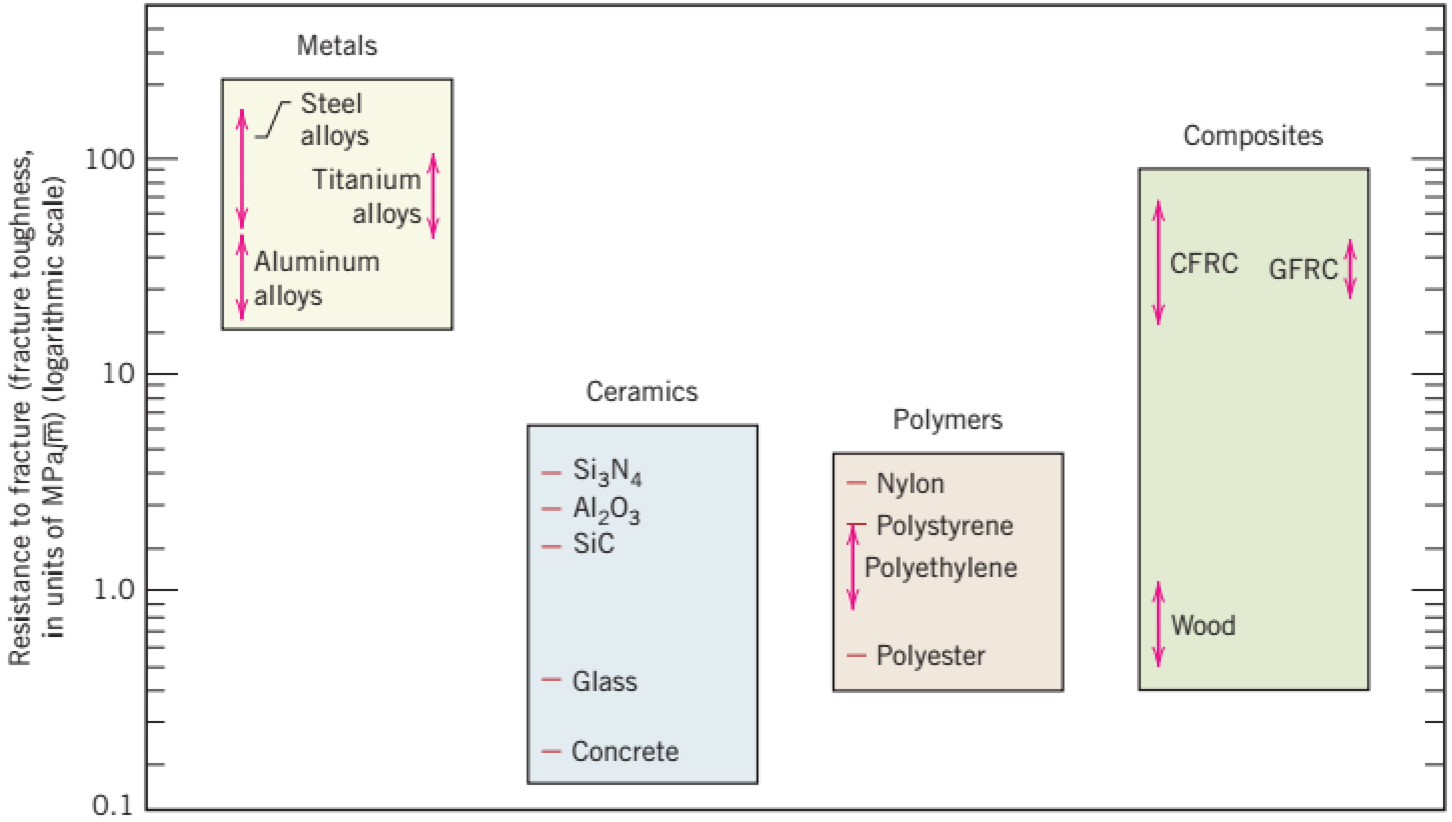
- With regard to mechanical characteristics, these materials are relatively stiff and strong, yet are ductile (i.e., capable of large amounts of deformation without fracture).





