

# Unit M3.3

## Physical Bases of Elastic Properties

Readings:

A & J 4, 5, 6

16.001/002 -- “Unified Engineering”  
Department of Aeronautics and Astronautics  
Massachusetts Institute of Technology

## LEARNING OBJECTIVES FOR UNIT M3.3

*Through participation in the lectures, recitations, and work associated with Unit M3.3, it is intended that you will be able to.....*

- ....**identify** the various types of atomic bonds and the factors involved in such
- ....**describe** the atomic/molecular structure of materials and the effects on basic material behavior
- ....**employ** an atomic model to estimate the elastic modulus of materials
- ....**explain** the make-up of a composite and the contributors to its elastic response

We have seen that we can characterize materials on a macroscopic basis using homogenized elastic properties. But these elastic properties do depend on the microscopic reality of the material and thus we look at the “structure of the material”.

Also will give us some idea as to how we might affect/control properties

At the most basic level, a material is made up of atoms, so let's first look at this level and consider the origin of the...

## Energy and Force: Atomic Bonds

There are two parts to the contribution atomic bonds make:

1. Strength/Stiffness of Bond -- depends on type of bond

Think of two atoms connected by a spring (often nonlinear):

**Figure M3.3-1 Representation of interatomic bond as atoms connected by spring**

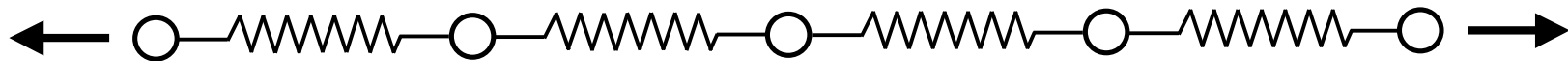


Stiffness of spring depends on type of bond

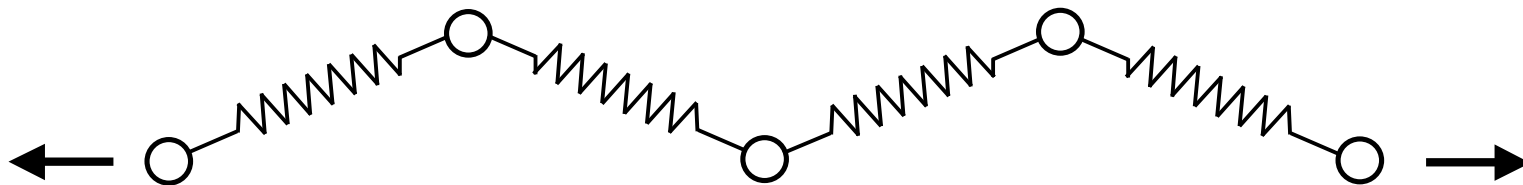
2. Arrangement of atoms and bonds

This is the “structure” of the material

**Figure M3.3-2 Atomic packing represented as array of springs**



*versus*



Top configuration will be stiffer than bottom configuration for same individual bond stiffnesses.

--> Let's first deal with the types of bonds. We can identify two generic types:

### Primary Bonds

- Ionic, covalent or metallic
- Have high melting temperatures (1000°K)
- e.g., metals, ceramics

### Secondary Bonds

- Hydrogen bonds, Van der Waals
- Have lower melting temperatures (100° - 500°K)
- e.g., polymers

There are often a mixture of bond types in one material

--> How does one obtain the bond energy of different types for different materials?

Quoted in chemistry databooks. Gives answer as to whether it is favorable to form bonds for particular situations.

--> Let's first consider each of the three types of...

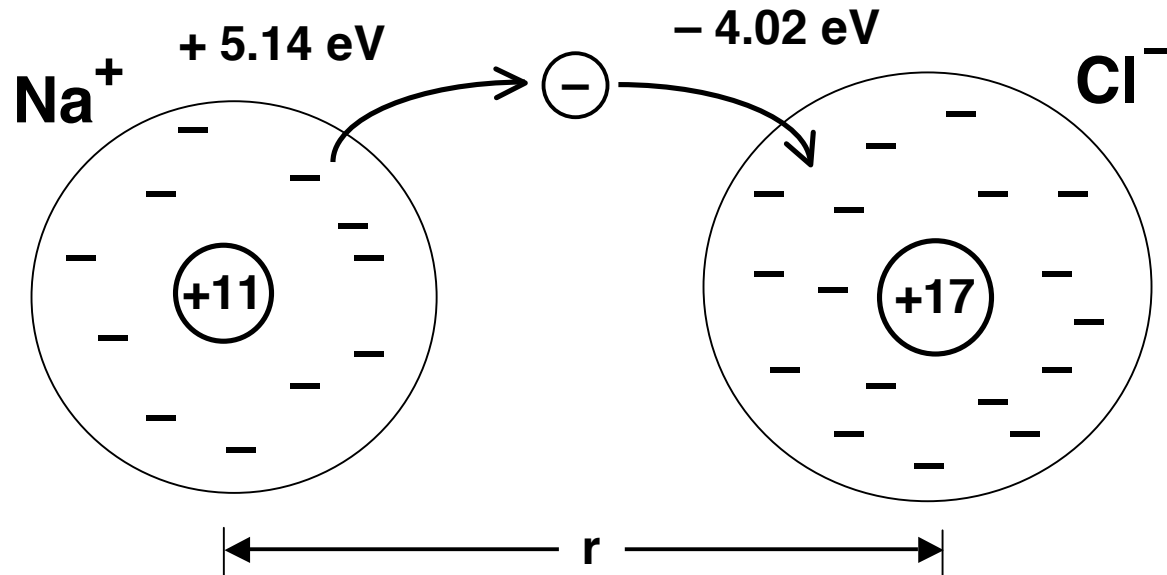
## Primary Bonds

### Ionic Bonding

(e.g., alkali halides, magnesia, alumina)

- Electrostatic attraction between ions
- Electron goes from positive ion to negative ion

**Figure M3.3-3 Example of Ionic Bond to form sodium chloride**



Energy associated with bond:

1. Work of Ionization (removal/gain of electrons) =  $U_i$

It takes  $5.14\text{eV} - 4.02\text{eV} = 1.12\text{eV}$  to make  $\text{Na}^+/\text{Cl}^-$  separate ions

## 2. Work to separate ions

$\text{Na}^+/\text{Cl}^-$  attract in an omnidirectional fashion with:

$$\text{Force} = F_{att} = \frac{q^2}{4\pi\epsilon_o r^2} \quad (\epsilon_o = \text{permittivity})$$

Force between charged particles

And the energy is the integral of the force needed to take these two ions from  $\infty$  (fully separated) to a distance  $r$  (the equilibrium distance):

$$\text{Energy} = U_{att} = \int_r^\infty F dr = \frac{-q^2}{4\pi\epsilon_o r}$$

## 3. Repulsive Energy

There is a repulsive force due to the electronic charge distributions in the atoms. This has the form:

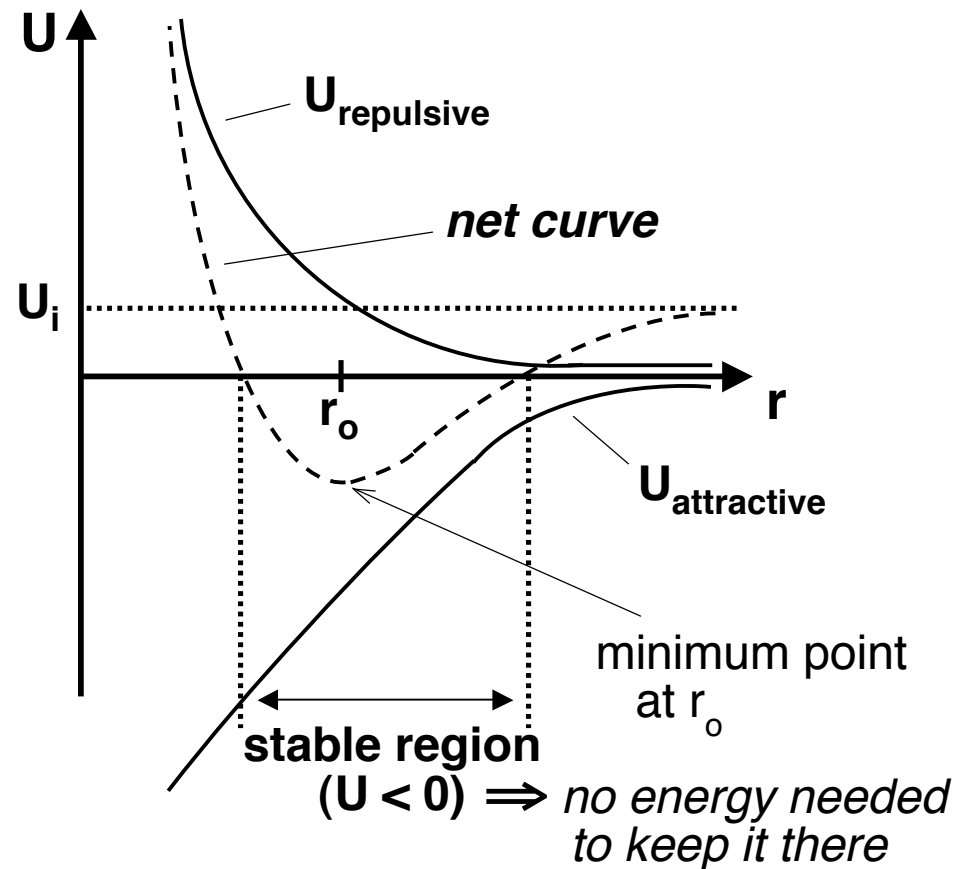
$$U_{rep} = \frac{B}{r^n}$$

Finally we add these parts to get the total energy:

$$U = U_i + U_{att} + U_{rep}$$

$$\Rightarrow U = \frac{-q^2}{4\pi\epsilon_0 r} + \frac{B}{r^n}$$

**Figure M3.3-4 Representation of energies associated with ionic bonding for NaCl**





Note: Ionic bonds are omni-directional -- charged particles attract equally in all directions

⇒ leads to isotropic behavior, but different sized ions lead to non-isotropic behavior

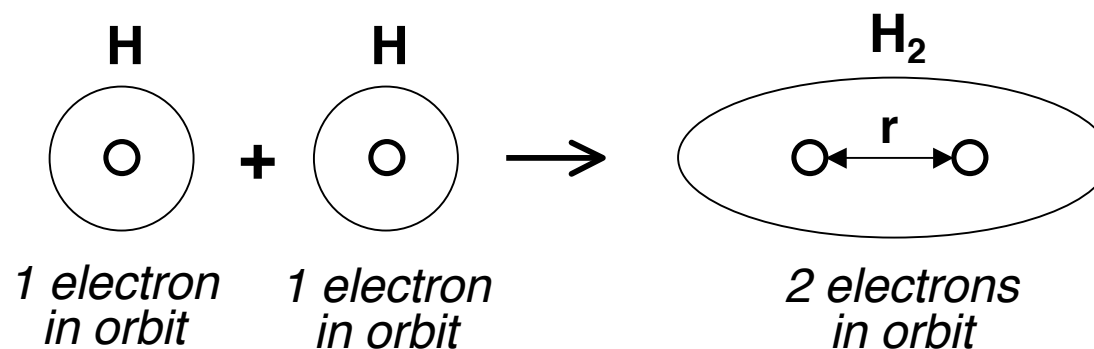
The next bond type is the....

--> Covalent Bonding

(e.g., diamond, silicon, glasses, some metals, also polymer chains)

- Electron shared by two (or more) atoms
- Very strong

**Figure M3.3-5 Example of covalent bond to form hydrogen molecule**

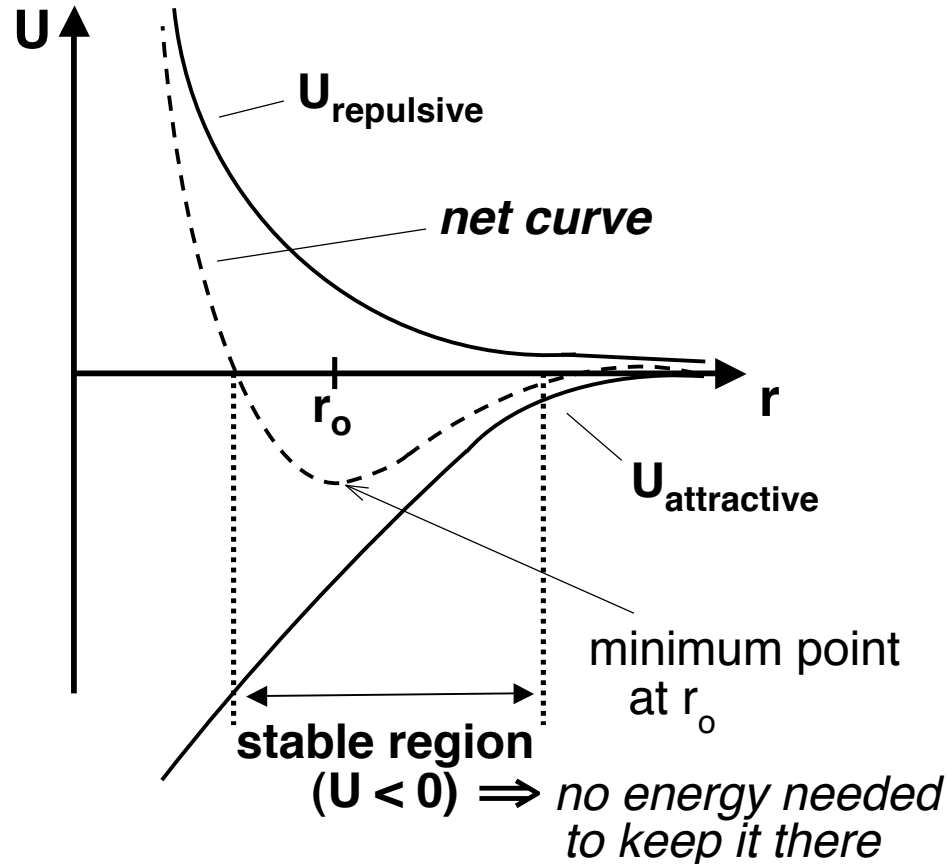


Shared electron goes to a new molecular orbit thereby reducing the energy.

The energy is again made of two parts (attractive and repulsive) and can be expressed empirically as:

$$U = \underbrace{-\frac{A}{r^m}}_{\text{attractive}} + \underbrace{\frac{B}{r^n}}_{\text{repulsive}} \quad \begin{array}{l} \text{(with } m < n) \\ \text{(} m > 2) \end{array}$$

**Figure M3.3-6 Representation of energies associated with covalent bond**



For most other atoms (e.g., diamond), the shared orbital paths have preferred directions and thus covalent bonds are generally highly directional.

Note: Generally ceramics are bonded by a mixture of ionic and covalent bonds.

