MSE160 Notes

QiLin Xue

February 8, 2021

Contents

1 Introduction

1.1 Types of Material

- There are three classes of material (though not all materials fall under these categories):
    - Metals
    - Ceramics
    - Polymers
- **Metals** (e.g. Fe, Cr, Cu, Zn, Al) are held together with *mellatic* bonds and is described by **bond theory**.
- **Ceramics** (e.g. poreclain, concrete) are held together with *ionic* bonds and are *brittle*. A lot of them are metal oxides.
- **Polymer** (Teflon®, Gore-tex®, polyethylene) *tend* to be from *covalent bonds*

> **Warning**: The word plastic actually describes a material property, and not a material type. There are plastics that are not polymers.

- Examples of materials that do not fall under this classification scheme include wood, skin, superconductors, and more.

1.2 Elastic Behaviour

- Hooke's law tells us that $F = -k\Delta x$, where Δx is the displacement from equilibrium.

- **Engineering stress** is defined as $\sigma = \dfrac{F}{A_0}$ where A_0 is the *initial* (unloaded) cross-sectional area.

  > **Warning**: Due to material properties, the cross sectional area of a spring can change as it elongates or compresses, so the engineering stress only refers to the initial cross sectyional area. The *true stress* refers to the force divided by the real area.

- **Engineering strain** is defined as $\varepsilon = \dfrac{\Delta \ell}{\ell_0}$ and the two are related via the **Young's Modulus**:

$$\sigma = E\varepsilon \tag{1}$$

- There are two possible definitions for elastic deformation. When viewing it from a macroscopic perspective:

  > **Definition**: During elastic deformation, the sample dimensions return to their original dimensions upon unloading.

  but it is also possible to view it from a microscopic perspective:

  > **Definition**: During elastic deformation, atoms return to their original positions upon unloading.

1.3   Simple Model for Bonding in solids

- A crudge (but quite accurate) model is to assume nearby atoms in a solid are connected by springs. (This is actually Einstein's model of solid, except he modeled the interactions as quantum harmonic oscillators)

  > **Idea**: A more realistic model would be using the Lennard-Jones potential, which gives the force between two atoms as:
  > $$V = -\frac{a_1}{r^{13}} + \frac{a_2}{r^7} \tag{2}$$
  > and is graphically represented below (here, $a_1 = 5$ and $a_2 = 3$ for illustration purposes only)

Lennard Jones Force
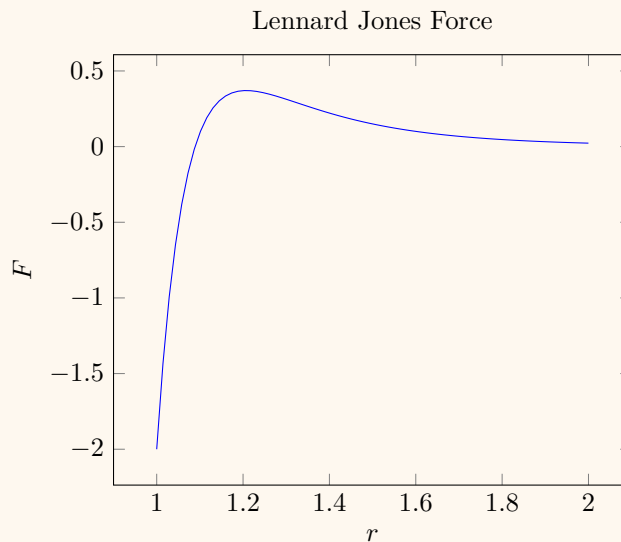
  When the two atoms are close to each other, the force scales roughly linearly with displacement, which is exactly the description of Hooke's Law.
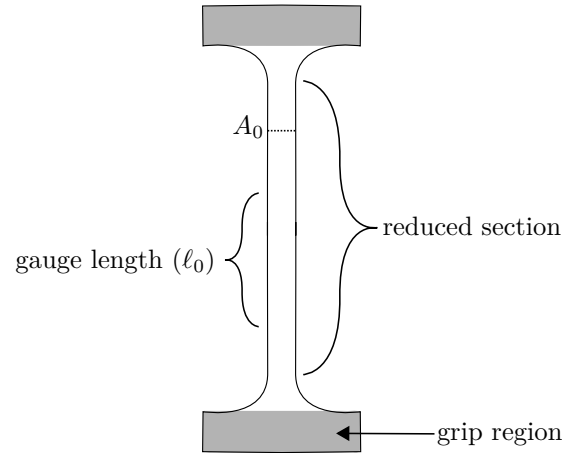
- Specifically, the Young's Modulus can be recovered by defining it as:

$$E \propto \left. \frac{dF}{dr} \right|_{r=r_0} \tag{3}$$

where r_0 is the equilibrium distance and is only dependent on the material. Permanently deforming a metal will not change its Young's Modulus.

1.4   Getting a stress-strain curve

- The tensile specimen is in a **dogbone** shape as illustrated below: and the test is performed by gripping the grip

regions and performing a uni-axial tension test.

1.5   Poisson's Ratio and Shear

- When a material deforms, it does not deform in only one direction. The **poisson's ratio** ν relates the strain in all three directions:

$$\nu = -\frac{\varepsilon_R}{\varepsilon_Z} = -\frac{\varepsilon_x}{\varepsilon_z} = -\frac{\varepsilon_y}{\varepsilon_z} \tag{4}$$

for a cylindrically symmetrical material.

- Shear stress is defined as

$$\tau = \frac{F}{A_0} \tag{5}$$

and shear strain is defined as:

$$\gamma = \frac{\Delta \ell}{\ell_0} \tag{6}$$

- Similarly, shear stress and strain is related via the shear modulus G:

$$\tau = G\gamma \tag{7}$$

- The Young's modulus and the shear modulus is related via the poisson ratio:

$$E = 2G(1 + \nu) \tag{8}$$

2   Inelastic Behaviour

- Permanent deformation can be defined in three ways:

  1. Upon unloading, sample does not return to original dimensions

  2. Strain does not return to zero

  3. Atoms move to new positions

  4. Occurs near the end of linear behaviour

- Plastic comes from the greek word *plastikos*, which means to shape or to sculpt. In this course, plastic does not refer to the material type but instead the permanent deformation.

- The **strength** of a material describes when the permanent deformation occurs.

> **Warning**: Strength depends on context and is not always defined as above.

- The stress strain curve for different materials resemble different shapes.
    - Polymers have a distinct yielding region
    - Metals start a concave down behaviour as soon as elastic deformation ends
    - Ceramics have linear behaviour all the way until they fracture
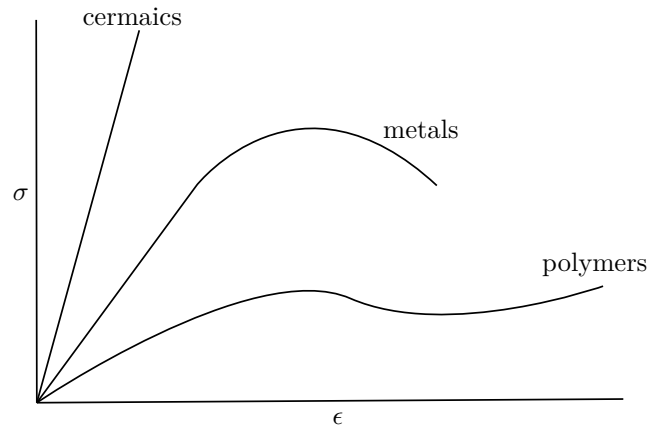
- For polymers, the use of *Young's Modulus* is misleading since the elastic behaviour depends on several different types of bonds, while Young's Modulus is related to the bahviour of a single bond. As a result, the term **elastic modulus** is used to describe polymers and composite materials.

