Materials Science

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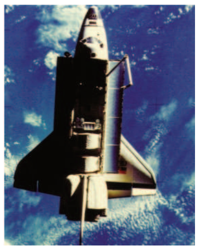
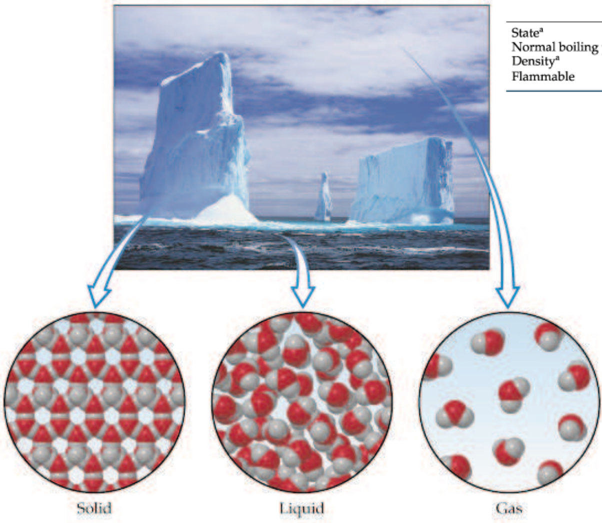
Materials Science

- Materials make modern life possible - from the polymers in the chair you're sitting on, the metal ball-point pen you're using, and the concrete that made the building you live or work in to the materials that make up streets and highways and the car you drive.
- Briefly defined, Materials Science is the study of "stuff". Materials Science is the study of solid matter, inorganic and organic.

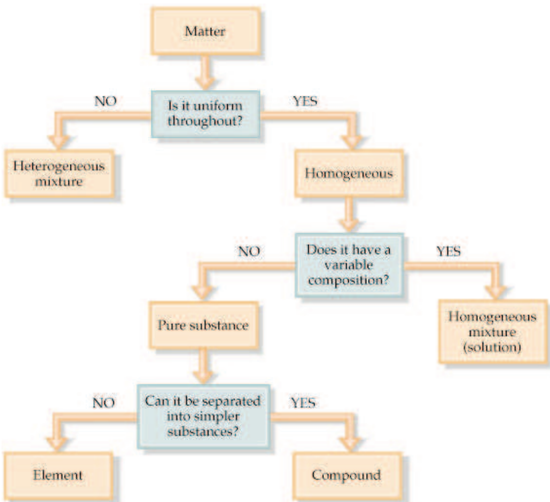


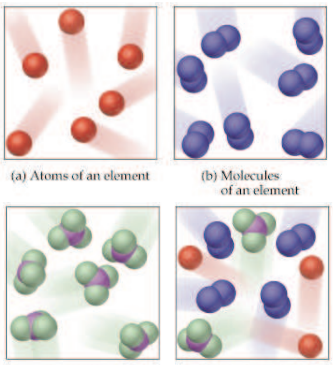
Physical Classification (State)



	Water	Hydrogen	Oxygen
State[a]	Liquid	Gas	Gas
Normal boiling point	100°C	−253°C	−183°C
Density[a]	1.00 g/mL	0.084 g/L	1.33 g/L
Flammable	No	Yes	No

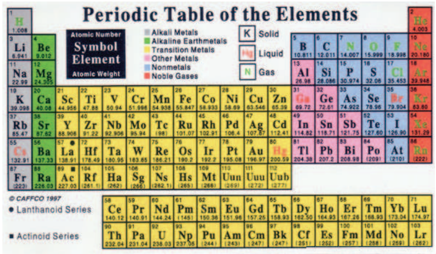
Chemical Classification (Composition)

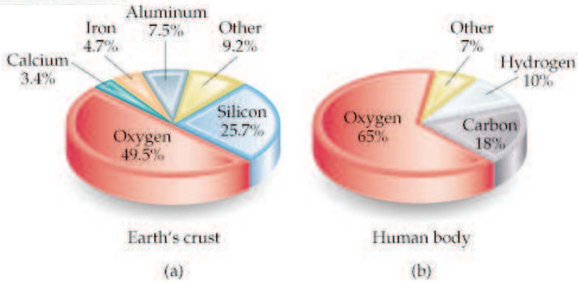




(a) Atoms of an element
(b) Molecules of an element
(c) Molecules of a compound
(d) Mixture of elements and a compound

