The Structure of Atoms

- Atoms are made of a dense nucleus consisting of protons and neutrons
- Electrons surround the nucleus
  - Play a significant role in determining engineering properties
  - Valence electrons are those electrons in the outermost shell that are involved with bonding
  - Elements with similar electron configurations in their outer shell have similar properties

A MOLECULE-INTEGRATION OF ATOMS

- A molecule-energy effective integration of atoms
- Connections between atoms are ionic or covalent
- Ionic bonding-exchange of electrons to form a maximal stable outer shell
- Covalent bonding –joint use of electron to develop maxum stability of the outer shell.

GASEOUS PHASE

- The integration depends on the temperature and pressure
- High T and low P-high kinetic energy of molecules
- Free motions of molecules, no intermolecular bonding-gase

LIQUID PHASE

- High P, lower T-no free motion, high vibrational energy
- Van-der-Waals forces
- Control of intermolecular distance, no control of moceles position

SOLID STATE

- Low T, High P-packaging of atom at the max density
- The only permitted motion-limited vibratio
- Atoms form a space structure
- Most important –lattice (crystal structure)

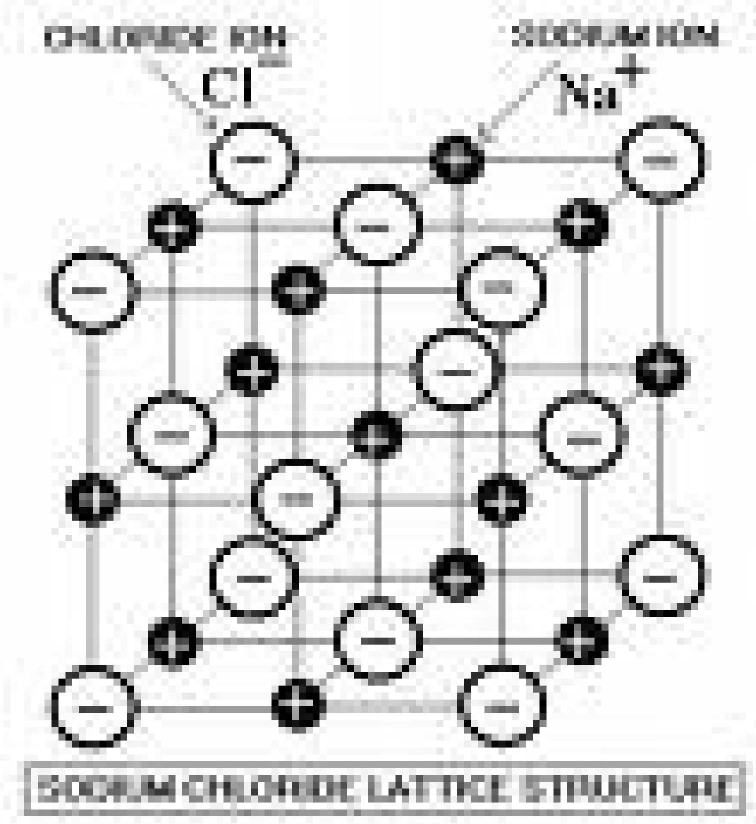
Atomic Bonding

- Three types of primary bonds
  - Ionic
  - Covalent
  - Metallic
- Ionic bonding
  - Electrons are transferred from positive ions to negative ions
  - The electrostatic attraction between the negative and positive ions forms a strong bonding force
  - Materials joined by ionic bonding have moderate to high strength, high hardness, brittleness, high melting point, and low electrical conductivity

Atom Arrangements in Materials

- Molecular structures
  - Distinct number of atoms that are held together by primary bonds
  - Weak attraction between a molecule and similar groupings
  - Examples: O_2, H_2O, and C_2H_4
- Crystalline structure
  - Solid metals and minerals
  - Atoms are arranged in a three-dimensional lattice
- Amorphous structures
  - Glass
  - Certain degree of local order

IONIC STRUCTURE



COVALENT STRUCTURE (DIAMOND)

- In diamond, each carbon shares electrons with four other carbon atoms - forming four single bonds.
- This is a *giant* covalent structure - it continues on and on in three dimensions.

