

# NATURE OF METALS AND ALLOYS

## Chapter 3

# NATURE OF METALS AND ALLOYS

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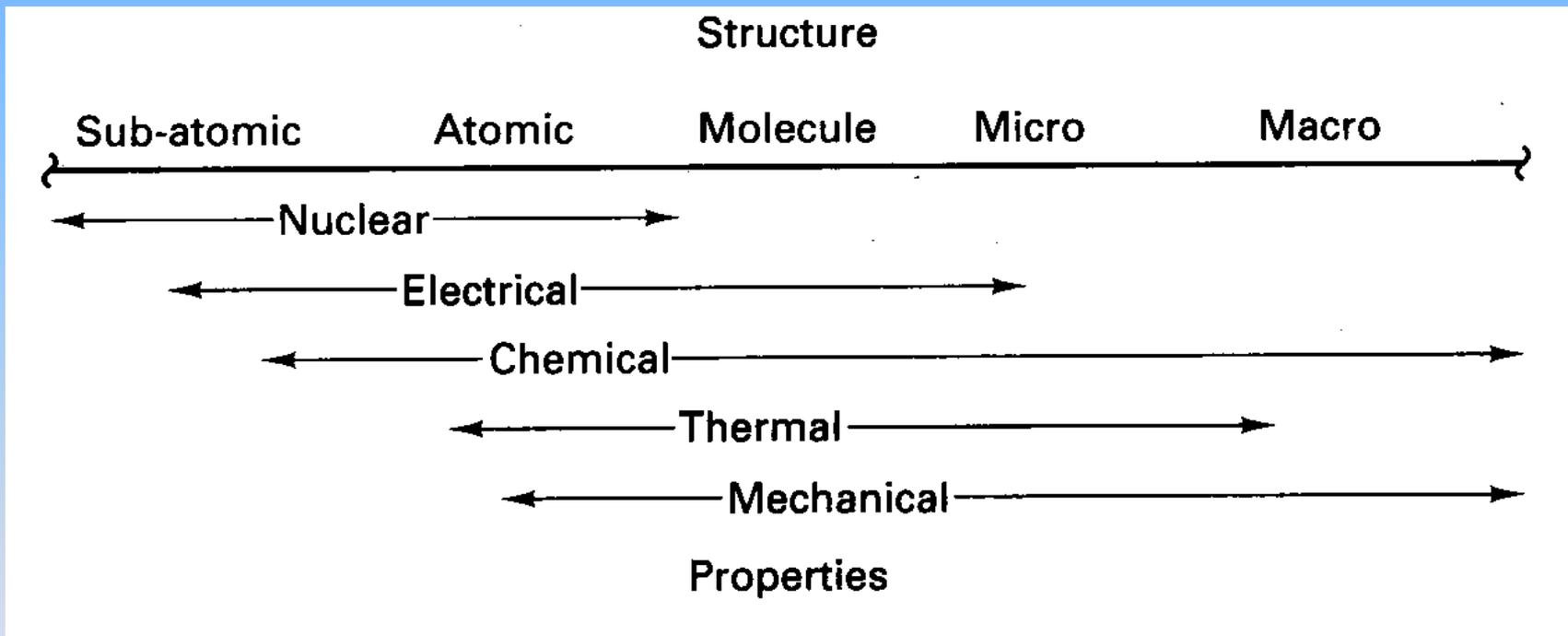
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Office Hours: Tuesday, 11:30 am-12:30 pm,  
Friday, 11:30 am-12:30 pm

# 3.1 Structure –Property-Processing- Performance Relationships

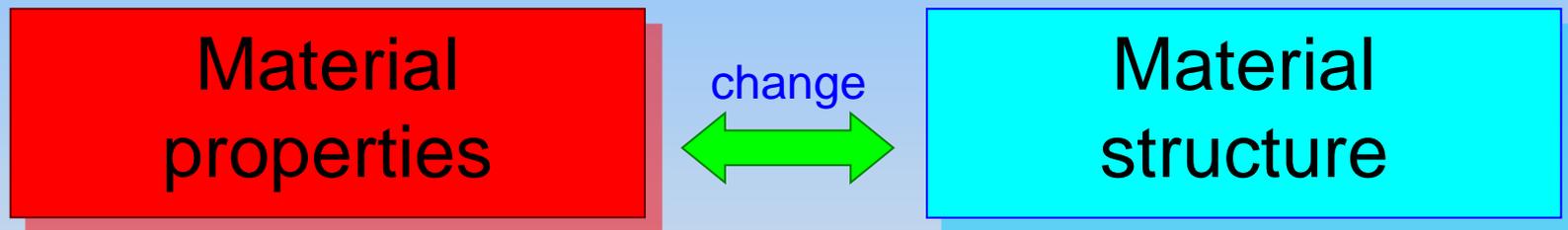
- Primitive cultures limited to naturally occurring sources;
- Civilization advancement & materials engineering;
- Properties must match specific requirements of the application;
- Material properties are direct result of structure:
  - **subatomic structure** (protons, neutrons, electrons);
  - **atom** is a basic unit of an element that can undergo chemical change;
  - **atomic bonding** (molecule, crystal, amorphous aggregate);
  - **microstructure** (observed on a microscopic scale).

# 3.1 Structural Level of Properties Relations



# 3.1 Structure –Property Relationships

- Interactive relation to yield improved materials engineering solutions



## 3.2 The Structure of Atoms

- Atom composition:
  - nucleus {protons (+), neutrons (neutral), high mass};
  - electron (-) cloud, equal number as protons, arranged in shells and sub-shells;
  - neutral charge balance;

## 3.2 The Structure of Atoms

- **Atomic number**; the number of protons in the nucleus of an atom of an element;
- **Electron shell**: a group of electrons with the same principal quantum number, **n**;
- **Electron shells**: shell-1 (two electrons); shell-2 (eight electrons); shell-3 (max. 32 electrons);
- **Stable configuration** with 8 electrons in 3<sup>rd</sup> shell and up;
- **Valence electrons**: electrons in the outermost shells which are most often involved in bonding;

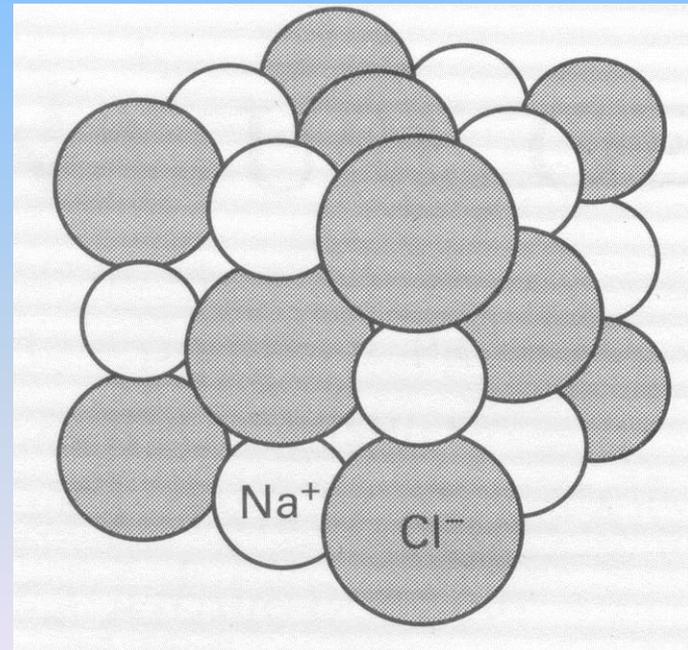
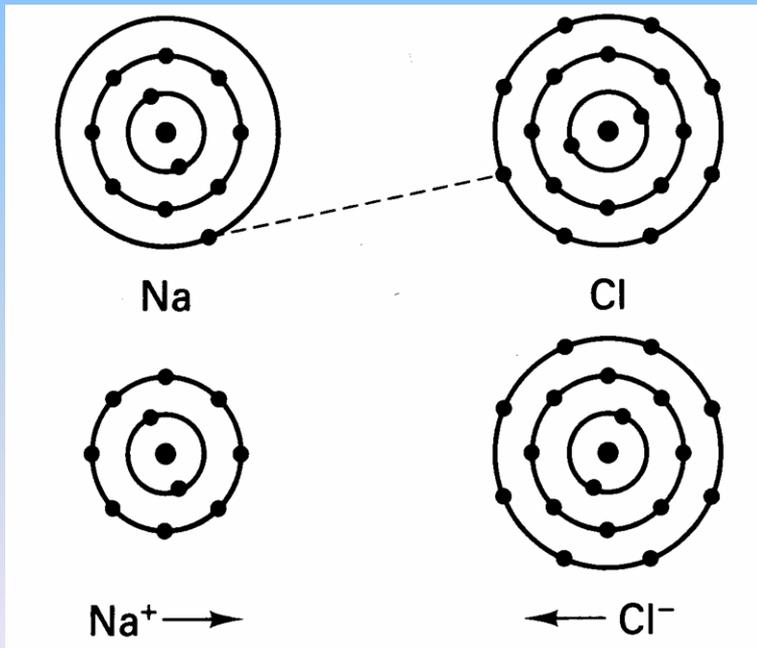
## 3.2 Charged Species

- **Negative ion:** formed by accepting an electron into vacant spot in his electron configuration and becomes negatively charged;
- **Positive ion:** formed by donating an excess electron into vacant spot of another atom's electron configuration to become positively charged;