Metals

- These materials are resistant to fracture, which accounts for their widespread use in structural applications.



Metals

- Metals are element substances which readily give up electrons to form metallic bonds and conduct electricity.
- **Some of the important basic properties of metals are:**

(a) Metals are usually good electrical and thermal conductors

(b) At ordinary temperature metals are usually solid

(c) To some extent metals are malleable and ductile

(d) The freshly cut surfaces of metals are lustrous

(e) When struck metal produce typical sound

(f) Most of the metals form alloys

Ceramics

- Ceramics are compounds between metallic and nonmetallic elements; they are most frequently oxides, nitrides, and carbides.
- The wide range of materials that falls within this classification includes ceramics that are composed of clay minerals, cement, and glass.
- With regard to mechanical behavior, ceramic materials are relatively stiff and strong—stiffnesses and strengths are comparable to those of metals.
- In addition, they are typically very hard.
- Historically, ceramics have exhibited extreme brittleness (lack of ductility) and are highly susceptible to fracture.

Ceramics

- However, newer ceramics are being engineered to have improved resistance to fracture; these materials are used for cookware, cutlery, and even automobile engine parts.
- These materials are typically insulative to the passage of electricity and heat, and are more resistant to high temperatures and harsh environments than metals and polymers.

Polymers

- Polymers include the familiar plastic and rubber materials.
- Many of them are organic compounds that are chemically based on carbon, hydrogen, and other nonmetallic elements (i.e., O, N, and Si).
- Furthermore, they have very large molecular structures, often chainlike in nature, that often have a backbone of carbon atoms.
- Some common and familiar polymers are PTFE (Polytetrafluoroethylene), polyethylene (PE), nylon, poly(vinyl chloride) (PVC), polycarbonate (PC), and silicone rubber etc.

Polymers

- These materials typically have low densities, whereas their mechanical characteristics are generally dissimilar to those of the metallic and ceramic materials—they are not as stiff or strong as other materials
- Many of the polymers are extremely ductile and pliable (i.e., plastic), which means they are easily formed into complex shapes.
- They are relatively inert chemically and unreactive in a large number of environments.
- They have low electrical conductivities and are nonmagnetic.
- One major drawback to the polymers is their tendency to soften and/or decompose at modest temperatures, which, in some instances, limits their use.

Composites

- Consist more than one kind of material; tailor made to benefit from combination of best characteristics of each constituent.
- Available over a very wide range: natural (*wood*) to synthetic (*fiberglass*).
- Many are composed of two phases; one is matrix – which is continuous and surrounds the other, dispersed phase.
- Classified into many groups: (1) Depending on orientation of phases; such as particle reinforced, fiber reinforced, etc. (2) Depending on matrix; metal matrix, polymer matrix, ceramic matrix.

