

MECHANICAL BEHAVIOR OF MATERIAL



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Mechanical Behavior of Material

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This text was compiled on 05/15/2026

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Chapter 1: Atomistic Structure of Materials

Topics Covered in this Class

Part I: Structure, Linear Elasticity, Stress and Strain Using Tensor Notation, Stress and Strain Transformations

Part II: Anisotropic Materials, Linear Viscoelasticity, Beams, Buckling, Plasticity

Part III: Strengthening Mechanisms, Creep, Deformation Mechanism Maps, and Fatigue and Fracture

The Materials Tetrahedron

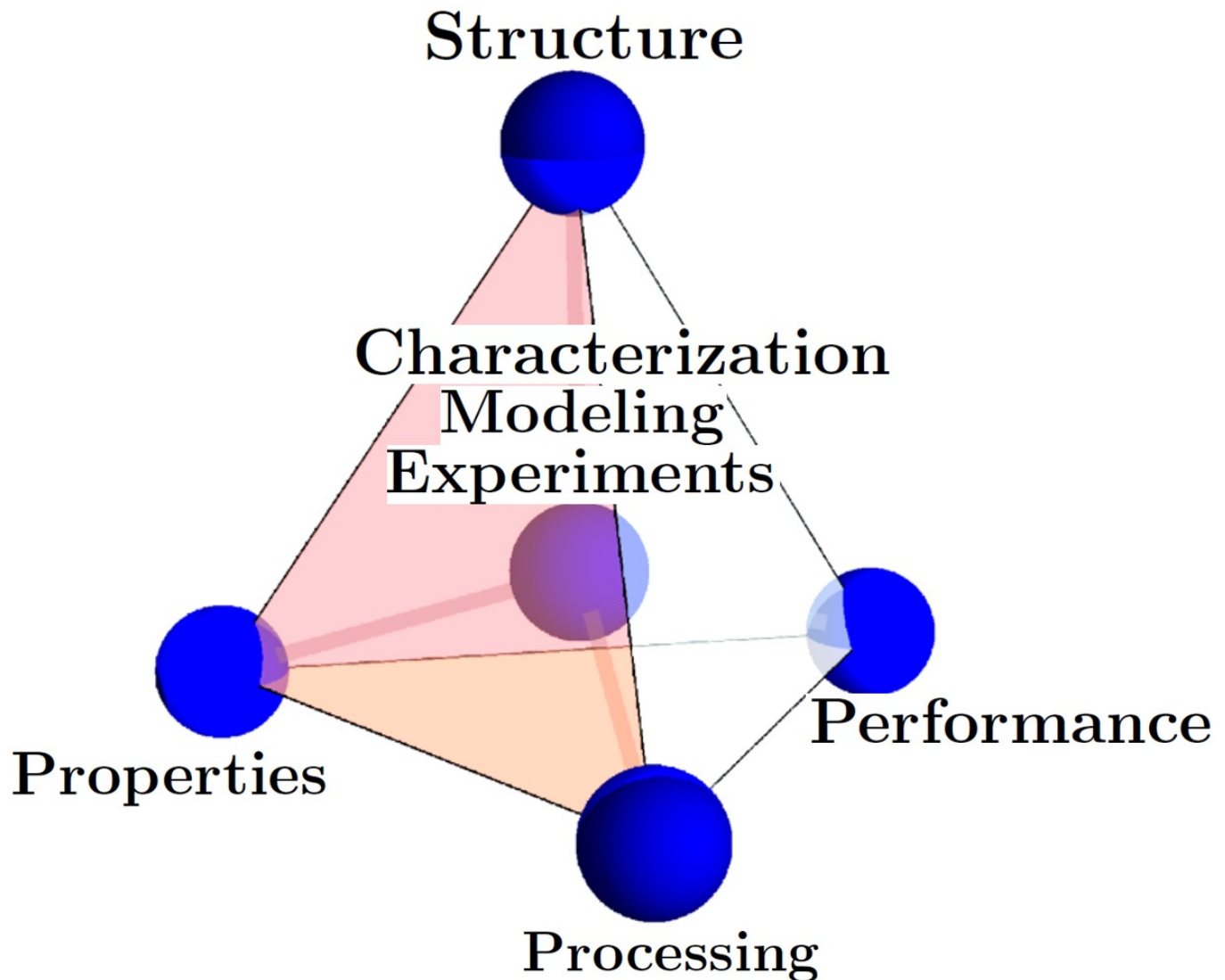


Figure *Chapter1.1*: Materials Tetrahedron

The four corners of the Materials Science and Engineering Tetrahedron are: Structure, Processing, Properties, Performance. At the center is a combination of Characterization/Modeling/Experimentation.

A couple of quick examples: if you process sheet metal by cold rolling you change the structure and induce more dislocations in the material. This in turn will change the yield strength (property) and thus the performance of that sheet metal in the application of interest. As materials scientists, at the core of what we do is try to characterize material with experimentation and simulation to better understand this materials tetrahedron and to eventually reach a point where we can begin to predict some material responses.

Different Types or Classifications of Materials

- Metals
- Polymers
- Ceramics
- Composites
- Active Matter
- Piezoelectric
- Shape Memory Alloys
- Ferromagnetic Materials

Material Properties

- Thermal
- Magnetic
- Optical
- Electrical
- Structure

In this course we are going to focus in particular on Mechanical Properties!! However, as you are about to see in Materials Science, many properties are interrelated. One of the fundamental concepts we will see illustrated over and over again in this class is that structure will dictate properties.

Intra and Inter Molecular Bonding

Intramolecular Forces/Interactions

When it comes to binding and types of intramolecular interactions it is all about the electrons. Elements that have no valence electrons or that have a completely filled outer shell are called the inert or noble gases. All other elements which do not have a completely filled outer shell have valence electrons and these electrons are the ones of import when it comes to bonding. Bonding is critically important as most of the structural, physical, and chemical properties are influenced or determined by the interatomic bonding.

For intramolecular interactions we will typically deal with:

- Covalent (5 eV or about 200 kT)
- Ionic (1–3 eV or ~80 kT)
- Metallic (0.5 eV or ~20 kT)

Let's talk a little bit about why bonding occurs. Well, it all goes back to Gibbs: the energy of the set of bonded atoms is lower than the isolated atoms.

Introduction to Thermodynamics

Ideally you have all taken one or two thermodynamics courses (the more the better). However we will take the time to review the essential concepts from thermodynamics that will be relevant to our discussion of the mechanical behavior of materials. Moreover, we will focus primarily on always keeping a strong physical intuition on what is occurring in a problem/process and how to relate that conceptually to concepts of thermodynamics and free energy. Thus, aside from this lecture, we will not spend a copious amount of time defining or deriving key thermodynamic quantities but instead focus on some key concepts and equations and relating how that impacts the mechanical properties of materials.

The Key Ideas for Thermodynamics in This Course

The fundamental equation that we will be working with when we talk about thermodynamics is Gibbs free energy:

$$G = U + PV - TS = H - TS \quad (\text{Chapter 1.1})$$

or more often we are interested in changes in Gibbs free energy:

$$\Delta G = \Delta H - T\Delta S \quad (\text{Chapter 1.2})$$

where U is the internal energy, T is the temperature, S is the entropy, G is the Gibbs free energy, P is the pressure, V is the volume, and H is the enthalpy.

One of the fundamental concepts in thermodynamics that we will continuously discuss is the competition between enthalpy and entropy. The competition between enthalpic interactions/contributions vs. the penalty or change in entropy will come up over and over again.

The focus of thermodynamic studies involves finding the state of a system/process at equilibrium. This occurs when the free energy is minimized, which occurs when the derivative of the free energy (with respect to externally applied forces) is set to zero.

When are we as humans at 0? When we are dead — we are non-equilibrium active matter!!

Also remember that a spontaneous process will occur when the change in free energy is less than zero.

Entropy Refresher

Now when thinking of entropy, typically the term that is often used to describe what entropy is physically is “disorder.” But this is a somewhat rudimentary way of conceptualizing entropy. As opposed to disorder, I would suggest to instead think of entropy (at least configurational or conformational, not vibrational yet) as the number of possible microstates that a system can exist in.

The entropy can be calculated using the following expression by Boltzmann (engraved on his tombstone):

$$S = k \ln \Omega \quad (\text{Chapter 1.3})$$

where Ω is the number of microstates or configurations.

First Law of Thermodynamics

To do this we need to go back to the First Law of Thermodynamics. The First Law of Thermodynamics states that the increment of change in the internal energy of a system is equal to the heat (either into or out of the system) plus the increment of work (performed on or by the system). The first law of thermodynamics is thus a law of energy conservation. Energy is never destroyed!

\$\$

$$\begin{aligned} dU &= \delta q + \delta w \\ dU &= dq + dw \end{aligned} \quad (\text{Chapter 1.4})$$

\]

where q is heat, and w is the work term. Note here that dQ is the exact differential but the δ is an inexact or imperfect differential, i.e. it is path dependent. As a result I will typically just use the exact differential form for this class. There is also some confusion on the sign of heat and work. In this class we will say that heat transferred into a system will have a positive value and work done on a system will also have a positive value.

Second Law of Thermodynamics

The second law of thermodynamics states that the total entropy of an isolated system can never decrease over time. The second law confirms the existence of state functions or path independent functions and is concerned with the direction of natural processes. There are a couple of statements about the second law of thermodynamics. Clausius states that heat never spontaneously flows from an object at a lower temperature to one at higher temperature. Kelvin states that it is impossible to continuously perform work by cooling a system below the temperature of its surroundings. And perhaps the key statement is that the entropy of the universe (system and surroundings) must increase in any spontaneous process. It will only remain constant in a reversible process. IT IS NEVER NEGATIVE!!!

Let's think about an example for hydrostatic pressure work where we push a plunger extremely slowly so that we are at equilibrium at all times. For this the process is reversible and we can evaluate the exact differential. And for reversible processes we can relate entropy to heat transfer via the following equation

$$dQ = TdS \quad (\text{Chapter 1.5})$$

where S is entropy. Now before we get back to writing the full differential forms of free energy let's talk about some different forms of work that we may encounter in this class.

Types of Work

Work of Hydrostatic Pressure:

$$dw = -P dV \quad (\text{Chapter 1.6})$$

where P is the hydrostatic pressure and V is the volume, this is relevant for processes like pushing on a plunger or more importantly volume expansion.

Chemical Work:

$$dw = \mu dn \quad (\text{Chapter 1.7})$$

where μ is the chemical potential and n is the number of moles, this is relevant for many diffusion processes.

Work of Surface Energy:

$$dw = \gamma dA \quad (\text{Chapter 1.8})$$

where γ is surface tension and A is the area, this is critically important for coarsening and Oswald ripening.

Mechanical Work:

$$dw = \phi dq \quad (\text{Chapter 1.9})$$

where ϕ is electrical potential and q is the electric charge, very important for battery applications.

Elastic Deformation Work:

$$dw = \sigma d\epsilon \quad (\text{Chapter 1.10})$$

where σ is stress and ϵ is strain, very important for mechanical problems and rubber elasticity.

Typically there will be many other work terms which modify the internal energy of the system. Work terms can be generalized as so:

$$dw = \alpha d\beta \quad (\text{Chapter 1.11})$$

where α can be thought of as a generalized force and $d\beta$ is a generalized displacement. Additionally, each work term will consist of an intensive and extensive variable. An intensive variable will not scale or change with the size of system unlike an extensive variable which will change with the size of a system. For example pressure, temperature, chemical potential, stress, and electrical potential would all be intensive variables and volume, entropy, strain, number of particles, and charge would all be extensive variables. Typically the generalized force will be the intensive variable and the generalized displacement will be the extensive variable.

Interatomic Potentials

There are forces of attraction and repulsion between electrons and protons. The force F is related to the potential energy U by

$$F = -\nabla U \quad (\text{Chapter 1.12})$$

where ∇ is the gradient operator and will take the partial derivative of the function with respect to the dimensionality of the problem. There are many different equations or potentials that describe the interactions between atoms such as Morse, Born-Mayer, Van der Waals, etc. One of the most common is the Lennard-Jones (LJ) Potential which approximates the interaction between a pair of neutral atoms. It is popular due to the computational simplicity.

\$\$

$$U_{\text{LJ}} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \\ = \epsilon \left[\left(\frac{r_o}{r} \right)^{12} - 2 \left(\frac{r_m}{r} \right)^6 \right]$$

\]

where ϵ is the depth of the potential well, σ is the distance at which the inter-particle potential is zero, r is the distance between particles, and r_m is the distance where the potential is minimized.

For ionic bonding Coulomb's law of electrostatic attraction can be helpful to describe the bonding and the force of coulombic attraction is given by

$$F_C = \frac{Ce^2}{r^2} \quad (\text{Chapter 1.13})$$

where e is the charge of an electron, $1.602 \times 10^{-19} \text{ C}$, and C is Coulomb's constant $8.988 \times 10^9 \text{ Nm}^2\text{C}^{-2}$. The potential would then be

$$U_C = \frac{-ACe^2}{r} + \frac{B}{r^n} \quad (\text{Chapter 1.14})$$

Now that this digression is over we can get back to talking about the different types of intramolecular interactions and how to distinguish between covalent, ionic, and metallic interactions. The key to determining which type of bonding occurs is the valence electrons, specifically if they are gained, lost, or shared.

