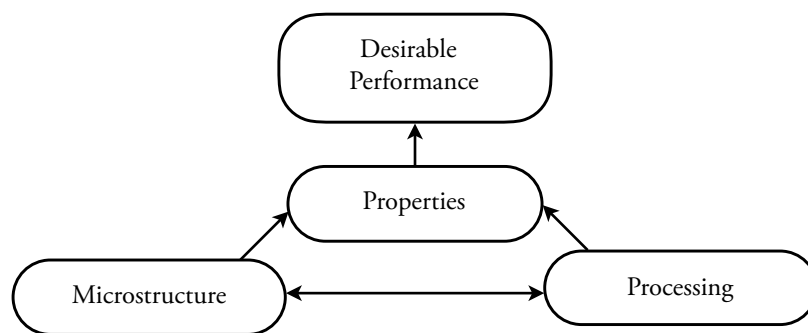


### Introduction to Properties, Application and Design

The materials selection criteria depends on some desired performance or function from industry. There is often some driving force, for example the aircraft industry wanting to use less fuel and have more energy efficiency. This would lead to a reduction in aircraft weight using a light structure that ensures the same mechanical performance. Other requirements include strength, stiffness, stability, corrosion resistance, durability (fatigue behaviour) etc. What is possible to make is *limited by material properties and manufacturing technology*.

Developing new materials requires examining their properties, which are dependent on their microstructure and processing. *Desirable performance* and *properties* make up the **materials selection criteria**, while **failure analysis of new materials** is made up of *properties, microstructure* and *processing*.



Developing new materials is done by **failure analysis**. **Failure** in this sense is considered as a change in desired performance, which can include changes in property or shape.

Mechanisms by which failure can occur:

- Mechanical properties
  - ▶ **Elastic deformation** does not usually cause failure, except for if **buckling**
  - ▶ **Plastic deformation** causes disfiguring and permanent change in the original design; in this case it is important to make sure the stress does not exceed yield stress
  - ▶ **Fracture** is a break in material which causes failure
  - ▶ **Fatigue** causes small geometrical changes over time, which is the most serious problem in industry and there are many challenges in predicting behaviour over what can be years
  - ▶ **Creep** causes small geometrical changes over time
- Microstructural changes
  - ▶ **Twinning**
  - ▶ **Phase transformations**
  - ▶ **Grain growth**
  - ▶ **Particle coarsening**

Other environmental changes (not covered in this course) include chemical or electro-chemical degradation (corrosion, oxidation) and physical degradation (wear, erosion).

A mismatch in materials is bad. For example, in a joint implant, it is crucial that the bone and steel work together as a strong interface without slipping. Compatibility conditions are thus necessary, such that strong steel protects weak bones.

Design or Failure Analysis prerequisite information needed:

1. Structural details (geometry and dimensions)
2. Load acted on structures
3. Material properties

The **factor of safety**  $X$  depends on  $\sigma$  (a function of load, geometry and environment) and  $\sigma_0$  (a function of microstructure and processing).

$$X: \sigma \leq \sigma_0$$

$$F.S. = \frac{\sigma_{fail}}{\sigma_{allow}}$$

### Materials Selection: Materials Performance Indices

The process of deriving material performance indices is detailed below. The purpose of this is to rank materials in order to tell a customer which is best. Four aspects (function, objective, constraints and free variables) are used, where the objective aspect for all is to minimise mass (weight) while the free variable is cross-sectional area. The mass (objective) is given as  $m = \rho LA$ . The free variable is then eliminated to obtain an expression including portions specified by application and portions that may be varied or minimised for small  $m$ . By convention, the material index is flipped from the varied parameters to obtain the highest (best) value.

<i>Function</i>	<i>Constraints</i>	<i>Constraint</i>	<i>Elimination</i>	<i>Specified</i>	<i>Varied</i>	<i>Material Index</i>
Cable (tensile)	Material must not fail under force	Strength: $F = \sigma A$	$m = FL \frac{\rho}{\sigma_f}$	$FL$	$\frac{\rho}{\sigma_f}$	$M = \frac{\sigma_f}{\rho}$
Cable (tensile)	Stiffness $S = F/\delta$ (must not elongate more than $\delta$ )	Stiffness: $\frac{F}{\delta} = \frac{\sigma A}{\epsilon L} = E \frac{A}{L}$	$m = \frac{FL^2 \rho}{\delta E}$	$\frac{FL^2}{\delta}$	$\frac{\rho}{E}$	$M = \frac{E}{\rho}$
Beam (bending)	Stiffness $S = F/\delta$ (must not elongate more than $\delta$ )	Stiffness: $I = \frac{A^2}{12}$ $\delta = \frac{Fl^3}{48EI}$ $S = \frac{F}{\delta} = \frac{48EI}{l^3} = \frac{48EA^2}{l^3}$	$m = \frac{(Sl^5)^{1/2} \rho}{2E^{1/2}}$	$\frac{(Sl^5)^{1/2}}{2}$	$\frac{\rho}{E^{1/2}}$	$M = \frac{E^{1/2}}{\rho}$

For the **specific strength** or **strength to weight ratio**  $M = \sigma_f/\rho$ , a high value means the structure has a low weight under the condition of the same strength.

$$M = \frac{\sigma_f}{\rho}$$

For the **specific modulus** or **modulus to weight ratio**,  $M = E/\rho$  for tension members and  $M = E^{1/2}/\rho$  for bending members, a high value means the structure has a low weight under the condition of the same stiffness.