Elements





Earth's crust (a)

Human body (b)

Types of Materials

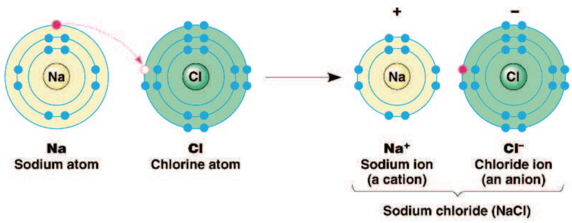
- Classification of materials: based on Nature and Applications.

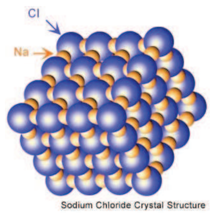
Table 1.1. Classification of materials based on nature and applications (Bever (1986)).

Nature	Applications
Ceramics	Industrial materials
Glasses	Electrical materials
Metals and alloys	Electronic materials
Other inorganic materials (including semiconductors)	Superconducting materials
Polymers	Magnetic materials
Elastomers	Nuclear materials
Fibres	Materials for other energy applications
Composite materials	Optical materials
Wood	Biomedical materials
Paper and paperboard	Dental materials
Other biological materials	Building materials

Bonding in Materials

- Ionic Bonding:
  - Between highly electropositive and electronegative elements.
  - Sodium (Na) atom radius = 0.192 nm; Chlorine (Cl) atom radius = 0.099 nm
  - Sodium ion (Na^+) ionic radius = 0.095 nm; Chloride ion (Cl^-) ionic radius = 0.181 nm.
  - The ions in an ionic solid must be arranged in a structure so that local charge neutrality is maintained.



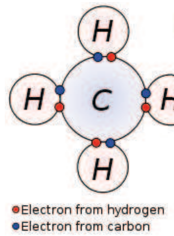


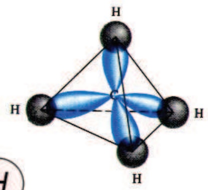
Bonding in Materials (Ionic Bonding)

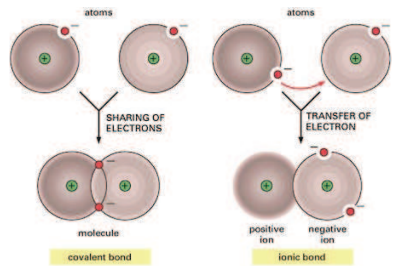
Property	Ionic Material Characteristics	Explanation
Melting Point	High letting points	Many strong electrostatic attractions to be broken
Conductivity	Conductors only when molten or in solution	The ions can carry the electric charge when they are free to move
Hardness	Hard but brittle	Ions are held rigidly in position in the lattice. Stress brings ions of the same charge in close proximity and the structure breaks along cleavage planes
Solubility	Mostly soluble	The charged ions can be carried off by the polar water molecules unless the electrostatic attractions within the lattice are too large
Structure	Giant lattice of repeating ions in three dimensions	Electrostatic attraction between oppositely charged ions causes the negative ions to surround the positive ions and vice versa.

Bonding in Materials

- Covalent Bonding:
  - Between atoms with small differences in electronegativity, and which are close to each other in the periodic table.
  - Atoms most commonly share their outer *s* and *p* electrons with other atoms so that each atom attains the noble-gas electron configuration.

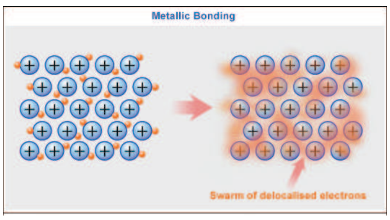


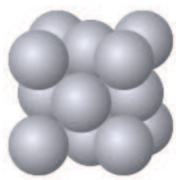


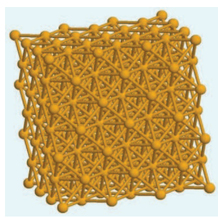


Bonding in Materials

- Metallic Bonding:
  - In the solid state, atoms are packed relatively close together in a systematic pattern or crystal structure.
  - In this structure the atoms are so close together that their outer valence electrons are attracted to the nuclei of their numerous neighbors.
  - The valence electrons are not associated with any particular nucleus, and are thus spread out among the atoms in the form of a low-density electron charge cloud, or "electron gas".