With covalent bonds there are valence electrons that are shared between adjacent atoms, which results in a pairing of electrons into localized orbitals and concentrating the negative charge between the positive nuclei. For ionic interactions we are typically dealing with atoms that have a different affinity for electrons, different electronegativities. A net transfer of charge can occur forming positively and negatively charged ions. These ions can form networks of ionic bonds held together by long-range coulombic interactions.

When the electronegativity is similar or the same between atoms the valence electrons are shared equally and the bond is purely covalent. When the electronegativity is very different the more electronegative atom withdraws nearly all the valence electrons and the bond is purely ionic. Thus electronegativity is how we distinguish between covalent and ionic interactions. In the intermediate case of electronegativity differences, bonds can have both covalent and ionic characteristics. We call these bonds polar covalent and one atom will have a partial positive and negative charge, as in HCl.

While there is no universally agreed upon cutoff value, in this class we will define an electronegativity difference of 0–0.4 to be non-polar covalent, 0.5–1.7 to be polar covalent, and greater than 1.7 to be ionic. In the case of metallic bonds, all atoms share their valence electrons and the nuclei form a positively charged array in a sea of delocalized electrons.

For soft matter the most common intramolecular interaction that we will deal with will be covalent interactions.

Intermolecular Forces/Interactions

As previously mentioned, intermolecular interactions are critical for many soft matter systems and there are several weak intermolecular interactions of interest, which include:

- Hard sphere potentials: the ability of atoms to effectively occupy space and repel at short length scales, quantum mechanical in nature
- Coulombic interactions: electrostatic attraction/repulsion between charged ions
- Lennard-Jones (LJ) potentials: induced dipole interactions between neutral atoms
- Hydrogen bonding: net dipole interactions
- The hydrophobic effect: a largely entropic interaction related to the structuring of water around hydrophobic interfaces
- Van der Waals force: includes London dispersion force, Debye force, and Keesom force which describe attraction and repulsion due to fluctuating polarization between nearby atoms/elements/particles, quantum mechanical in nature. Van der Waals forces decay as d^{-6}

If you are interested in the origin of these interactions there is an excellent book by Israelachvili that I can recommend. The key thing to focus on is that all of these interactions have energies on the order of 1 kT, so thermal fluctuations can potentially break these bonds.

Structure of Crystalline Materials

A crystal structure is a periodic array of atoms that repeats over large distances. There is long-range periodic order, both long range translational and orientational order, in addition to short range order. Before we analyze crystal structures we first have to start off

with a primitive lattice, lattice constants, interaxial angles, symmetries, point groups, and Bravais lattices.

Lattice, Primitive Unit Cell, Basis Vectors, Lattice Constants

A lattice is a periodic array of points (atoms) in 1D, 2D, or 3D. Those points are lattice points. Let's start with the 2D case. A 2D lattice can be described by a primitive or unit cell which in turn is described by two lattice constants (a , b), two basis vectors (a_1 and a_2), and an interaxial angle γ . Once we have defined this we can pick any point in our 2D lattice as an origin and we can describe any point in our lattice with the previous values.

When we pick our basis vectors we pick the shortest lattice translation as a_1 and the second to shortest translation as a_2 . The lattice constants are given by $a = |a_1|$ and $b = |a_2|$. The interaxial angle γ is then defined. This also defines our primitive cell which will only contain a single lattice point.

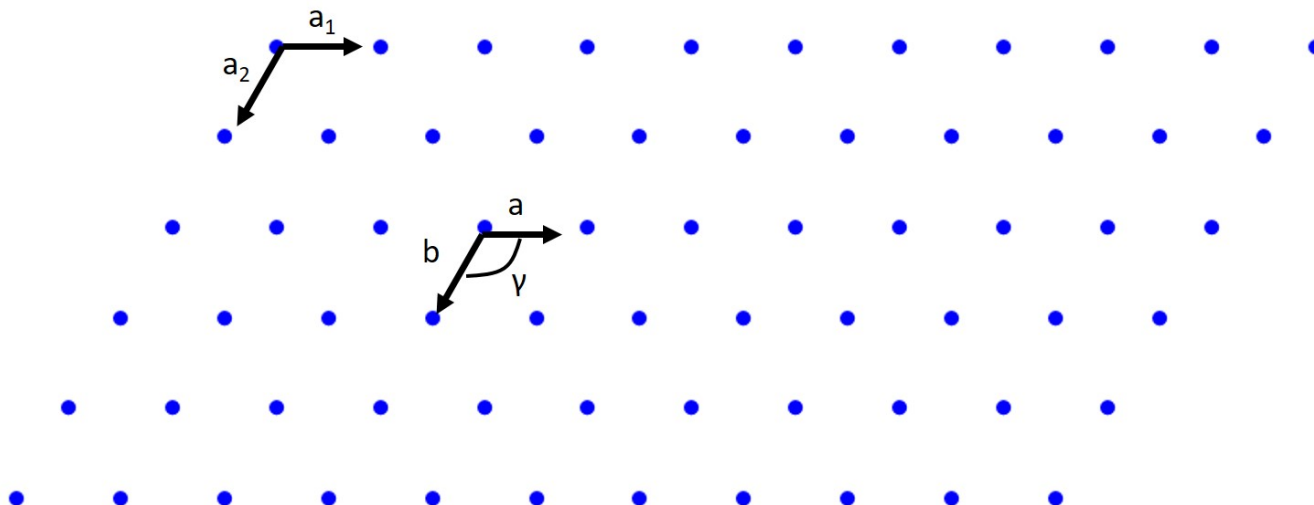


Figure Chapter1.2: Lattice with Parallelogram Cell

How about a rectangular lattice?

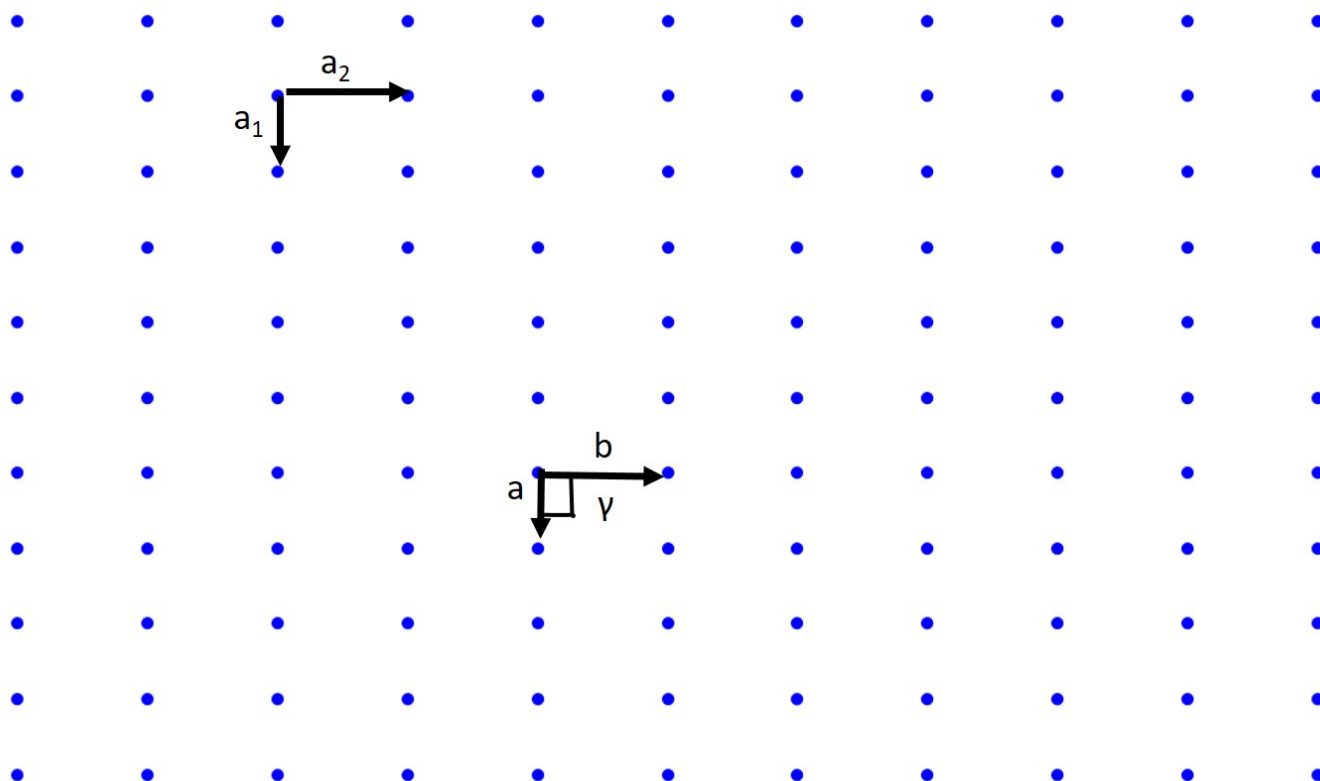


Figure Chapter1.3: Lattice with Rectangular Cell

Associated with crystallography is a myriad of symmetry operations and we have just dealt with translational symmetry. There are also reflection or mirror symmetry, glide symmetry, rotational symmetry, and more. These topics are all important but we are not a crystallography class so we will not be covering them in detail, but you should know these concepts exist. There are also 230 space groups, 32 crystallographic point groups, 14 Bravais lattices, and 6 crystal systems.

Crystal Systems: Simple Cubic, BCC, FCC, HCP

We are going to focus on the 6 crystal systems: triclinic, monoclinic, orthorhombic, tetragonal, hexagonal, and cubic. We will describe the unit cell, the primitive lattice vectors, and the interaxial angles.

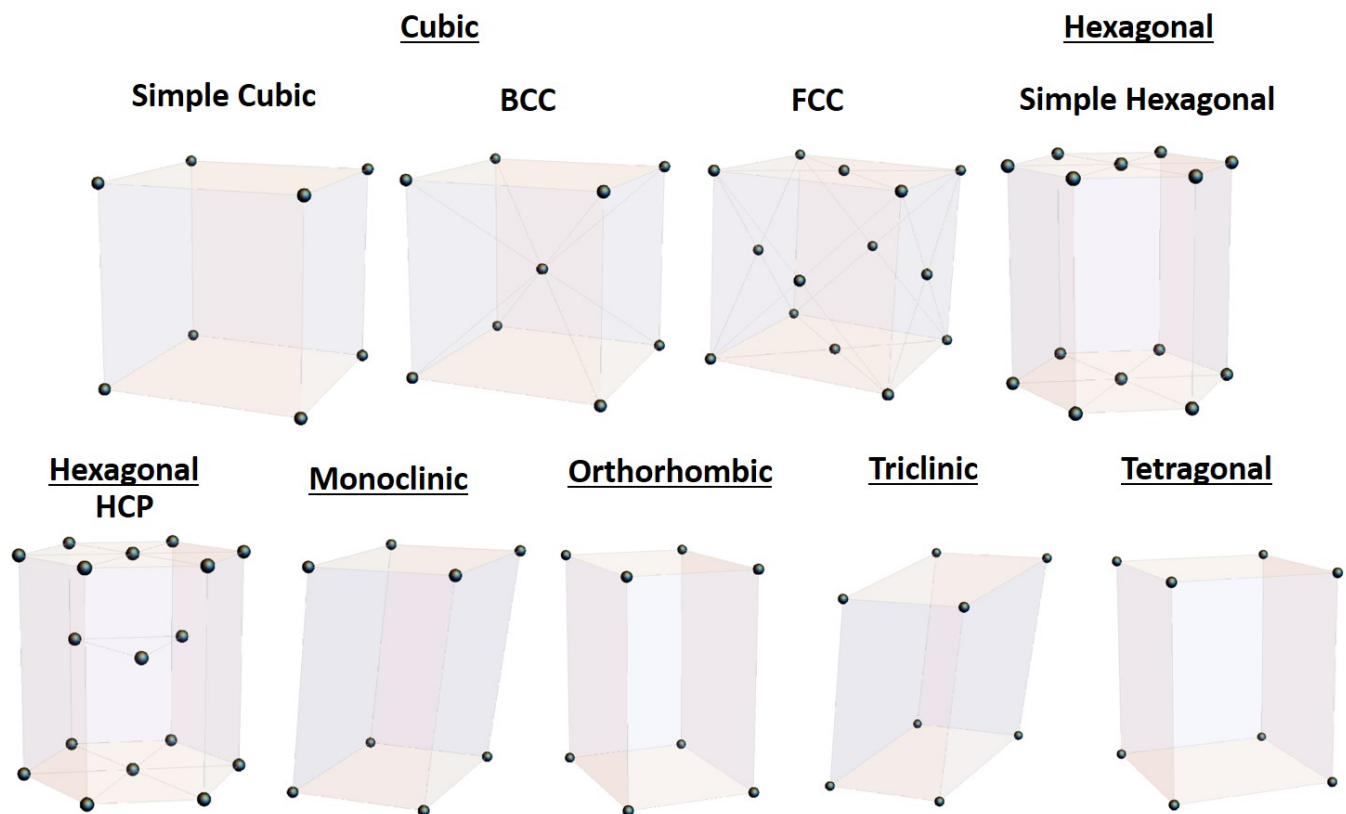


Figure Chapter 1.4: 6 Crystal Lattice Systems

You can see the rules and relationships between the lattice constants and the interaxial angles on the lecture slides.