COVALENT STRUCTURE (GRAPHITE)

- Each carbon atom uses three of its electrons to form simple bonds to its three close neighbours.
- The fourth electron in the bonding level.
- The "spare" electrons in each carbon atom become delocalised 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 delocalised 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 delocalised electrons in one sheet and those in the neighbouring sheets.
- The atoms within a sheet are held together by strong covalent bonds – stronger than in diamond
- So what holds the sheets together?
- Van der Waals forces holds together sheets

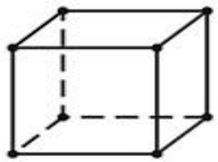
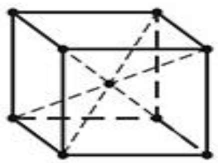
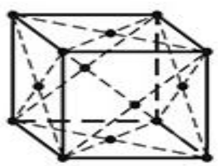
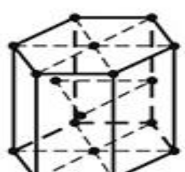
POLYMERS

- 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.

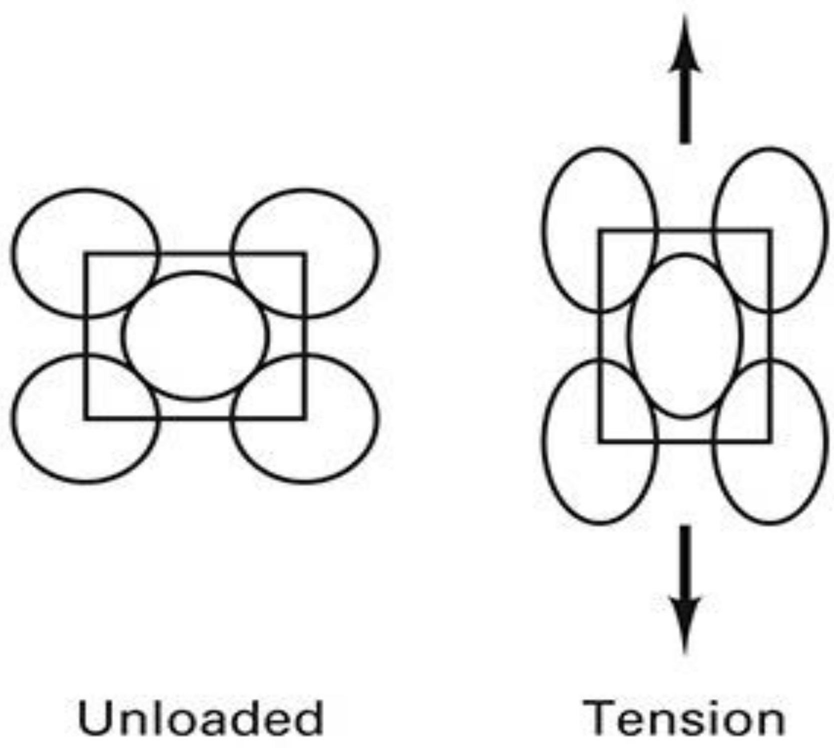
CERAMICS

- 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.