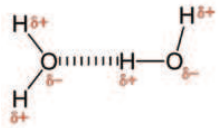






Bonding in Materials

- Intermolecular forces:
  - Hydrogen bonding.
  - Dipole-dipole interactions.
  - Van der Waals forces: A weak attractive force between atoms or nonpolar molecules caused by a temporary change in dipole moment arising from a brief shift of orbital electrons to one side of one atom or molecule, creating a similar shift in adjacent atoms or molecules



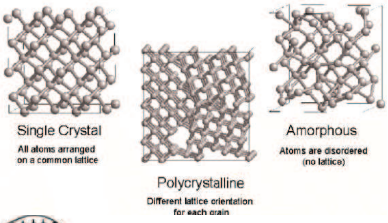
Bonding in Materials

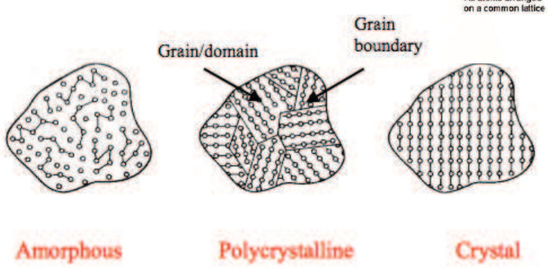
- A summary of physical properties associated with interatomic bonds:

Property	Ionic	Covalent	Metallic	Van der Waals
	Nondirectional; Structures of high coordination	Directional; structures of low coordination and low density	Nondirectional structures of high coordination and high density	Analogous to metallic bond
Mechanical	Strong, hard crystals	Strong, hard crystals	Variable crystals	Weak, soft crystals
Thermal	High melting point, low expansion coefficient	High melting point, low expansion coefficient	Range of melting points, extended liquidus range	Low melting point, large expansion coefficient
Electrical	Weak insulator, conduction by ion transport when liquid	Insulator in solid and liquid state	Conduction by electron transport	Insulator
Optical	Absorption and other properties mainly of the individual ions	High refractive index, absorption different in solid or gas	Opaque, with similar properties in liquid state	Properties of individual molecules

Structure of Solids

- Structure of Solids (2D and 3D Views)





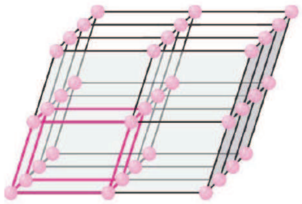
No recognizable long-range order

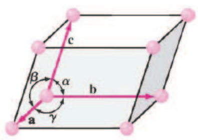
Completely ordered In segments

Entire solid is made up of atoms in an orderly array

Crystal (Space Lattice)

- Atomic arrangements in crystalline solids can be described with respect to a network of lines in three dimensions.
- The intersections of the lines are called "lattice sites" (or lattice points). Each lattice site has the same environment in the same direction.
- A particular arrangement of atoms in a crystal structure can be described by specifying the atom positions in a repeating "unit cell".

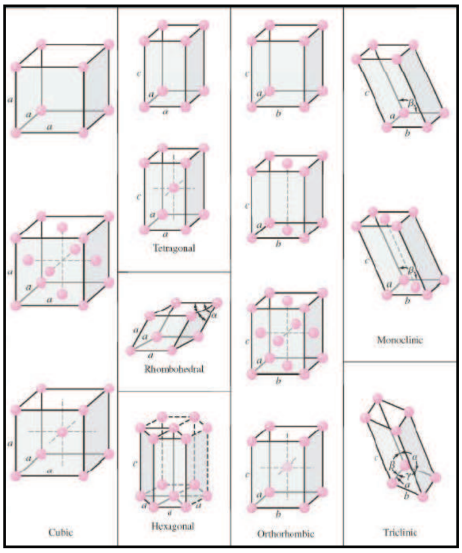




Crystal (Regular Pattern)