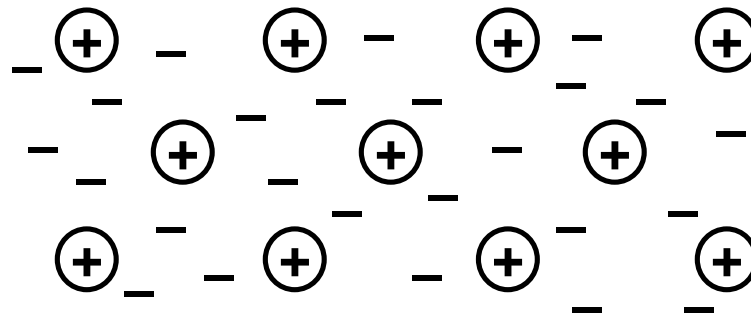
the final primary bond type is the.....

--> Metallic Bond

(dominant in metals and alloys)

- A “sea” of free electrons which have “left” highest energy atoms (making them ions)

**Figure M3.3-7 Representation of free electrons in metallic bonding**



⊕ = ions

- = free electrons

There is attraction and repulsion in this mix of positive and negative charges. This can be best represented by an expression of the same form as for a covalent bond:

$$U = - \underbrace{\frac{A}{r^m}}_{\text{attractive}} + \underbrace{\frac{B}{r^n}}_{\text{repulsive}} \quad (m < n)$$

Notes:

- Easy movement of electrons leads to high electrical conductivity of metals
- No directionality of this configuration (with regard to bonds)  $\Rightarrow$  “*omni-directional*”

Now let's quickly consider....

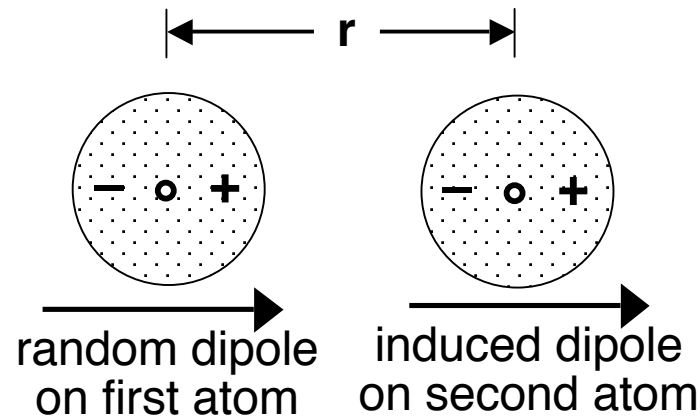
## Secondary Bonds

First consider....

--> Van der Waals Bonding

- Dipolar attraction between uncharged atoms
- Instantaneous position of outer electrons induces change in neighboring atoms (distribution of charge due to motion of atom)

**Figure M3.3-8 Representation of Van der Waals bonding**

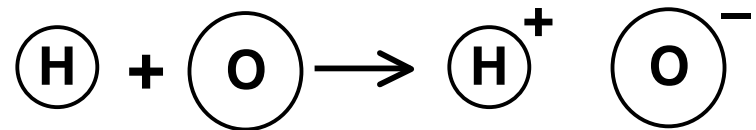


next....

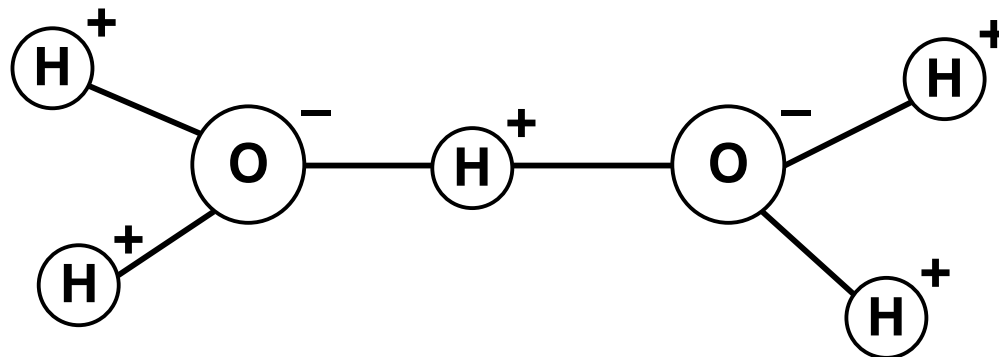
--> Hydrogen Bonding

- Hydrogen atom gives up charge to nearest oxygen atom
- Occurs in water and other polar liquids

**Figure M3.3-9 Representation of hydrogen bonding**



and the neighboring  $\text{H}^+$  acts as a bridging bond between neighboring  $\text{O}^-$  's



This forms repetitive and cross pattern ( $\text{H}_2\text{O}$ )

Note: for both secondary bonds, the energy is again empirically distributed as the sum of two parts:

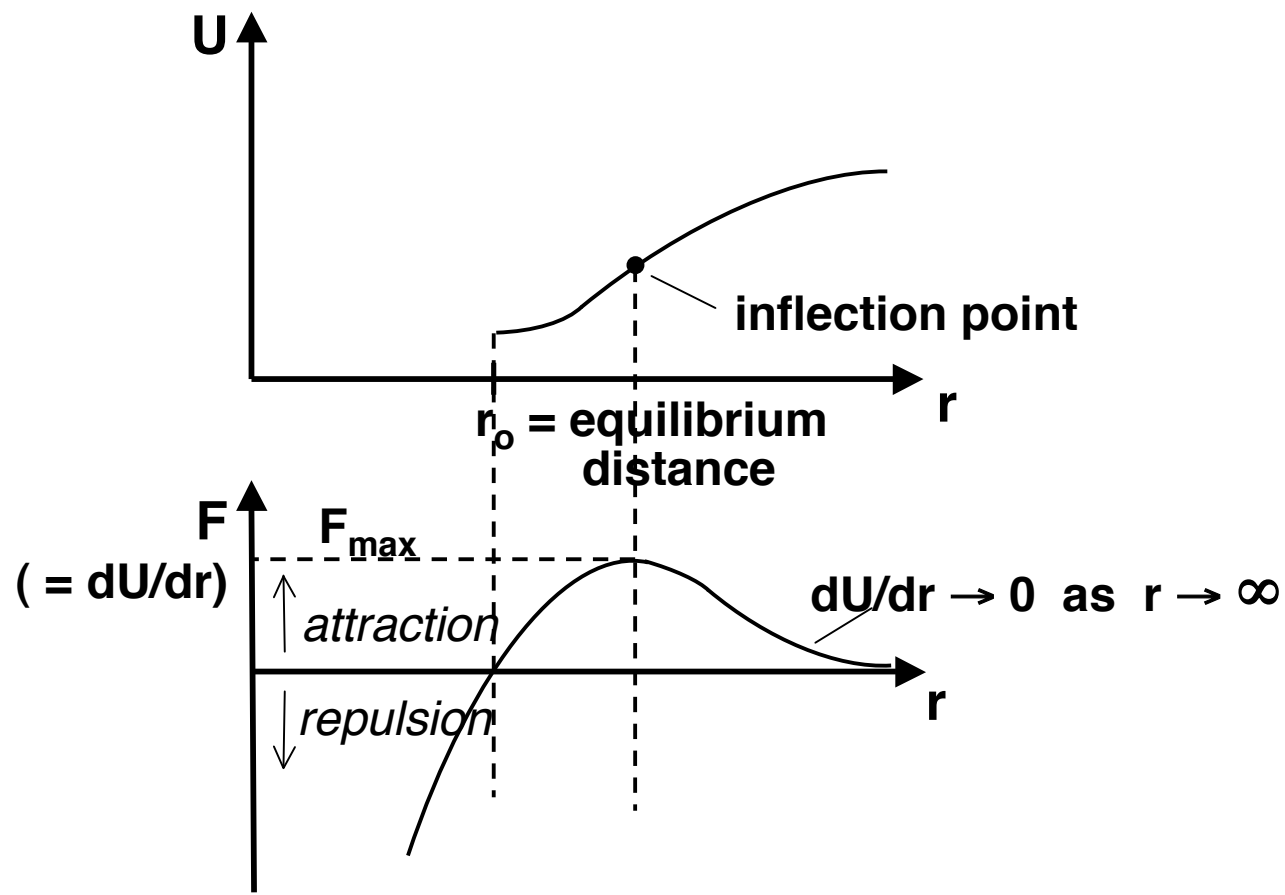
$$U = \underbrace{-\frac{A}{r^m}}_{\text{attractive}} + \underbrace{\frac{B}{r^n}}_{\text{repulsive}} \quad (m < n)$$

with the value of  $m$  for secondary bonds being larger than the value for primary bonds.