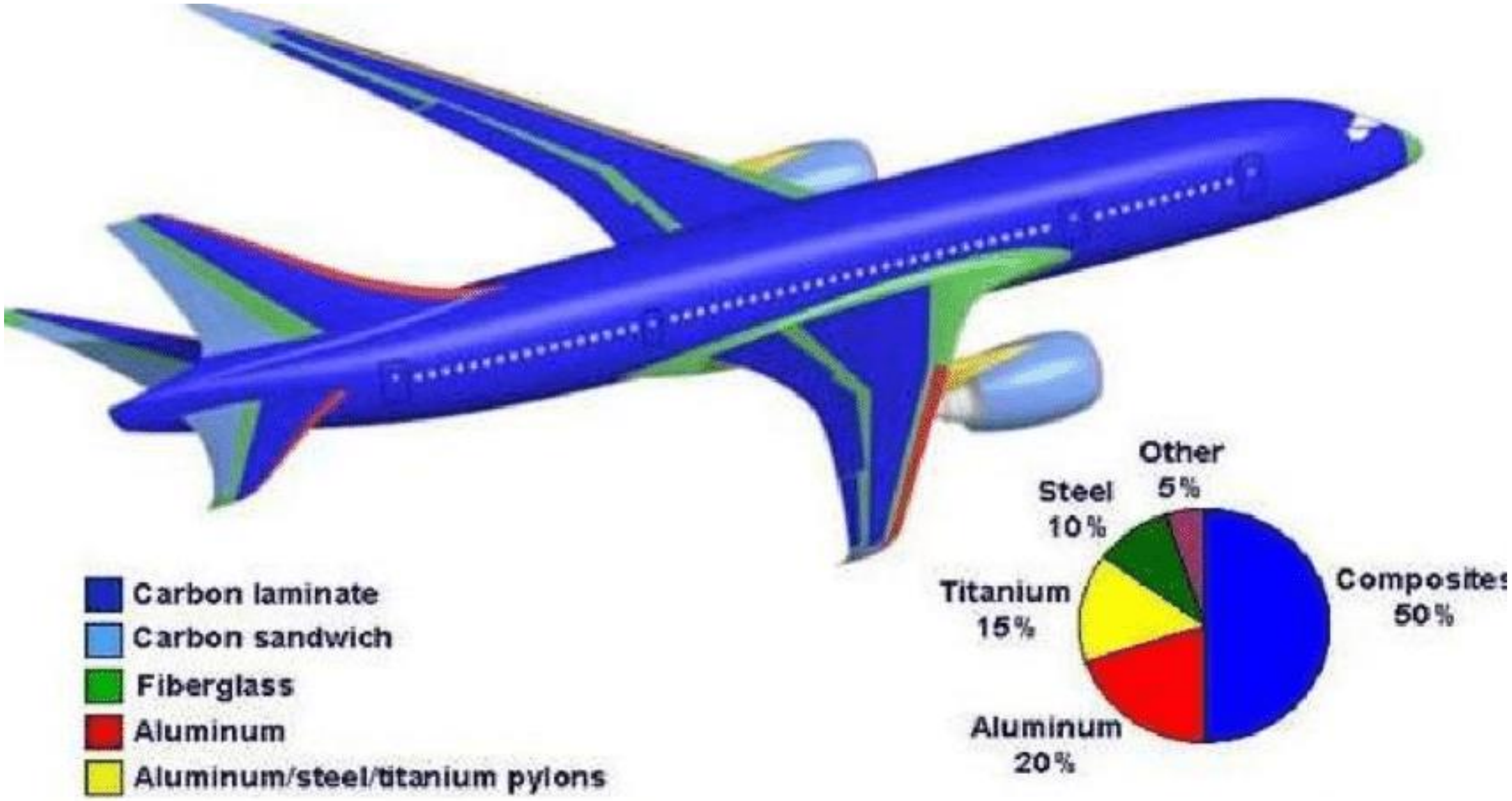
fiberglass surfboards

- For example: Cement concrete, Fiberglass, special purpose refractory, bricks, plywood, etc.