2.1   Ceramics

- Ceramics are not typically tested in tension because:
    1. It is difficult to grip because it crumbles easily
    2. It is difficult to shape it into a dogbone shape
    3. Machine alignment is difficult to achieve.
- Instead, we test them by **3-point bending**:
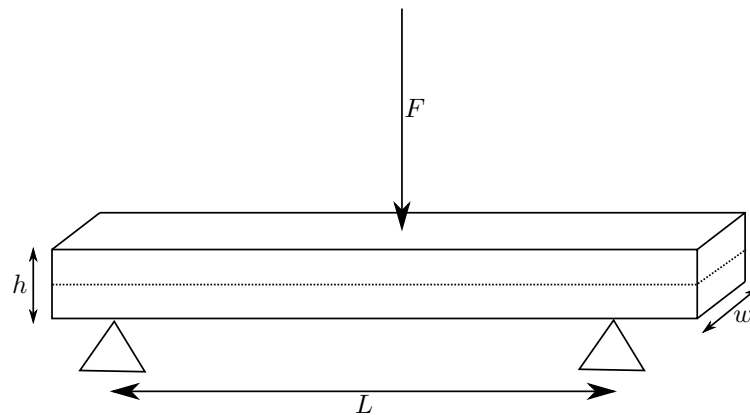
- The dotted line is the neutral axis and since it is weak in tension, the plate will break in the lower half at a stress value of:

$$\sigma = \frac{3FL}{2wh^2} \tag{9}$$

2.2   Tempered Glass

– **Tempered glass** has a very high strength and is relatively "safe" when it fractures (small pieces instead of large ones)

> **Idea:** Initially, tempered glass is very hot in a large volume. However, as it rapidly cools, the surfaces cool faster than the center. Since glass is made of silica bonded to four oxygen, it forms a very complex network structure. Therefore, during this rapid cooling, it "fixes" in excess volume.
>
> The regions in the middle that are cooling more slowly is trying to contract but is constrained by the outer surface that it goes into tension. The fast cooling regions on the other hand will be in tension.

– When the glass bends, the opposite side of the window can still be in considerable compression even though for a regular ceramic it should be in tension. This increases the strength.
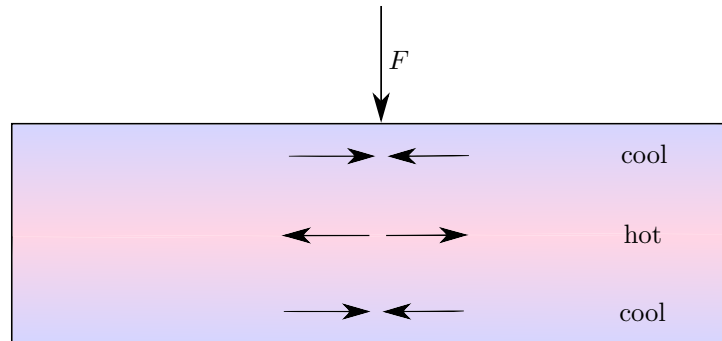
– The stress distribution creates **residual stress** which results in stored strain energy. When the glass gets fractured, the stored strain energy gets transformed into **surface energy**.

– Since surface energy is proportional to surface area, this means that the fractured pieces are smaller.

– **Chemical processes** can also be used to create tempered glass, usch as gorilla glass. Ions with a larger size diffuse into the surface and take up a larger space in the network resulting in an increase in volume at the surface.

3   Structure Property Relationship

• If we plot the relationship between the Young's Modulus and the density, we find that there are no materials with a high Young's Modulus and a low density and that most materials fall on a single line.

• The **materials performance index** MPI for a beam is defined as:

$$MPI = \frac{E^{1/2}}{\rho} \tag{10}$$

Proof. The deflection of a beam takes the form of:

$$\delta = \frac{FL^3}{CEA^2} \implies A = \left(\frac{FL^3}{CE\delta}\right)^{1/2} \tag{11}$$

and using the equation:

$$m = AL\rho \tag{12}$$

we are able to retrieve the equationa bove.   □

• If we were to plot the Young's Modulus against the density on a log-log scale and draw out the curve:

$$\log E = 2\log\rho + \log MPI \tag{13}$$

then materials on the same line would have the same materials performance index. If we shift this line to the left, the performance index of the material improves.

- For a beam, performing this analysis will give us composites such as carbon fibre. Ceramics also belong in this category but because they are susceptible to catasctophic brittle fracture, we can ignore them.

- For a loaded plate, the MPI is:

$$MPI = \frac{E^{1/3}}{\rho} \tag{14}$$

  and the best in this category is wood.

- **Polycrystalline** refers to materials made of crystals, typically around the micron scale.

- Most metals and some ceramics are crystalline (e.g. sapphire), but not everything is. **Amorphous** materials are not organized, an example being window glass.