--> One can get force by noting that force is the derivative of energy:

$$F = \frac{dU}{dr}$$

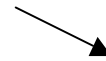
**Figure M3.3-10 Relationship of (bonding) energy and force**



--> Note that the stiffness of an individual bond is the derivative of the force of the bond

$$\text{Stiffness of bond} = S_{bond} = \frac{dF}{dr} = \frac{d^2U}{dr^2}$$

This is linear in a region near the equilibrium distance  $r$



will return to this point (i.e., linear elastic modulus)

--> Let's now consider material types and how atoms are arranged (structure) and the types of bonds as well....

## Metals and Ceramics: Atomic Packing

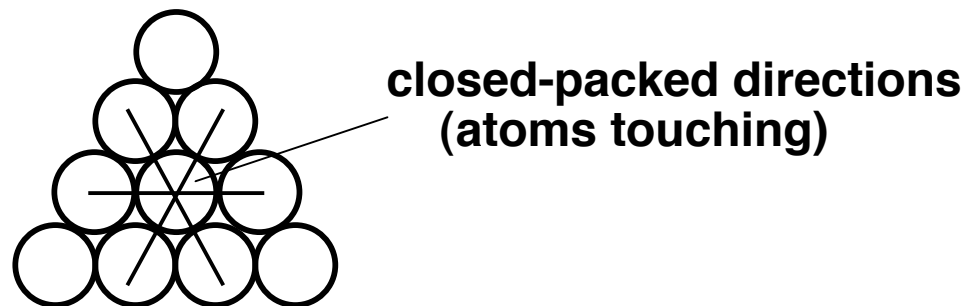
- Many engineering materials composed of small crystals-grains
- Atoms become arranged in certain sequences known as “packing”.
- When the material is crystalline, the atomic structure is the one that minimizes the energy of the crystal



- > Simplification: think of atoms as hard spheres (e.g., pool balls)
- packing in plane
  - stacking of plane to give 3-D crystal

In the plane, often have a “close-packed plane” as a model where spheres take up least space (minimizes energy)

**Figure M3.3-11 Representation of close-packed plane**

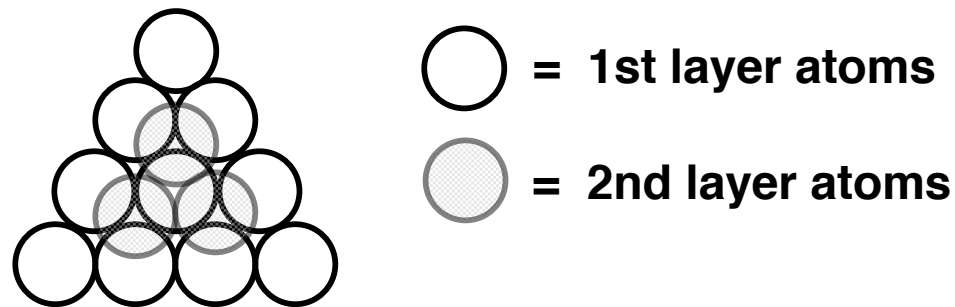


⇒ Each atom has 6 nearest neighbors in-plane

Out of plane, these close-packed planes stack up.

The second layer will logically occur such that the 2nd-layer atoms fit in the gaps of the 1st-layer atoms

**Figure M3.3-12 Representation of 3-D stacking of two adjacent close-packed planes**

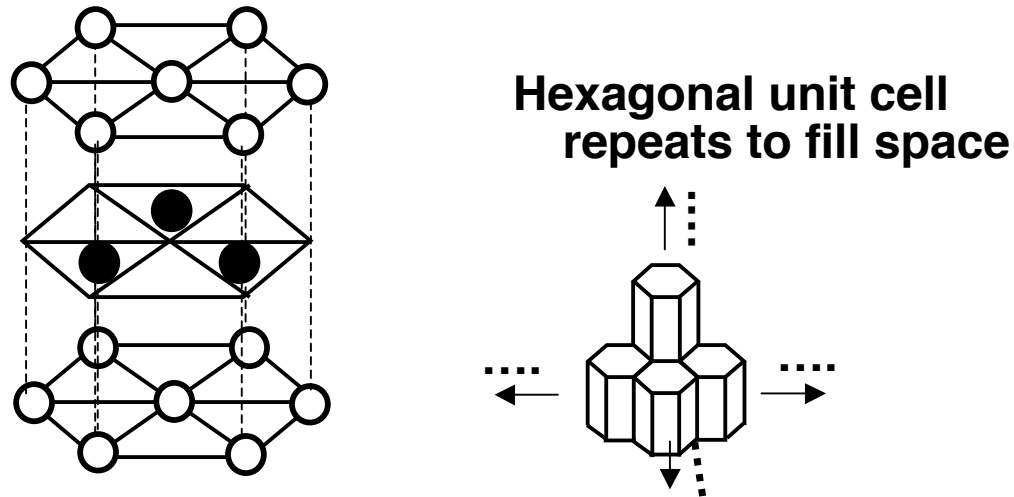


There are then two possibilities for the 3rd layer:

--> Possibility 1: Repeat 1st layer  
 1 - 2 - 1 - 2 - 1 arrangement

Yields close-packed hexagonal: 1 - 2 - 1 - 2 - 1

**Figure M3.3-13 Representation of hexagonal close-packed structure**

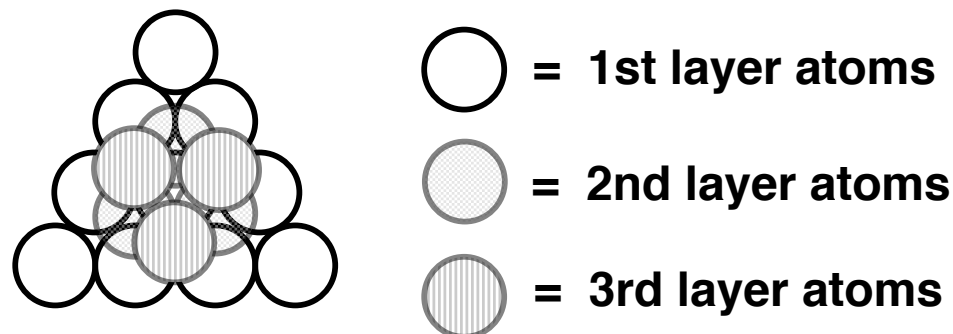


Magnesium (Mg), Zinc (Zn), Titanium (Ti)