Composites

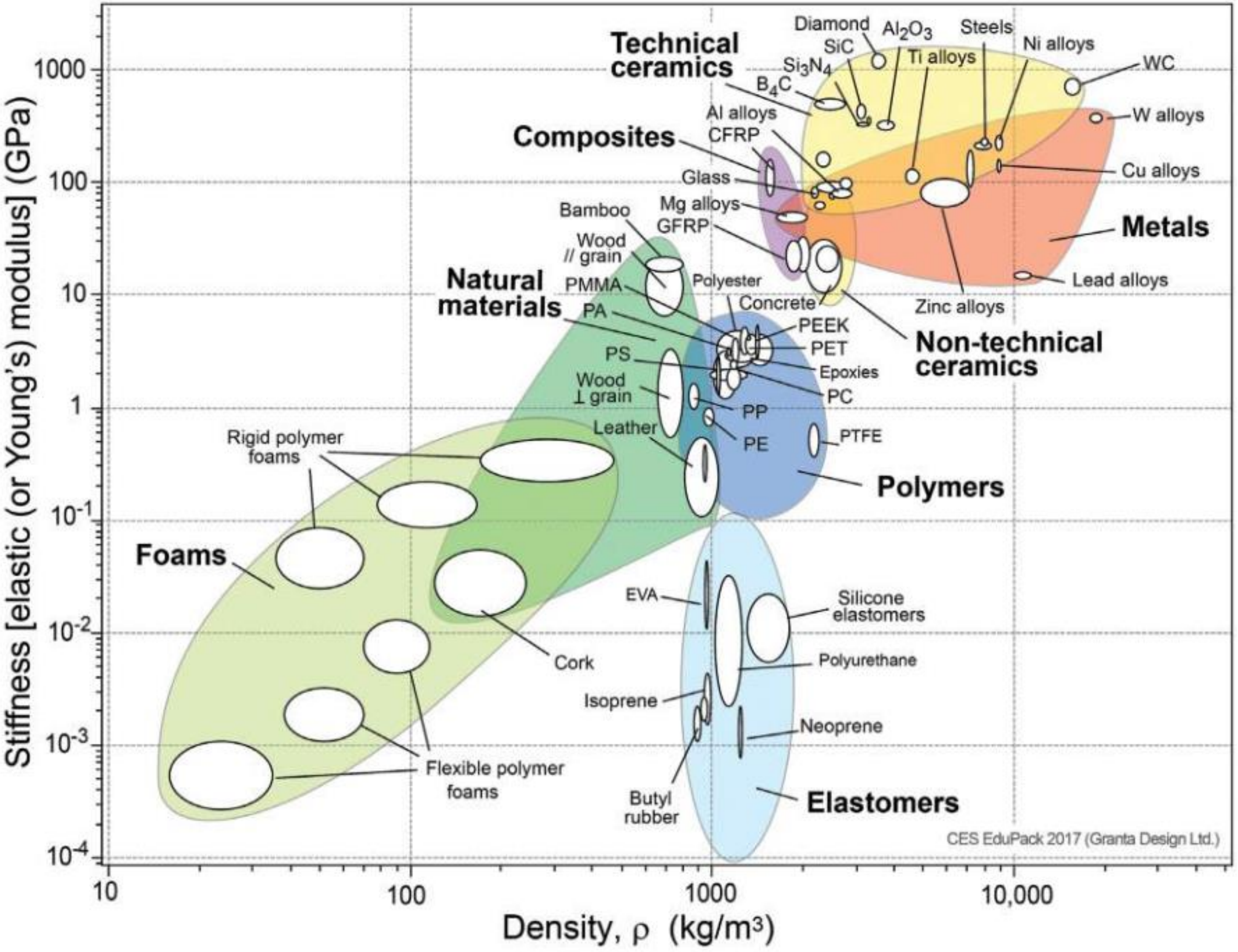
- Another technologically important material is the carbon fiber–reinforced polymer (CFRP) composite—carbon fibers that are embedded within a polymer.
- These materials are stiffer and stronger than glass fiber–reinforced materials but more expensive.
- CFRP composites are used in some aircraft and aerospace applications, as well as in high-tech sporting equipment (e.g., bicycles, golf clubs, tennis rackets, skis/ snowboards) and recently in automobile bumpers.
- The new Boeing 787 fuselage is primarily made from such CFRP composites.

Composites



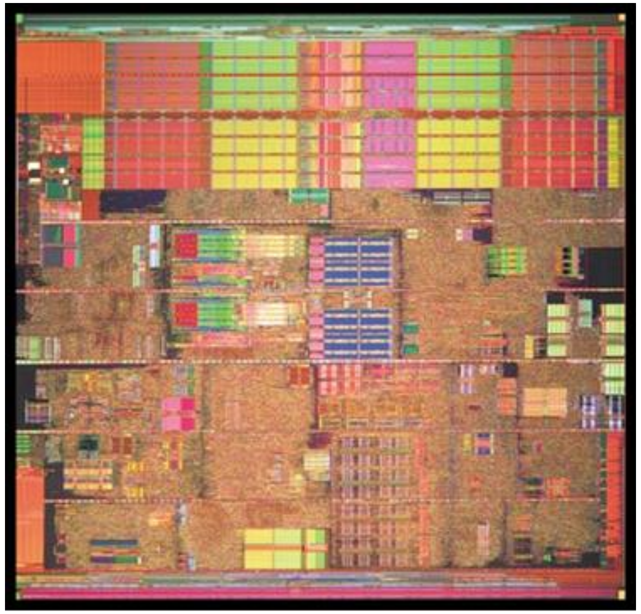
Carbon laminate
Carbon sandwich
Fiberglass
Aluminum
Aluminum/steel/titanium pylons
Other
5%
Steel
10%
Titanium
15%
Composites
50%
Aluminum
20%