# 3.3 Atomic Bonding

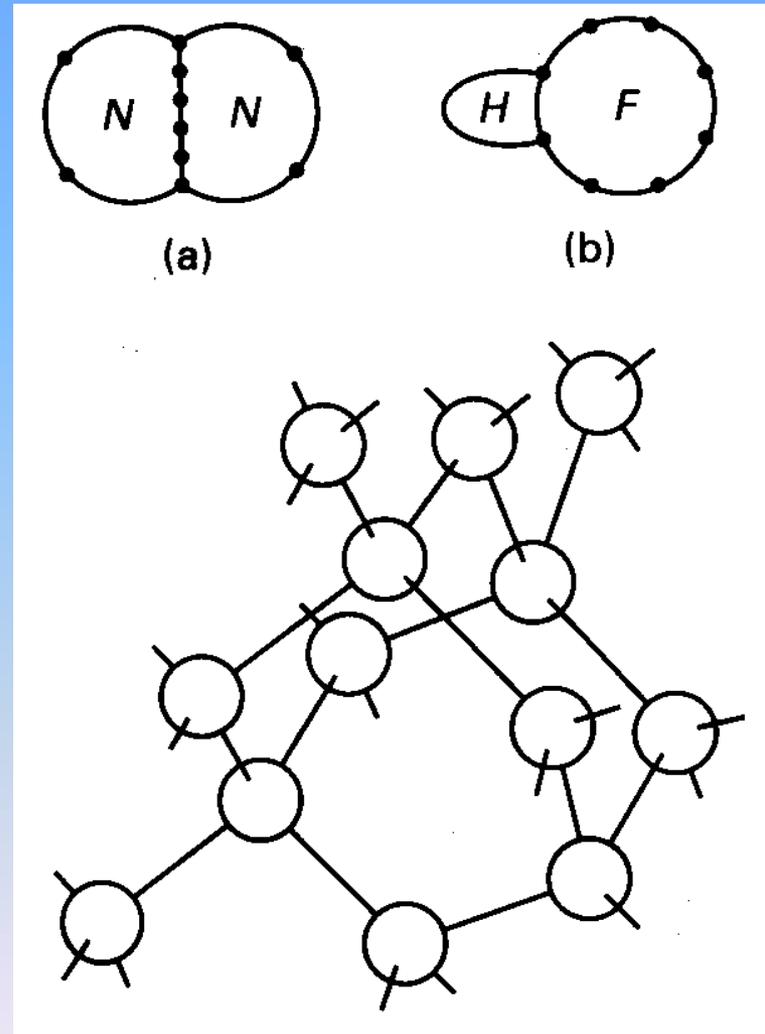
- Primary bonds:
  - **Ionic bond** resulting from the electrostatic attraction of oppositely charged ions, it is non-directional (e.g. NaCl crystal);
  - **Covalent bond** resulting from the sharing of electrons. Mostly by overlapping of half filled orbitals of two atoms. It is a directional bond;
  - **Metallic bond** resulting from sharing of delocalized outer shell electrons (electron charge cloud) by an aggregate of metal atoms. It is non-directional bond (e.g. elemental sodium);

# Ionic Bonding of Sodium Chloride

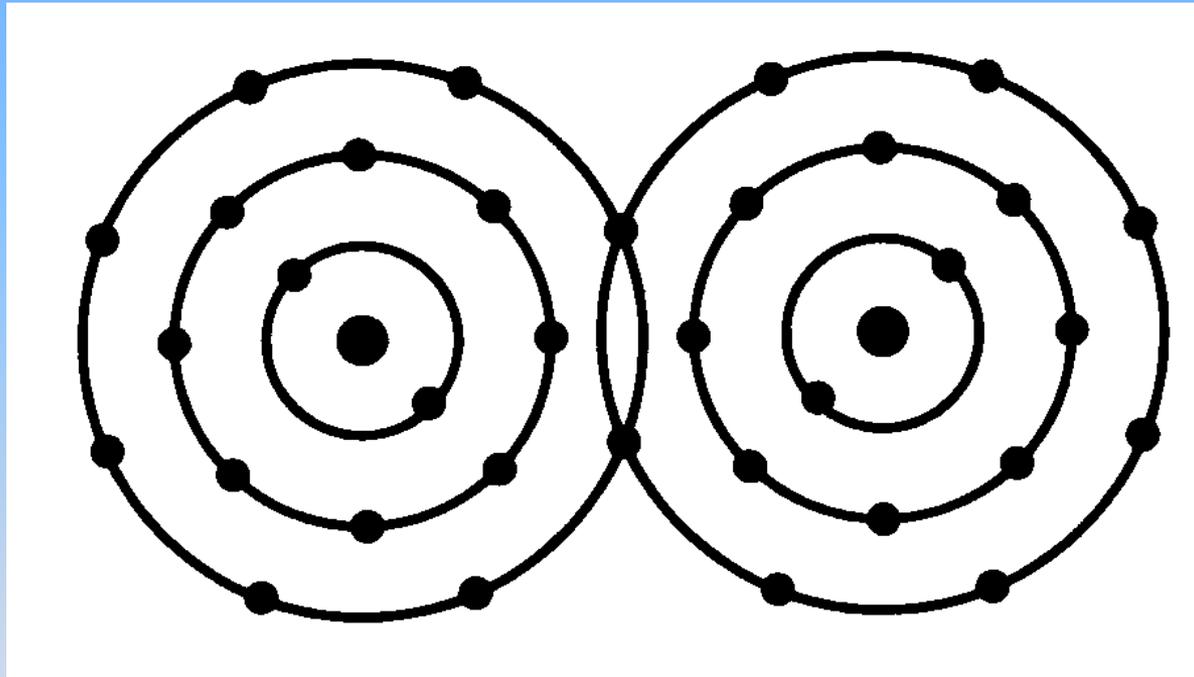


# Covalent Bonding

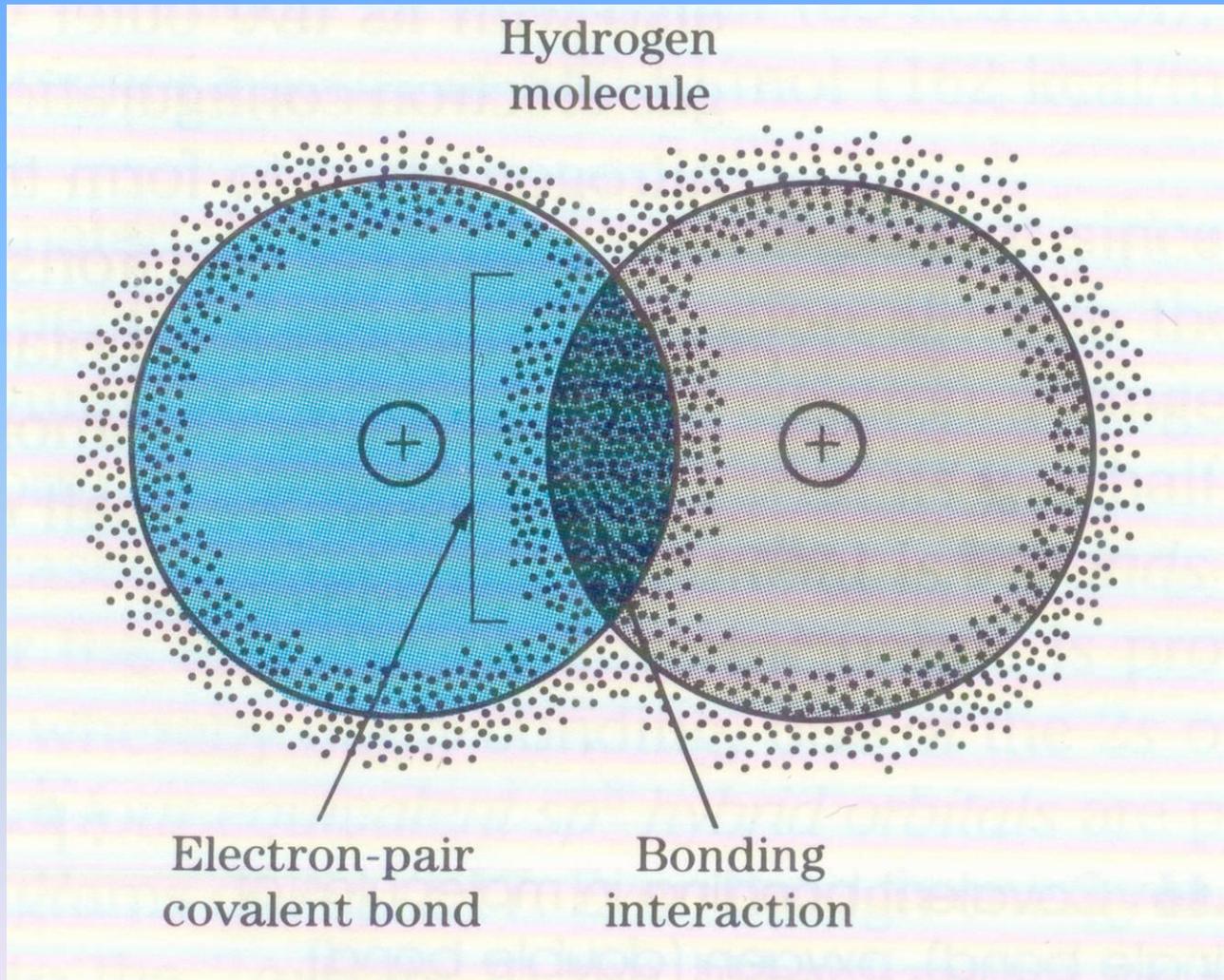
- a) Stable 2-atom molecule of Nitrogen (multiple electron sharing);
- b) Hydrogen-Fluoride (different species);
- c) 3-D structure of Diamond (carbon with four electrons in valence shell where one atom shares electrons with four neighboring atoms)



# Chlorine Molecule Covalent Bonding



# Hydrogen Bonding



# Covalent Structure (Graphite)

- Each carbon atom uses three of its electrons to form simple bonds to its three close neighbors.
- The fourth electron is in the bonding level.
- The "spare" electrons in each carbon atom become delocalized over the whole of the sheet of atoms in one layer.
- They are no longer associated directly with any particular atom or pair of atoms.
- Are free to wander throughout the whole sheet.