<u>Simple Cubic</u> $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	<u>Orthorhombic</u> $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	<u>Hexagonal</u> $a = b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma = 120^\circ$
<u>Tetragonal</u> $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	<u>Monoclinic</u> $a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$	<u>Triclinic</u> $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$

Figure Chapter 1.5: 6 Crystal Systems

Crystallographic Directions

When discussing crystals we will also have to specify crystallographic directions and planes. In order to refer to specific crystallographic planes or directions we need a labeling system to index them. This system is called Miller indices. A crystallographic direction is a vector denoted by $[u\ v\ w]$. u , v , and w are integers which correspond to the reduced projections along the x , y , and z axes, respectively. We always use $[]$ for directions.

Example: draw the $[100]$ direction. To draw the direction of a vector, pick an origin for the vector tail (the side without the arrow), then pick the ending point for the vector (the arrow). Subtract the arrow point from the tail point and the resultant vector must coincide with the direction you are trying to draw. Typically pick the origin as your origin.

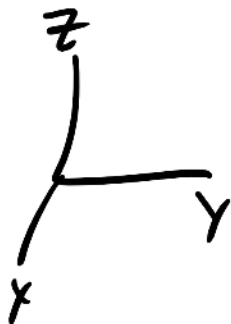
How about the $[111]$ direction?

What about $[100]$?

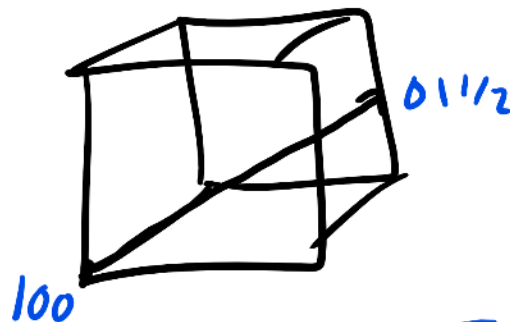
What about $[1\ -1\ 0]$?

What about $[222]$?

Now a little more complicated: what is the vector below?



What direction?



$$0\ 1\ 1/2 - 100 = 1\ 1\ 1/2$$

$$[2\ 2\ 1]^R$$

Figure Chapter1.6: What direction is this?

Crystallographically Equivalent Directions $\langle hkl \rangle$

For a number of crystal structures there are several nonparallel directions with different indices that are crystallographically equivalent. This means that the spacing and number of atoms along each direction is the same. In cubic crystals $[100]$, $[-100]$, $[010]$, $[0\ -10]$, $[001]$, and $[00\ -1]$ are all crystallographically equivalent so we group them in a family denoted by angled brackets $\langle 100 \rangle$.

Crystallographic Planes

For crystallographic planes we use Miller indices $(h\ k\ l)$ which correspond to the x , y , and z axes respectively. Notice again that $()$ are for planes and $[]$ are for directions. $\langle \rangle$ is for families of directions. Families of planes are denoted with $\{ \}$.

To draw planes, determine the intercepts. The intercepts are the inverse of the Miller indices. For example, the (111) plane:

(111) Plane
Intercepts $\rightarrow x = \frac{1}{1} \quad y = \frac{1}{1} \quad z = \frac{1}{1}$

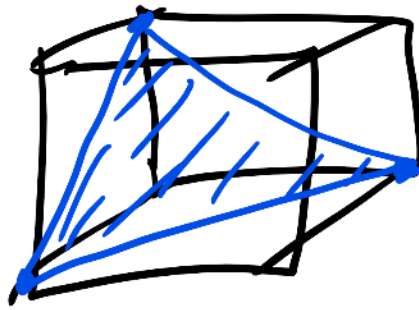


Figure Chapter1.7: (111) plane

For the (110) plane, if the inverse gives infinity, that means the plane is parallel to that axis. So the plane looks like this:

(110) Plane
Intercepts $\rightarrow x = \frac{1}{1} \quad y = \frac{1}{1} \quad (z = \frac{1}{0} = \infty \text{ Parallel!!})$

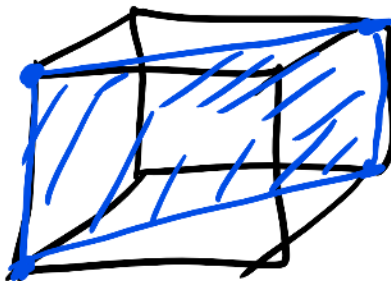
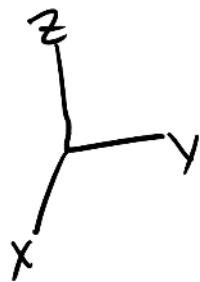
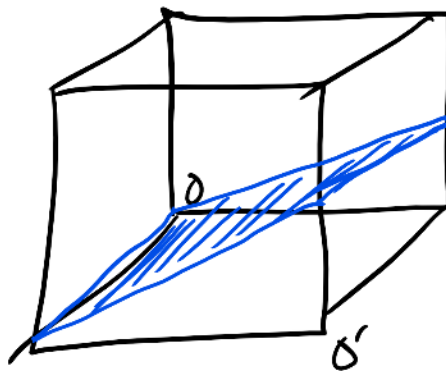


Figure Chapter1.8: (110) plane

Another tricky problem is when the plane passes through the origin:



What is the Plane?



Intercepts origin!
Redefine $0'$

Intercepts
 $x = \text{none}$ $y = -1$
 $z = 1/2$
(012)

Figure Chapter1.9: Plane Passing Through Origin

When a plane intersects the origin you must choose a different origin and repeat the procedure to determine intercepts and then Miller indices. Families of planes are denoted with $\{hkl\}$.

Here is a nice demonstration to visualize the Crystallographic Planes:

<https://demonstrations.wolfram.com/C...CubicLattices/>

Isotropic and Anisotropic

Up to now we have often assumed that material properties are the same in every direction. If materials behave in such a manner they are said to be isotropic materials. For many problems and theories in this course we will assume isotropy. This can often be the case for cubic structures. However, many materials are anisotropic, meaning that some material properties (mechanical, optical, kinetic, etc.) are different depending on the crystallographic direction you are investigating. For example titanium exhibits a larger modulus along the z -axis in the HCP structure than in the basal plane. This presents a significant problem when trying to superplastically form very thin titanium foil. A similar issue arises with magnetic properties of HCP materials as well. Also, real materials are not perfect single crystals — they are polycrystalline, made of many grains.

Simple Cubic (SC)

The simple cubic (SC), also called primitive cubic, is the structure for oxygen, fluorine, and others. It is described by the primitive lattice vectors a_1 , a_2 , and a_3 and interaxial angles α , β , γ . In SC all angles are 90° and $a = b = c = 2R$ where R is the atomic radius.

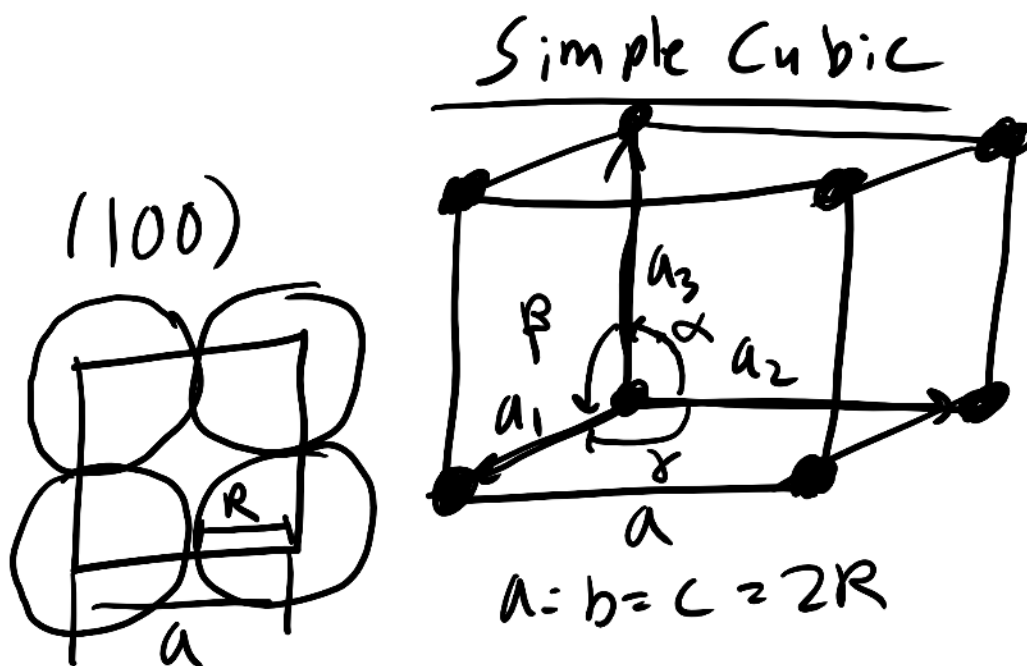


Figure Chapter1.10: Simple Cubic

How many atoms are contained in a simple cubic cell?

Answer: 1 atom (corner atoms shared by 8 unit cells).

How many nearest neighbors (NN)? 6.

How many second nearest neighbors (NNN)? 12.

What is the NN distance? $2R$.

What is the NNN distance? $2R\sqrt{2}$.

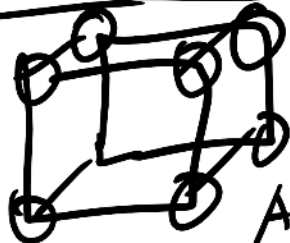
Atomic packing factor (APF): ratio of atom volume to unit cell volume. For SC:

$$APF_{SC} = \frac{\pi}{6}$$

(Chapter 1.15)

Atomic Packing Factor (APF)

SC (1 atom)



$$APF = \frac{1 \times (4/3\pi R^3)}{8R^3} \approx \pi/6$$

$$a = 2R$$

$$APF = \frac{\# \text{ atom} \times \text{atom volume}}{\text{Volume of cell}}$$

APF = 0.74
close packed
for spheres
equal
size !!!

Not close packed

Figure Chapter 1.11: SC APF

Body-Centered Cubic (BCC)

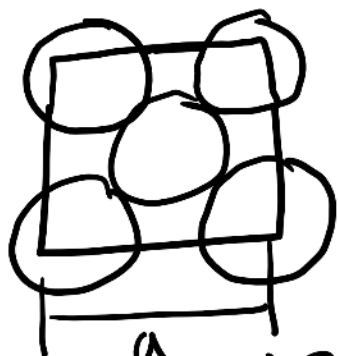
The BCC structure is found in Li, Fe, V, Mo. It is described by lattice vectors $a_1 = (a/2)[1 \ -1 \ 1]$, $a_2 = (a/2)[1 \ 1 \ -1]$, $a_3 = (a/2)[-1 \ 1 \ 1]$. Angles are 90° . Geometry shows that

$$a = \frac{4R}{\sqrt{3}}$$

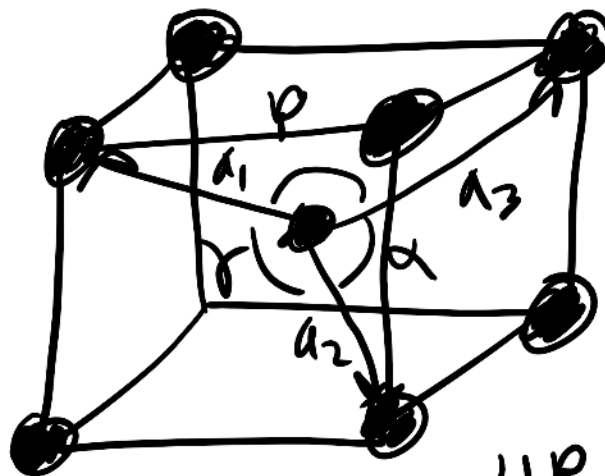
(Chapter 1.16)

Body-Centered Cubic (BCC)

(110)



$$a \approx 2R$$



$$a > 2R$$

$$a = \frac{4R}{\sqrt{3}}$$

Figure Chapter1.12: Body Centered Cubic

How many atoms per cell? 2 (1 inside + 8 corners shared).

How many NN? 8.

How many NNN? 6.

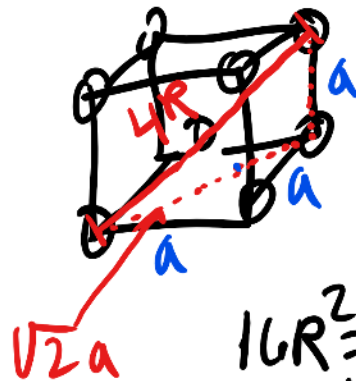
NN distance = $2R$.

NNN distance = $\frac{4R}{\sqrt{3}}$.

APF = 0.68.