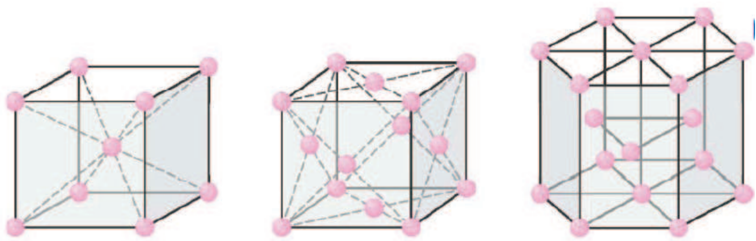
- 14 Bravis Lattices.
- Auguste Bravis (1811-1863).

Crystal System	Possible Variations	Axial Distances (edge lengths)	Axial Angles	Examples
Cubic	Primitive, Body centred, Face centred	a = b = c	α = β = γ = 90°	NaCl, Zinc Blende, Cu
Tetragonal	Primitive, Body centred	a = b ≠ c	α = β = γ = 90°	White tin, SnO_2, TiO_2, $CaSO_4$
Orthorhombic	Primitive, Body centred, Face centred, End centred	a ≠ b ≠ c	α = β = γ = 90°	Rhombic Sulphur, KNO_3, $BaSO_4$
Hexagonal	Primitive	a = b ≠ c	α = β = 90°, γ = 120°	Graphite, ZnO, CdS
Rhombohedral (tetragonal)	Primitive	a = b = c	α = β = γ ≠ 90°	Calcite ($CaCO_3$, Cinnabar (HgS)
Monoclinic	Primitive, End centred	a ≠ b ≠ c	α = γ = 90°, β ≠ 120°	Monoclinic Sulphur, $Na_2SO_4.10H_2O$
Triclinic	Primitive	a ≠ b ≠ c	α ≠ β ≠ γ ≠ 90°	$K_2Cr_2O_7$, $CuSO_4.5H_2O$, H_3BO_3



Principle Metal Crystal Structures

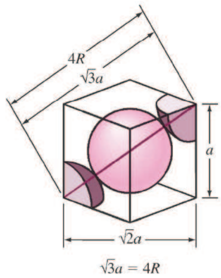
- There are three principle crystal structures for metals:
  - Body-Centered Cubic (BCC)
  - Face-Centered Cubic (FCC)
  - Hexagonal Close-Packed (HCP)

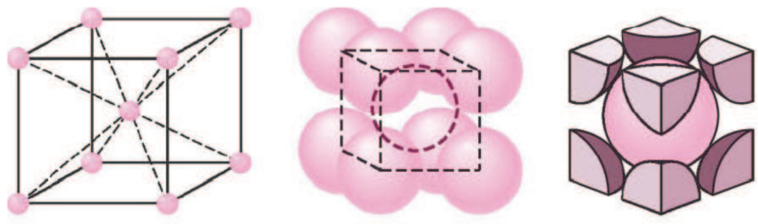


(a) (b) (c)

Body-Centered Cubic (BCC)

- Elements with BCC: Cr, Fe, K, Li, Mo, Na, Ta, and W.
- Atoms per cell:
- No. of nearest neighbors:
- Nearest neighbor distance:

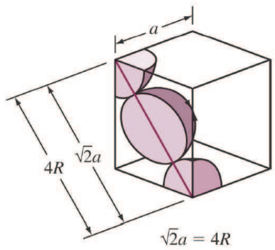


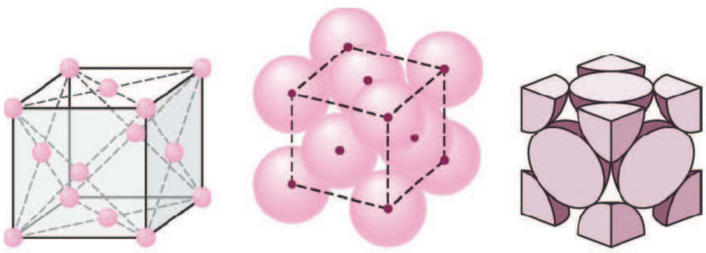


(a) (b) (c)