# Covalent Structure (Graphite II)

- The delocalized electrons are free to move anywhere within the sheet –
- Each electron is no longer fixed to a particular carbon atom.
- There is no direct contact between the delocalized electrons in one sheet and those in the neighboring sheets.
- The atoms within a sheet are held together by strong covalent bonds –stronger than in diamond
- So what does hold the sheets together?
- Van der Waals forces hold the sheets together.

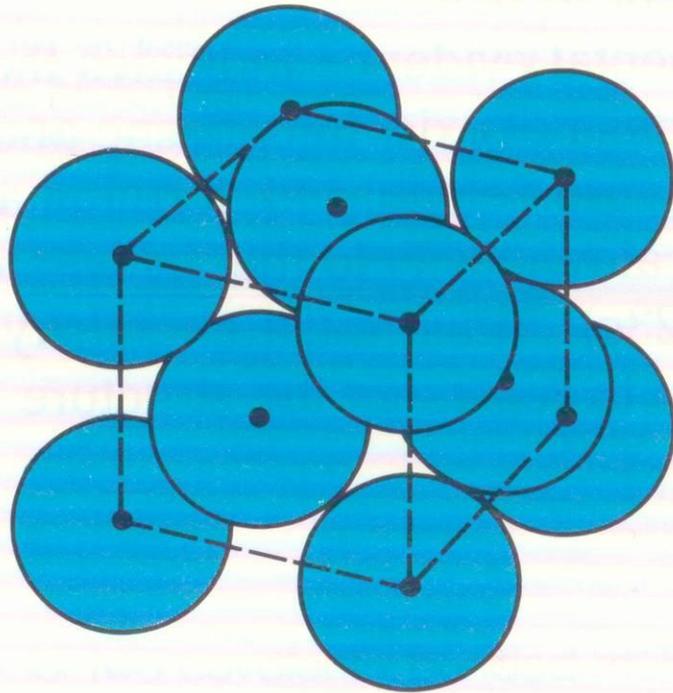
# Polymers

- A polymer is composed of many simple molecules that are repeating structural units called monomers.
- A single polymer molecule may consist of hundreds to a million monomers and may have a linear, branched, or network structure.
- Covalent bonds hold the atoms in the polymer molecules together
- Secondary bonds then hold groups of polymer chains together to form the polymeric material.
- Copolymers are polymers composed of two or more different types of monomers.

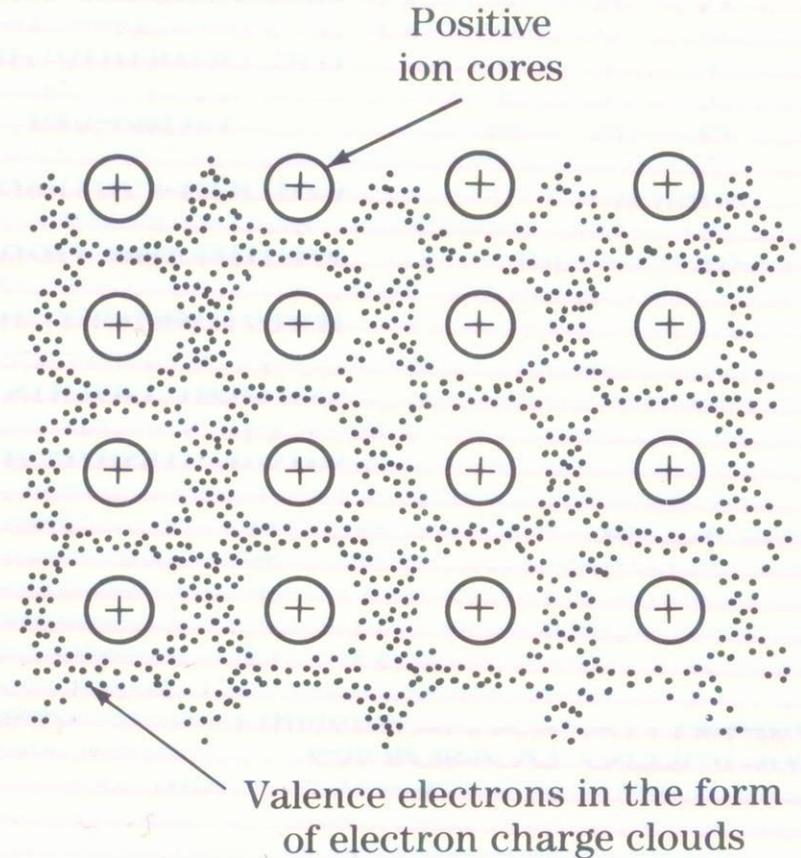
# Ceramics

- A ceramic is “an inorganic, nonmetallic solid that is prepared from powdered materials and is fabricated into products through the application of heat.
- The two most common chemical bonds for ceramic materials are covalent and ionic.
- Thus ceramics have high hardness, high compressive strength, and chemical inertness.
- Also low ductility and low tensile strength.
- The absence of free electrons is responsible for making most ceramics poor conductors of electricity and heat.

# Metallic Bonding in Copper Crystal



(a)



(b)

# 3.3 Atomic Bonding

- **Ionic bonding** produces electrically neutral structure by adopting the most stable configuration (moderate to high strength, high hardness, brittleness, high melting point, low electrical conductivity, atom or ion movement needed for charge transport)
- **Covalent bonding** produces materials with high strength and high melting point, brittle. Electrical conductivity depends on bond strength (e.g. conductive tin-weak bond, semiconductive silicon, insulating diamond);
- **Metallic bonding** produces highly conductive (E/T) materials (mobile pool of electrons), variety of bond and/or material strengths, nontransparent (opaque), deformation by atom movement mechanism (no breaking of discrete bonds) so deformed material is as strong as original;

## 3.4 Secondary Bonds

- **Van der Waals force:** intermolecular force (weak force) of attraction between molecules caused by the electrons in the bonds between two atoms being attracted to the positive nucleus of another atom (e.g. layers of C-atoms in graphite held together);
- **Permanent dipole bond:** created by attraction of molecules which have permanent dipole moments. Each molecule have (+)&(-) charge centers separate by a distance.

# 3.5 Interatomic Distances and Size of Atoms

- Space occupied by electrons much smaller than electron shells space (vacant space).
- Bonding forces pull atoms together, but repelling forces between neighboring nuclei exist as well.
- Equilibrium distance=Sum of atomic radii to assign distinct size to atoms.
- Removing valence shell (bonding) reduces size of atom.
- Atoms oscillate around their equilibrium positions.

## 3.6 Atom Arrangements in Materials

- Atoms bond together to form aggregates.
- **Molecular structure**: takes place when distinct number of atoms are held by primary bonds ( molecules are free to move around ) low melting and boiling point, eg. O<sub>2</sub>, H<sub>2</sub>O, and C<sub>2</sub>H<sub>4</sub>.
- **Crystalline structure**: solid metals & most minerals. Atoms arranged in geometric array called **lattice** (**unit block** repeated in space called **unit cell**).
- **Amorphous structure**: certain degree of local order, eg. glass, chalk.

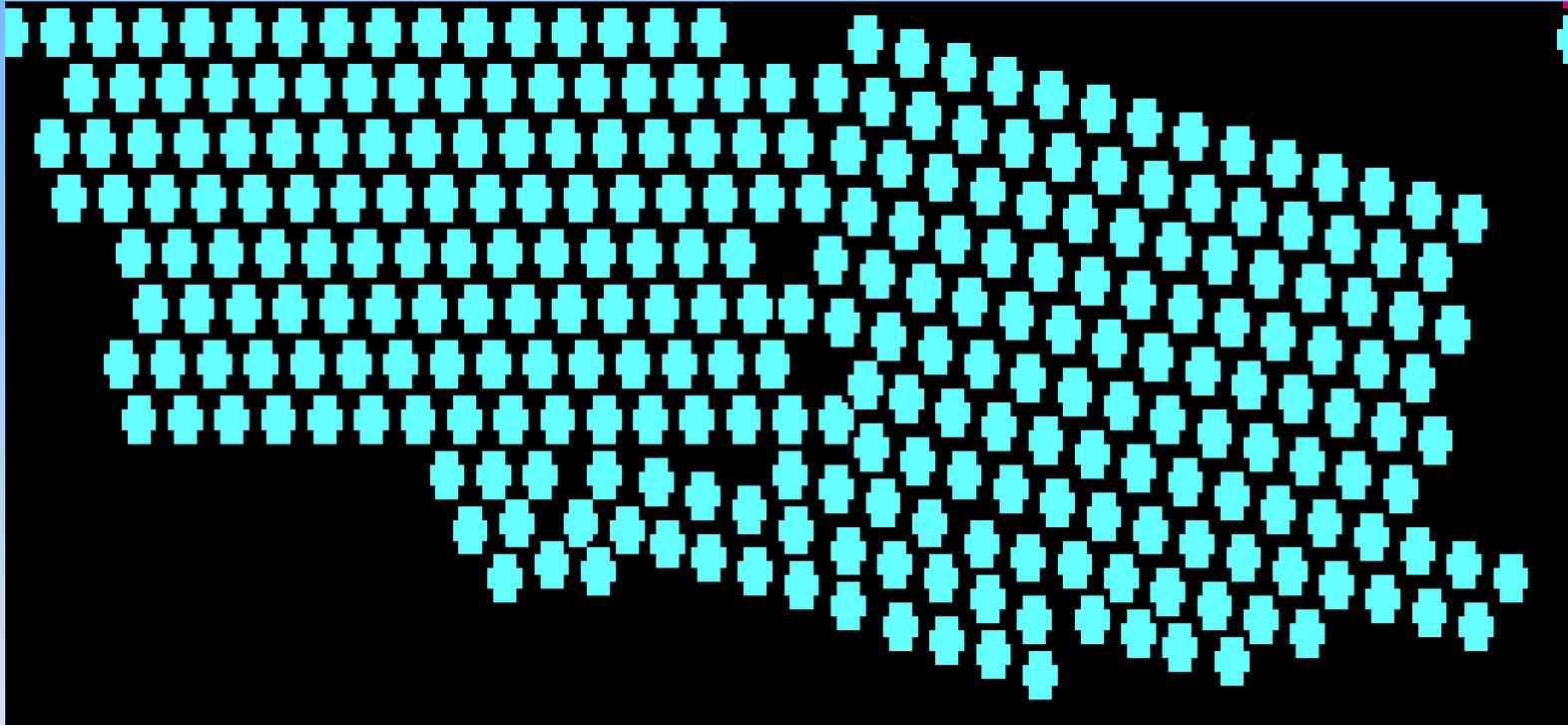
## 3.6 Atom Arrangements in Materials

- In an **amorphous structure** such as glass atoms have some degree of local order (with respect to neighbors), but as an aggregate the structure lacks orderly arrangement of atoms such as crystal structure.

