Chemmat 121

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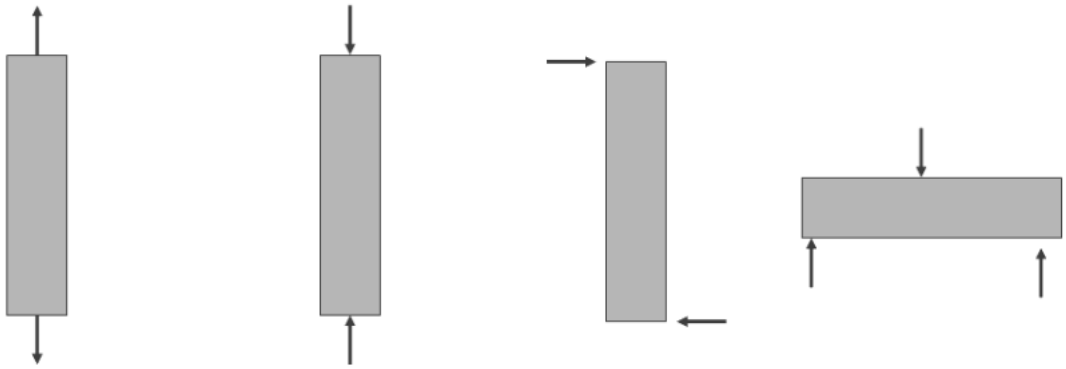
1 Deformation and structure of solids

1.1 Strength

How much force can a material withstand before it fails? That's a materials strength. A material can fail in several ways but the two most common are fracturing and permanent deformation.



Some types of force that a material/object can undergo
From left: Tension, Compression, Shear and a Combination.

1.2 Stress

Engineers typically talk about stress instead of forces because stress is just a force proportional to its area. Stress is represented by the greek letter sigma (σ) and is given by the force (F) divided by the cross-sectional area (A).

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

Cross-sectional area is the area that is perpendicular to the applied force

Example

Given: $m = 25\,\text{kg}, d = 10\,\text{mm}$

$$A = \pi r^2$$

$$A = \pi \times \frac{(0.01)^2}{2}$$

$$F = 25 \times 9.81$$

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

$$\sigma = 3,120,000\,\text{Pa}$$

$$\sigma = 3.12\,\text{MPa}$$

1.3 Strain

Strain is how long something gets compared to its original size. Stress and strain are related very closely and the stress against strain graph is a very important thing to materials engineering. Strain is given by the change in length over the original length.

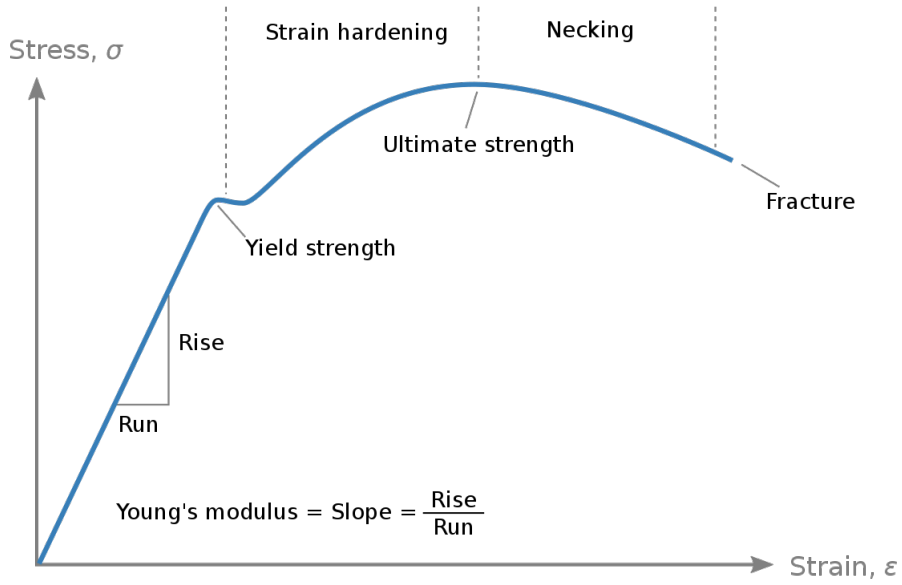
$$\epsilon = \frac{\Delta L}{L_o}$$

Strain is unitless but is commonly expressed as a percentage (%).

Example

$$\begin{aligned}
\epsilon &= \frac{\Delta L}{L_o} \\
&= \frac{100.32\,\text{mm} - 100\,\text{mm}}{100\,\text{mm}} \\
&= \frac{0.32\,\text{mm}}{100\,\text{mm}} \\
&= 0.0032 \\
&= 0.32\%
\end{aligned}$$

1.4 Stress-Strain Curve



The area under the curve is $F \times d$ and gives the 'toughness' which is approximately the energy required.