Atomic Packing Factor (APF)

BCC



$$APF = \frac{2 \times \left(\frac{4}{3} \pi R^3 \right) (3)^{3/2}}{64 R^3} \approx 0.68$$

Not CP!!!

$$16R^2 = a^2 + 2a^2$$

$$a = \frac{4R}{\sqrt{3}}$$

Figure Chapter1.13: BCC APF

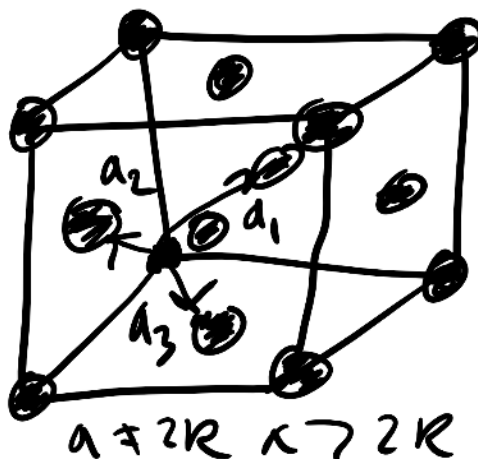
Face-Centered Cubic (FCC)

The FCC structure is found in Ni, Cu, Ca. Lattice vectors $a_1 = (a/2)[0 \ 1 \ 1]$, $a_2 = (a/2)[1 \ 0 \ 1]$, $a_3 = (a/2)[1 \ 1 \ 0]$. Angles 90° . In FCC:

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

(Chapter 1.17)

Face - Centered Cubic (FCC)



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

Figure Chapter1.14: Face Centered Cubic

Atoms per cell = 4 (8 corners shared + 6 faces shared).

Nearest neighbors = 12.

Second nearest neighbors = 6.

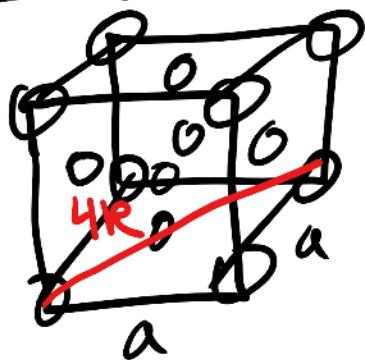
NN distance = $2R$.

Second NN distance = $2\sqrt{2} R$.

APF = 0.74 (the maximum possible packing for spheres of equal diameter).

Atomic Packing Factor (APF)

FCC 4 atoms



$$2a^2 = 16R^2 \quad a = 2\sqrt{2}R$$

$$APF = \frac{4 \times \left(\frac{4}{3}\pi R^3\right)}{\left(\frac{4}{2}\right)^{3/2} R^3} \approx$$

$$\boxed{0.74 \text{ CP!!!}}$$

Figure Chapter1.15: FCC APF

Close-Packed Structures and Atomic Packing Factor

HCP and FCC both achieve the maximum APF of 0.74 and are called close-packed structures. FCC stacks ABCABC... indefinitely while HCP stacks ABAB... indefinitely.

Close-Packed Planes and Planar Density

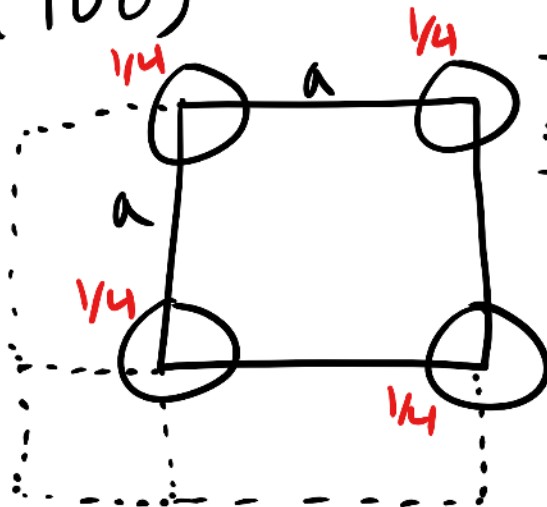
A close-packed plane has a packing density ≈ 0.9069 . Example: planar density of SC (100), BCC (110), FCC (111). Only close-packed structures can achieve close-packed planes, but often we care about the most closely packed plane even if not exactly 0.9069.

Close Packed Planes (CCP)

SC (100)

$$a = 2R$$

$$a^2 = 4R^2$$



Packing density =

$$\frac{\# \text{circles} \times \text{area}}{\text{plane area}}$$

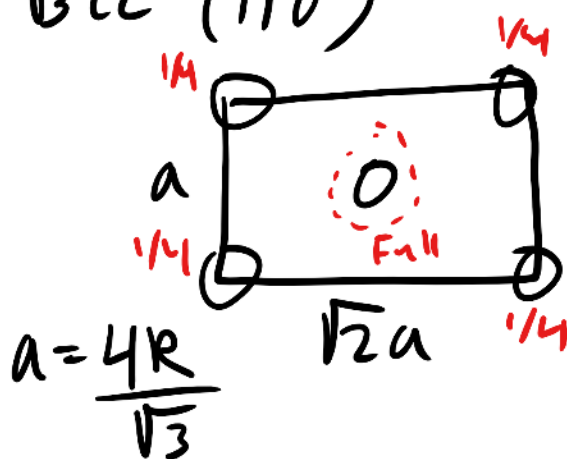
$$= \frac{1 \times \pi R^2}{4R^2}$$

$$= \frac{\pi}{4} \text{ Not CCP}$$

Figure Chapter1.16: Planar density SC (100)

Close Packed Planes (CCP)

BCC (110)



Packing density:

$$\frac{2 \times \pi R^2}{a^2 \cdot 2}$$

$$\frac{2 \times \pi R^2 \cdot 3}{32 \cdot R^2} \approx 0.589$$

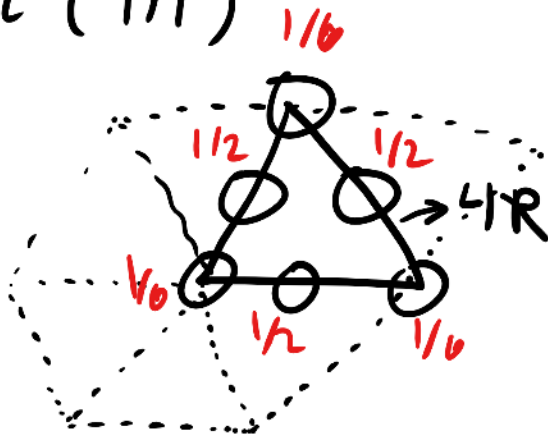
Not CCP!!

Figure Chapter1.17: Planar density BCC (110)



Close Packed Planes (CCP)

FCC (111)



Packing

$$\frac{2 \times \pi R^2}{\sqrt{3}/4 a^2} =$$

$$\frac{2 \pi R^2 \cdot 4}{\sqrt{3} 16 R^2} = 0.9069 \text{ CCP!!}$$

Figure Chapter1.18: Planar density FCC (111)

Close-Packed Directions

SC: $\langle 100 \rangle$

BCC: $\langle 111 \rangle$

FCC: $\langle 110 \rangle$

Polymorphism/Allotropy

When materials have more than one crystal structure they are polymorphic. In elemental solids this is called allotropy. Examples: carbon (diamond, graphite, fullerenes, graphene), iron (BCC and FCC), titanium (HCP and BCC). Polymorphism is common and important in materials science.

Structure of Non-Crystalline Materials: Semi Crystalline and Amorphous

Examples include polymers, liquids, glasses, gases, liquid crystals, and many more. Up to this point we have focused only on crystalline materials because they are the simplest to characterize in terms of structure. However, many materials do not adopt a crystalline structure with short-range, long-range translational, and long-range orientational order.

With crystalline materials we were able to translate a unit cell to essentially infinity because we had short range order, long range translational order, and long range orientational order. In polymers, glasses, and liquid crystals typically we only have short range order (SRO) and perhaps some degree of long range order either translational or orientational but not both.

To describe these non-crystalline materials we use the dimensionless pair distribution function (PDF) or radial distribution function (RDF). This is also called the pair correlation function. It is our key descriptor for quantifying the SRO present in a material.

The PDF or RDF is defined as:

$$g(r) = \frac{1}{\langle \rho \rangle} \frac{dn(r, r + dr)}{dv(r, r + dr)} \quad (\text{Chapter 1.18})$$

where ρ is the average particle number density, dn is the number of particles counted in a small spherical shell sampling volume element of size dv at each distance r from a particle chosen as the origin. The number of particles in each shell is counted at each subsequent dr shell.

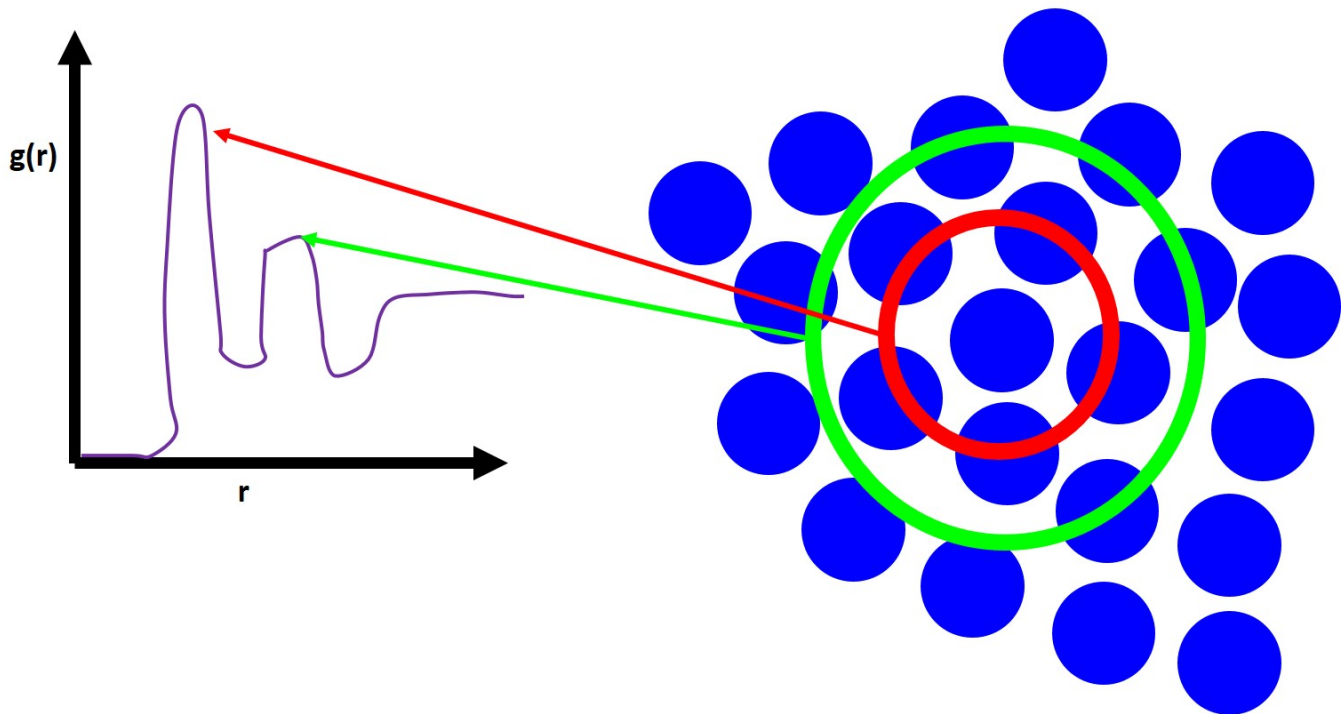


Figure Chapter 1.19: Pair distribution function schematic

To get a smooth curve you want to pick dr much smaller than the particle radius and average over multiple origins. For perfect crystals the PDF shows sharp discrete peaks at interatomic spacings corresponding to the structure. For liquids you see a large first peak and then smaller peaks. The first peak corresponds to nearest neighbors, which can be calculated:

$$\langle NN \rangle = \langle \rho \rangle \int_{\text{peak}} g(r) 4\pi r^2 dr \quad (\text{Chapter 1.19})$$

PDF can also be used to quantify SRO for glasses. Example: silica glass (also applies to thermoset polymers).