Face-Centered Cubic (FCC)

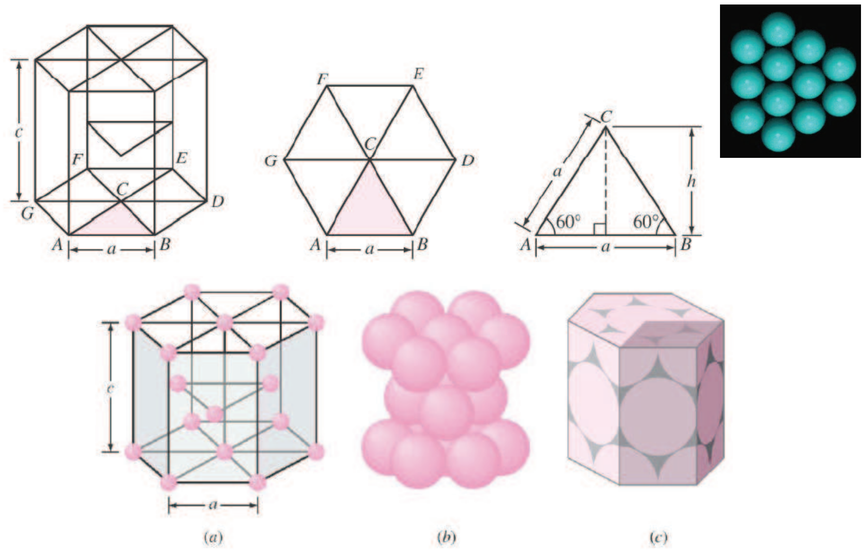
- Elements with FCC: Al, Ag, Ca, Cu, Ni, Pb, and Pt.
- Atoms per cell:
- No. of nearest neighbors:
- Nearest neighbor distance:





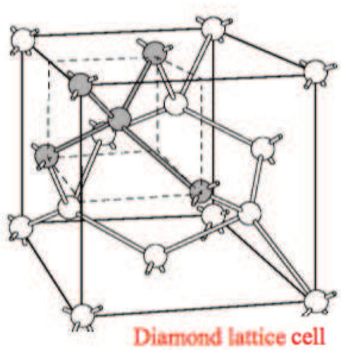
(a) (b) (c)

Hexagonal Close-Packed (HCP)

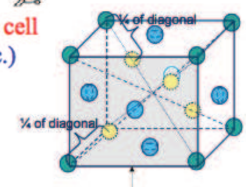


Diamond Lattice

- Two interleaving FCC cells offset by 1/4 of the cube diagonal form the lattice.
- Atoms in diamond lattice have four nearest neighbors (covalent bonds).



Diamond lattice cell
(C, Si, Ge, etc.)



(100) Plane

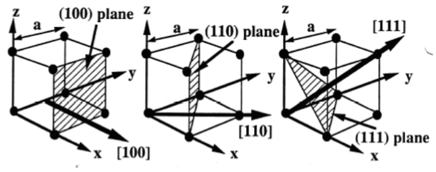
- Atoms per cell: 8
- No. of nearest neighbors: ?
- Nearest neighbor distance: ?

Miller Indices

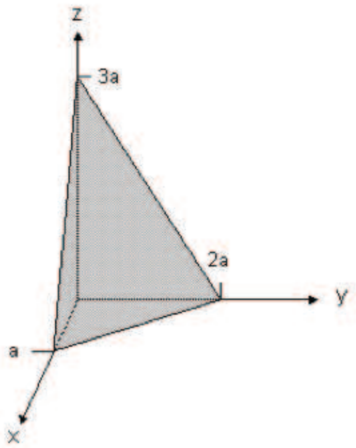
- Crystal orientation is important in micro/nano fabrication processing.
- Certain material properties can depend on the orientation of the crystal lattice.
- Certain processing techniques must consider the orientation of the crystal lattice.
- Miller indices provide a conventional method to specify planes and directions in a crystal.