A Common Diagram



Semiconductors

- Semiconductors have electrical properties that are intermediate between electrical conductors and electrical insulators.
- The electrical characteristics are extremely sensitive to the presence of minute amounts of foreign atoms.
- Found many applications in electronic devices over decades through integrated circuits.
- It can be said that semiconductors revolutionized the electronic industry for the last few decades.



Intel Pentium 4

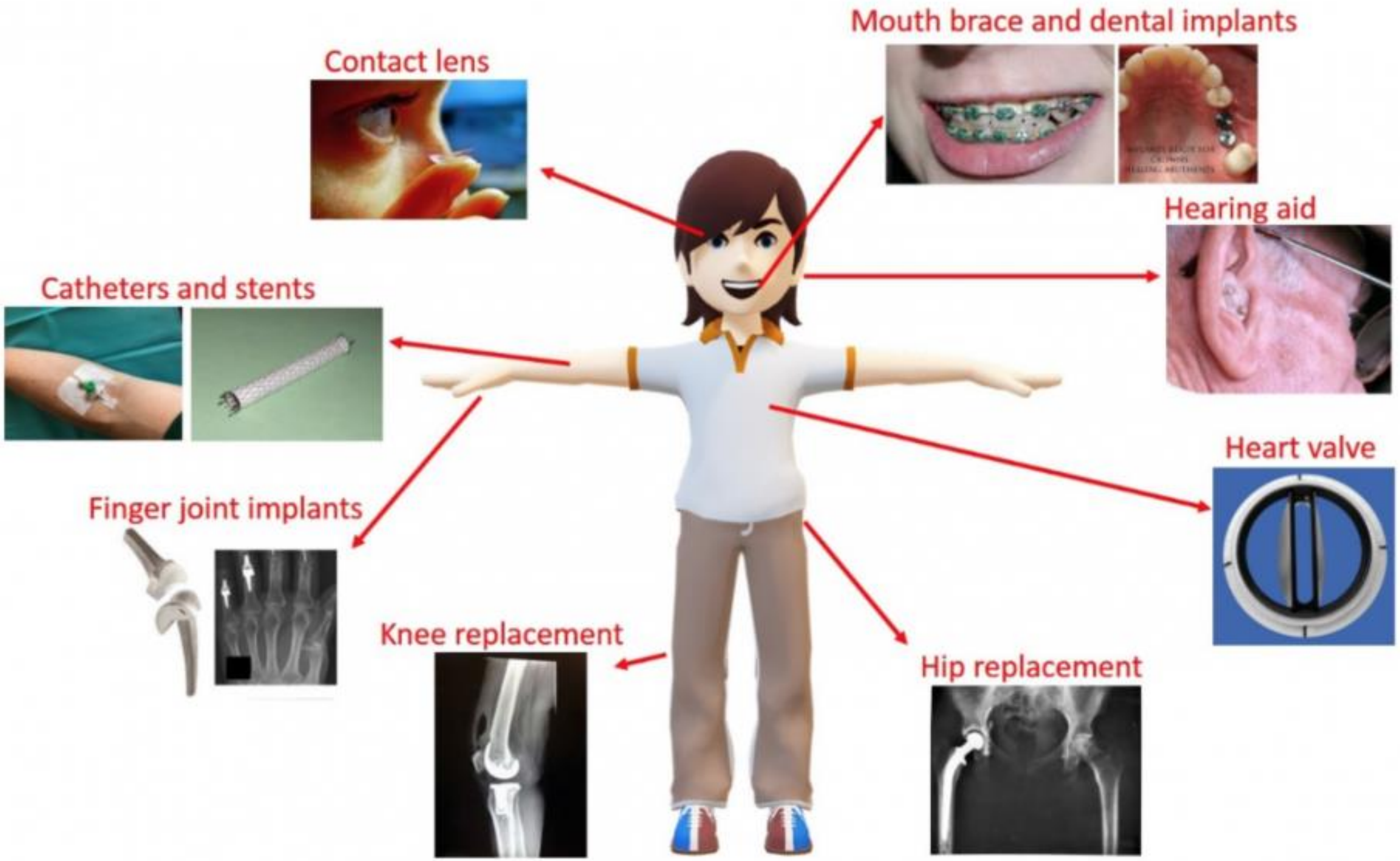
Biomaterials

- These are used for the replacement of damaged or diseased body parts.
- **Primary requirements: must be biocompatible with body tissues, must not produce toxic substances.**
- Important materials factors: ability to support the forces, low friction and wear, density, reproducibility and cost.

- All the previous materials can be used as biomaterials depending on the application.
- A classic example: hip joint.

hip replacement

Biomaterials



Smart Materials

- Smart (or intelligent) materials are a group of new and state-of-the-art materials now being developed that will have a significant influence on many of our technologies.
- The adjective *smart* implies that these materials are able to sense changes in their environment and then respond to these changes in predetermined manners—traits that are also found in living organisms. In addition, this smart concept is being extended to rather sophisticated systems that consist of both smart and traditional materials.

Smart Materials

- These are either traditional materials with enhanced properties or newly developed materials with high performance capabilities. Thus, these are relatively expensive.
- Components of a smart material (or system) include some type of sensor (which detects an input signal) and an actuator (which performs a responsive and adaptive function).
- Actuators may be called upon to change shape, position, natural frequency, or mechanical characteristics in response to changes in temperature, electric fields, and/or magnetic fields.

Smart Materials

- **Four types of materials used as actuators:**

a) **Shape memory alloys:** The two most prevalent shape-memory alloys are copper-aluminium-nickel and nickel-titanium (NiTi)

b) **Piezoelectric ceramics:** Barium Titanate, Potassium Niobate, Sodium Tungstate.

c) **Magnetostrictive materials:** Fe-Ni (Permalloy), Co-Ni, Fe-Co, and Co-Fe-V (Permendur); several ferrites ($CoFe_2O_4$ and $NiFe_2O_4$).

d) **Electro-/Magneto-rheological fluids:** Oleic acid, tetramethylammonium hydroxide, citric acid.

Smart Materials

- **Materials/Devices used as sensors:**

  - Optical fibers

  - Piezoelectric materials

  - Micro-electro-mechanical systems (MEMS)