--> Possibility 2: 3rd layer fits above unfilled gaps of 1st layer

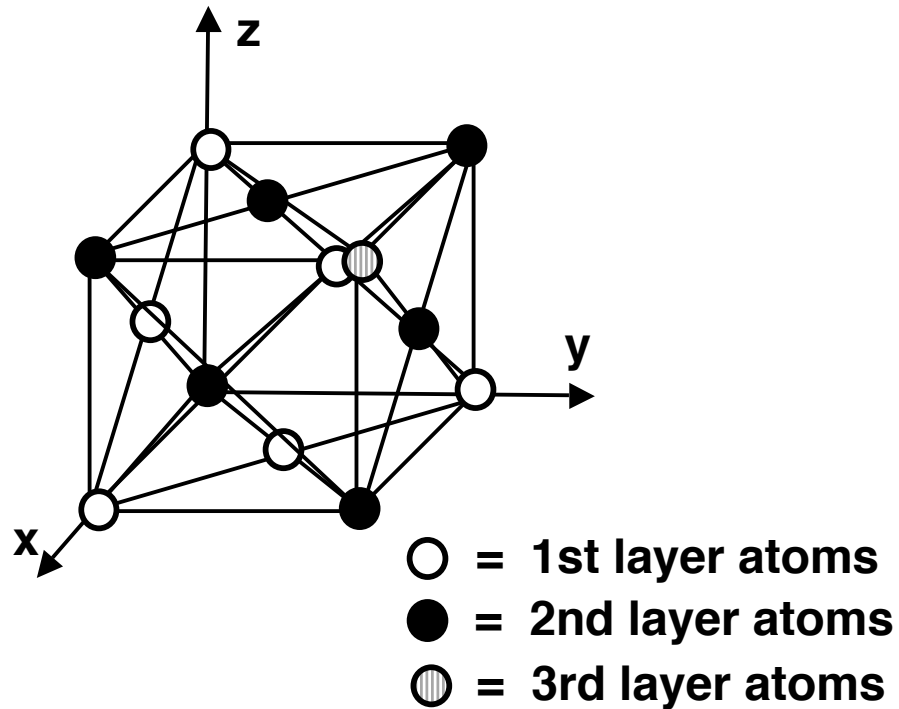
1 - 2 - 3 - 1 - 2 - 3 arrangement

**Figure M3.3-14 Representation of 3-D stacking of three adjacent close-packed planes**

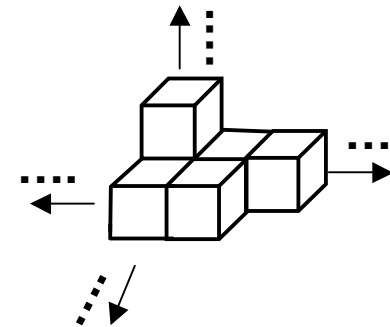


Yields Face-centered-cubic: 1 - 2 - 3 - 1 - 2 - 3

**Figure M3.3-15 Representation of face-centered cubic structure**



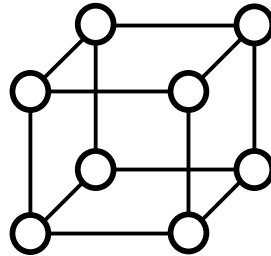
**Cubic unit cell  
repeats to fill space**



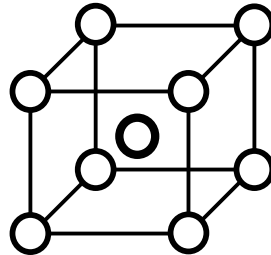
Copper, Gold, Aluminum, Nickel

--> Other arrangements (not close-packed)

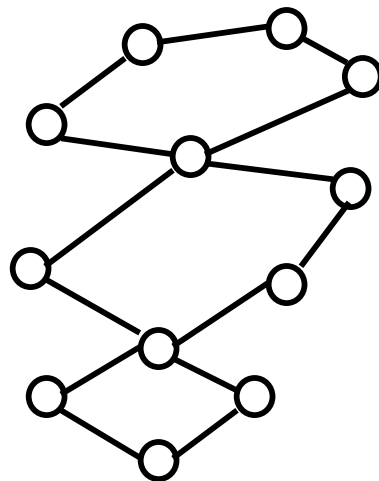
- Cubic (e.g., NaCl)



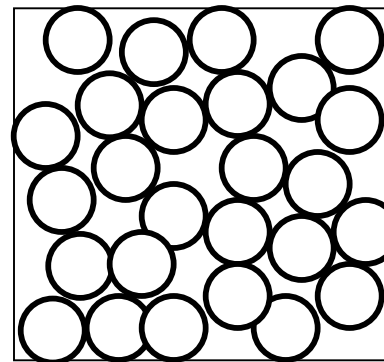
- Body-Centered Cubic (e.g., Iron)



- Random packing (e.g., glasses, amorphous metals)



*in cross-section*



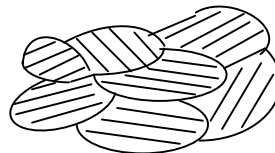
## Notes:

- Packing is not necessarily close-packed (have directional bonds, different sized atoms)
- A material can have more than one structure depending on temperature and mixture (e.g., tin)
- Density of solid reflects mass of atoms and density of packing

--> Finally, let's consider general characteristics of the two material classes:

### Metals:

- metallic bonds (strong and stiff)
- dense packing
- mobile electrons allow good thermal and electrical conductivity
- crystals form grains which make up the bulk material



grains have different orientations overall having no preferred direction

## Ceramics:

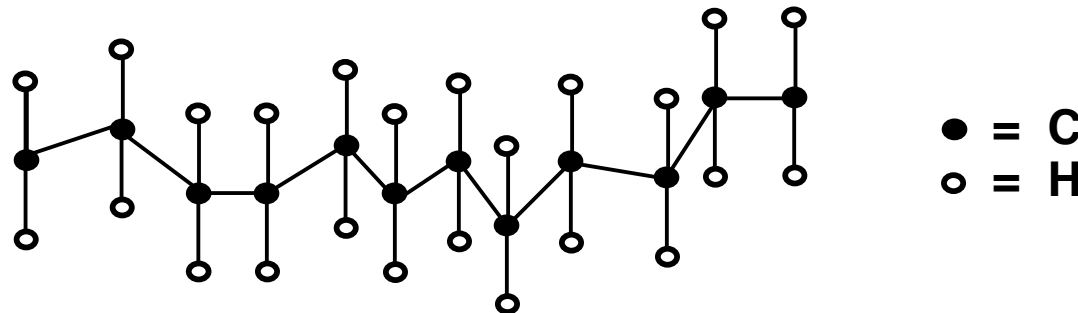
- ionic or covalent bonds (stiff but brittle)
- chemically stable (primary bonds very stable)
- electrons not mobile  $\Rightarrow$  low thermal and electrical conductivity

Now consider....

## Polymers and Their Structures

- Basic structural unit is atoms linked in long chains by covalent bonds (strong). (1000+ carbon atoms)

**Figure M3.3-16 Representation of polymer hydrocarbon chain**

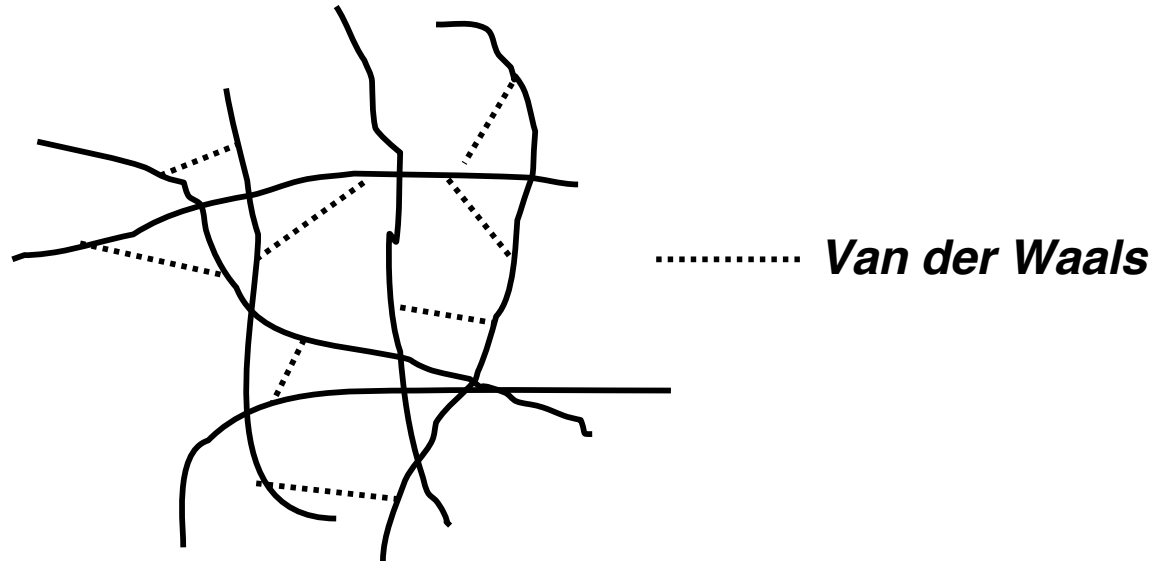


chains are “spaghetti-like” (not straight)