Miller Indices of a Plane

- Establish the coordinate axes along the edges of the unit cell.
- Note where the plane intercepts the axes.
- Divide each intercept by the unit cell length along the respective coordinate axis.
- Record the normalized intercepts in x, y, z order.
- Compute the reciprocal of each intercept.
- Multiply the intercepts by the smallest overall constant that yields whole numbers.

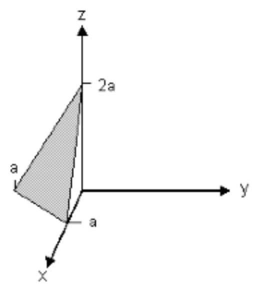


Miller Indices of a Plane



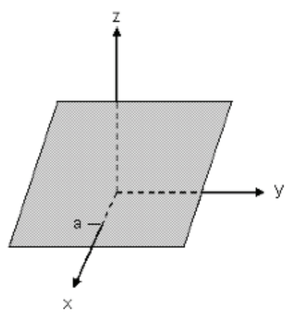
- Normalized intercepts:
  - 1,2,3
- Reciprocals:
  - 1, 1/2, 1/3
- Multiplier is 6
- Miller indices for this plane:
  - (6,3,2)

Miller Indices of a Plane



Place a bar over negative intercept.

Miller indices: $(2,\bar{2},1)$



When a plane does not intersect an axis the intercept is infinity and the miller index is zero.
Miller indices: (1,0,1)

Miller Indices of a Vector

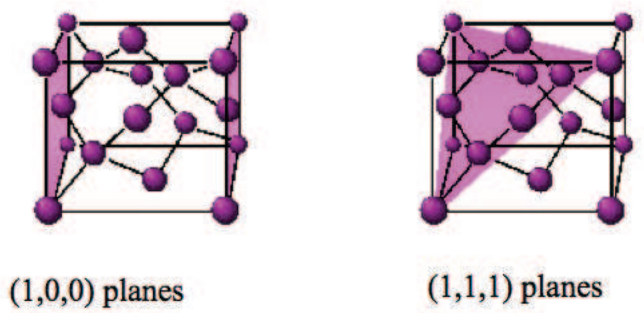
- Establish the coordinate axes along the edges of the unit cell.
- Draw a vector in the direction of interest.
- Decompose the vector into components by projecting it onto the coordinate axes.
- Record the components in x, y, z order.
- Multiply the components by the smallest overall constant that yields whole numbers.
- Miller indices of a vector are enclosed in brackets.
- A plane has the same Miller indices as its normal vector.

Miller Indices

- (100) for planes.
- {100} for all equivalent planes, where in diamond lattice the following six planes are equivalent owing to lattice symmetry: (100), (010), (001), and negative ones.
- [100] for vectors.
- <100> for equivalent vectors.
- In cubic materials, (hkl) and [hkl] are perpendicular.

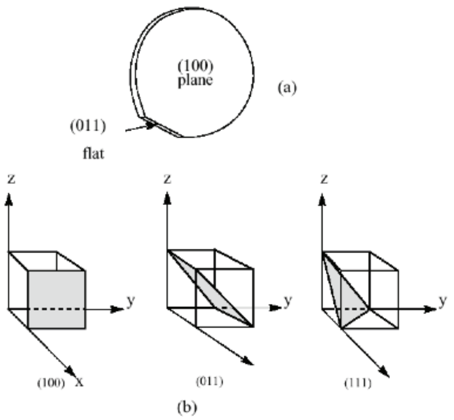
Crystal Planes

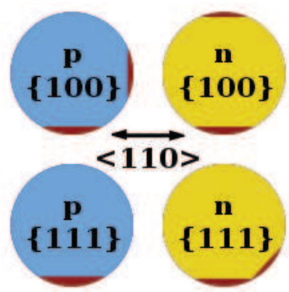
- Different chemical and electrical properties.
- For example: oxidation rate, interface density, capacitances, and currents.