Necking is a localised reduction in thickness, which reduces diameter, which reduces area, increasing stress. This causes it to fail.

1.5 Poisson's Ratio

Poisson's ratio is the relationship between deformation for a given material. It is a measure of the Poisson effect, that describes the expansion or contraction of a material in directions perpendicular to the direction of loading. It has no units and is represented by the greek character 'nu' (ν). For most materials $\nu \approx 0.3$.

$$\nu = \frac{-\epsilon_x}{\epsilon_z}$$

1.6 Young's Modulus

The Young's Modulus of a material is a measure of the 'stiffness'. It is the gradient of the elastic part of the stress-strain curve for a given material. It has units of Pascals (Pa) and is represented by the capital letter E.

$$E = \frac{\Delta\sigma}{\Delta\epsilon}$$

1.7 Steel

Steel has what is called a 'discontinuous yield'. This means at the yield strength there is a bit of 'noise' and it moves a little randomly before becoming nonlinear.

1.8 0.2% Proof Stress

The 0.2% Proof Stress of a material is a geometrical construct that is used when the yield stress of a material cannot be properly determined. It is a very slight overestimate (generally) that can be calculated by drawing a line parallel to the actual curve at a strain of 0.002 and finding the intersection with the original curve. This stress value is the approximation.

1.9 Safety Factor

The safety factor is a scalar value that demonstrates how much more stress a material can hold relative to the requirement. I.e. if, for example, $F \approx 1000\,\mathrm{N}$ the engineers might pretend $F = 2000N$. This would gie a safety factor of 2. When the conditions of the material are more uncertain, you would want a higher safety factor.

1.10 Engineering Stress vs Real Stress

In engineering, we draw a stress-strain graph as going 'down' after the ultimate tensile strength. In reality, because of the effect of necking, it goes up after this. As engineers, we use the model because it is easier to handle theoretically.

1.11 Ductility

Ductility is a measure of how much something can deform elastically (with 100% recovery / without permanent deformation). The stress-strain graph of a ductile material will have a longer elastic section while a more brittle material (less ductile) will have a shorter one. It is generally described by one of two equations:

$$\textbf{Percentage Elongation} = \frac{\Delta L}{L_o} \times 100\%$$

$$\textbf{Percentage Reduction in Area} = \frac{\Delta A}{A_o} \times 100\%$$

2 Microstructure and mechanical properties

2.1 Crystal Structure

> If a material is crystalline, the atoms of a material have **LONG RANGE ORDER**. This means the material is made up of a crystal lattice made of repeating units called 'unit cells'.

There are 14 possible crystal arrangements but this course will only look at three. We describe arrangements by looking at the unit cell. The unit cell is a tessellating shape that has all the information to describe the entire lattice. The unit cell has 4 important properties:

- Number of atoms
- Co-ordination Number (The number of neighbours for the unit cell)
- Unit Cell Dimension (The length of each side of the cell written 'a')
- Atomic Packing Factor (Amount of space taken up by the atoms)

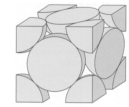
$$a = \text{ Atomic Packing Factor } = \frac{\text{volume of atoms}}{\text{volume of unit cell}}$$

2.1.1 Body Centered Cubic

Body Centered Cubic (BCC) has one atom at each corner of a cube and one right in the middle.

- Number of Atoms $= 2 = 1 + 8 \times \frac{1}{8}$
- Co-ordination Number $= 8$
- Unit cell dimension $= \frac{4R}{\sqrt{3}}$
- APF $= 0.68 = 0.68\%$

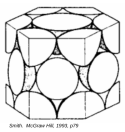
2.1.2 Face Centered Cubic



Face Centered Cubic (FCC) has one atom at each corner of a cube and one in the middle of each face of the cube.

- Number of Atoms = 4
- Co-ordination Number = 12
- unit cell dimension = $\frac{4R}{\sqrt{2}}$
- APF = 0.74 = 0.74%

2.1.3 Hexagonal Close Packed



Hexagonal Close Packed (HCP) is a prism shape with hexagonal arrangements of atoms layered up.

- Number of Atoms = 6
- Co-ordination Number = 12
- APF = 0.74 = 0.74%

2.2 Density

Density is the degree of compactness of a substance. The amount of mass you get for a given volume. The density of a material is its mass divided by its volume.

$$\rho = \frac{n.A}{V_c.N_a}$$

Where n is the number of atoms per unit cell, A is the atomic mass of the material, V_c is the volume of the unit cell (a^3) and N_a is Avrogado's Number.