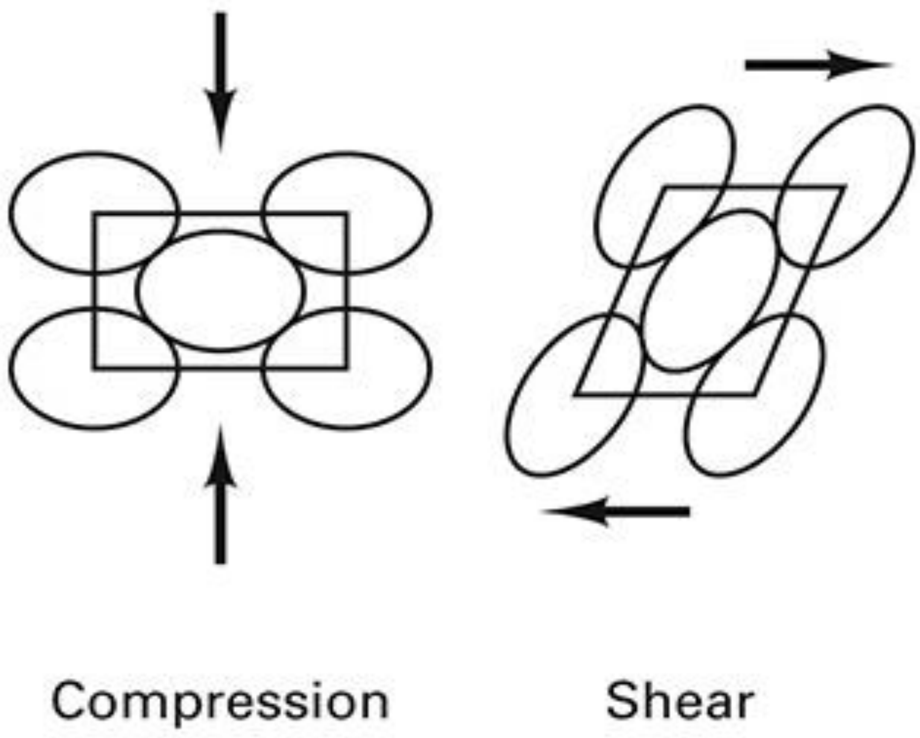
CRYSTAL STRUCTURE

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

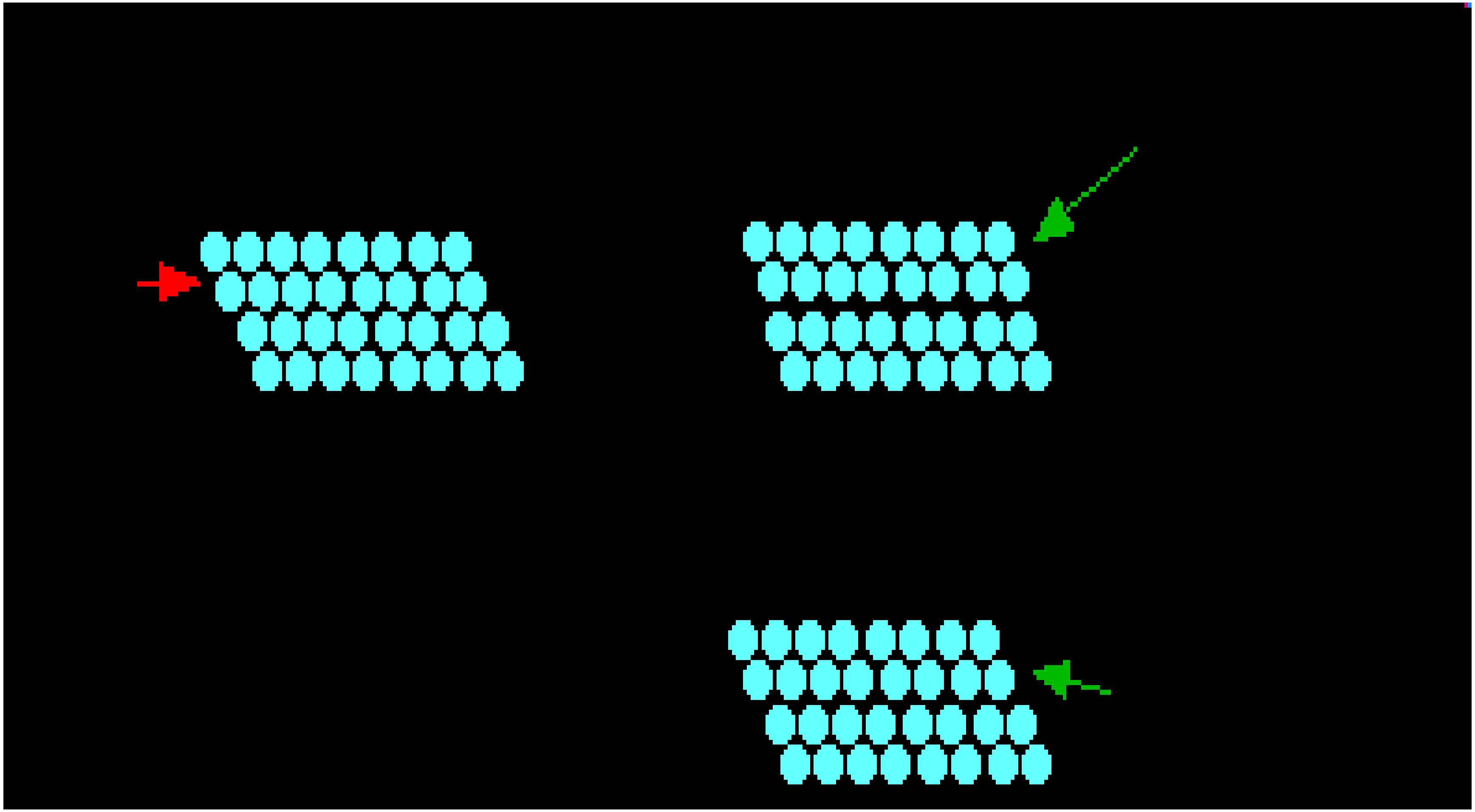
ELASTIC DEFORMATION



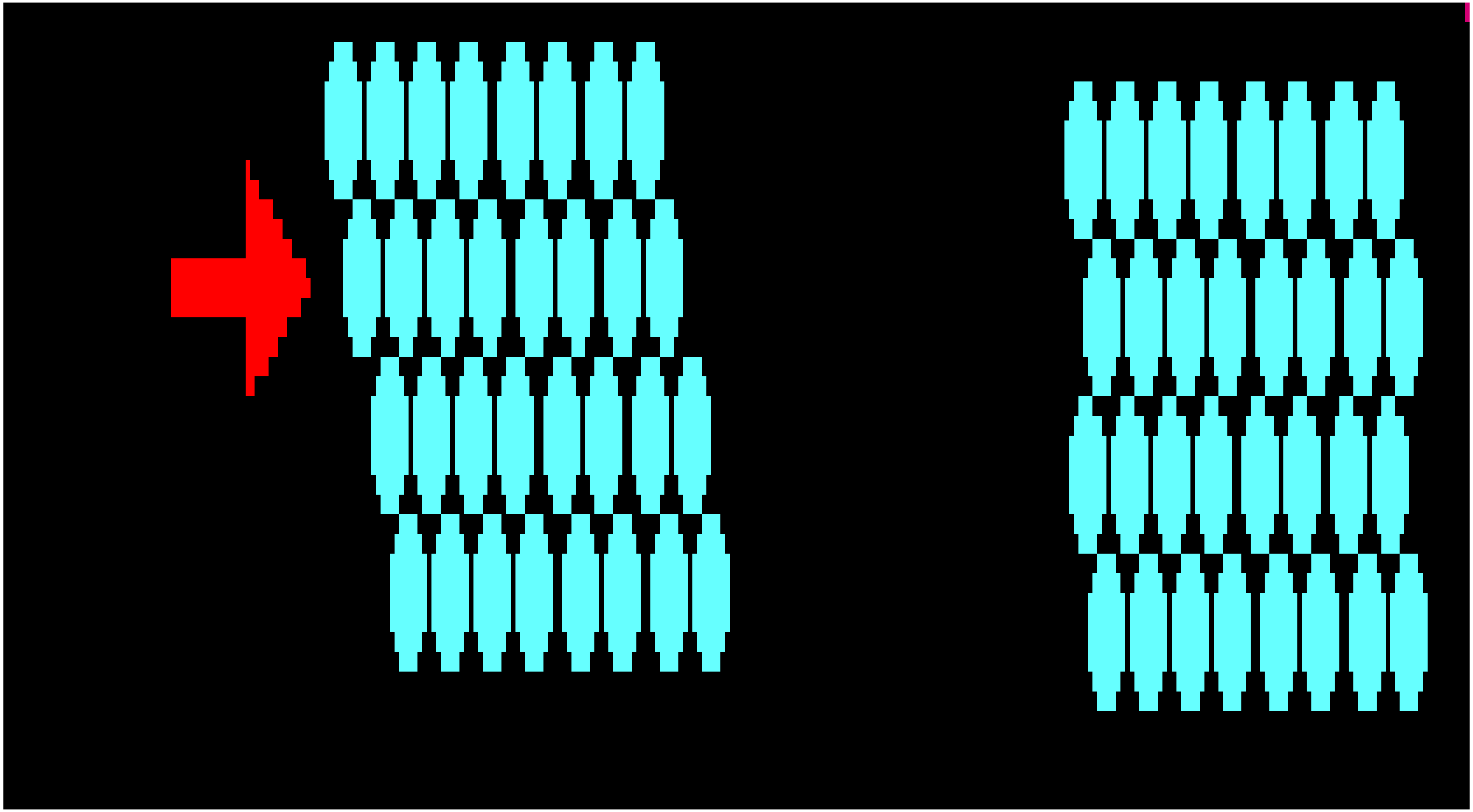
ELASTIC DEFORMATION