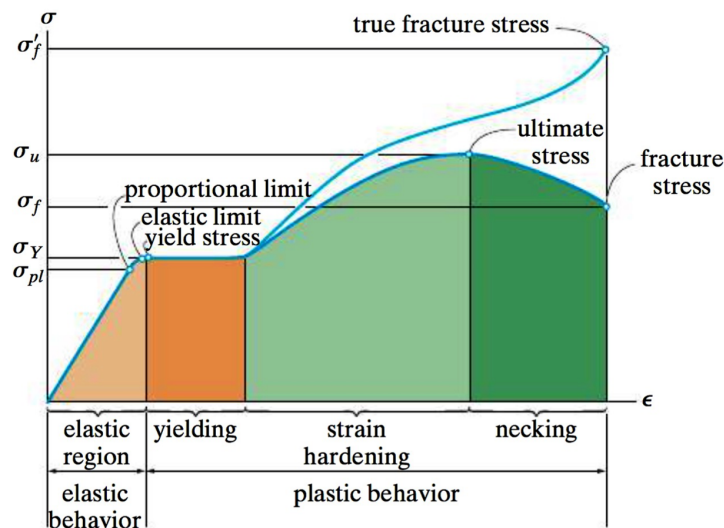
$$M = \frac{E}{\rho} \quad ; \quad M = \frac{E^{1/2}}{\rho}$$

For example, stiffness may be a design requirement. Two materials can be compared with a mass target, with the purpose of stating the area required to achieve that material property. For instance, if we have four times the strength, we only need a quarter of the area to achieve the same requirement.

A table can be used for comparison:

Material	$E$	$\rho$	Area Design		Mass		Material Index	
			Tensile	Bending	Tensile	Bending	Tensile	Bending
			$E/\rho$	$E^{1/2}/\rho$	$E/\rho$	$E^{1/2}/\rho$	$E/\rho$	$E^{1/2}/\rho$
1	16	16	$A_0/4$	$A_0/2$	$m_0$	$m_0$	1	0.25
2	4	4	$A_0$	$A_0$	$m_0$	$m_0$	1	0.5

### Basic Mechanical Properties of Engineering Materials



Conventional and true stress-strain diagrams for ductile material (steel) (not to scale)

- **Elastic behaviour:** Stress is proportional to strain and the material is **linear elastic**. The point at which the linear relationship begins to bend and flatten is the **proportional limit**. Up until the **elastic limit**, if the load is removed, the specimen will still return to its original shape. The total deformation here is elastic deformation.
- **Yielding:** Yielding is when a slight increase in stress above the elastic limit results in permanent or **plastic deformation**. The total deformation here is the elastic plus plastic deformation. **Yield stress**, or the point at which 0.2% or 0.002 of strain has occurred, causes this. An initial upper yield point is often followed by a sudden decrease in load-carrying capacity to a lower yield point. Once this point is reached, the specimen will continue to elongate without any increase in load, and is often called **perfectly plastic**.
- **Strain Hardening:** When yielding has ended, an increase in load can be supported by the specimen, resulting in a curve that rises continuously but flattens until it reaches a maximum or **ultimate stress**. The rise in the curve in this manner is called **strain hardening**.
- **Necking:** Up to the ultimate stress, as the specimen elongates, its cross-sectional area will decrease. This decrease is fairly uniform over the gauge length; however, just after, at the ultimate stress, the cross-sectional area will begin to decrease in a localised region. A constriction or “neck” tends to form as the specimen elongates further. Here, the stress–strain diagram tends to curve downward until the specimen breaks at the **fracture stress**.

**Nominal** or **engineering stress** is obtained by dividing the applied load by the specimen's original cross-sectional area.

$$\sigma = \frac{F}{A}$$

**Nominal** or **engineering strain** is obtained by dividing the change in the specimen's gauge length by the specimen's original gauge length.

$$\varepsilon = \frac{\Delta L}{L}$$

Hooke's Law

**Hooke's Law** defines the linearity between stress and strain within the elastic region. The **modulus of elasticity** or **Young's modulus**,  $E$ , can only be used if a material has linear-elastic behaviour.

$$\sigma = E\varepsilon$$

Poisson's Ratio

When a deformable body is stretched by a tensile force, not only does it elongate but it also contracts laterally, that is, it contracts in two other dimensions. Likewise, a compressive force acting on a deformable body causes it to contract in the direction of the force while its sides expand laterally.