Metal PDF/RDF

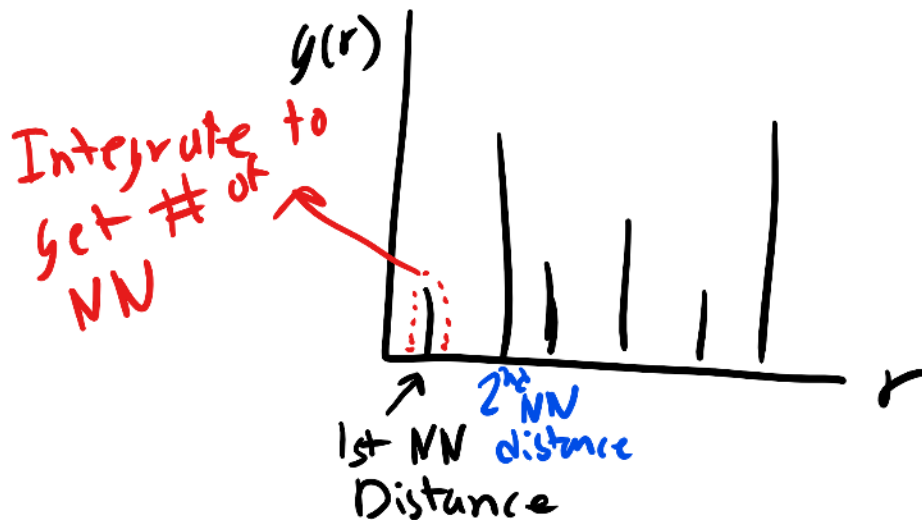


Figure Chapter1.20: Metal RDF interpretation

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Chapter 10: Creep, Fracture, and Fatigue

Time-Temperature Dependent Plasticity

We have previously been investigating the phenomenon of plastic deformation at low temperatures and particularly we have observed plastic deformation through the phenomenon of dislocation glide (DG). However, as temperature increases as we discussed previously dislocations are able to move via dislocation climb and multiple and an insidious phenomenon known as creep can come into play in particular for metals creep becomes a relevant mechanism once $T > 0.3T_m$ and for ceramics when $T > 0.5T_m$. Additionally as we will see the creep strain depend principally on the applied stress and temperature of the system.

We have previously discussed creep in relation to polymer LVE. Creep is time or temperature dependent plastic deformation in crystalline materials. Creep is particularly insidious because the stress where creep ensues is much much less than the reported or measured yield stress of a material. This is extremely problematic as we see in our LVE lecture if we were working with a linear elastic material if we applied a stress $\sigma < \sigma_y$ we should expect that the strain remain constant but at high enough temperatures the strain increases with time. Now when dealing with creep there are typically three regimes characterized by the plot below.

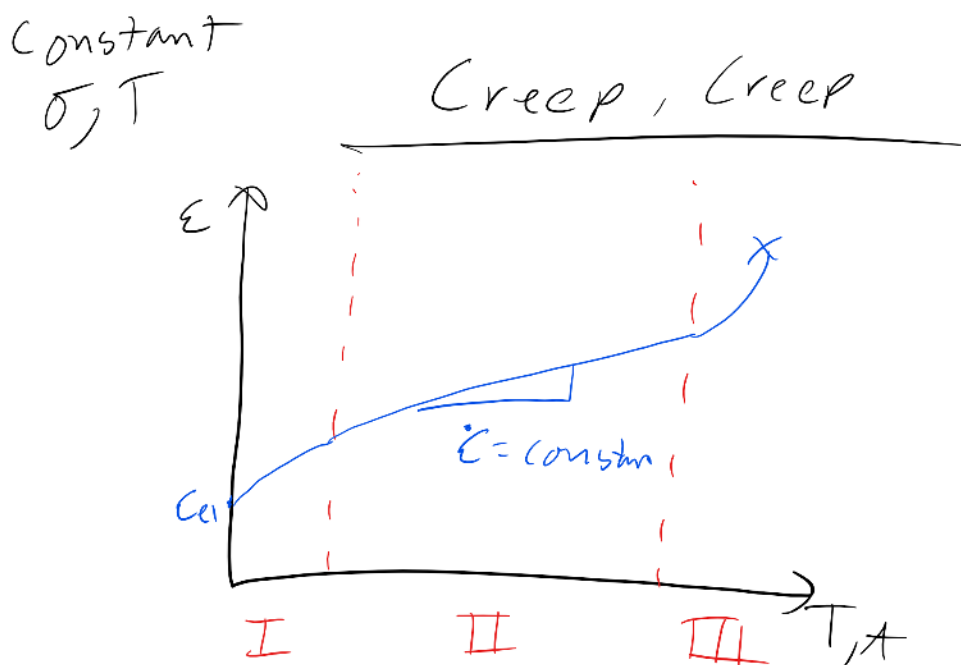


Figure Chapter10.1: Creep stages.

1. Primary or Transient Creep
2. Secondary or Steady State Creep
3. Tertiary or Runaway Creep

In the primary or transient creep regime the strain growth is relatively slow however once we reach the secondary creep regime we see the the strain grows at a constant strain rate $\dot{\epsilon}_c$. This leads to large strains and can be a limiting factor in design. Now in the tertiary regime the strain increases extremely fast and this also known as runaway creep, no way to stop creep in this regime and it typically leads to failure. Creep is a critically important phenomenon in high temperature application like turbine blades, power stations, hot forming operations, and many others.

Again as materials scientists we want to focus on predicting the creep strain rate, $\dot{\epsilon}_c$, so that we can determine the expected creep strain in our application and we can predict when the material may fail in an application. For example in an turbine engine we need to make sure the turbine blades to creep to an extent where they contact the turbine engine enclosure, that can be very bad!!

So when considering how we design applications to consider creep we have to ensure the following:

- The total creep strain is less than the allowable strain for a particular application
- The strain to failure must be greater than both the total creep strain and allowable strain for an application
- The time for the application must be less than the time to failure for creep

These may seem like obvious design criterion but both creep and fatigue are often the most overlooked phenomenon in application design and lead to most catastrophic failure in applications.

Now in addition to thermally activated diffusion we can also observe creep and diffusion that is driven by a mechanical force as well. Consider the following scenario if there is no applied force than in the image below atoms A and C are equally likely to diffuse into the vacancy B but if a material is loaded it is much more likely that A moves into B than C. Thus we have effectively introduced an energy potential into this system and thus biased the diffusion in a particular direction.



Figure Chapter10.2: Mechanisms of creep diffusion.

Let's talk about some more mechanisms in detail now to get an atomistic perspective before zooming out the macro scale.

Atomistic Mechanisms of Creep

Now before we get into our macroscopic view point and look at some beautiful equations and deformation mechanism maps let us consider creep at the atomistic length scale and one mechanism of how creep can occur is via diffusion. Now we have just had a thorough discussion of diffusion but we will see that several of the mechanisms of creep will occur via dislocation climb which is a thermally activated diffusion process. Now what is interesting in creep is that we are dealing with crystalline materials primarily when we discuss creep (creep also occurs in polymers which are viscoelastic materials but we can discuss creep in polymers more if people are interested) and there are actually multiple diffusive pathways in crystalline materials. Remember that most crystalline materials are poly-crystalline so there regions of perfect crystal which we will refer to as the bulk there are also multiple grain boundaries in polycrystalline materials and materials can also diffuse along grain boundaries as well as in or around other defects like dislocations, point defects, and even free surfaces. As we saw in our brief diffusion refresher typically atoms will diffuse faster when there is more available free space so atoms will diffuse faster in grain boundaries than in the bulk and this is because there is more open space and thus the activation energy for diffusion is lower in the grain boundaries than in the bulk $Q_{GB} < Q_B$.

Bulk Diffusion

When we consider Bulk diffusion we will typically see atoms that move via vacancy diffusion into a site. Now there are other modes of diffusion where atoms can move into an interstitial site or a tetrahedral, octahedral, split-dumbell, and many other sites

but for most metals, ionic crystals, and ceramics this is the most likely diffusion pathway.

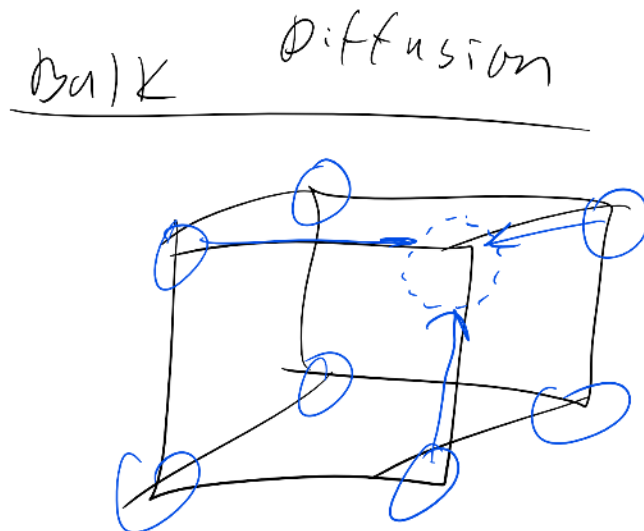


Figure Chapter10.3: Bulk diffusion.

Grain Boundary Diffusion

As we have mentioned previously grain boundaries meet when the crystal orientation is offset by some angle and as we discussed previously these can be high or low angles. In addition to this change in angle there will also typically be some width to the grain boundary and the structure will be more open than the rest of the crystal. Now typically this grain boundary width δ will be at least two atomic diameters or around $5\text{\AA}$ or very close to a nm so this distance is significant. Now at this point you may ask well if the grain boundary diffusion is so much faster than the bulk why are we even considering the contribution of the bulk? Well that is because even though the grain boundary diffusion is much faster its total contribution to creep depends on how much grain boundary is available to diffuse into and through so thus it depends on both the δ and the grain diameter d_g . We can actually compare the relative areas for grain boundary and bulk diffusion as follows we imagine a circular grain and let's neglect constants for now but for bulk diffusion the area will be approximately $\left(\frac{d_g}{2}\right)^2$ whereas for a grain boundary it will be approximately $\frac{\delta d_g}{2}$ so if we divide the area for grain boundary diffusion by that for bulk we get

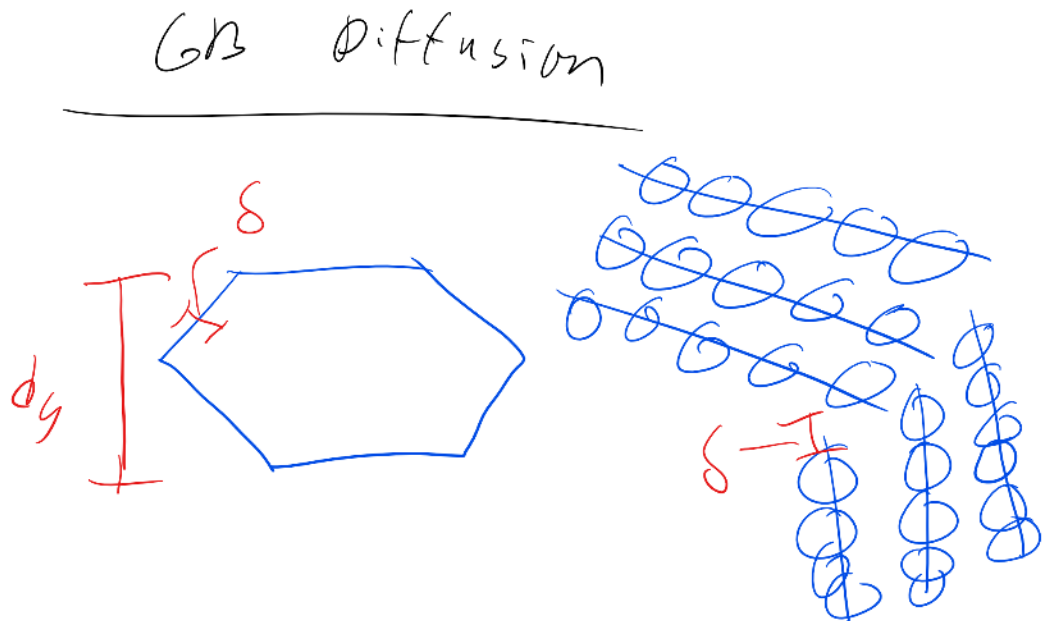


Figure Chapter10.4: Grain boundary diffusion.

$$\frac{2\delta}{d_g}$$

(Chapter 10.1)

this is a very very important expression. We see that the relative areas depend inversely with grain size. The width of the grain boundary will not change appreciable but grain size can vary from 100s of μm to 10s of nm or less. That is a 4 order of magnitude change and it makes sense intuitively. As the grain size decreases due to conservation of volume there will be more crystalline grains and thus diffusion along grain boundaries will begin to dominate as there are more diffusive paths relative to large grain sizes and the enhanced diffusion will make this type of dislocation mechanism dominate the overall behavior. Vice versa can be said as grain size increases.

Power Law Creep Dislocation Climb

One more mechanism that we will delve into is just a bit is power law creep through dislocation climb. In this scenario there can be obstacles to dislocation climb i.e. point defects, precipitates, dislocations, which prevent or seriously inhibit dislocation glide. One method to move around these obstacles is for the dislocation to climb around the obstacles so the dislocation can continue to climb. This force can initiate the diffusion of atoms from the dislocation core as that is where stress is the largest. This process repeats to allow the dislocation to move through the material. Now remember that typically dislocation climb is a thermally activated process but we discussed previously that this assumption held for relatively small applied stresses. However, at high stresses this is not necessarily the case and as described above climb can be initiated.