Example

Iron

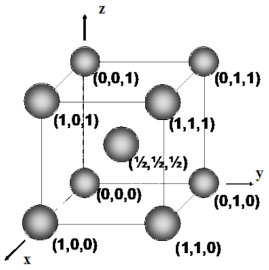
$$a = 0.286\,\text{nm}, n = 2$$
$$\rho = \frac{2 \times 55.85}{(2.86 \times 10^{-8})^3 \times 6.023 \times 10^{23}}$$
$$\rho = 7.92\,\text{g.cm}^{-3}$$

The real density of iron is $7.87\,\text{g.cm}^{-3}$ so this is a good estimate.

2.3 Polymorphism

Materials that can exist in more than one crystal form (can have lattices made up of different unit cells) are called polymorphic. For example, Iron at room temperature has a BCC structure but at 912°C it has an FCC structure.

2.4 Planes, Directions and Positions



Navigation around our crystal structures is based on a typical x,y,z orthogonal axis. We can denote the postition of an atom using a typical three dimensional vector. By convention, positions are denoted with round brackets.

2.4.1 Directions

Directions in the lattice are defined with square brackets $[u, v, w]$.

1. Draw a vector from the origin for the direction
2. Project the length of the vector onto the unit cell axes
3. Put this in terms of the coefficients
4. Convert to integers (multiply by a constant)
5. Put in square brackets

Example

Projecting the length of the vector onto axes: $1a\ 0b\ \frac{1}{2}c$
Put this in terms of co-efficients: $1\ 0\ \frac{1}{2}$
Convert to integers (multiply by two): 2 0 1
Put in square brackets: [201]

Note: Negative directions will have a bar over them (read 'bar').

$$[1\bar{1}0]$$

2.4.2 Planes

Planes in the lattice are defined by **Miller Indices** (h, k, l).

1. Work out the intercepts of the plane on the unit cell
2. Take reciprocals of the intercepts
3. Convert to integers (multiply by a constant)
4. Put in round brackets

Example

Intercepts: $1\ -1\ \infty$
Reciprocals: $1\ -1\ 0$
Integers: $1\ -1\ 0$
Round Brackets: $(1\bar{1}0)$

2.4.3 Families

You can denote the 'family' of a plane (all of the planes made up with these values). Families of planes are denoted with curly brackets e.g. Cube Faces $\{100\}$. Families of directions are denoted with angle brackets e.g. $< 100 >$.

2.5 Slip, Theoretical Strength and Defects

Recall that there are two types of deformation: Elastic and Plastic (In-elastic). Elastic Deformation springs back (recovers), Plastic Deformation does not. At the atomic level, Elastic Deformation is merely stretching the atomic bonds. Any further deformation is permanent (plastic, past the yield point) and results from a process called **slip**. In plastic deformation, atomic bonds are broken (and remade).

2.5.1 Theoretical Strength

We can can calculate the *theoretical* strength of a material by evaluating the amount of energy needed to break and remake the atomic bonds. This is not a very good approximation. For example, the theoretical shear strength of pure iron is 10,000MPa but the measured shear strength of pure iron is 20MPa... Why is this? Imperfections.

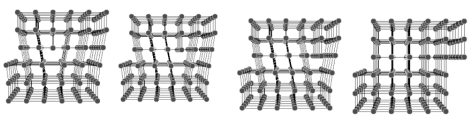
2.6 Imperfections

There are a number of a different imperfections that DO happen within a lattice containing millions of atoms. This is what causes our theoretical strength and theoretical density to be off. It is EXTREMELY difficult to get 'pure' anything so this is true for any sample.

- Point Defects
  - Vacancy
  - Substitution
  - Interstitial Atom
- Planar Defects (Dislocations, $\perp$)
  - Edge Dislocation
  - Screw Dislocation

A vacancy is simply a missing atom in the lattice. A substitution is when a different atom is in the place of the atom that should be there. Interstitial atoms are atoms that occupy a normally unoccupied site in a crystal lattice.

2.7 Slip



Explaining how Slip works is a common exam question. Draw these!

The model of slip we will use is the movement of dislocations. The movement of dislocations means that slip can occur more easily than in a perfect arrangement of atoms. Easy slip means that a material is easily plastic deformed, this means it is *ductile*.

2.7.1 Slip Systems

Slip (dislocation movement) occurs most easily on closepack planes and in closepacked directions. Not all systems have closepacked planes so slip happens on the *closest* packed plane

A slip system is a combination of planes and directions. For FCC, the closepacked planes are $\{111\}$[1]. The closepacked directions on these planes are $< 110 >$[2].

Hence, the main slip system for FCC is: $\{111\} < 110 >$

The main slip system for BCC is: $\{110\} < 111 >$

HCP structures have closepacked planes but they are all parallel. Slip is very difficult so HCP metals are often brittle.

[1] *A family of planes*

[2] *A family of directions*

3 Phase diagrams and Alloying

4 Strengthening mechanisms

5 Engineering ceramics and glasses

6 Polymers

7 Failure of materials

8 Corrosion of metals

9 Engineering composites