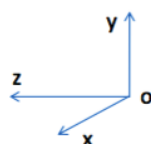
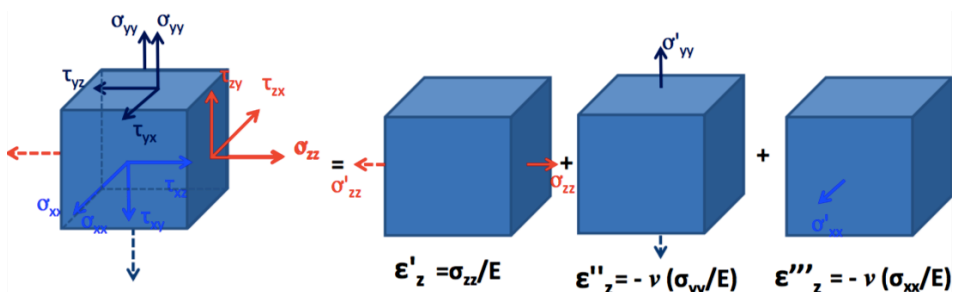
$$\varepsilon_{axial} = \frac{\delta}{L}$$

$$\varepsilon_{lateral} = \frac{\delta_r}{r}$$

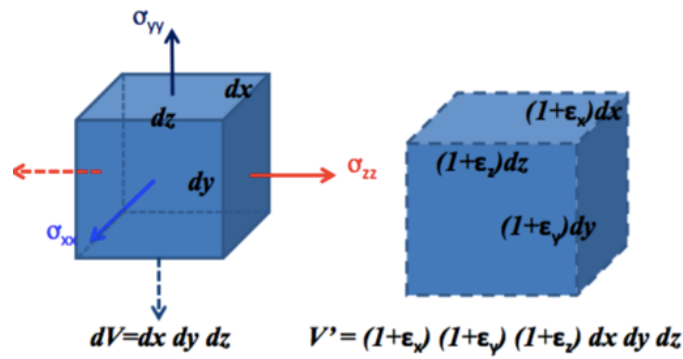
Poisson's ratio is a constant. Lateral strain is the same in all lateral directions. Usually,  $0 \leq \nu \leq 0.5$ . For most linearly elastic materials,  $\nu \approx 0.3$ .

$$\nu = -\frac{\varepsilon_{lateral}}{\varepsilon_{axial}}$$

Using a tensile model under tensile conditions in three directions, strain can be calculated by superposition. Stress in other directions will cause strain in one direction.



$$\begin{aligned} \varepsilon_z &= \varepsilon'_z + \varepsilon''_z + \varepsilon'''_z = [\sigma_{zz} - \nu(\sigma_{yy} + \sigma_{xx})]/E \\ \varepsilon_x &= [\sigma_{xx} - \nu(\sigma_{yy} + \sigma_{zz})]/E \\ \varepsilon_y &= [\sigma_{yy} - \nu(\sigma_{xx} + \sigma_{zz})]/E \end{aligned}$$



$$\delta V = (1+\epsilon_x)(1+\epsilon_y)(1+\epsilon_z) dx dy dz - dx dy dz$$

$$= (\epsilon_x + \epsilon_y + \epsilon_z) dx dy dz$$

**Volume Strain:**  $e = \frac{\delta V}{dV} = \epsilon_x + \epsilon_y + \epsilon_z = \frac{1-2\nu}{E}(\sigma_{zz} + \sigma_{yy} + \sigma_{xx})$

$$\sigma_{zz} = \sigma_{yy} = \sigma_{xx} = p$$

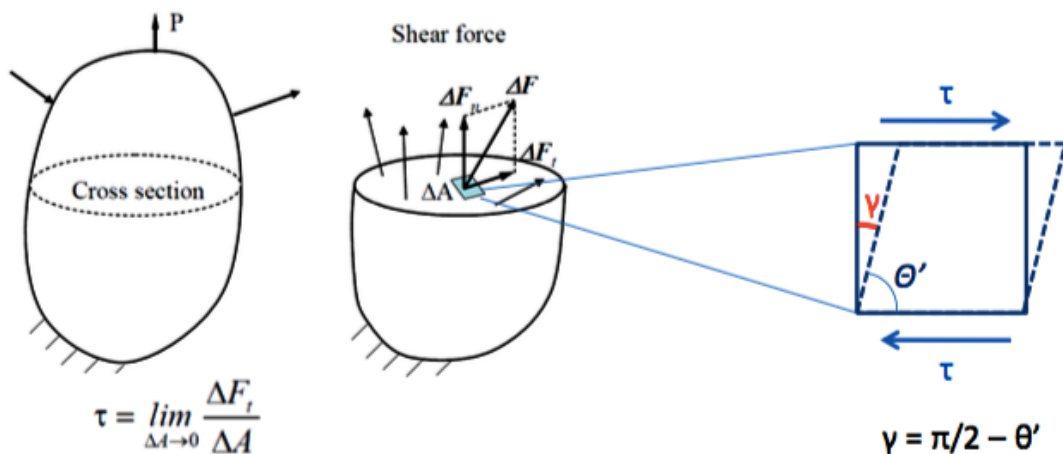
The **volume modulus of elasticity**, also called the **bulk modulus** is hence derived.