ELASTIC DEFORMATION



PLASTIC DEFORMATION



Plastic Deformation

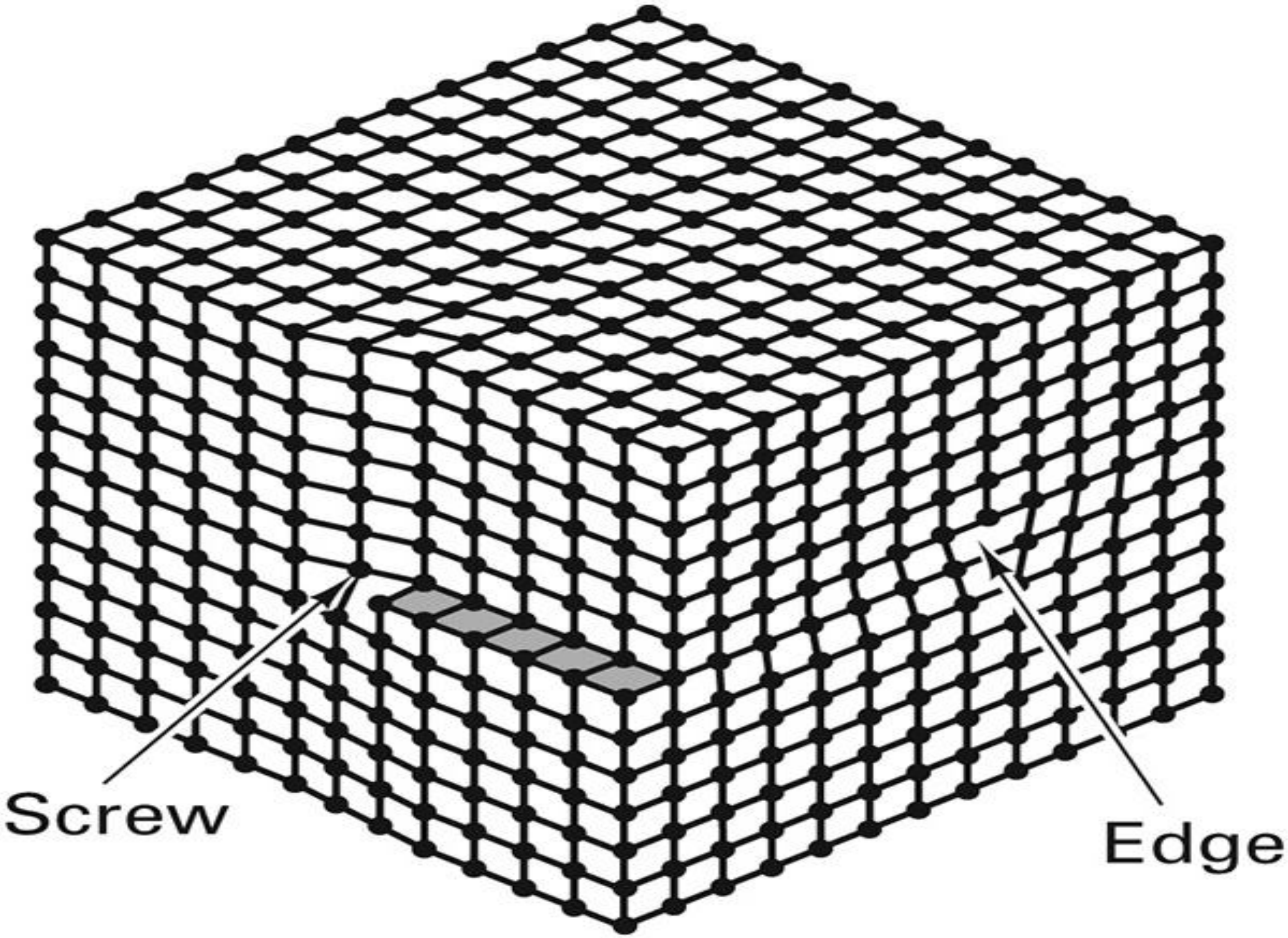
- As a load is applied to a material, distortion increases until
  - Bonds are broken to produce a fracture
  - Atoms slide over one another to reduce the load
- Results in a permanent change in shape in the material that does not deteriorate its properties
- Plastic deformation occurs by the sliding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