    – Long-range order refers to a organization at a distance well beyound the nearest neighbour

    – Short-range order refers to organization at only the first or second nearest neighbour.

- One such highly organized material has a **face-centered cubic** (FCC) structure. Many metals have this organization:
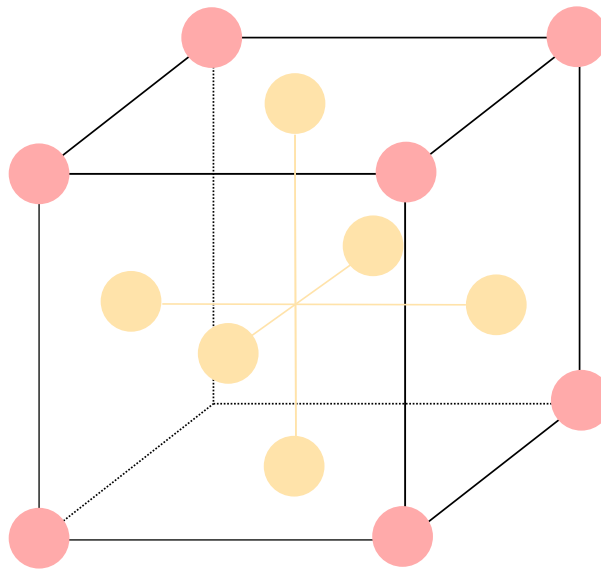
- Each of the eight corners have $\frac{1}{8}$ of an atom and each of the six faces have $\frac{1}{2}$ of an atom, which gives: $n_{\text{FCC}} = 4$ atoms in a unit cell.

- Given n, we can calculate the density of an FCC material such as alunium, via:

$$\rho = \frac{nA}{a^3 N_A} \tag{15}$$

  where a is the length of the unit cube known as the **lattice parameter**, A is the molar mass, and N_A is Avocado's number.

- Based off of the hard sphere model, we treat atoms in ordered solids as hard spheres that make contact with their nearest neighbours. However, this is very hard to draw so we will go by the *reduced sphere* model by drawing atoms smaller.

Example 1: Suppose we wish to find the theoretical density of Aluminum, which is a FCC structure. We are given:

$$A = 26.892\,\text{g mol}^{-1}$$
$$R = 143\,\text{pm}$$

The lattice parameter is given by:

$$a = 2\sqrt{2}R \tag{16}$$

which gives us:

$$\rho = \frac{nA}{(2\sqrt{2}R)^3 N_A} = 2.71\,\text{g cm}^{-3} \tag{17}$$

- The **atomic packing factor** is given by:

$$\text{APF} = \frac{V_\text{spheres}}{V_\text{unit cell}} \tag{18}$$

Since the unit cell is a cube with volume a^3, we have:

$$\text{APF} = \frac{4\pi R^3 n}{3a^3} \tag{19}$$

and for FCC:

$$\text{APF} = \frac{16\pi R^3}{3a^3} \tag{20}$$

We can also relate the R and a together via:

$$a = 2\sqrt{2}R \tag{21}$$

for FCC packing, which yields:

$$\text{APF}_\text{FCC} = \frac{\pi}{3\sqrt{2}} \approx 0.74 \tag{22}$$

which is the highest possible value. The maximum fraction that a volume can be filled up is 74%.

4 Crystallographic Planes and Directions

- We develop a set of notation to describe directions. It comes with a set of rules:
    - Translate vector, if it simplifies things.
    - Determine projection onto x, y, z.
    - Reduce to lowest integers.
    - Enclose in square brackets (negative signs are moved above, no commas)

Example 2: We can find the crystallographic directions of both the blue and the red vectors in the figure below.
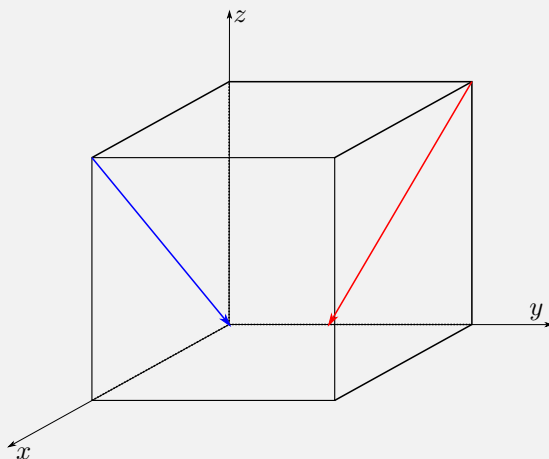
For the blue vector, we first let the tail by the origin. The vector travels 1 in the negative x direction, 0 in the y direction, and -1 in the negative z direction, which gives $[\bar{1}\,0\,\bar{1}]$.