$$k = \frac{p}{e} = \frac{E}{3(1-2\nu)}$$

All three components are positive in this case, thus the bulk modulus  $k$  should be positive. To make sure it is positive,  $\nu$  should not exceed 0.5. If  $\nu$  is higher than 0.5, the bulk modulus will be negative, i.e. when stretched, the specimen tends to shrink and when pressed in all directions, it tends to expand, which is wrong. For engineering materials, if  $\nu = 0.3$ ,  $k$  will be equal to a linear Young's modulus.

### Shear Stress and Shear Strain

Shear strain is the deformation created by shear stress. It is defined as the change in angle of the element and is a non-dimensional quantity.



$$\tau = \lim_{\Delta A \rightarrow 0} \frac{\Delta F_t}{\Delta A}$$

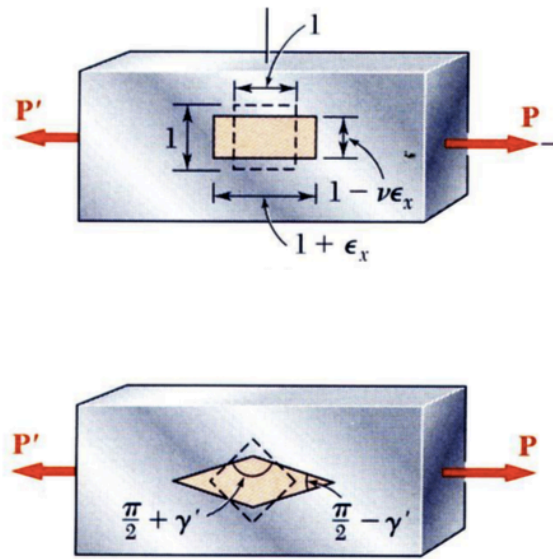
$$\gamma = \pi/2 - \theta'$$

### Hooke's Law for Shear

The **shear Hooke's Law** uses  $G$ , the **shear modulus of elasticity** or shear modulus or **modulus of rigidity**.

$$\tau = G\gamma$$

Relation Among  $E$ ,  $\nu$  and  $G$



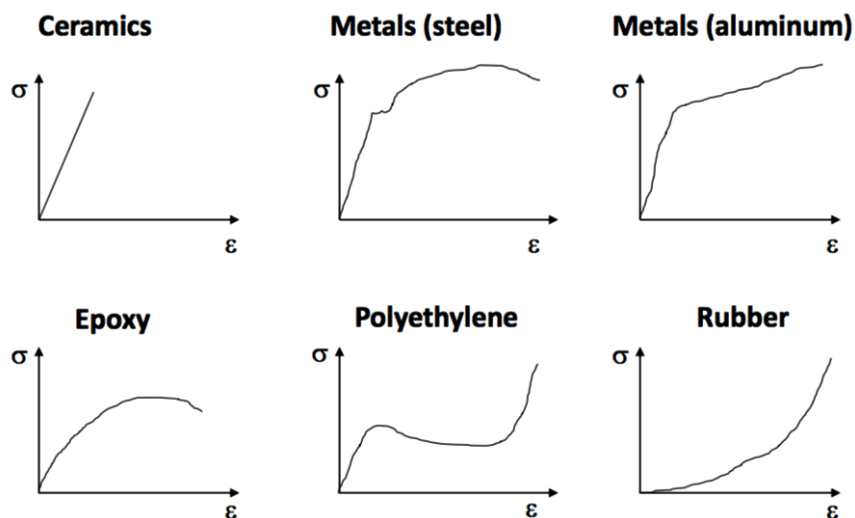
- An initially cubic element oriented as in the top figure will deform into a rectangular parallelepiped. The axial load produces a normal strain ( $E$ )
- An axially loaded slender bar will elongate in the axial direction and contract in the transverse directions ( $\nu$ )
- If the cubic element is oriented as in the bottom figure, it will deform into a rhombus. Axial load also results in a shear strain ( $G$ )

Components of normal and shear strain are related by the following expression.