Dislocation Theory of Slippage

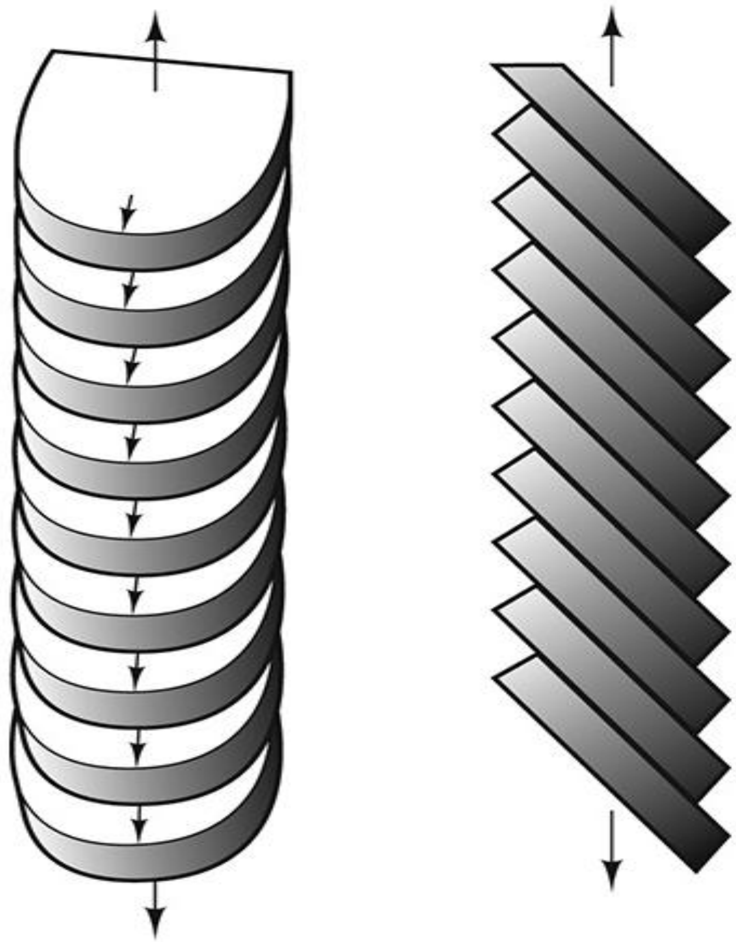
- Deformation is the result of the progressive slippage of a localized disruption known as a dislocation
- Localized imperfections
  - Edge dislocation
    - Edges of extra half-planes of atoms
  - Screw dislocation
    - Partial tearing of the crystal plane