### 3 behaviors:

#### --> Thermoplastics

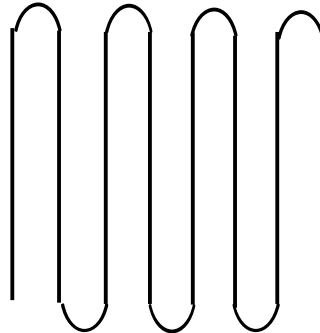
- chains linked by Van der Waals bonds (weak) via side atoms
- chains are generally randomly distributed



results in amorphous behavior



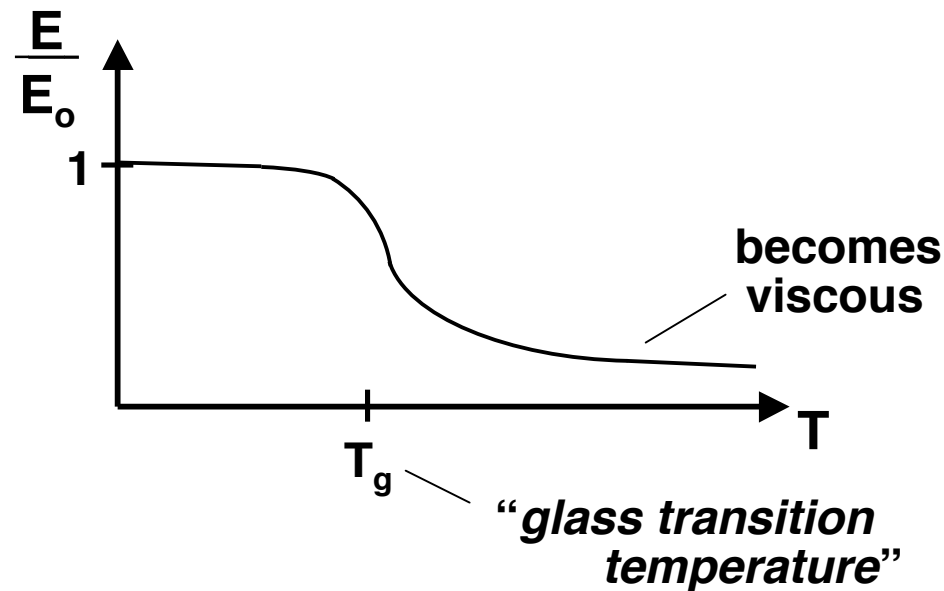
- can have regions where chains align



results in crystalline (region) behavior

Note: As temperature increases, Van der Waals bonds break down reducing stiffness

**Figure M3.3-17 Modulus variation with temperature**



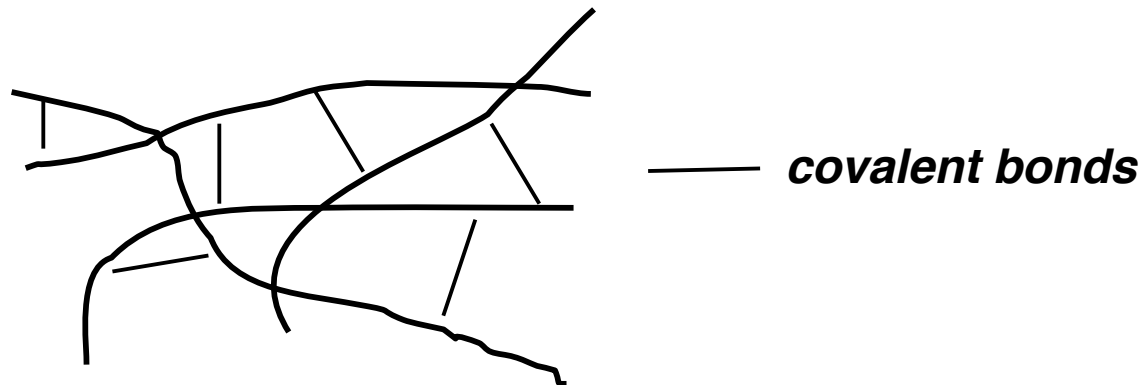
--> Van der Waals limits modulus as these are not stiff bonds

--> Elastomers (Rubbers)

Basically a thermoplastic above  $T_g$  (i.e., no Van der Waals bonds) but with a few covalent crosslinks

--> Thermosets

Carbon chains with covalent crosslinks



There are more covalent bonds  $\Rightarrow$  stiffer behavior

- Typical of epoxies
- As temperature increases, some softening but more breakdown (no recovery as in thermoplastics)

--> Additionally, there are oriented polymers



strong and stiff (e.g., stiffness of C-C band gives modulus of 100 GPa)