$$\frac{E}{2G} = (1 + \nu)$$

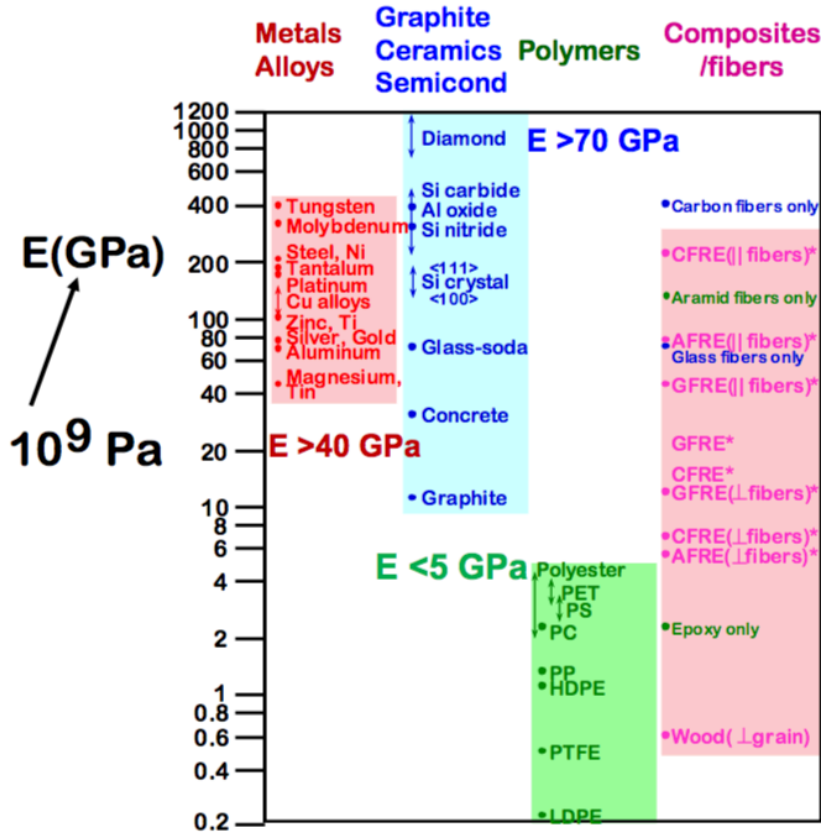
Material Selection: Engineering Materials

*Typical Stress-Strain Curves*



Most engineering materials, excluding rubber and soft polymers, have a unit of GPa for the Young's modulus.

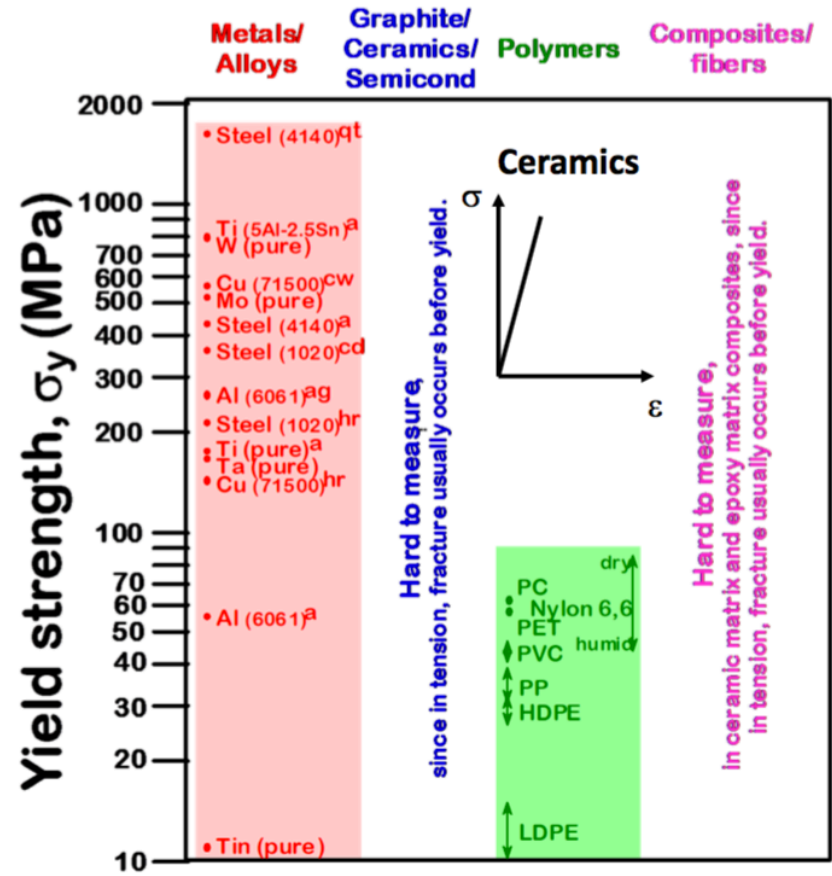
Young's Modulus



**Eceramics**  
**> Emetals**  
**>> Epolymers**

Composite data based on reinforced epoxy with 60 vol% of aligned carbon (CFRE), aramid (AFRE), or glass (GFRE) fibers.