Figure 3-16 Schematic representation of screw and edge dislocations.

SCREW AND EDGE DISLOCATION



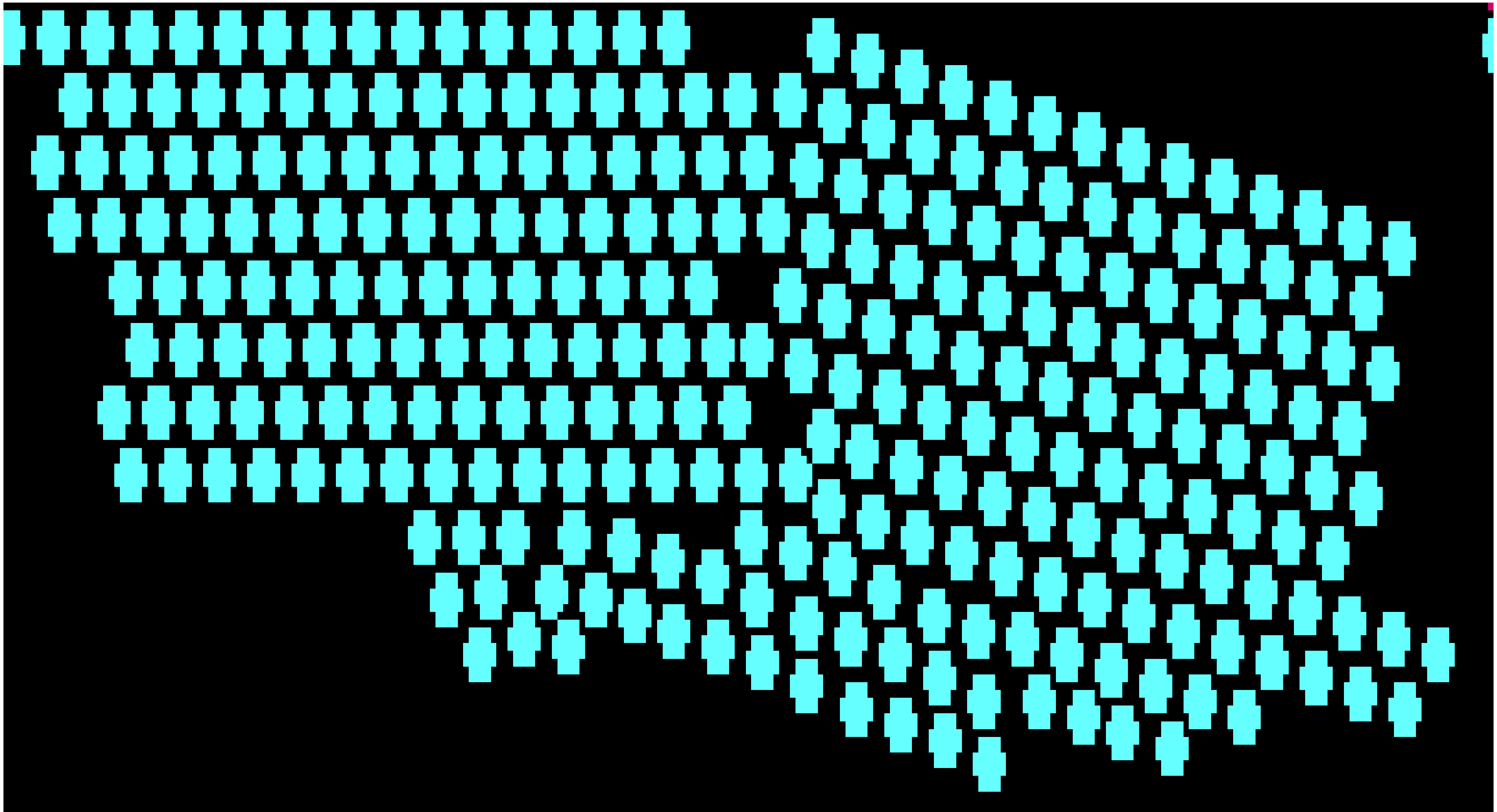
SCHEMATIC OF PLASTIC DEFORMATION



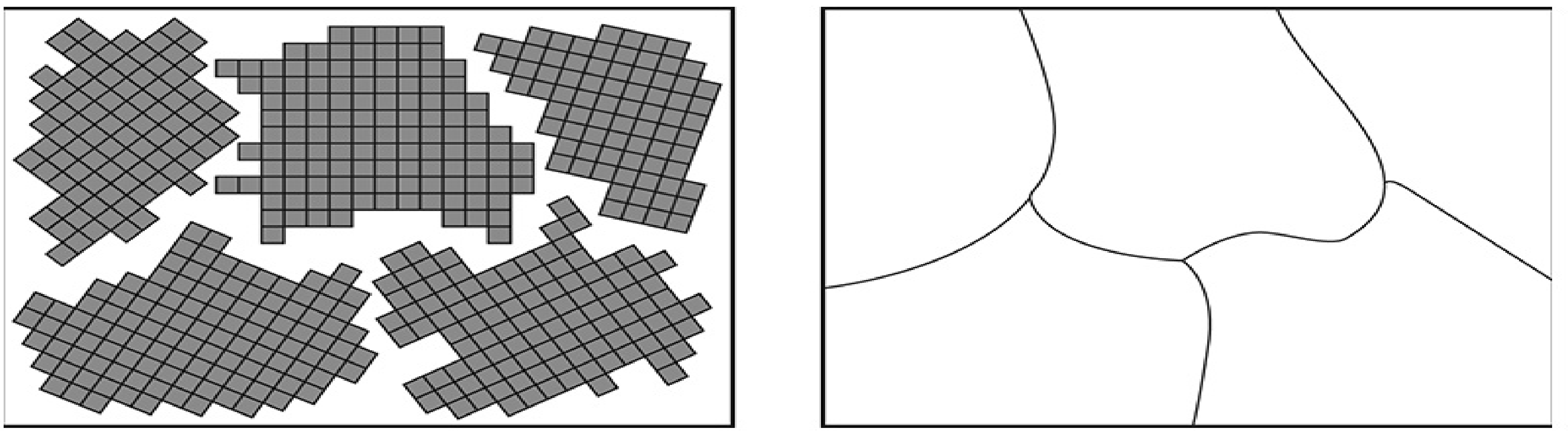
Grain Growth

- 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

CRYSTAL STRUCTURE



CRYSTAL GROWTH



Grain Shape and Anisotropic Properties

- 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

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

GRAIN SIZE VS PROPERTIES

- For low carbon steels and aluminum the grain size less than 1 μm, the materials usually exhibit high strength and low uniform elongation.
- In the grain size greater than 10 μm, 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 bestfor 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 POLYCRYSTAL MATERIALS

- Single crystal materials are occasionally used as structural materials,
- Polycrystalline materials are commonplace.
- The differences between single crystal and polycrystalline materials are 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 POLYCRYSTAL 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

SINGLE VS POLYCRYSTAL MATERIALS,III

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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