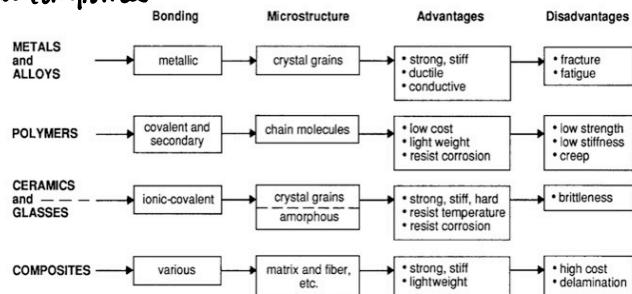


Structure, Defects, and Deformation in Materials

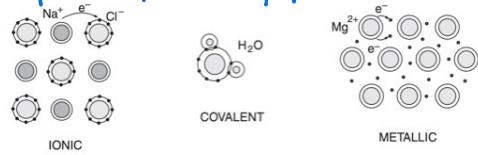
Engineering materials are used in applications where resistance to mechanical loading is necessary and are broadly classified as metals + alloys, polymers, ceramics and glasses, and composites



- strong chemical bonding in ceramics and glasses imparts mechanical strength and stiffness (high E), and also temp + corrosion resistance, but causes brittle behavior
- many polymers are relatively weakly bonded between the chain molecules, in which case the material has low strength and stiffness and is susceptible to creep deform.

Bonding in Solids

Primary bonds - ionic, covalent, + metallic; strong + stiff, don't easily melt w/↑ temperature
• responsible for bonding of metals + ceramics, provide the relatively high elastic mod. E

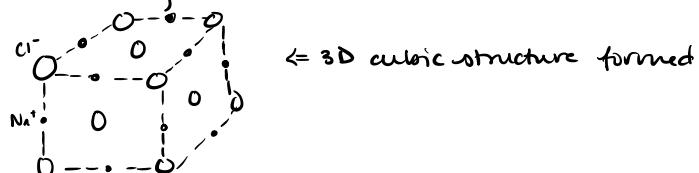


Ionic bonding involves xfer of 1 or more e^- between atoms of different types (remember that the outer shell of e^- surrounding an atom is stable if it contains 8 e^- ; except 2 for H + He)

ex. atom of metal Na w/only 1 e^- in its outer shell can donate to an atom of Cl⁻ which has an outer shell of 7 e^-

→ atoms become charged ions such as Na^+ or Cl^- which attract one another due to their opposite electrostatic charges

→ collection of charged ions forms an electrically neutral solid by arrangement into a regular crystalline array



many common salts, oxides, and other solids have bonds that are mostly or partially ionic and these materials tend to be hard and brittle

Covalent bonding involves the sharing of e^- and occurs where the outer shells are half full or more than half full; shared e^- can be thought of as allowing both atoms involved to have stable outer shells of 8 (or 2) e^-

ex. 2 H each share an e^- w/ O to make H_2O ; 2 Cl share e^- to make diatomic Cl_2

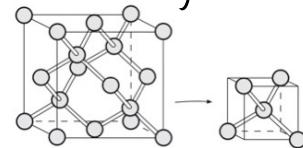
→ tight covalent bonds make molecules relatively independent of one another, so collection of them tend to form liquids or gases at ambient temp

Metallic bonding is responsible for the usually solid form of metals and alloys

- for metals, outer shell of e^- usually $< \frac{1}{2}$ full; each atom donates its outer-shell e^- to a "cloud" of $e^- \Rightarrow$ thus are shared in common by all of the metal atoms which have become \oplus charged ions as result of giving up e^-
 \rightarrow ions thus held together by their mutual attraction to the e^- cloud

Discussion of P bonds

- covalent bonds only have property of being strongly directional; this arises from covalent bonds being dependent on the sharing of e^- with specific neighboring atoms (while ionic + metallic solids held together by electrostatic attraction involving all neighboring ions)
- continuous arrangement of covalent bonds can form a 3D network to make a solid
- carbon in the form of diamond (shown) in which each C shares an e^- w/ 4 adjacent C and these atoms are arranged at equal angles to one another in 3D space
 \rightarrow as a result of the strong and directional covalent bonds, diamond (in its diamond cubic crystal structure of carbon) has the highest melting temp, highest hardness, and highest elastic mod E of all known solids
- many solids, such as SiO_2 and other ceramics, have chemical bonds that have a mixed ionic-covalent character ... note that mixed bonding is most common
- metals of more than 1 type may be melted together to form an alloy (metallic bonding)

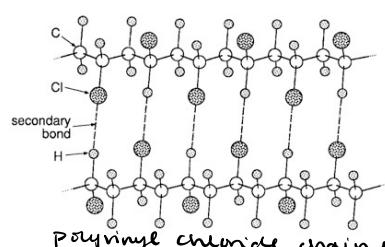


Secondary bonds (van der Waals and H-bonding) occur due to the presence of an electrostatic dipole which can be induced by a primary bond