Yield Strength

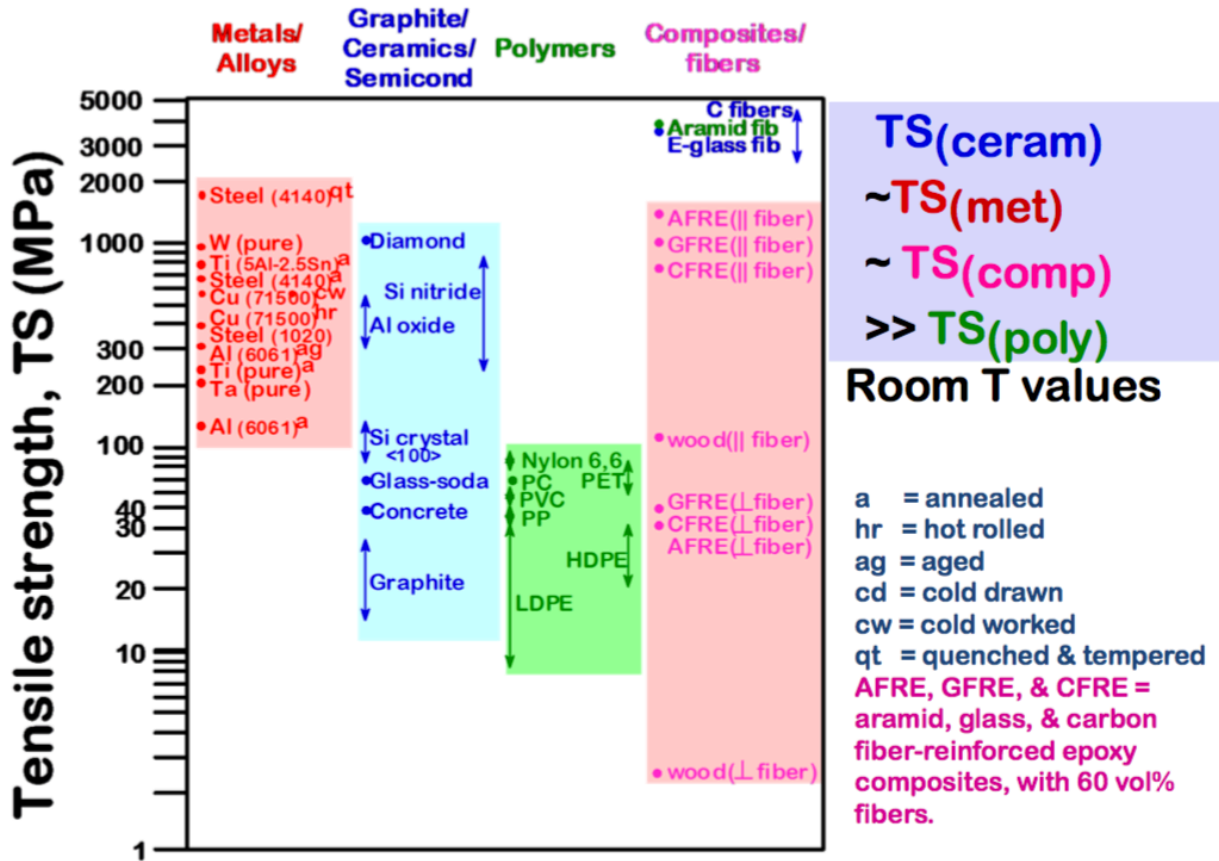


**σy(ceramics)**  
**>> σy(metals)**  
**>> σy(polymers)**

Room T values

- a = annealed
- hr = hot rolled
- ag = aged
- cd = cold drawn
- cw = cold worked
- qt = quenched & tempered

## Tensile Strength



## Mechanical Properties of Typical Structural Alloys

For alloys, lower density is an advantage as it causes lower weight. This is present in the aluminium alloy, used for light structures. Titanium is even lighter and stronger. The ratio of strength to density is important, where a higher ratio is favourable. The geometrical constraints such as size and area must also be taken into account, as well as the values of stress and load.