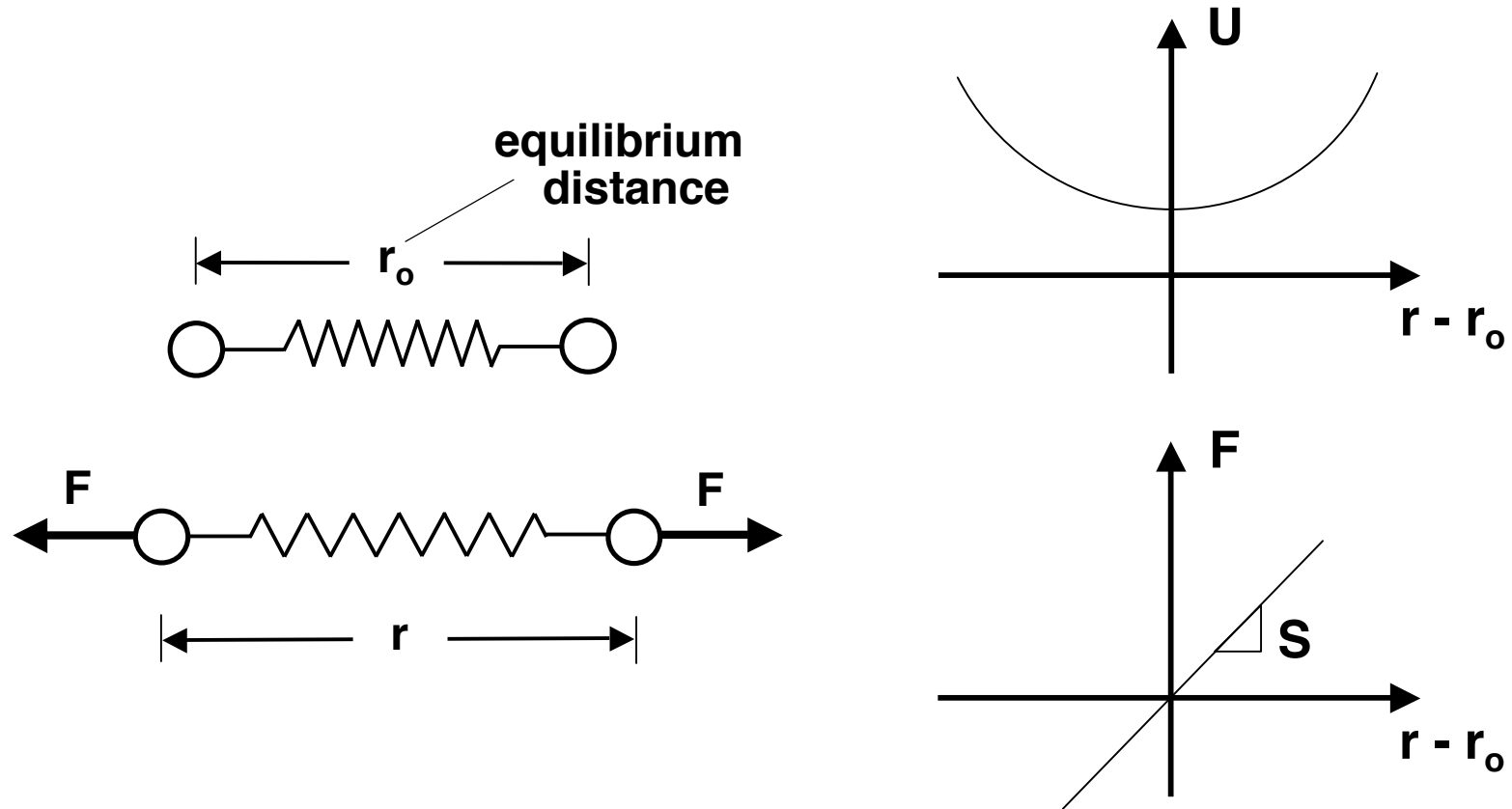
Example: Kevlar fiber

Now that we've described the basic material classes and their structure(s), let's return to the issue of modulus based on the microstructure.....

## Estimate of Moduli

Earlier we looked at atomic bonds, their energy, resulting force and stiffness.

**Figure M3.3-18 Model of a bond as two atoms joined by a spring:**



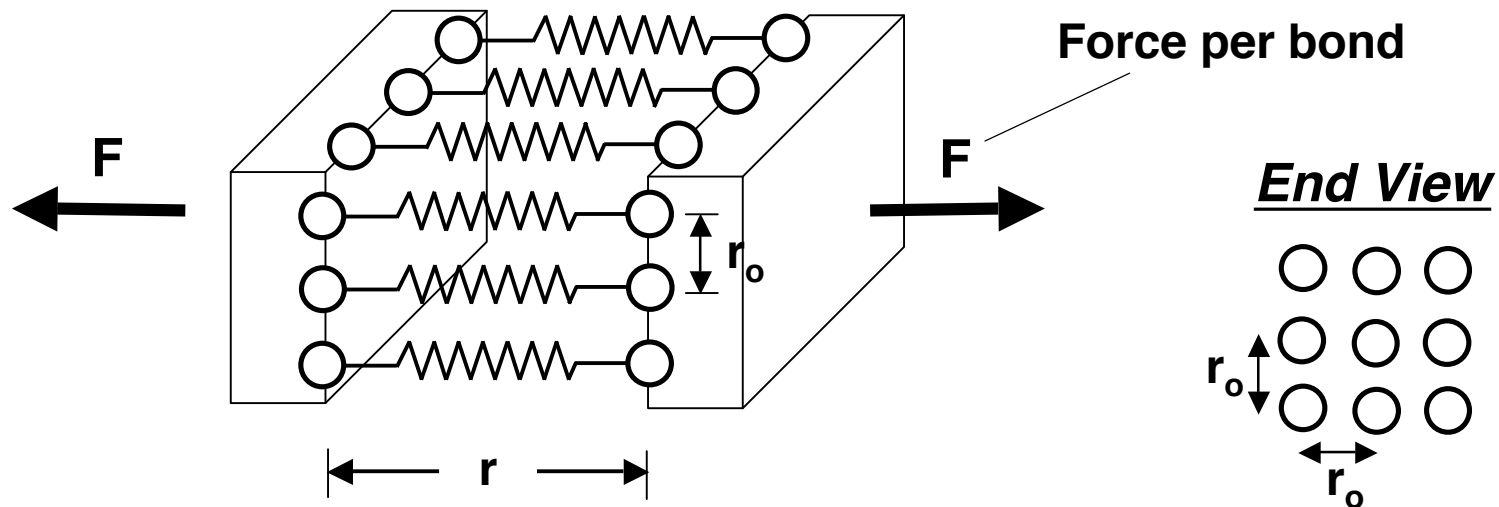
We had:

$$S_0 = \left( \frac{dF}{dr} \right)_{r=r_0} = \left( \frac{d^2U}{dr^2} \right)_{r=r_0}$$

$$\text{So near } r_0: F = S_0 (r - r_0)$$

Now consider (for simplicity), a material with a cubic lattice (atoms at corner of cube with sides of  $r_0$ )

**Figure M3.3-19 Model of material as cubic lattice**



The stress carried by each atom/bond is:

$$\sigma = \frac{F}{A} \quad \text{where } A \text{ is overall area of the face}$$

$$\Rightarrow \sigma = \frac{F}{r_0^2} \quad \text{per atom/bond} = r_0^2$$

And from our previous picture:

$$\delta = r - r_0$$

$$\Rightarrow \varepsilon = \frac{\delta}{r_0} = \frac{r - r_0}{r_0} \quad \text{since } r_0 \text{ is original length}$$

Recall:

$$F = S_0 (r - r_0)$$

$$\Rightarrow \sigma r_0^2 = S_0 (r - r_0)$$

$$\Rightarrow \sigma = \frac{S_0}{r_0} \left( \frac{r - r_0}{r_0} \right)$$

or:

$$\sigma = \frac{S_0}{r_0} \varepsilon$$

Recalling Hooke's law ( $\sigma = E\varepsilon$ ) and comparing gives:

$$\boxed{E = \frac{S_0}{r_0}}$$

$\Rightarrow$  an estimate for Young's modulus based on atomic considerations

--> So if we know the expression for  $U$ , we can differentiate and get  $S_0$

NOTE: generally quite complicated

Recall for “relatively simple” case of an ionic bond:

$$U = U_i - \frac{q^2}{4\pi\epsilon_0 r} + \frac{B}{r^n}$$

$$\text{with } B = \frac{q^2 r_0^{n-1}}{4\pi n \epsilon_0}$$

$$\Rightarrow U = -\frac{q^2}{4\pi\epsilon_0 r} + \frac{q^2 r_0^{n-1}}{4\pi n \epsilon_0 r^n}$$

$$F = \frac{dU}{dr} = \frac{q^2}{4\pi\epsilon_0 r^2} - \frac{q^2 r_0^{n-1}}{4\pi \epsilon_0 r^{n+1}}$$

(NOTE:  $F = 0$  at  $r = r_0$ )

$$S_0 = \frac{dF}{dr} = \frac{d^2U}{dr^2} = \frac{-2q^2}{4\pi \epsilon_0 r^3} + \frac{(n+1) q^2 r_0^{n-1}}{4\pi \epsilon_0 r^{n+2}}$$

evaluate at  $r = r_0$

$$\Rightarrow S_0 = -\frac{2q^2}{4\pi \epsilon_0 r_0^3} + \frac{q^2(n+1)}{4\pi \epsilon_0 r_0^3} = \boxed{\frac{\alpha q^2}{4\pi \epsilon_0 r_0^3} = S_0}$$

with  $\alpha = (n-1)$

Since there are atomic interactions between more than just one neighbor, actually find various values of  $\alpha$ .