Silicon Wafer and Crystal Planes

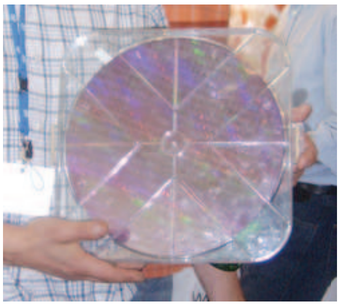
- Silicon wafer cut at the (100) plane with a (011) flat to help orient the wafer during microfabrication.

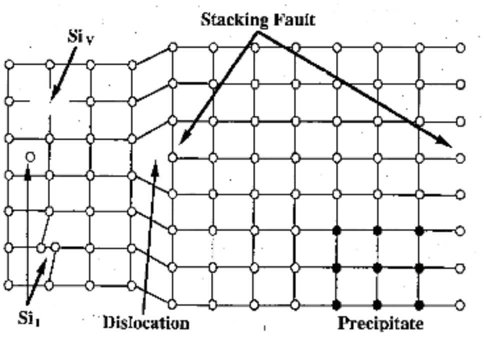




Ultra-Pure Silicon Wafer

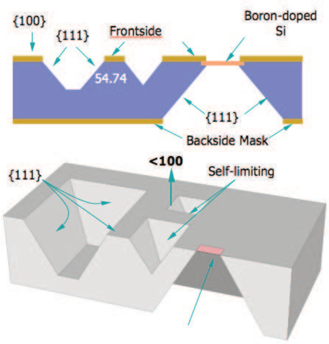
- Si or GaAs crystals must be ultrapure in order to yield desirable material properties.
  - Parts per Billion (PPB) unwanted impurities.
  - No Crystal defects.

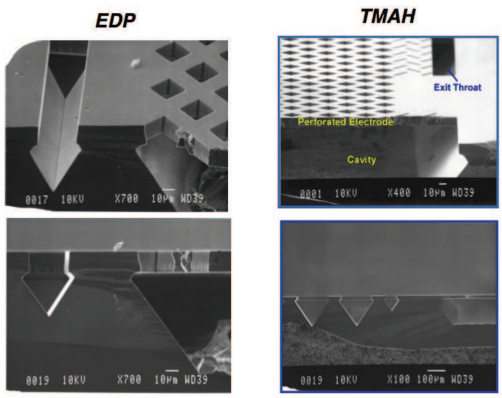




Anisotropic Silicon Etching

- Different atomic surface density (cm^{-2}) on (100), (110), and (111) planes.
- Etching is a process that removes atoms from a material surface.





Metals

- The wide use of metal in the creation of structures, machines and tools is also closely correlated with the industrial revolution of the 18th and 19th centuries and could be seen as the foundation of our modern society. As an overview, metals often exhibit the following general properties:
  - Metals are **dense, strong, hard, ductile, shiny,** and **lustrous**
  - Metals are **good conductors** of electricity, heat, and sound

Plastics

Plastics can be further classified as;
•Thermoplastic
•Thermoset
•Elastomers

Thermoplastics	Thermosets	Elastomers
Acrylics	Epoxy resins	Rubbers
Nylons	Phenolic	Silicones
PVC	Polyesters	Polyurethanes
Polyethylene		

Ceramics

- A **ceramic** is an inorganic, nonmetallic solid prepared by the action of heat and subsequent cooling. Ceramic materials may have a crystalline or partly crystalline structure, or may be amorphous (e.g., a glass). Because most common ceramics are crystalline, the definition of ceramic is often restricted to inorganic crystalline materials, as opposed to the noncrystalline glasses.
  - Oxides (alumina – insulation and abrasives, zirconia – dies for metal extrusion and abrasives)
  - Carbides (tungsten-carbide tools)
  - Nitrides (cubic boron nitride, 2nd in hardness to diamond)

Composites

- A composite is a combination of two or more chemically distinct materials whose physical characteristics are superior to its constituents acting independently.
- Because of their high strength/stiffness to weight ratio they are widely used in the;
  - Aerospace industry
  - Offshore structures
  - Boats
  - Sporting goods

Nanomaterials