For the red vector, it travels in the negative y direction for 0.5 and in the negative z direction for 1 so we get, after getting rid of fractions: $[0\,\bar{1}\,\bar{2}]$.

- To denote a family of directions, we can use braket notation. All face diagonals can be written as:

$$< 0\,1\,1 > \tag{23}$$

  which includes:

$$[0\,1\,1], [0\,\bar{1}\,1], [0\,1\,\bar{1}], [1\,0\,1], \ldots \tag{24}$$

- To determine crystallographic planes, we use **crystallographic planes**. It uses the following set of rules:

    - Translate plane so origin is not on the plane (defining new origin).

    - Determine distance to intercept plane by travelling along each axis, from the origin.

    - Take the reciprocol of the distance.

    - Enclose in parentheses (use h, k, ℓ). Negatives go above, no commas.

Example 3: We can represent the following plane using Miller indices:
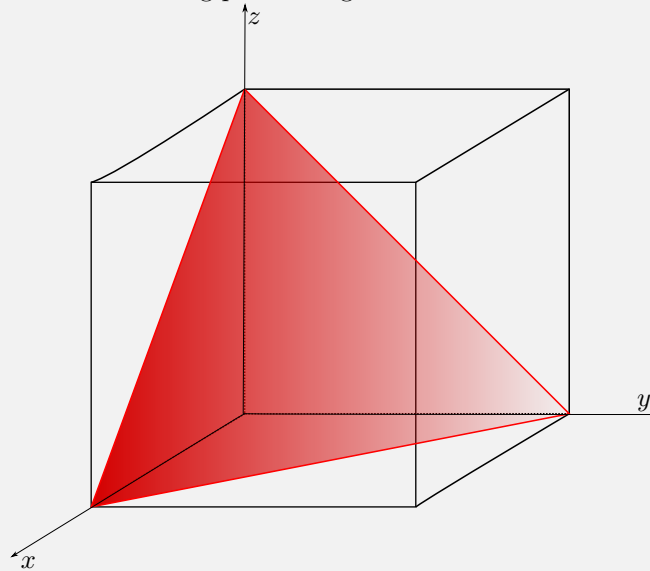
We can start from the origin and travel a length of 1 in both the positive x, y, and z direction. Taking the reciprocal, we still have $1, 1, 1$, so the final miller index is $(1\,1\,1)$.