(Good value = 0.58)

$$q = 1.6 \times 10^{-19} \text{ C}$$

$$\epsilon_0 = 8.854 \times 10^{-12} \text{ Fm}^{-1}$$

For ionic materials,  $r_0 \approx 2.5 \times 10^{-10} \text{ m}$



Table with estimates based on this:

Bond Type	$S_o$ [N/m]	Approximate E [GPa]
Covalent C-C	180	1000
Ionic	9-21	30-70
Metallic	15-40	30-150
H-Bond	2	8
Van der Waals	1	2

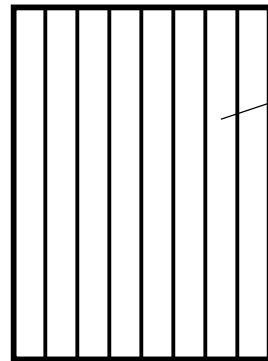
(Remember, can mix bond types in one material)

Finally, we consider what happens if we mix material types on a larger scale and deal with, for example.....

## (Fiber) Composites

A composite is a combination of more than one type of material (beyond atomic level). Often seen in fibrous form:

--> Aligned/Unidirectional



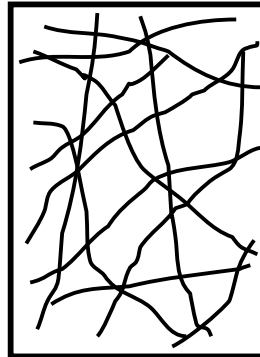
**fibers ( ceramic -- graphite, glass  
polymer -- kevlar  
metal -- boron )**

*in*

**matrix ( ceramic -- carbon  
polymer -- epoxy  
metal -- aluminum )**

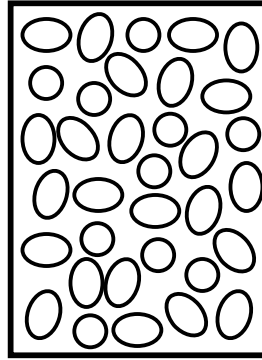
gives orthotropy

--> Random (long or chopped)



generally gives isotropy

--> Particulate



- gives isotropy
- gain in properties but not as much as fibrous

Consider aligned case and resulting modulus (homogenized at ply level -- do not recognize individual fibers and matrix)

Define:

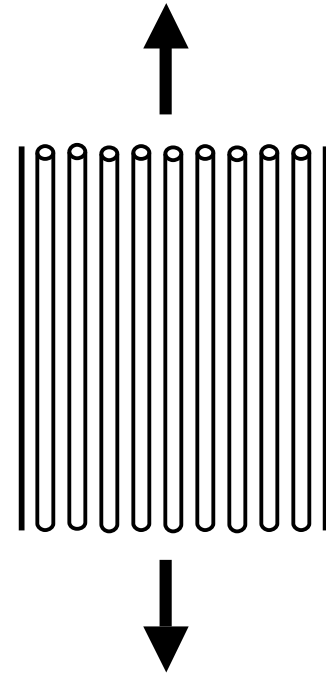
volume fraction of fibers =  $v_f$

volume fraction of matrix =  $v_m = 1 - v_f$

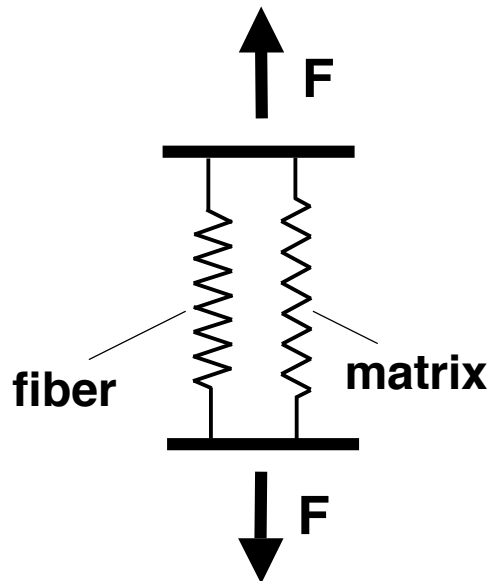
To determine effective moduli, use “Rule of Mixtures”

--> along fibers:

- fibers are stiff springs, matrix is soft springs.
- bonded well together so they deform same amount (*combined action*)



**Figure M3.3-20 Model of fibers and matrix as springs in parallel**



results in:  $\epsilon_{\text{fiber}} = \epsilon_{\text{matrix}}$

So:

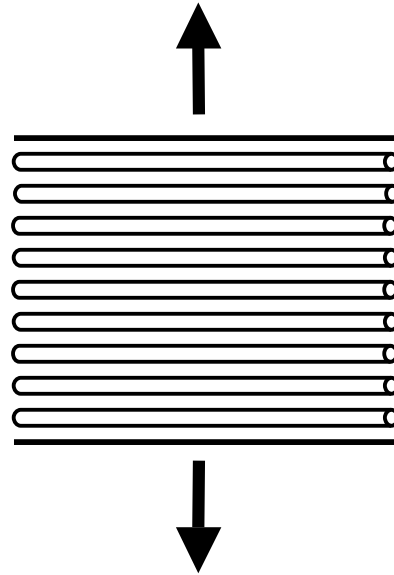
$$\begin{aligned}\sigma_{\text{total}} &= \sigma_{\text{fiber}} v_f + \sigma_{\text{matrix}} (1 - v_f) \\ &= E_{\text{fiber}} \epsilon v_f + E_{\text{matrix}} \epsilon (1 - v_f)\end{aligned}$$

longitudinal  
(parallel to fibers)  $\Rightarrow E_{L\text{comp}} = \frac{\sigma}{\epsilon} = E_f v_f + E_m (1 - v_f)$

Rule of Mixtures is a weighted average  
(same for density)

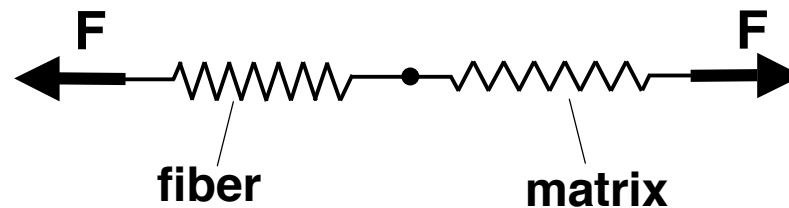
--> transverse to fibers

- fibers and matrix must carry same load



$$\Rightarrow (\sigma_f = \sigma_m = \sigma_{\text{comp}})$$

**Figure M3.3-21 Model of fibers and matrix as springs in series**



total strain is sum of two strains (deformation) weighted by fraction of each:

$$\varepsilon_{comp} = v_f \varepsilon_f + v_m \varepsilon_m$$

$$\Rightarrow \varepsilon_{comp} = v_f \frac{\sigma_{comp}}{E_f} + (1 - v_f) \frac{\sigma_{comp}}{E_m}$$

$$E_{Tcomp} = \frac{1}{\frac{v_f}{E_f} + \frac{(1 - v_f)}{E_m}} = \frac{E_f E_m}{E_m v_f + E_f (1 - v_f)}$$

transverse

(perpendicular to fibers)

Note the very large (potentially) difference between the two values (orthotropy).

Depends on:

$$\begin{array}{l} E_f \\ E_m \\ v_f \end{array}$$


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Now that we've looked at the (micro) structure of materials, let's go back and look at our description of the macroscopic stress-strain behavior and explain it based on the microstructure.