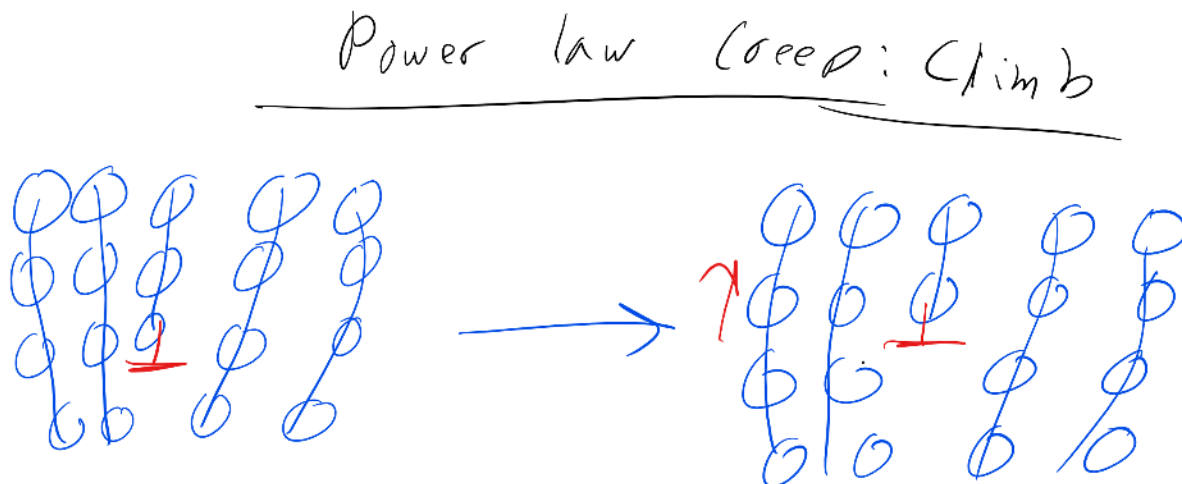


Figure Chapter10.5: Power law creep via dislocation climb.

General Creep Strain Rate Expression

Luckily we have developed a nice framework for describing creep in the secondary regime, we typically will neglect the first regime and once we reach the tertiary regime there is nothing we can do. So we can use the following general expression to describe the creep strain rate

$$\dot{\epsilon}_c = K_c \sigma^x d_g^y D_c = K_c \sigma^x d_g^y D_o \exp\left(\frac{-Q_c}{kT}\right) \quad (\text{Chapter 10.2})$$

where K_c is an empirical material specific creep constant, σ is the applied stress, d_g is the grain diameter, D_c is the creep diffusivity, and Q_c is the activation energy for that creep mechanism. Now those diffusion mechanisms are diffusion of vacancies through the lattice or bulk diffusivity, diffusion of vacancies along grain boundaries, and diffusion of vacancies to dislocations.

Lattice/Volume/Bulk Diffusion: Nabarro-Herring Creep

We have our equation for Nabarro-Herring Creep below:

$$\dot{\epsilon}_{NH} = \frac{K_{NH} \sigma D_o \exp\left(\frac{-Q_L}{kT}\right)}{d_g^2} \quad (\text{Chapter 10.3})$$

The key things to see in this equation is the activation energy for lattice diffusion and the scaling behavior with the grain size. Also note that this creep describes diffusion in the bulk and it is linear with stress. This mechanism will dominate at high temperatures, larger grain sizes, and intermediate to low stresses.

Grain Boundary Diffusion: Coble Creep

Here the number of diffusive pathways increases as the grain size decreases and remember that the activation energy for grain boundary diffusion is lower than for bulk.

$$\dot{\epsilon}_{CC} = \frac{K_{CC} \sigma D_o \exp\left(\frac{-Q_{GB}}{kT}\right)}{d_g^3} \quad (\text{Chapter 10.4})$$

The noticeable relationships here are that again we have a linear relationship with stress a strong dependence on grain size, even stronger than for NH creep. Also we see that the diffusion we describe here is grain boundary diffusion. Now this regime will get considerably larger and dominate when the grain size is small. Also this regime will tend to dominate at lower temperatures than NH creep. Why is this? Because remember the activation energy for diffusion in the grain boundary is lower than that for the bulk so we need less energy to get equivalently fast diffusion.

Power Law Creep

Here the net motion of dislocation cores moves in direction of applied stress, i.e. macroscopic creep. The dependence on applied stress is critical as you can see the scaling behavior in the equation below. Additionally dislocation climb is the rate-limiting process.

$$\epsilon_{DLC} = K_{NH} \sigma^{4-6} D_o \exp\left(\frac{-Q_L}{kT}\right) \quad (\text{Chapter 10.5})$$

We can now take a look at some key aspects of creep and in particular the scaling behavior of creep:

Unknown environment 'tabular'

We can see that PLC will dominate at high temperatures and high stress and Coble creep will dominate at lower temperatures compared to NH.

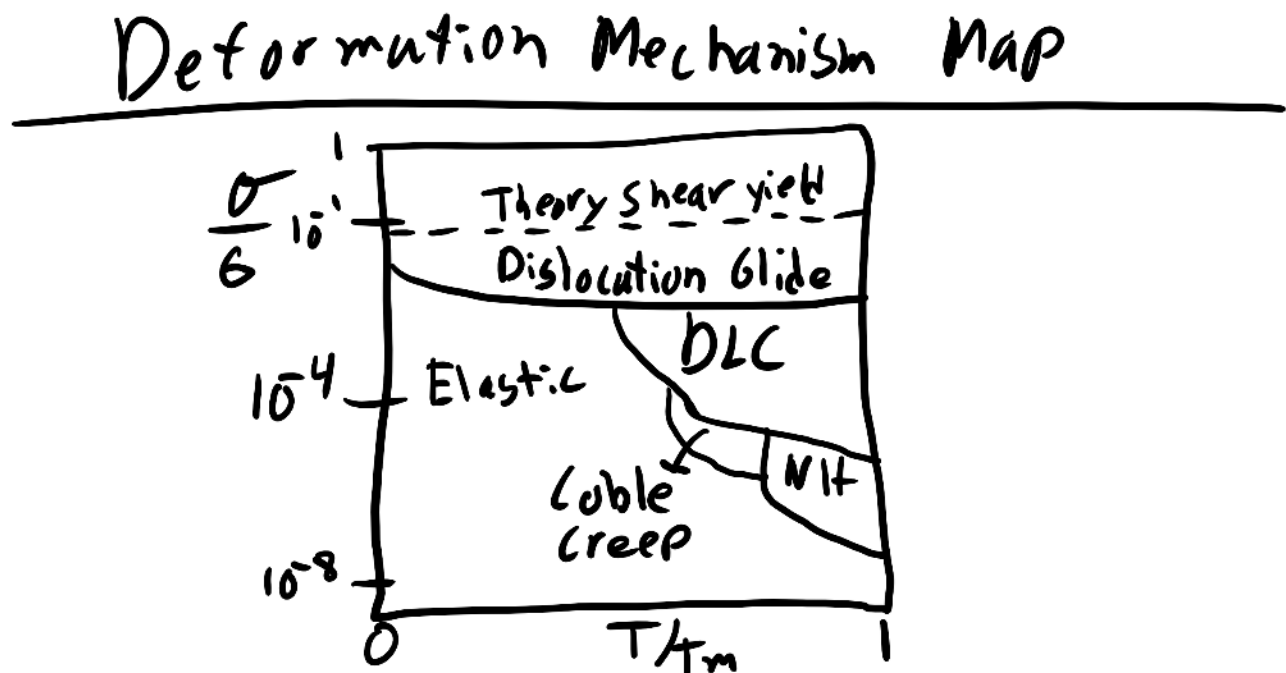


Figure Chapter10.6: Deformation mechanism maps. Visualize and explain why certain mechanisms are predominant.

You will notice that there are other distinct regions in this deformation mechanism map which shows the various mechanism of deformation. Note that on this plot the x-axis is a plot of the homologous temperature which is a dimensionless number which plots temperature divided by the melting temperature and we also have stress on the y-axis normalized by the shear modulus. In addition to our creep mechanisms we also have

- Theoretical Yield Strength: The dashed line is completely flat and indicates the theoretical yield strength of a material which is approximately $\sigma_{theory} = \frac{G}{10}$. This line will never change location regardless of material.
- Elastic: Deformation that is purely elastic and dominates at low temperatures and stress, must be below the dislocation glide line which indicates the yield strength at different temperature conditions.

- Dislocation Glide: Deformation that is plastic and deformation occurs exclusively through dislocation glide. The stress is above the yield stress of the material which is indicated by the solid black line.

One of the ways to mitigate or prevent creep is typically close packed structures are more creep resistant also if one solute strengthens, precipitate strengthens, or increasing grain size as it slows creep due to fewer diffusive pathways along grain boundaries. Superalloys typically leverage this technique through the precipitating strengthening and anti-phase boundaries (APB). Also many high temperature applications will even use single crystal materials to avoid CC creep.

Fracture Regime

Finally Fracture!!

Fracture is the last resort for material deformation mechanisms when all other elastic/plastic mechanisms are exhausted. Energy is dissipated by bond breaking. In uniaxial loading, the stress required to break the material in two pieces, at the stress fracture. Again as in the case of yielding the theoretical stress required to fracture materials (Steel 4340 65GPa, Al 20GPa, Si 7GPa) is orders of magnitude higher than the actual stress required to fracture materials (Steel 4340 ~3GPa, Al ~0.7GPa, Si ~0.3GPa). This is because real materials typically contain cracks (inside, at surface, or at interfaces) and these micro-cracks act as stress concentrators. For an elliptical hole we can define the stress as a function of the distance from the stress concentrator as:

$$\sigma = \sigma_o \left(1 + 2\sqrt{\frac{a}{R}} \right) \quad (\text{Chapter 10.6})$$

and R at the tip of the crack is $\frac{b^2}{a}$. Brittle fracture occurs when the stress concentration at a pre-existing crack tip is so high that the material will break catastrophically.

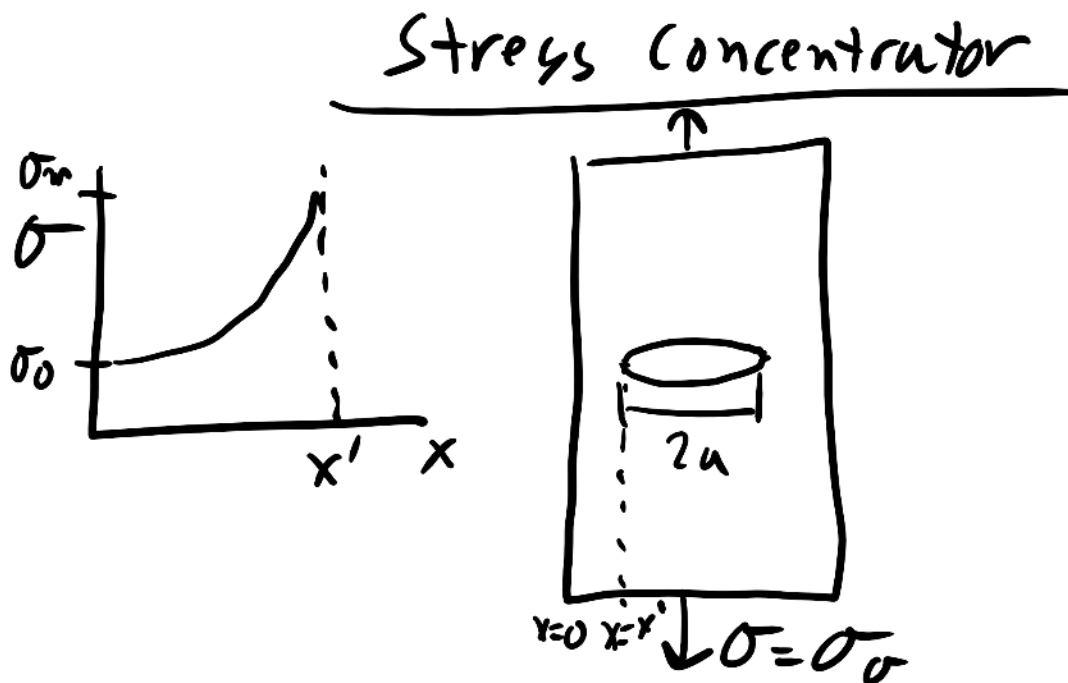


Figure Chapter10.7: Stress Concentrator.

Griffith's Theory of Brittle Fracture

We can develop an equation for brittle fracture from Griffith by considering the surface area created as the crack grows and the stored elastic energy that is relieved. Note that this derivation is particularly valid for very brittle materials like glasses and ceramics.

When considering fracture, the two energy contributions are: creating surface area (energy penalty) and relieving elastic strain energy (energy release). Creating surface area results in a positive energy contribution that resists crack growth, while relieving

strain energy provides a negative contribution that drives crack propagation. Fracture will proceed when the reduction in elastic strain energy equals or exceeds the energy required to create new surfaces.

Relieving Stored Elastic Energy

We know that we can calculate the stored elastic strain energy in a material as:

$$U_{ESE} = \int \sigma d\epsilon = \frac{\sigma^2}{2E} \quad (\text{Chapter 10.7})$$

Note here that we are assuming the material is very brittle, so $\sigma = E\epsilon$. This is the energy per unit volume, so to obtain the total energy, we multiply by the volume of the elliptical crack, approximated as:

$$\Delta U_{el} = -\frac{\pi a^2 t \sigma^2}{2E} \quad (\text{Chapter 10.8})$$

The negative sign indicates that this term represents a reduction in energy as the crack grows.