Example 4: We can represent the following plane using Miller indices:
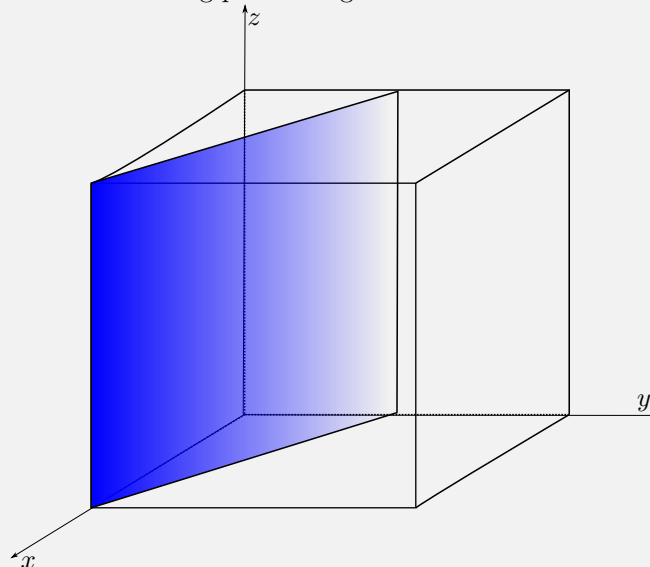
We can start from the origin and travel a length of 1 in the x direction, $1/2$ in the y direction, and ∞ in the z direction. Taking the reciprocal we get $(1\,2\,0)$.
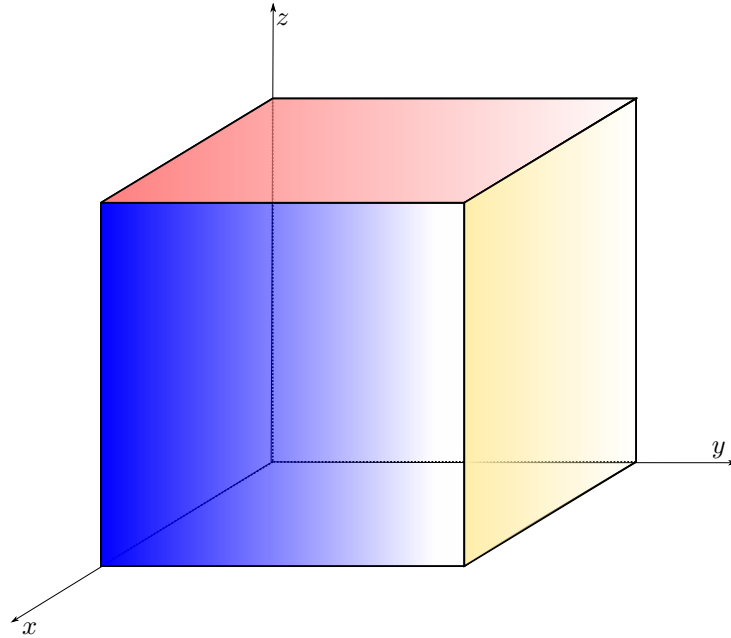

- We can represent **families of planes** using curly braces. For example, faces of a cube can be represented by:

$$\{0\,0\,1\} \tag{25}$$

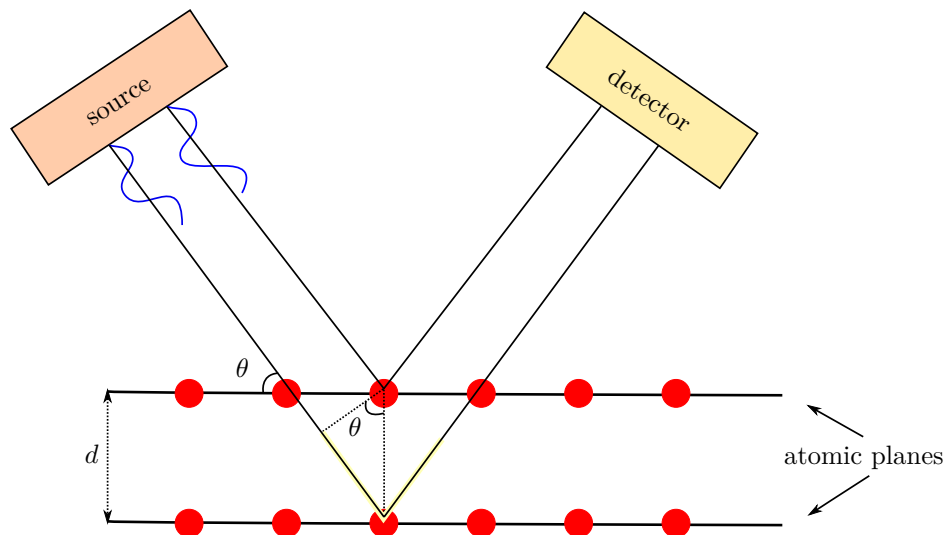 which represent the following planes:

$$(1\,0\,0),\ (0\,1\,0),\ (0\,0\,1) \tag{26}$$

  corresponding to the below blue, yellow, and red plane respectively:

5 X Ray Diffraction

- Suppose there is an x-ray source that reflects off a sample and hits a detector at a certain angle θ. If we plot the intensity as a function of θ, we see that it peaks at very specific values.

- This is a result of constructive interference where the peaks of both wavelengths add up at the detector.

- This will only occur if the extra distance (shown in yellow) is an integer multiple of the wavelength λ. Mathematically:

$$2d\sin\theta = n\lambda \tag{27}$$

  known as **Bragg's Law**, where n is an integer.