### Steel Alloy (1040) Annealed:

- 1 – Indicates whether it is a carbon steel (1) or alloy steel (2 or above); 0 – Modification in alloy (none) i.e. plain carbon; 40 – Carbon content is 0.40%

### Aluminium Alloy (6061 T6):

- 6 – Alloy group includes magnesium and silicon; 061 – ~0.6% Silicon and ~1% Magnesium; T6 – Solution heat-treated and artificially aged

### Titanium Alloy (Ti-6Al4V):

- 6A – ~6% Aluminium; 4V – ~4% Vanadium

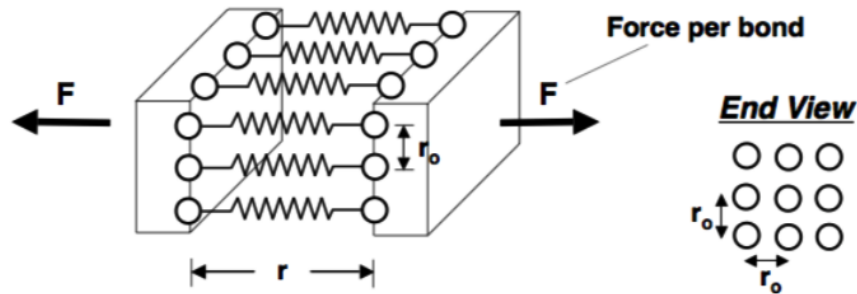
Material	Density (g/cm <sup>3</sup> )	Young's Modulus (GPa)	Yield Strength (MPa)	Tensile Strength (MPa)
Steel Alloy (1040) Annealed	7.85	207	355	520
Steel	7.9	210	200	400
Aluminium Alloy (6061 T6)	2.7	69	276	310
Aluminium	2.7	71	75	101
Titanium Alloy (Ti-6Al4V)	4.4	115	850	950
Titanium	4.5	120	170	240



## Young's Modulus (Elasticity) – Stiffness

The **Young's Modulus** is a measure of stiffness. It is based on physics experiments. Down to the atomic scale in solids, atoms are bonded together closely (overcoming their own weight such that they don't fall apart). Two things are important in determining the modulus:

1. The forces that hold atoms together (the **interatomic bonds**), which act like little springs, linking one atom to the next in the solid state
2. The ways in which atoms pack together (the **atom packing**), since this determines how many little springs there are per unit area, and the angle at which they are pulled



The springs have a certain stiffness and the initial distance between them is  $r_0$ . The overall area of the face per atom/bond is thus  $r_0^2$ . The stress represents the intensity of a certain area. Then, once the area approaches zero (the limit being the size of the individual atom), stress is finally taken by a single element at the smallest area possible.

Stress being geometrically independent is the foundation of finite element analysis. FEA can be valid for different areas and sizes, and is mostly done by software.

$r$  is the new length of the spring once stretched. The equation for stiffness  $S$  can then be recalled, where  $S_0$  is the stiffness property of the material.

$$\sigma = \frac{F}{A} = \frac{F}{r_0^2}$$

$$\delta = r - r_0$$

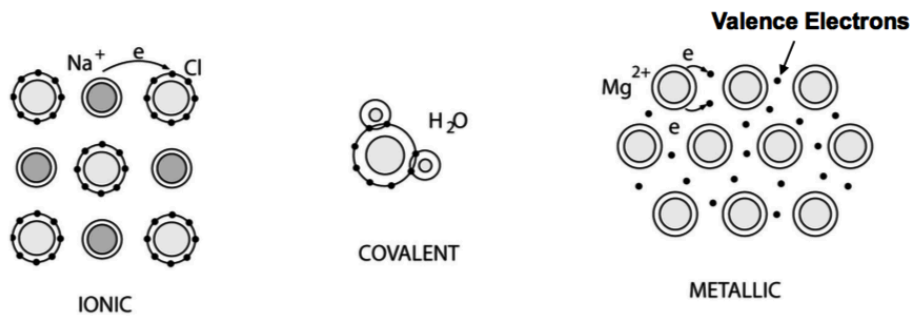
$$\epsilon = \frac{\delta}{r_0} = \frac{r - r_0}{r_0}$$