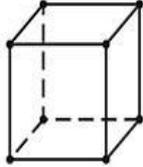
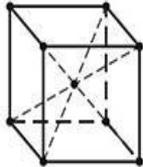
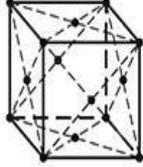
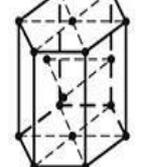
# 3.7 Crystal Structures of Metals

- More than 50 known chemical elements are metals;
- High strength, good E/T conductivity, luster, high deformability without fracture, high density;
- Existing in more than one lattice form (depending on P&T). They are allotropic or polymorphic.
- Allotropic transformation: the change from one to another lattice form to another;
- 14 types of basic crystal structures (**lattices**);
- Most of commercial metals solidify in: BCC, FCC and HCP.

# 3.7 Crystal Structure



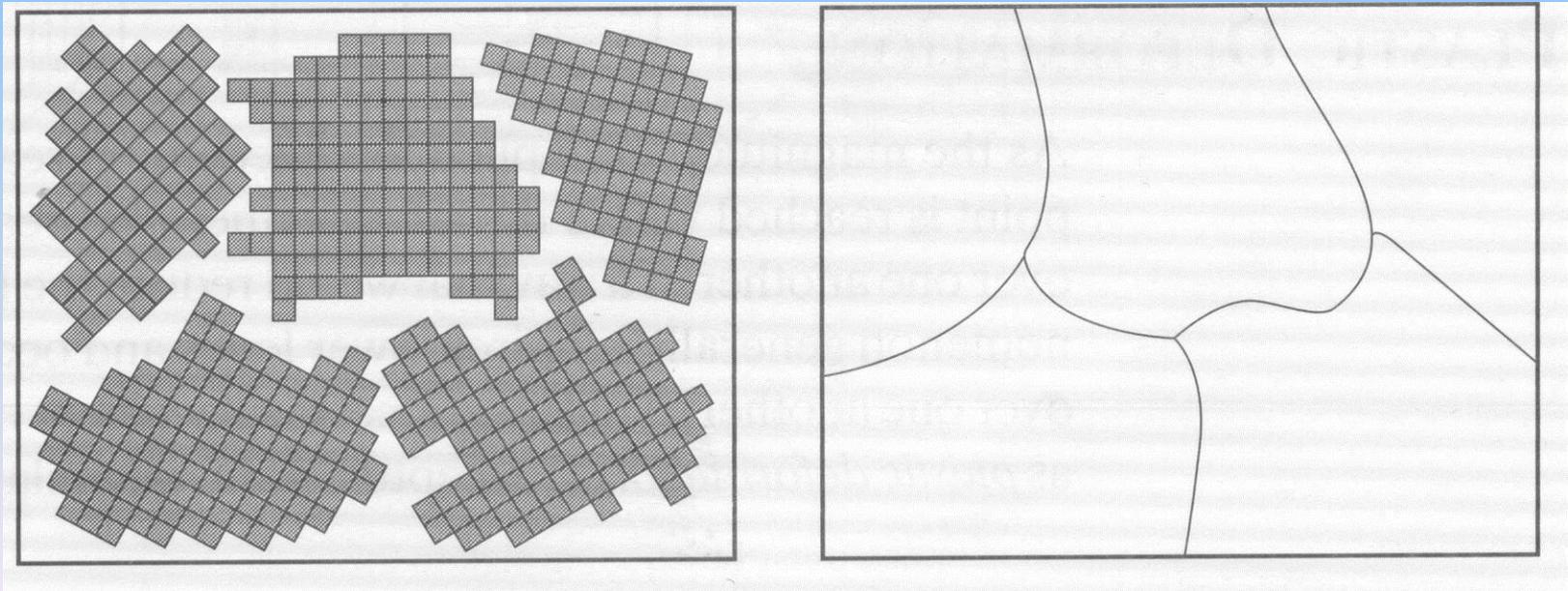
# 3.7 Common Crystal Structures

	Lattice structure	Unit cell schematic	Ping-Pong ball model	Number of nearest neighbors	Packing efficiency	Typical metals
<i>a</i>	Simple cubic			6	52%	None
<i>b</i>	Body-centered cubic			8	68%	Fe, Cr, Mn, Cb, W, Ta, Ti, V, Na, K
<i>c</i>	Face-centered cubic			12	74%	Fe, Al, Cu, Ni, Ca, Au, Ag, Pb, Pt
<i>d</i>	Hexagonal close-packed			12	74%	Be, Cd, Mg, Zn, Zr

# 3.7 Development of a Grain Structure

From the pool of molten metal many small particles having lattice parameters of given material form (**nucleation**).

**Crystal growth** follows up until interference with neighbors forming **grain boundaries** upon solidification completion.



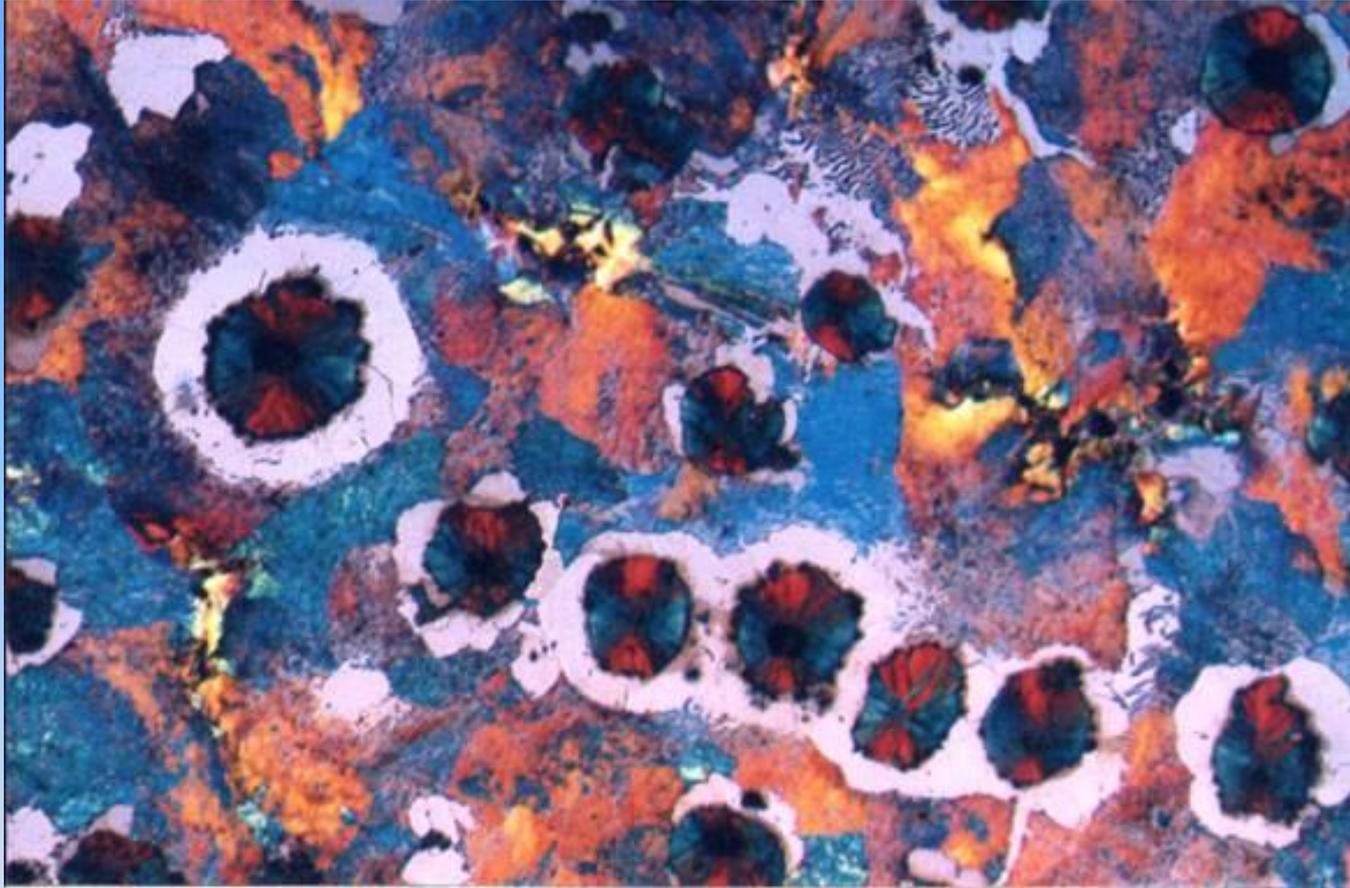
# 3.7 Grain Growth

- If a metal is held above its recrystallization temperature for a while, the grains will increase in size
- Mechanical properties decrease as grain size increases
- Temperatures should be controlled during processing so that the grain growth and therefore property changes are retarded