- in H_2O , the side of H atom away from the covalent bond to O atom has a positive charge due to the sole e^- being predominantly on the side toward the O atom
 \rightarrow conservation of charge over the entire molecule then requires a negative charge on the exposed portion of the O atom \Rightarrow the dipoles formed cause an attraction between adjacent molecules, enabling the formation of liquid H_2O
 \hookrightarrow these are termed "permanent dipole bonds" and though relatively weak, nevertheless sufficient to bind materials into solids (water being ice)
- where the 2° bond involves H, such as in H_2O , it's stronger than other dipole bonds and is called hydrogen bonding

Van der Waals bonds arise from fluctuating positions of e^- relative to an atom's nucleus \Rightarrow uneven distribution of electric charge that occurs causes a weak attraction between atoms or molecules ... such fluctuating dipole bonds affect the behavior of some liquids and allow the inert gases to form liquids + solids @ low temp

- in polymers, covalent bonds form the chain molecules and attach H and other atoms to the C backbone; H bonds and other 2° bonds occur between the chain molecules and tend to prevent them from riding past one another
 \rightarrow polyvinyl chloride
 \rightarrow relative weakness of 2° bonds accounts for low melting temp and low strength and low stiffness



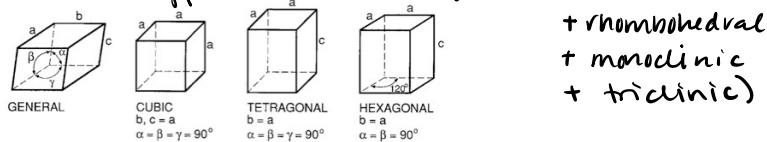
Structure in Crystalline Materials

- metals + ceramics composed of aggregation of small grains, each of which is an individual crystal
- glasses have an amorphous or noncrystalline structure
- polymers are composed of chainlike molecules, sometimes arranged in regular arrays in a crystalline manner

BASIC CRYSTAL STRUCTURES

arrangement of atoms (or ions) in crystals can be described in terms of the smallest grouping, called a **unit cell**, that's considered to be a building block for a perfect crystal

→ 7 basic types of unit cells (shown + orthorhombic



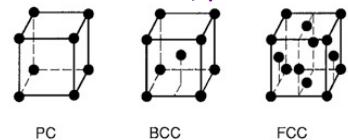
+ rhombohedral
+ monoclinic
+ triclinic)

- 3 crystal structures having a cubic unit cell are the **primitive cubic (PC)**, **body-centered cubic (BCC)**, and **face-centered cubic (FCC)** structures

→ PC rare

→ BCC in many common metals: chromium, iron, molybdenum, sodium, tungsten

→ FCC also common in metals: silver, aluminum, lead, copper, nickel



- the **hexagonal close-packed (HCP)** crystal structure also common in metals; 2 parallel planes called basal planes have atoms @ corners and center of hexagons and there's three additional atoms halfway between these planes
ex. beryllium, magnesium, titanium, zinc

- a given metal may change its crystal structure w/ temp or pressure, or w/ addition of alloying elements

MORE COMPLEX CRYSTAL STRUCTURES

- compounds formed by ionic or covalent bonding, such as ionic salts and ceramics, have more complex crystal structures than elemental materials due to necessity of accommodating more than one type of atom and to the directional aspect of even partially covalent bonds

→ however, structure can often be thought of as an elaboration of one of the basic crystal structures

→ in diamond cubic structure of C, $1/2$ atoms form FCC, other $1/2$ sit at intermediate positions also forming FCC

- polymers may be amorphous (irregular tangle of chain molecules) while portions may have chains arranged in a regular manner (shown)



Defects in Materials

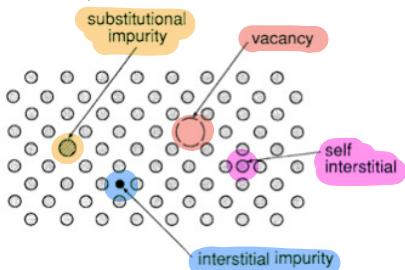
DEFECTS IN CRYSTALS

POLYCRYSTALLINE MATERIALS are composed of crystalline grains separated by grain boundaries and grain sizes vary widely

→ even w/in grains, crystals are not perfect, w/defects occurring that are classified as