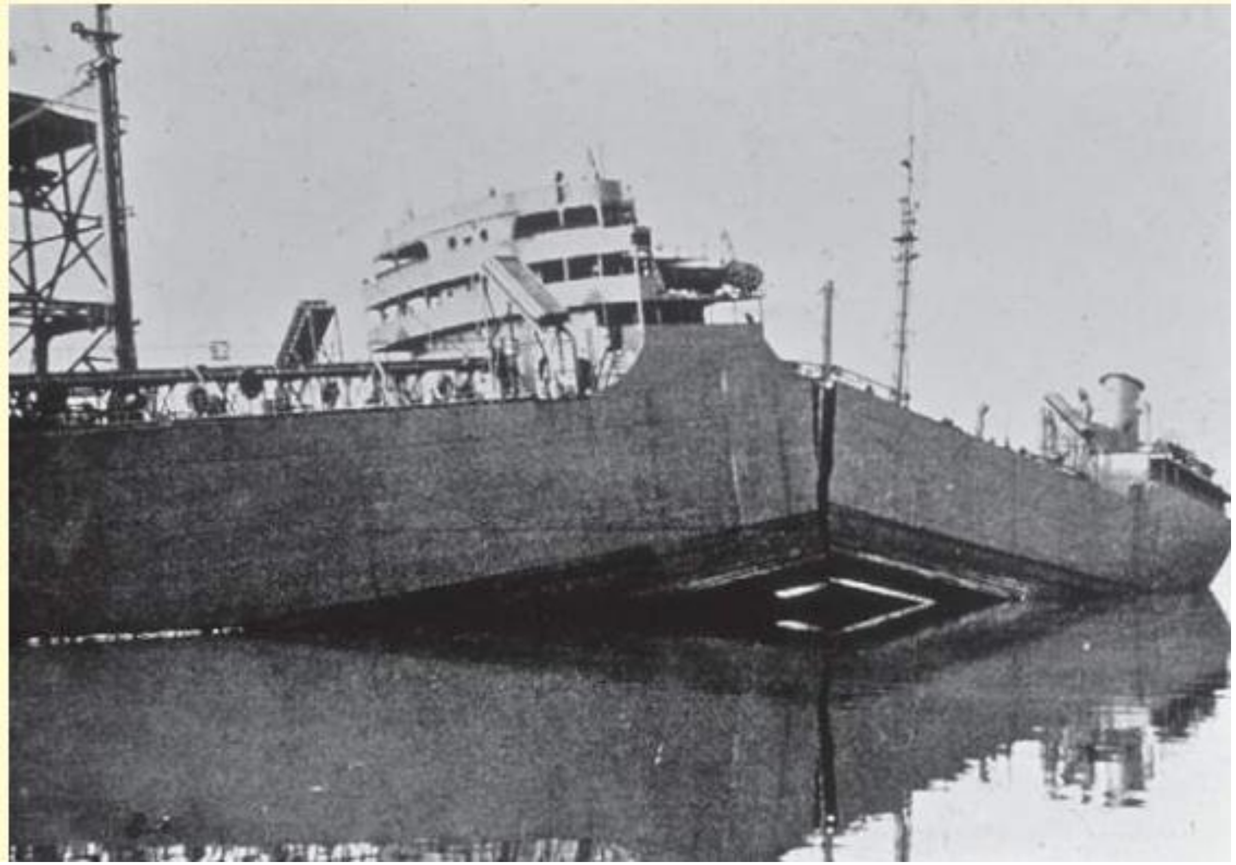
- One type of smart system is used in helicopters to reduce aerodynamic cockpit noise created by the rotating rotor blades. Piezoelectric sensors inserted into the blades monitor blade stresses and deformations; feedback signals from these sensors are fed into a computer-controlled adaptive device that generates noise-canceling antinoise.

Modern Materials' Needs

- Engine efficiency increases at high temperatures; requires high temperature structural materials.
- Use of nuclear energy requires solving problems with residue, or advance in nuclear waste processing.
- Hypersonic flight requires materials that are light, strong and resist high temperatures.
- Optical communications require optical fibers that absorb light negligibly.
- Structures: materials that are strong like metals and resist corrosion like plastics. Materials for Civil construction – materials for unbreakable windows.

Case Studies

Liberty Ship Failures



- When some normally ductile metal alloys are cooled to relatively low temperatures, they become susceptible to brittle fracture—that is, they experience a ductile-to-brittle transition upon cooling through a critical range of temperatures.

- The corner of each hatch (i.e., door) was square; these corners acted as points of stress concentration where cracks can form.

Carbonated Beverage Containers

- The material used for this application must satisfy the following constraints: (1) provide a barrier to the passage of carbon dioxide, which is under pressure in the container; (2) be nontoxic, unreactive with the beverage, and, preferably, recyclable; (3) be relatively strong and capable of surviving a drop from a height of several feet when containing the beverage; (4) be inexpensive, including the cost to fabricate the final shape; (5) if optically transparent, retain its optical clarity; and (6) be capable of being produced in different colors and/or adorned with decorative labels.