# 3.7 Microstructure Specification

- Rate of **nucleation** & rate of **solidification**;
- Mech./Phys. properties depend on **grain structure**
- ASTM ( American Society for Testing and Materials);
- Grain size number:  $N = 2^{n-1}$
- N-number of grains per square inch at 100x;
- n- ASTM grain size number;

# Microstructure

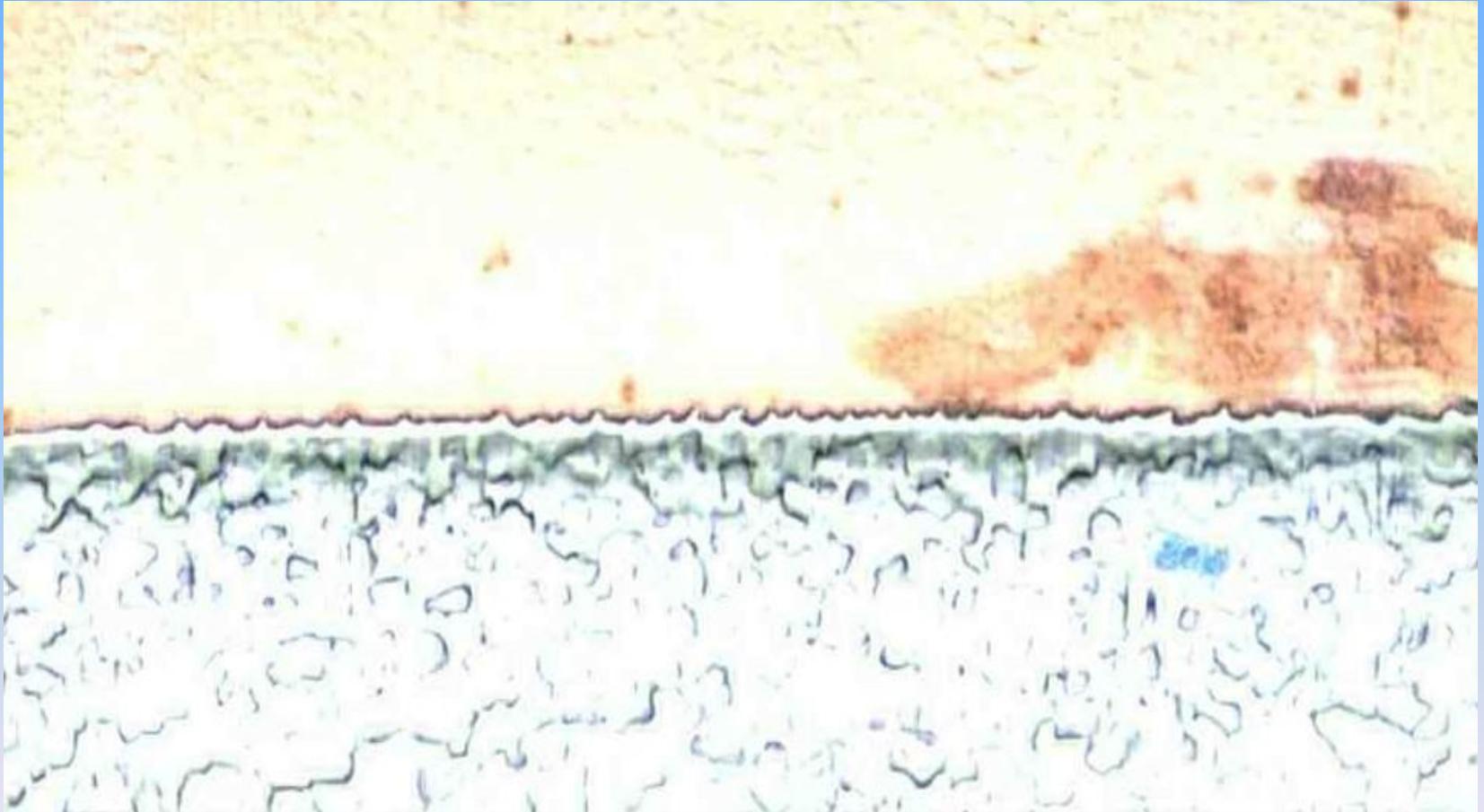


- Globular cast iron

# Copper-Copper bonded area



# Copper-Ni-Alloy bonded area

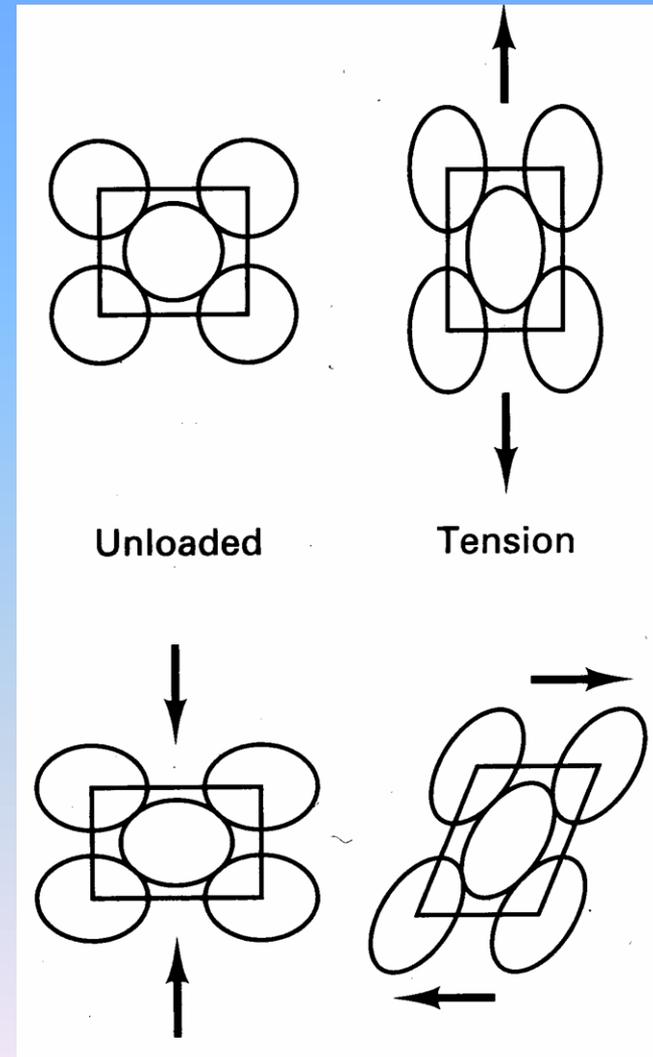


## 3.8 Elastic Deformation

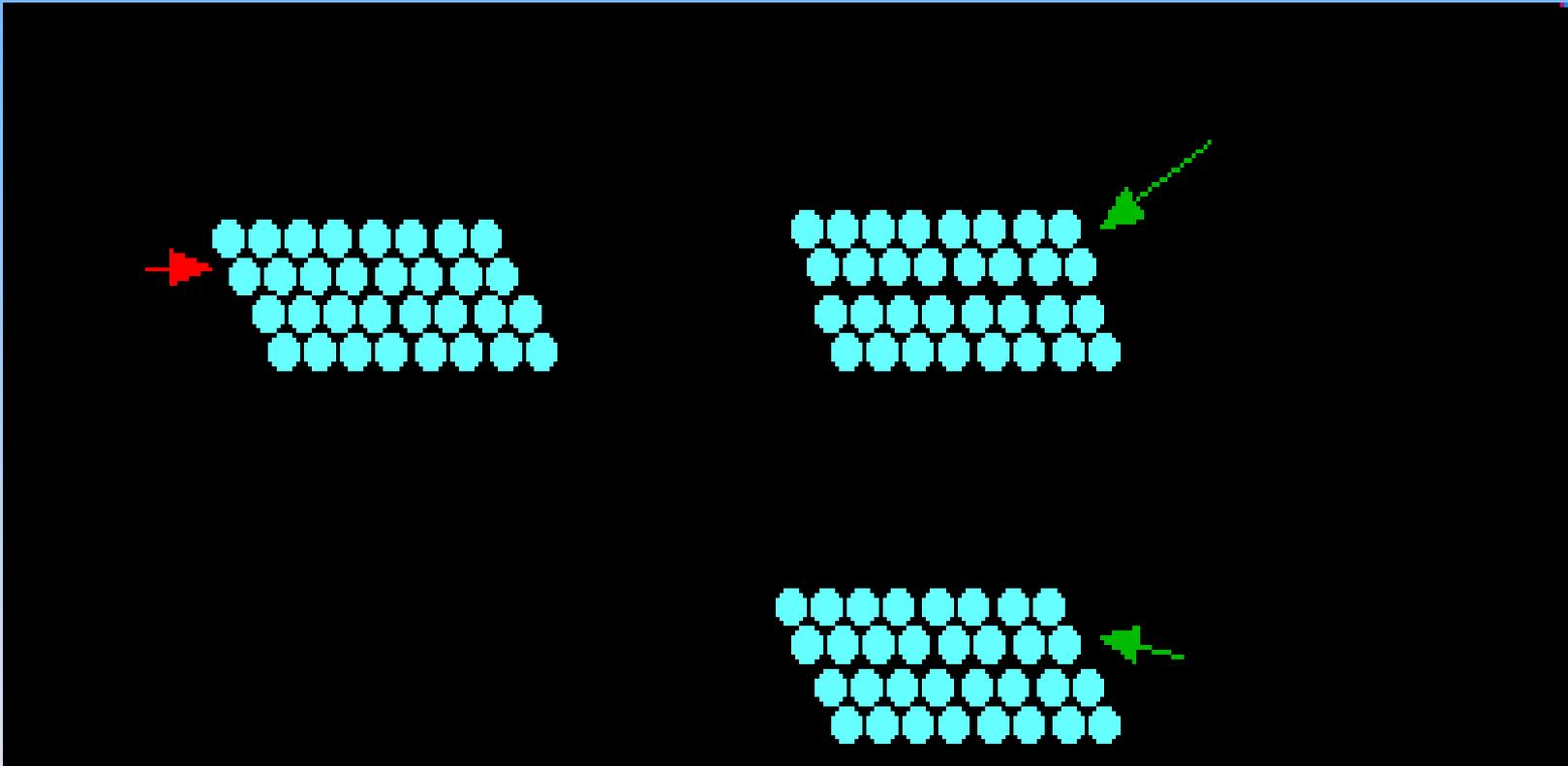
- Mechanical behavior depends on: lattice type, interatomic forces (bond strength), spacing between adjacent planes of atoms and the density of atoms on the various planes.