1. point defects
2. line defects
3. surface defects

Four Types of (1) Point Defects



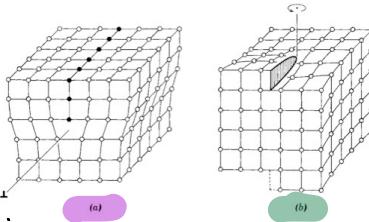
substitutional impurity occupies a normal lattice site but is an atom of different element than bulk material
vacancy is the absence of an atom at a normally occupied lattice site
an **interstitial** is an atom occupying a position between normal lattice sites; if interstitial is of same type as bulk material, called a **self interstitial**, and if another kind it's called an **interstitial impurity**

- relatively small impurity atoms often occupy interstitial sites in materials w/larger atoms (ex. C in Fe)
- if impurity atoms are of similar size to those of bulk material, more likely to appear as substitutional impurities (normal when 2 metals are alloyed, that is melted, together)

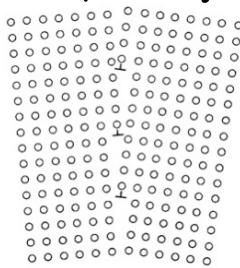
most important class of (2) Line Defects are **dislocations**

- where a line of crystal disruption occurs relative to a normal arrangement of lattice planes

Edge dislocation can be thought of as an extra $\frac{1}{2}$ -plane of atoms residing within an otherwise perfect crystal (note that the dislocation line is shown as the edge of the extra plane)



Screw dislocation can be visualized by assuming that a perfect crystal is cut as shown, then the crystal is displaced parallel to the cut and finally reconnected into the configuration shown; the dislocation line is the edge of the cut, and hence the line where the disruption originates



Grain boundaries can be thought of as a class of (3)-surface defect where the lattice planes change orientation by a large angle

- within a grain there may also be **low-angle boundaries** where an array of edge dislocations can form such a boundary (shown)
- several low angle boundaries may exist within a grain, separating regions of slightly different lattice orientation, called **subgrains**

→ other surface defects: **twin boundary** separates 2 regions of a crystal where the lattice planes are a mirror image of one another ... if lattice planes are not in the proper sequence for a perfect crystal, a **stacking fault** is said to exist

OTHER DEFECTS

Defects not closely related to the crystal structure include pores, inclusions, cracks, + slip bands

Pores are voids in an otherwise solid material

- strength + stiffness of material decreases for greater volume fractions of porosity
ex. engineered ceramics from sintering, metal parts from casting, molding, welding

Inclusions are particles within the crystal structure that are not soluble in the parent material

- if large number of inclusions, performance of material decreases

Cracks obvious defects that may start from pores, inclusions, surface scratches, or surface roughness, as a result of these features acting as local stress concentrators when stresses applied to material

- cyclic stresses especially likely to cause cracks

slip band riding may occur along certain planes within a crystal grain and this arises from dislocation motion

Elastic Deformation + Theoretical Strength

ELASTIC DEFORMATION

- remember: elastic deformation is associated with stretching, but not breaking, the chemical bonds between the atoms in a solid

- if an external stress is applied to a material, the distance between the atoms changes by a small amount that depends on the material and the details of its structure and bonding

- if the atoms in a solid were far apart, there wouldn't be forces between them

- as distance x between atoms \downarrow , attraction according to the type of bonding that applies \uparrow

- a repulsive force also acts that's associated w/ resistance to overlapping of the e^- shells of the 2 atoms

- the repulsive force is smaller than the attractive force at relatively large distances, but it increases more rapidly, becoming larger at short distances

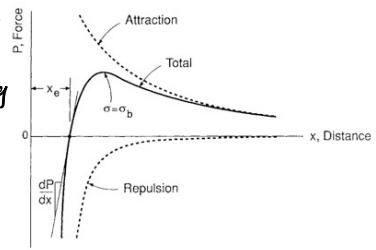
- \Rightarrow the total force is thus attractive at large distances, repulsive at short distances, and zero at one particular distance x_e which is the equilibrium atomic spacing (this is also the pt of min. potential energy)

$$\sigma = \frac{F}{A} \quad \varepsilon = \frac{x - x_e}{x_e} \quad E = \left. \frac{d\sigma}{d\varepsilon} \right|_{x=x_e} = \frac{x_e}{A} \left. \frac{dP}{dx} \right|_{x=x_e}$$

* from image:

\rightarrow the slope dP/dx at equilibrium spacing x_e is proportional to the elastic modulus E

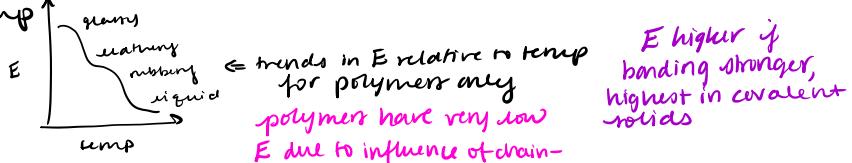
\rightarrow the stress σ_b , corresponding to the peak in total force, is the theoretical cohesive strength