Creating Surface Area as Crack Grows

When a crack grows, two new surfaces are created, with a total area approximated as:

$$\Delta U_{surf} = 4at\gamma \quad (\text{Chapter 10.9})$$

Now the crack reaches its critical length when the total energy is minimized:

$$\Delta U_{tot} = \Delta U_{surf} + \Delta U_{el} = 0 \quad (\text{Chapter 10.10})$$

This gives us Griffith's expression for the critical stress for fracture:

$$\sigma_f = \sqrt{\frac{2\gamma E}{\pi a_{crit}}} \quad (\text{Chapter 10.11})$$

Note that this derivation assumes the stress is constant at the crack tip, which is an approximation.

Orowan Theory of Ductile Fracture

There are a number of materials, metals and polymers, which will not fracture in a completely brittle manner but instead through the formation of a small plastic zone prior to each crack elongation. For these materials, Orowan proposed a theory for ductile fracture:

$$\sigma_f = \sqrt{\frac{EG_c}{\pi a}} \quad (\text{Chapter 10.12})$$

where G_c is the strain energy release rate.

Stress Intensity Fracture and Fracture Toughness

We can relate the Griffith criterion for fracture to useful material parameters such as the stress intensity factor and fracture toughness.

Rewriting Griffith's equation:

$$\sigma\sqrt{\pi a} = \sqrt{2\gamma E} \quad (\text{Chapter 10.13})$$

The left-hand side represents the applied conditions (loading), and the right-hand side represents material properties. We define the stress intensity factor as:

$$K_I = f\sigma\sqrt{\pi a} \quad (\text{Chapter 10.14})$$

where f is a geometric correction factor. The subscript "I" indicates the fracture mode (Mode I: opening mode). Modes II and III correspond to in-plane shear and out-of-plane shear, respectively.

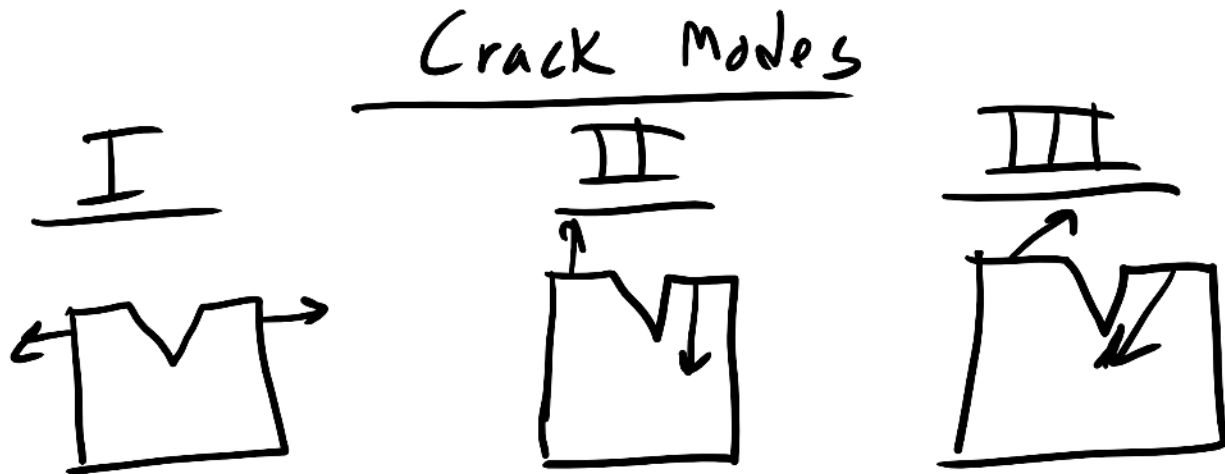


Figure Chapter10.8: Modes of Cracking.

The fracture toughness is defined as a material property:

$$K_{IC} = \sqrt{EG_c} \quad (\text{Chapter 10.15})$$

with units of $\text{Pa}\sqrt{m}$. Fracture occurs when:

$$K_I = K_{IC} \quad (\text{Chapter 10.16})$$

If $K_I < K_{IC}$, the material will not fracture. This criterion can also be used to determine the critical crack length or the stress required for fracture.

Now, we previously mentioned that a plastic zone develops near the crack tip. Because the stress at the crack tip theoretically approaches infinity, a small region undergoes yielding, forming a plastic zone of radius r_p .

The Griffith equation is only valid when this plastic zone is small, specifically when:

$$\frac{r_p}{a} < 0.02 \quad (\text{Chapter 10.17})$$

If this condition is not met, the Griffith approach cannot be used.

To estimate r_p , we assume a plane stress condition. The local stress field near the crack tip can be approximated by:

$$\sigma_{local} \approx \frac{\sigma\sqrt{\pi a}}{2\pi r} \approx \frac{K_I}{2\pi r} \quad (\text{Chapter 10.18})$$

Equating this to the yield stress gives:

$$\sigma_y = \frac{K_I}{\sqrt{2\pi r_p}} = \frac{\sigma\sqrt{\pi a}}{\sqrt{2\pi r_p}} \quad (\text{Chapter 10.19})$$

Thus, the plastic zone size is:

$$r_p = \frac{K_I^2}{2\pi\sigma_y^2} \quad (\text{Chapter 10.20})$$

This provides a good approximation for many materials.

Mechanisms of Fracture

Typically when we want to obtain a physical understanding of fracture we must understand that fracture is somewhat stochastic in that cracks will typically initiate where stress is concentrated the most, typically at microcracks, and these cracks are distributed stochastically and will propagate in a manner that follows the lowest energy path, i.e. to relieve elastic strain energy the most.

For ceramics and glasses, which are very brittle, cracks will propagate quite easily with minimal plastic deformation. Additionally, the fracture surface of these materials will be quite smooth and flat, again exhibiting little to no plastic deformation. This flat surface comes from the cleaving of atomic planes.

Most metals will typically fracture in a ductile manner and will have some plastic zone, but at certain temperature conditions may fracture in a brittle manner. The fracture surface for ductile metals will be much more rough due to this plastic deformation, and as you may imagine, materials with a larger yield strength will typically have a smaller plastic zone, whereas materials that exhibit a smaller yield stress will have a larger plastic zone.

Fracture for ductile metals often starts near inclusions within a metal, which are chemical compounds where the metal reacts with impurity atoms; this is a large problem in industry. The plastic flow typically will take place around these inclusions, leading to elongated cavities that line up and turn a sharp crack into a blunt one. Blunting a crack tip is the key to obtaining high toughness, and the ability of these inclusions to blunt crack propagation is important.

Polymers are much more complicated and can fracture in a ductile or brittle manner depending on temperature, time, and strain rates. Also, the toughness of these materials can increase by including rubber precipitates or by developing composites which blunt crack propagation.

Ductile to Brittle Transitions

Often metals and other materials can exhibit a ductile to brittle transition, and this transition depends on several parameters, specifically the yield stress and the size of the plastic zone.

Additionally, the yield stress also depends on temperature and strain rate as described by the following expression:

$$\sigma_y = \sigma_y^o \left(1 - \frac{kT}{Q_b} \ln \frac{\dot{\gamma}}{\dot{\gamma}_o} \right) \quad (\text{Chapter 10.21})$$

where σ_y^o is the yield strength at 0K, Q_b is the energy per bond, $\dot{\gamma}$ is the shear strain rate, and $\dot{\gamma}_o$ is a material parameter.

Additionally, remember that we have:

$$r_p \approx \left(\frac{K_I}{\sigma_y} \right)^2 \quad (\text{Chapter 10.22})$$

These expressions lead us to the following general relationships that are somewhat intuitive: as temperature decreases, the yield strength increases and plastic zone size decreases, thus the material becomes more brittle. Equivalently, the same occurs as the strain rate increases. This highlights a very important relationship — Time-Temperature Equivalence. This ductile-to-brittle transition is most notably observed as the cause for the fracture of liberty ships during World War II.

Creep Fracture

Fracture can also occur as a result of secondary creep and tertiary creep. Creep fracture typically occurs intergranularly, i.e. along the grain boundaries as opposed to trans- or intragranularly. The way that creep fracture occurs is via the coalescence of voids due to diffusion of material away from the grain boundaries, i.e. vacancies left behind as material moves along grain boundaries. This eventually causes rupture and can be described by some empirical relationships, specifically the Monkman-Grant equation and/or the Larson-Miller parameter.

Increasing Toughness by Blunting Crack Tip Propagation

There are multiple ways to increase the toughness of a material and reduce brittle fracture. One of the ways this is done in polymer blends is by including rubbery or soft inclusions, by blending a brittle polymer with a more rubbery polymer. This is most

noticeable in High Impact Polystyrene (HIPS), where we blend polystyrene (PS) with a rubbery polymer, polybutadiene (PB), in order to increase the toughness of the material while paying a cost in stiffness.

We can also create self-healing materials which seek to heal cracks and close them as they propagate. This is commonly done with microcapsules that activate an epoxy or a chemical reaction which fuses the crack. Additionally, depending on the diffusivity of the material, some can actually self-heal via diffusion.

Composites are also excellent examples of methods to increase the toughness of materials as they are typically composed of a brittle and more ductile component. Even if the composite is made of two brittle components, as the crack interacts with the different component it tends to be blunted and stops propagating.

Fatigue

Fatigue (cyclic) loading occurs at applied stresses that are much lower than the stress at fracture or even the yield stress but again, like creep, can lead to catastrophic failure at these low applied stresses.

Fatigue can occur in components or applications where there is no pre-existing crack and it can also occur where there is a pre-existing crack. Now typically most materials will have some pre-existing or microcracks, but there are certain applications like small components such as gear teeth where there may not be significant microcracks.

Let's consider the scenario where there are no pre-existing cracks first.

Fatigue: No Pre-existing Cracks

With a fatigue-type loading scenario, we will assume some type of cyclical loading with a particular number of cycles N , a number of cycles to failure N_F , and a maximum stress σ_{max} , and minimum stress σ_{min} as seen below.

Note that the change in stress is described as $\Delta\sigma = \sigma_{max} - \sigma_{min}$ and the mean stress is described as $\sigma_m = \frac{\Delta\sigma}{2}$.

For systems that have no pre-existing cracks we can describe the fatigue in two regimes: low-cycle and high-cycle fatigue. Typically, low-cycle fatigue will fail at fewer than 10^4 cycles and high-cycle fatigue will fail at more than 10^4 cycles.

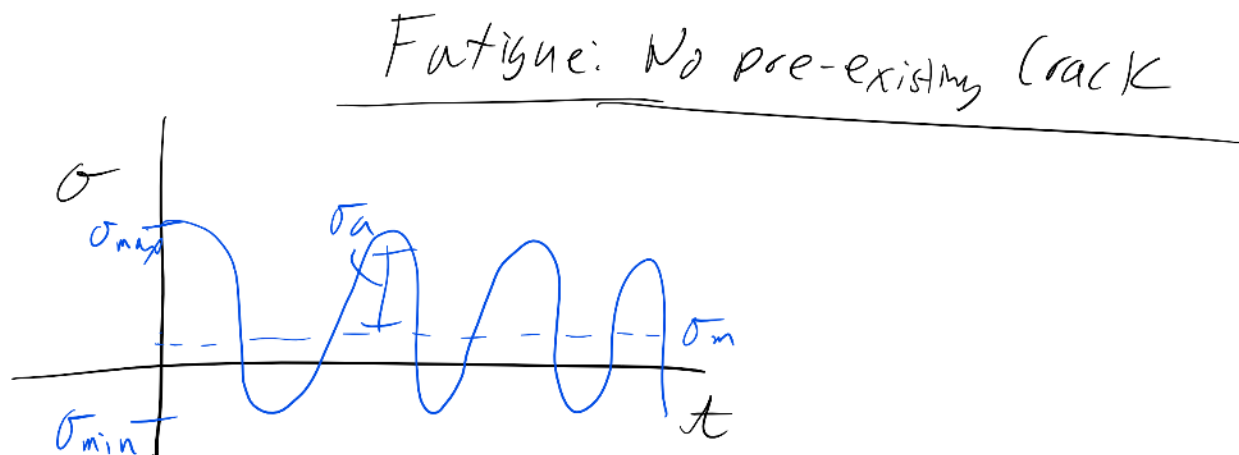


Figure Chapter10.9: Fatigue with no pre-existing crack.

We can actually develop a relationship that describes the change in stress to the number of cycles to failure as follows for high-cycle fatigue, and this is known as Basquin's Law:

$$\Delta\sigma N_f^a = C_1 \quad (\text{Chapter 10.23})$$

where a and C_1 are material properties and typically $\frac{1}{15} < a < \frac{1}{8}$. The low-cycle fatigue instead relates the change in plastic strain to the number of cycles to failure as described by the Coffin-Manson law:

$$\Delta\epsilon^p N_F^b = C_2 \quad (\text{Chapter 10.24})$$

where b will typically vary from 0.5–0.6.

Also, if $\Delta\sigma$ varies over the lifetime we can apply Miner's rule of cumulative damage to determine when the number of cycles to failure has been met using the following relationship:

$$\sum \frac{N_i}{N_{f,i}} = 1 \quad (\text{Chapter 10.25})$$

where $N_{f,i}$ is the number of cycles to fracture for each region i , and the ratio represents the fraction of lifetime used up after N_i cycles in that region.