# 3.8 Elastic Deformation

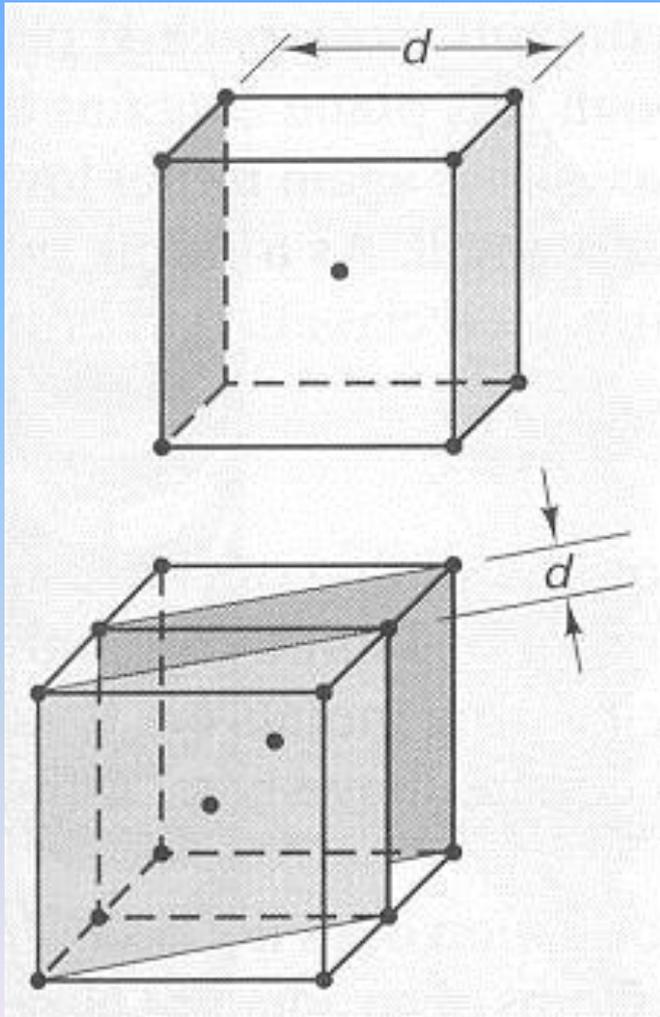
- Relatively low loads;
- Stretching or compressing of interatomic distance;
- Upon removal of load atoms resume original positions;
- Ratio of lateral contraction to axial tensile strain is **Poisson's ratio**.



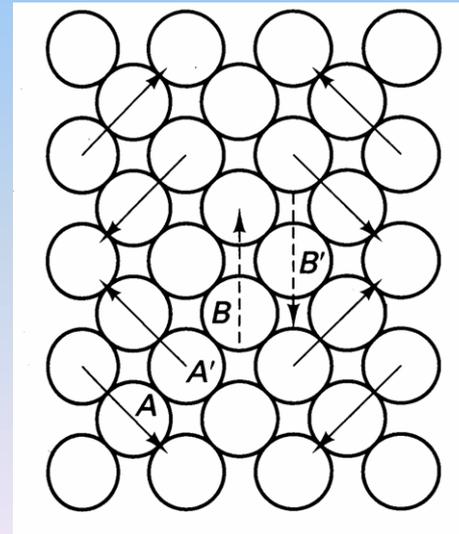
# 3.8 Elastic Deformation



# 3.9 Plastic Deformation



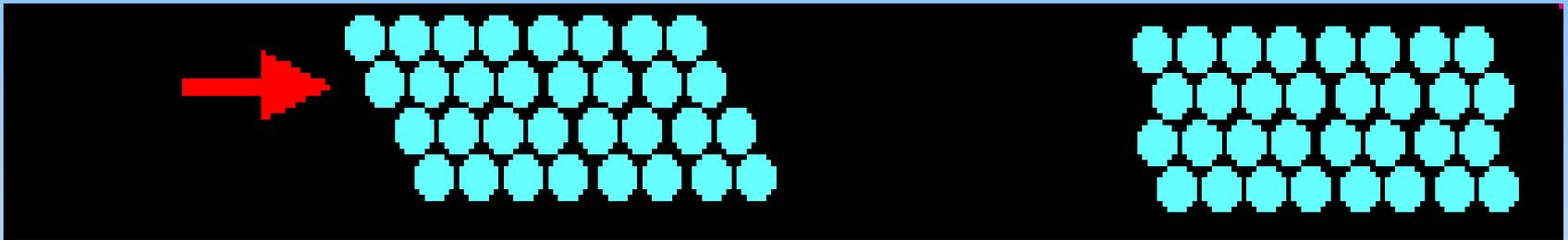
- Permanent shift of atom positions is plastic deformation;
- Takes place along planes having the highest atom densities.



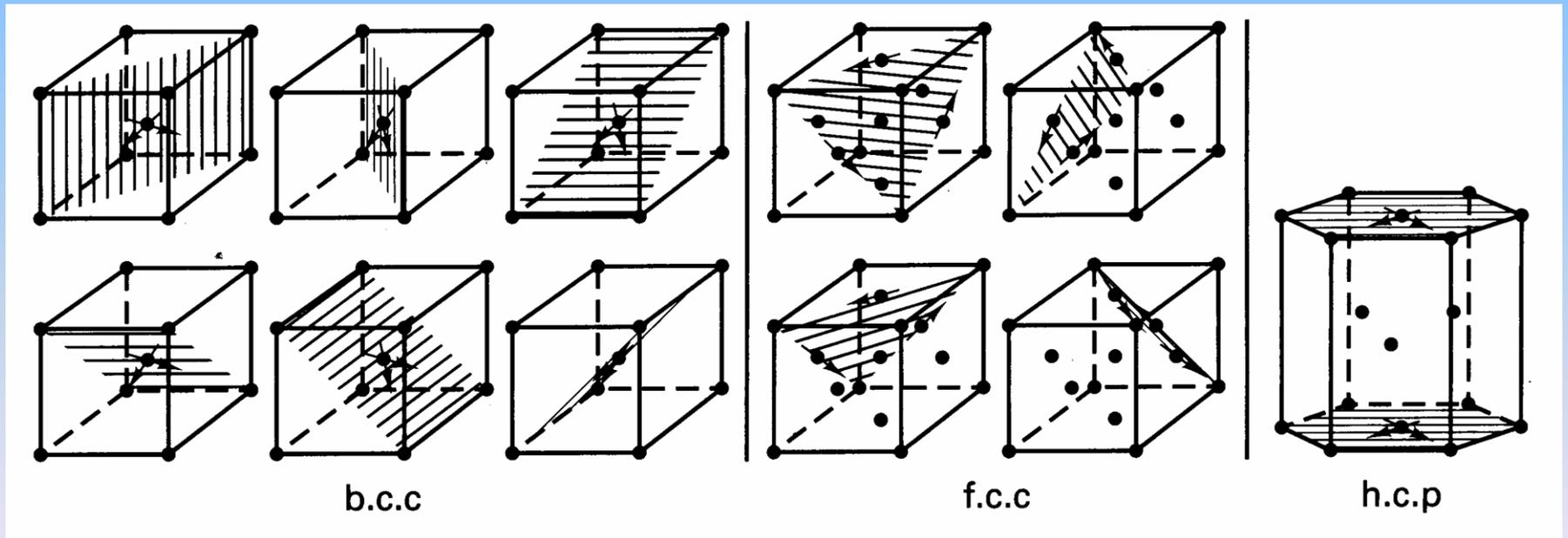
# 3.9 Plastic Deformation

- As a load is applied to a material, distortion increases until (bonds are broken to produce a fracture and atoms slide over one another to reduce the load).
- Results in a permanent change in shape in the material that does not deteriorate its properties.
- Plastic deformation occurs by the sliding of maximum-density planes in directions of closest packing (specific combination of a plane and direction is a slip system and resulting shear deformation is known as slip).