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

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

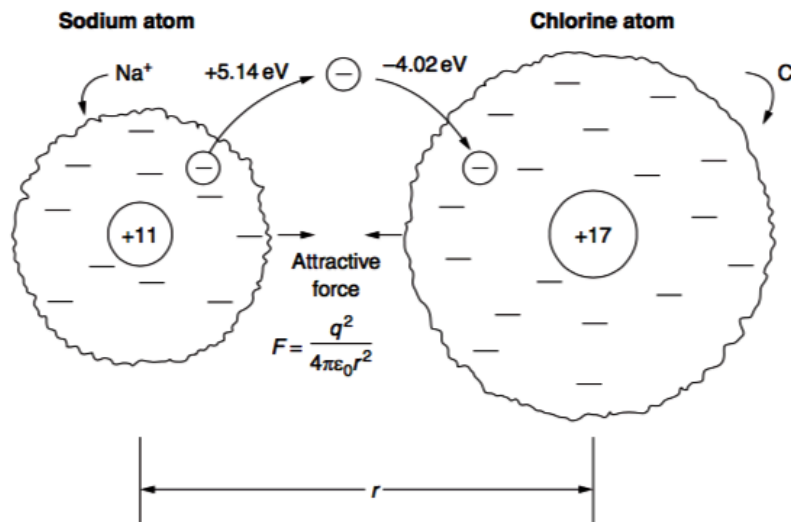
$$E = \frac{S_0}{r_0}$$

**Primary chemical bonds** include **ionic** (ceramics), **covalent** (metals, ceramics, polymers) and **metallic bonds** (metals). These strong, stiff bonds give high moduli. **Secondary bonds** include the **Van der Waals Bond** (dipolar attraction between uncharged atoms), **Dipoles** and **Hydrogen Bond** (binds polymer chains together to give solid polymers, keeping water liquid at room temperature). These are relatively weak. Many atoms are really bound together by bonds that are a hybrid of the simpler types (**mixed bonds**).



The **ionic bond** is typified by cohesion in sodium chloride (NaCl). The sodium atom has a nucleus of 11 protons and 12 neutrons, which is surrounded by 11 electrons. While the electrons are attracted to the nucleus by electrostatic forces, therefore having negative energies, their energies are not all the same. Those furthest from the nucleus naturally have the highest (least negative) energy and can most easily be removed from the sodium atom by expending 5.14 eV of work. This electron can be transferred to a vacant position on a distant chlorine atom, giving back 4.02 eV of energy.

Once bonded,  $F_{att}$  will be the force to separate the bond (attractive force). The energy analysis method is favoured.



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

$$5.14 \text{ eV} - 4.02 \text{ eV} = 1.12 \text{ eV}$$

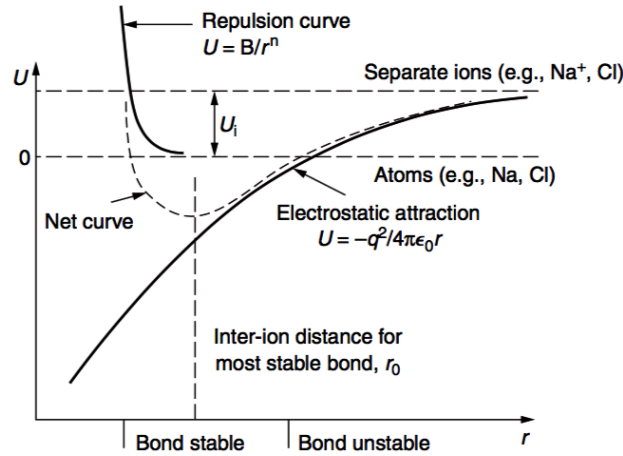
2. Work to separate ions ( $\epsilon_o$  = the permittivity of vacuum);  $F_{att}$  is the force between two oppositely charged particles;  $r$  is the separation of the ions

$$F_{att} = \frac{q^2}{4\pi\epsilon_o r^2}$$

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

3. Repulsive Energy ( $n \approx 12$ )

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



When the ions get close enough together, the electronic charge distributions start to overlap one another, and this causes a very large repulsion. This in turn causes a potential energy increase and explains why  $r$  does not decrease indefinitely, releasing more energy and ending in the fusion of the two ions. The ionic bond lacks directionality because there is considerable freedom in the way that the approximately spherical ions can be packed around each other, but the total charge must add up to zero and the positive ions are always separated from the negative ions.

4. Therefore,  $A/r^m$  is the attractive part and  $B/r^n$  is the repulsive part in the **empirical equation** for the potential energy of two atoms:

$$U = -\frac{A}{r^m} + \frac{B}{r^n}, \quad (m < n)$$

$$U(r) = U_i + U_{att} + U_{rep}$$

Noting that  $F = 0$  at  $r = r_0$ ,

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

$$U(r) = U_i - \frac{q^2}{4\pi\epsilon_0 r} + \frac{B}{r^n}, \quad B = \frac{q^2 r_0^{n-1}}{4\pi n \epsilon_0}$$

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

Evaluating at  $r = r_0$ ,

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

$$S_0 = \frac{\alpha q^2}{4\pi\epsilon_0 r_0^3}, \quad \text{where } \alpha = (n-1)$$

In this case,  $\alpha = 0.58$ ,  $q = 1.6 \times 10^{-19}$  C,  $\epsilon_0 = 8.854 \times 10^{-12}$  Fm<sup>-1</sup>. For ionic materials,  $r_0 \approx 2.5 \times 10^{-10}$  m.

**Covalent bonding** appears in its pure form in diamond, silicon and germanium. The simplest example of this type of bonding is the hydrogen molecule. The proximity of the two nuclei creates a new electron orbital, shared by the two atoms, into which the two electrons go. This sharing leads to a reduction in energy and a