TRENDS IN ELASTIC MODULUS VALUES

- strong primary chemical bonds are resistant to stretching and so result in a high value of E

- ex. strong covalent bonds of diamond $E=1000$ GPa vs. weaker metallic bonds in metals give values generally w/in a factor of 3 of 100 GPa vs. polymers whose E changes w/temp



THEORETICAL STRENGTH

- the theoretical cohesive strength of a solid can be obtained by using solid-state physics to estimate the tensile stress necessary to break primary chemical bonds, which is the stress σ_b corresponding to the peak value of force

- rather than bonds being pulled apart in tension, another possibility is shear failure

Theoretical shear strength τ_b

is maximum value as γ varies $\tau = \tau_b \sin\left(\frac{2\pi x}{b}\right)$ * the initial slope is then the shear modulus G (displacement $\gamma = x/b$) $G = \left. \frac{d\tau}{d\gamma} \right|_{x=0} = \left. \frac{h\partial\tau}{\partial x} \right|_{x=0}$

with x

thereby obtaining $\frac{d\tau}{dx}$ and substituting its value at $x=0$ gives τ_b :

$$\tau_b = \frac{Gb}{2\pi h}$$

the ratio b/h varies with the crystal structure, generally around 0.5 to 1

→ in a tension test, the maximum shear stress occurs on a plane 45° to the direction of uniaxial stress and is $\frac{1}{2}$ as large

∴ theoretical estimate of shear failure in a tension test is : $\sigma_b = 2\tau_b = \frac{Gb}{\pi h}$

small whiskers of crystals can be made that are nearly perfect single crystals. also, thin fibers and wires may have a crystal structure such that strong chemical bonds are aligned w/ the length direction

→ tensile strengths in such cases are much high than for larger and more imperfect samples of material

Inelastic Deformation

* inelastic deformation that occurs almost instantly as the stress is applied is called plastic deformation, as distinguished from creep deformation, which occurs only after passage of time under stress

PLASTIC DEFORMATION BY DISLOCATION MOTION

- single crystals of pure metals experience plastic deform. by shear at very low stresses such as through edge dislocation
 - plastic deform. proceeding one line of atoms at a time, does not occur simultaneously over an entire plane
- the plane in which the dislocation line moves is called the **slip plane** and where the slip plane intersects a free surface, a **slip step** is formed
- dislocations in real crystals are usually curved and thus have both **edge** and **screw** character, plastic deform. actually occurs by a combination of the 2 types of dislocation motion
- plastic deform. often concentrated in bands called **slip bands** and these are regions where numerous dislocations move on several adjacent planes

* for a given crystal, slip is easier on certain planes and w/in these planes in certain directions

- preferred planes are those on which the atoms are relatively close together, called **close-packed planes**, such as the basal plane for HCP
- similarly, the preferred slip directions w/in a given plane are the **close-packed directions** in which the distances between atoms is smallest

* process of plastic deformation by incremental motion of dislocations results in slip, aka relative sliding of crystal planes

→ various methods can be employed to ↑ the stress required for dislocation motion, and hence the yield strength

- such strengthening methods include cold work, grain size refinement, alloying, and introducing hard particles or other discontinuities into the crystal structure

CREEP DEFORMATION

- in addition to elastic & plastic deformation, materials deform by mechanisms that result in markedly time-dependent behavior called **creep**
- under constant stress, the strain varies w/time
 - there's initial elastic deformation ϵ_e
 - then strain slowly ↑ as long as stress maintained
 - if stress removed, elastic strain is quickly recovered, portion of creep strain may be recovered slowly w/time; rest remains @ permanent deformation
- distinguishing characteristic of creep is that deformations can occur at stresses below the yield strength
- in crystalline materials (metals, ceramics) an important mechanism of creep that occurs at low stresses is due to the **diffusional flow** of vacancies (vacancies previously introduced as defect associated w/moving atom at a crystal lattice site)
 - vacancies tend to form in crystal locations where atoms are elastically stretched in response to a tensile stress, and tend to be deficient in regions where interatomic spacings are less than the equilibrium spacing, due to compression
 - thus an uneven distribution of vacancies will exist in a sample or component subjected to a stress, resulting in vacancies diffusing (moving) from regions of high concentration to regions of low
 - * movement of a vacancy in one direction is equivalent to the movement of an atom in the opposite direction
 - accumulated movement of vacancies ↑ over time and is strongly temp dependent
 - overall effect is change in shape of grain that ↑ over time
- another creep mechanism is **dislocation creep** where dislocation motion can occur in time-dependent manner @ stresses below the yield strength
- time-dependent creep deformation especially likely at temperatures approaching melting
 - ↪ in polymers, get sliding of chain molecules