# 3.8 Plastic Deformation

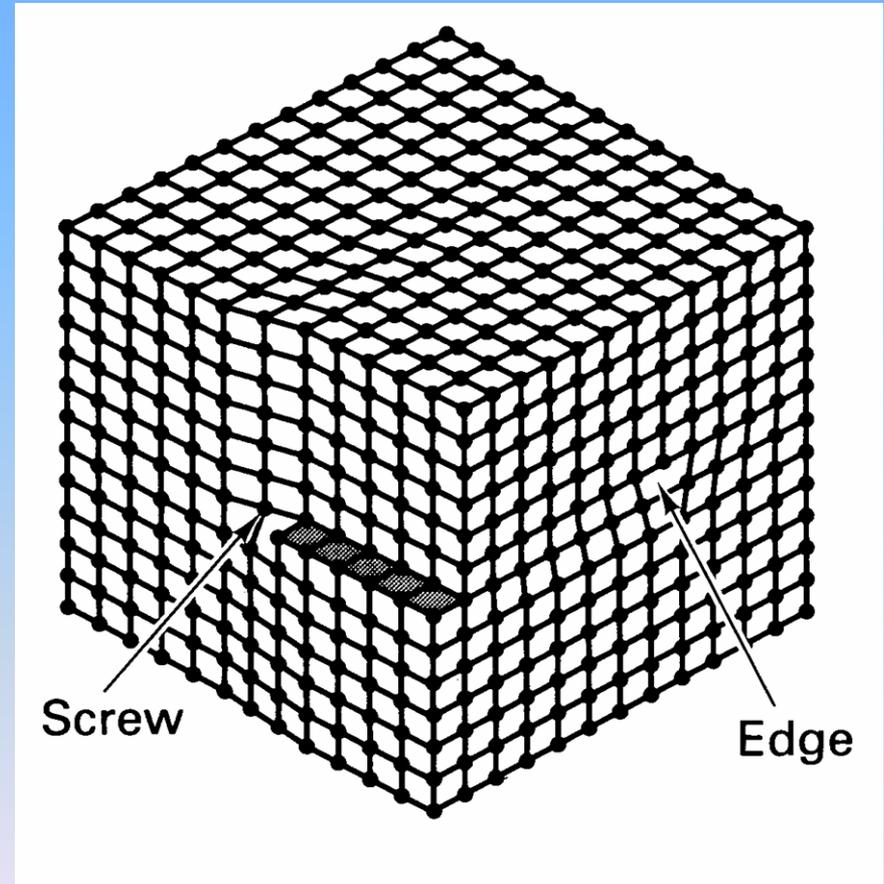


# 3.9 Slip Planes of the Various Lattice Types

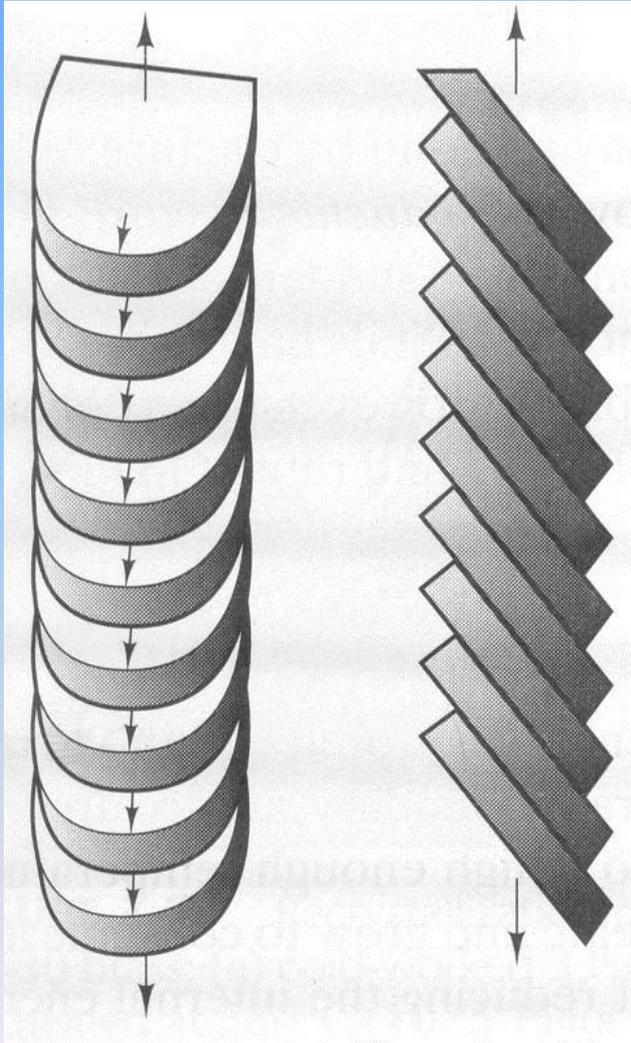


# 3.10 Dislocation Theory of Slippage

- Deformation results as progressive slippage of localized (disruption) dislocation;
- Edge dislocation: edge of extra half plane of atoms;
- Screw dislocation: parallel tearing of crystal plane;
- Barriers to dislocation motion: interstitials, substitutions, grain boundaries or free surface.



# 3.11 Strain or Work Hardening



- Phenomenon of material strengthening by plastic deformation;
- Slip & rotation (like skewed deck of cards);
- The structure changes so it would obstruct further dislocation movement;
- Further deformation occurs on alternative systems.

# 3.13 Grain Shape and Anisotropy

- As a metal is deformed, the grains elongate in the direction of metal flow.
- Properties that vary with direction are called anisotropic.
- Properties that are uniform in all directions are called isotropic.
- Anisotropic behavior can create problems during manufacturing.
- Further manufacture of metal sheets that have been rolled may exhibit this problem.

# 3.13 Grain Shape and Anisotropy

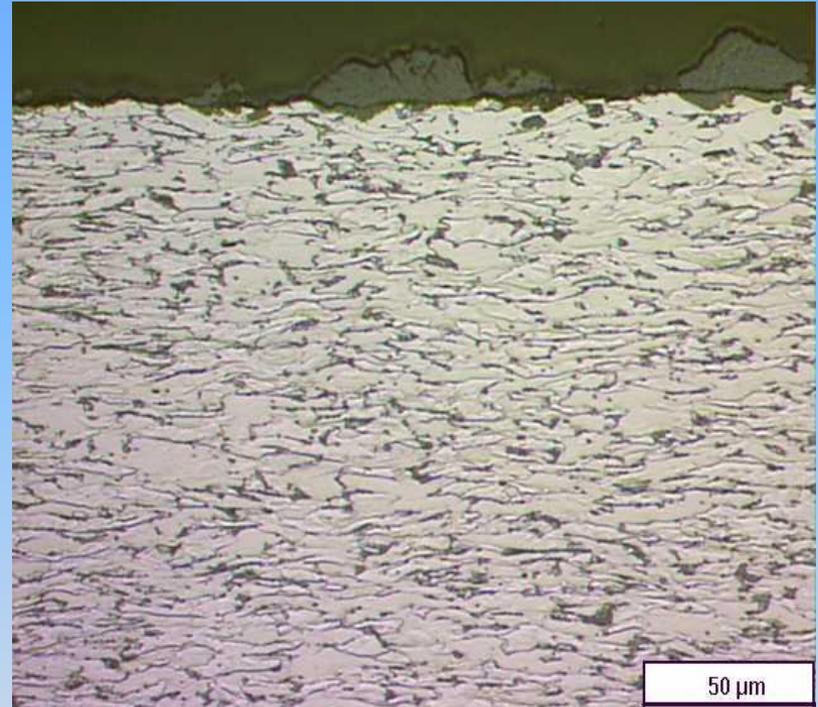
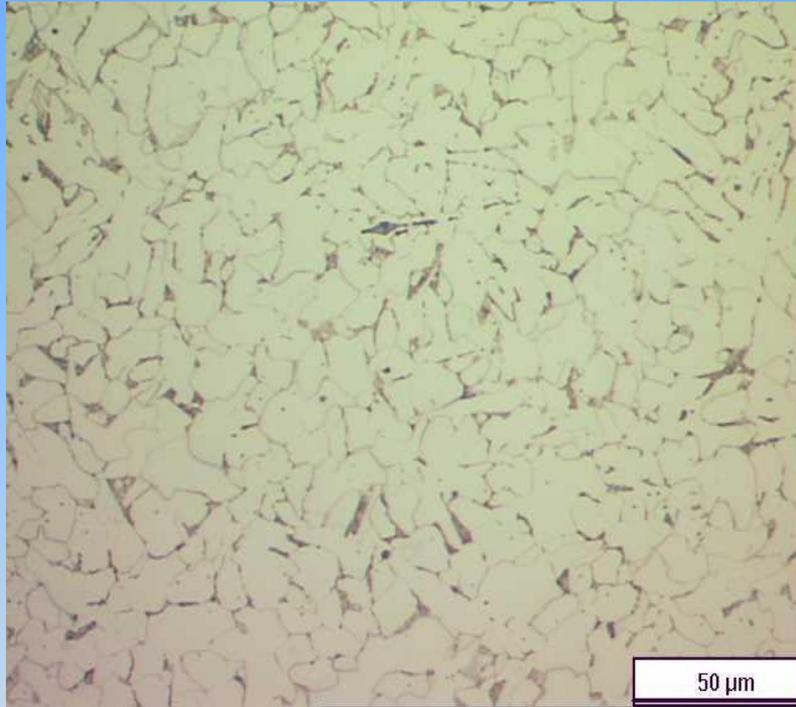
- Anisotropy
  - fiber alignment
  - anisotropy
  - inherent anisotropy
  - grain alignment
- High *strength to weight* ratio



# 3.14 Fracture of Metals

- If the material undergoes too much plastic deformation, a fracture will occur.
- In a ductile fracture, plastic deformation occurs before the material breaks.
- In a brittle fracture, the break occurs before plastic deformation.

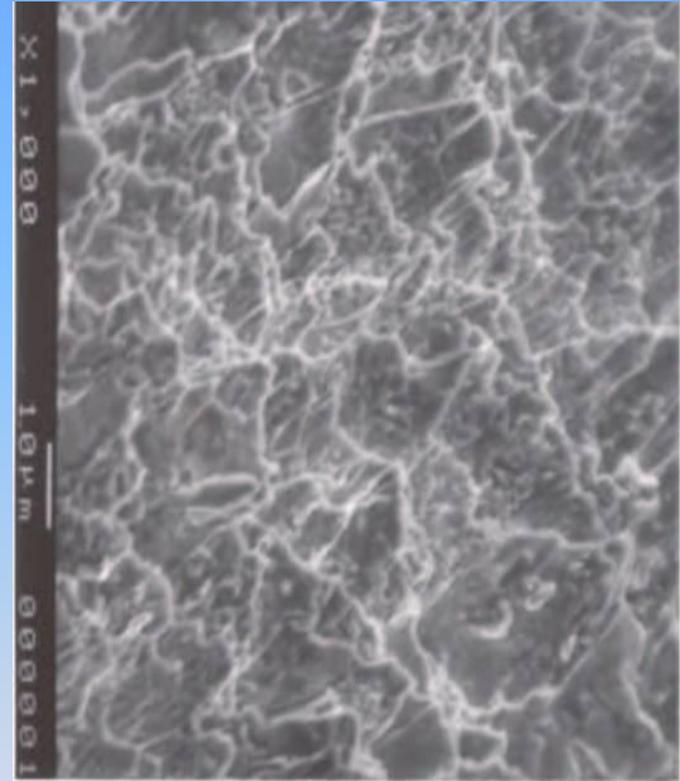
# 3.13 Grain Shape & Anisotropic Properties



- Left: deformed microstructure (A36 steel) round or slightly deformed inclusions, 50X
- Right: Fragment densely packed elongated grains (no oxide) 50X

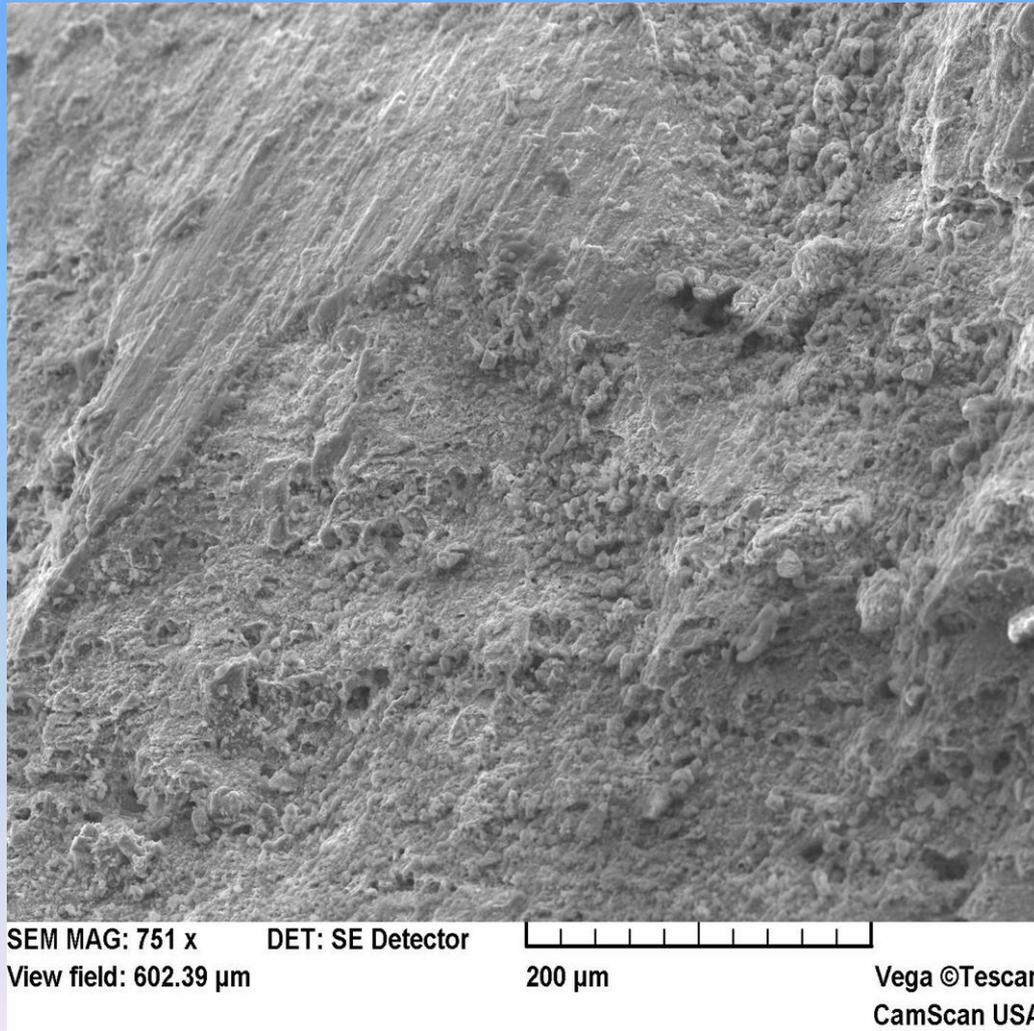
# 3.14 Fracture of Metals

## SEM Fractography Analysis

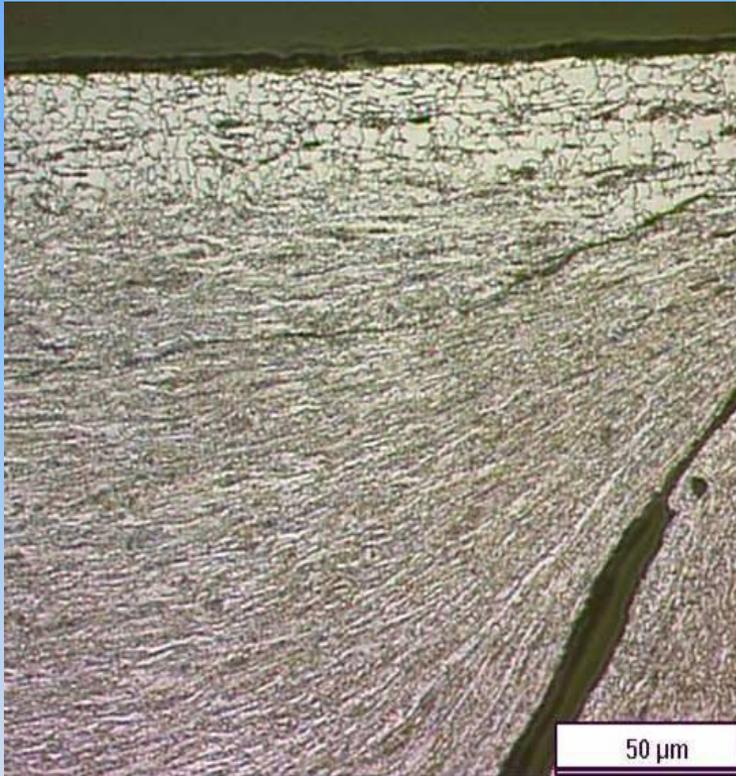


- Left: A36 steel sample (ductile overload failure)
- SEM fractograph (750X)

# 3.14 Aluminum Fracture



# 3.15 Recrystallized Oxidized Fragment



- Left: heavily deformed and recrystal. regions, 50X
- Right: recovered oxidized fragment (t=390 deg C)

# 3.15 Cold Working, Recrystallization, and Hot Working

- Reducing of internal energy through forming of new crystals.
- Cold working: Plastic deforming below recrystallization temp.
- Hot working: Plastic deforming above recrystallization temp.

# 3.17 Alloys and Alloy Types

- Alloy: composed of metal and another solid substance ( usually another metal);
- Constituents can be insoluble in each other;
- Solid solution (interstitial, substitutional);
- Intermetallic compounds: alloying element interact with atoms of base metal in definite proportion and definite geometric relationships.

# Grain Size vs. Properties

- For low carbon steels and aluminum the grain size less than 1 micron, the materials usually exhibit high strength and low uniform elongation.
- In the grain size greater than 10 micron, the materials usually exhibit low strength and high elongation.
- In either case the toughness is low.
- In the grain size of several micrometers, the toughness is the highest.
- The metallic materials with grain size of several micrometers are the best for structural applications.

# Properties vs. Microstructure

- Properties can be deduced from the microstructure.
- Microstructure the crystalline structure and all imperfections, including their size, shape, orientation, composition, spatial distribution, etc.
- Point defects (vacancies, interstitial and substitutional solutes and impurities).
- Line defects (edge and screw dislocations).
- Planar defects (stacking faults, grain boundaries), second phase particles and dispersoids or relatively large amounts of other phases.
- Grain size determines yield strength, (Hall-Petch relationship),

# Single vs. Polycrystalline Materials

- Single crystal materials are occasionally used as structural materials.
- Polycrystalline materials are commonplace.
- The differences between single crystal and polycrystalline materials are due to the presence of grain boundaries and to a randomization of the orientation of individual crystals.
- Though microscopically their properties are anisotropic due to preferred slip directions orientation of individual crystal was random.
- This randomization makes them appear macroscopically to be isotropic.

# Single vs. Polycrystalline Materials II

- The influence of the grain boundaries on properties can also be significant.
- At low temperatures grain boundaries act as barriers to dislocation motion, thus strengthening the material.
- At elevated temperatures grain the opposite is true, grain boundaries can lower strength by providing an alternate path for both diffusion and dislocation motion.
- Impurities tend to segregate to grain boundaries, altering the properties of the grain boundary.

# Summary

- Atomic structure and bonding dictates material properties (electrons involved in bonding determine properties)
- Grain structures and defects impact material properties (Can be controlled or changed through proper processing selection)