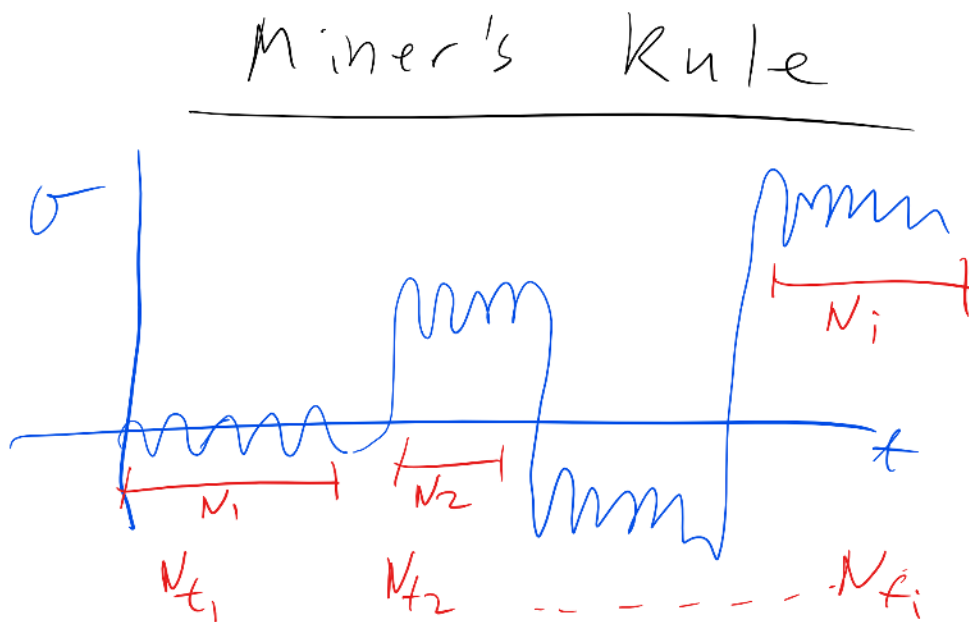


Figure Chapter10.10: Miner's rule.

Fatigue with Pre-Existing Cracks

The more common scenario you will most likely encounter is when we work with fatigue for a material that has pre-existing cracks. First you may be asking how can we tell if a material has pre-existing cracks? Well, have you ever seen people at the airport with a handheld device pressed near the exterior of the plane?

Those people are non-destructively looking for the presence of micro-cracks using ultrasound. You can also use X-rays for this, but using these techniques we can measure the distribution of crack sizes in a material and then use the following formalism to determine the number of cycles to failure for an initial crack length.

Fatigue failure is fracture due to crack growth every cycle of loading or the crack growth increment per loading cycle, defined below:

$$\frac{da}{dn} \quad (\text{Chapter 10.26})$$

where a is the crack length and n is the number of loading cycles.

We will deal with Static Fatigue and Cyclic or Classical Fatigue. Static fatigue occurs when a material is placed under a static or constant load and the crack faces of a material interact with the environment. The crack tip becomes embrittled due to interaction with the environment (stress corrosion cracking), the crack tip sharpens, the crack propagates, and the process repeats.

The more common fatigue scenario is cyclic or classical fatigue, where a material is under a cyclic load or stress. We need to define the cyclic applied stress, specifically the frequency of the applied load, f , which is $\frac{1}{\tau}$, where τ is the period of the applied stress. We also want to quantify the stress ratio, R :

$$R = \frac{\sigma_{min}}{\sigma_{max}} \quad (\text{Chapter 10.27})$$

As materials scientists we want to avoid catastrophic failure, and for fatigue that involves trying to estimate the number of cycles to failure, N_f , which is the number of cycles to grow a crack from initial length a_o to the critical or catastrophic crack length a_c .

There are three distinct regimes of fatigue crack growth: I) The Slow-Growth Rate or Near-Threshold Regime, II) Mid-Growth Rate or the Paris Regime, and III) High-Growth Rate Regime.

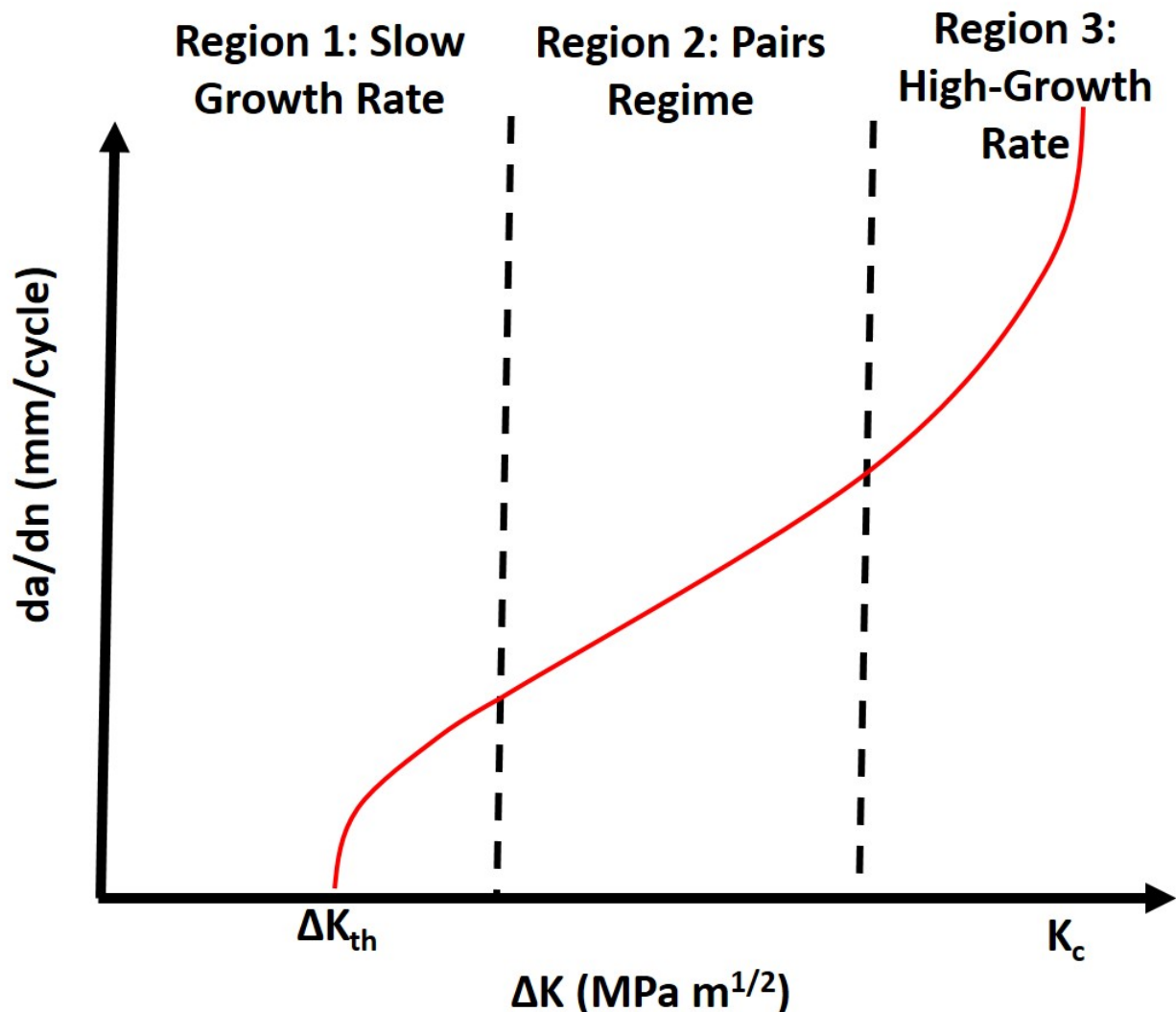


Figure Chapter10.11: Fatigue Regimes.

I) Slow-Growth Rate or Near-Threshold Regime

In the slow-growth rate regime the crack won't grow initially until the threshold stress intensity factor, ΔK_{th} , is reached where:

$$\Delta K = f \Delta \sigma \sqrt{\pi a} \quad (\text{Chapter 10.28})$$

Typically we say that when the rate of crack growth is 10^{-8} mm/cycle or less, the crack is dormant or growing at a near-undetectable rate. Once the threshold stress intensity factor is reached, the crack growth rate will increase but still the growth rate is extremely slow, still below one lattice spacing per cycle, until we reach the Mid-Growth Rate or the Paris Regime.

II) Mid-Growth Rate or Paris Regime

In the Mid-Growth Rate or Paris Regime we actually have an equation or law to describe fatigue crack growth, aptly named the Paris Law:

$$\frac{da}{dN} = C\Delta K^m \quad (\text{Chapter 10.29})$$

where C and m are empirical constants which depend on the material, the applied stress, frequency, and R . Typically for metals m will approach 3 or 4.

We can use the Paris Law to predict the number of cycles to failure, N_f :

$$\int_0^{N_f} dN = \int_{a_o}^{a_c} \frac{da}{C(f\Delta\sigma\sqrt{\pi a})^m} \quad (\text{Chapter 10.30})$$

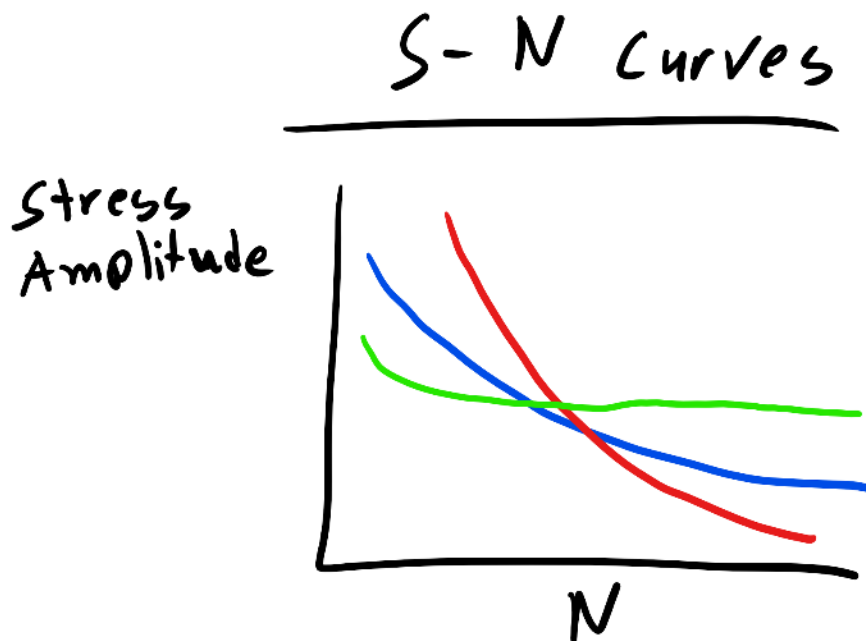


Figure Chapter10.12: S-N Curve.

which leads to:

$$N_f = \frac{1}{C(f\Delta\sigma\sqrt{\pi})^m} \left[\frac{a_c^{1-\frac{m}{2}} - a_o^{1-\frac{m}{2}}}{1 - \frac{m}{2}} \right] \quad (\text{Chapter 10.31})$$

Fatigue cracks are marked via striations on the fracture surface.

III) High-Growth Rate Regime

The last stage, the high-growth rate regime, is characterized by an orders-of-magnitude increase in the crack growth rate and additional cleavage in the material or microvoid coalescence. This is the end region where catastrophic crack failure will occur throughout the material. We need to take the material out of service before we reach this regime.

One way that we can try to predict the lifetime of materials is by looking at empirically determined S-N curves. S is the stress amplitude (the difference between the maximum and minimum applied stress). N is again the number of cycles. We can look at the

curve and determine when the material will fail.

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Chapter 2: Defects in Materials

"Crystals are like people, it is the defects in them which tend to make them interesting! - Professor Sir Colin Humphreys"

A crystal is at a state of thermodynamic equilibrium when its free energy $G = H - TS$ is minimized. When are we (humans) at equilibrium?

We have two knobs that we can tune to lower the free energy of the system above and that is entropy and enthalpy. At low temperatures our entropy knob becomes negligible and energy is minimized by minimizing H . This is done via binding and forming the ordered structures that we discussed previously. At the limit of $T = 0$ that perfect crystal is the equilibrium configuration. When temperature increases the free energy is minimized by adopting a less well-ordered atomic/molecular arrangement because that increases the entropy. Entropy increases when imperfections exist so when the temperature is not zero the equilibrium state will most likely contain imperfections. We can calculate the equilibrium concentration by looking at the change in free energy ΔG and the ΔS by adding imperfections and the enthalpic ΔH_f cost of forming those defects.

Crystalline Point Defects (0D)

Vacancies

A vacancy exists when a site that is normally occupied in the perfect crystal is unoccupied. This can occur in many ways for example, forcing an atom onto an interstitial site, into a dislocation core, or to a grain boundary or free surface. You can see a couple of examples of a vacancy below

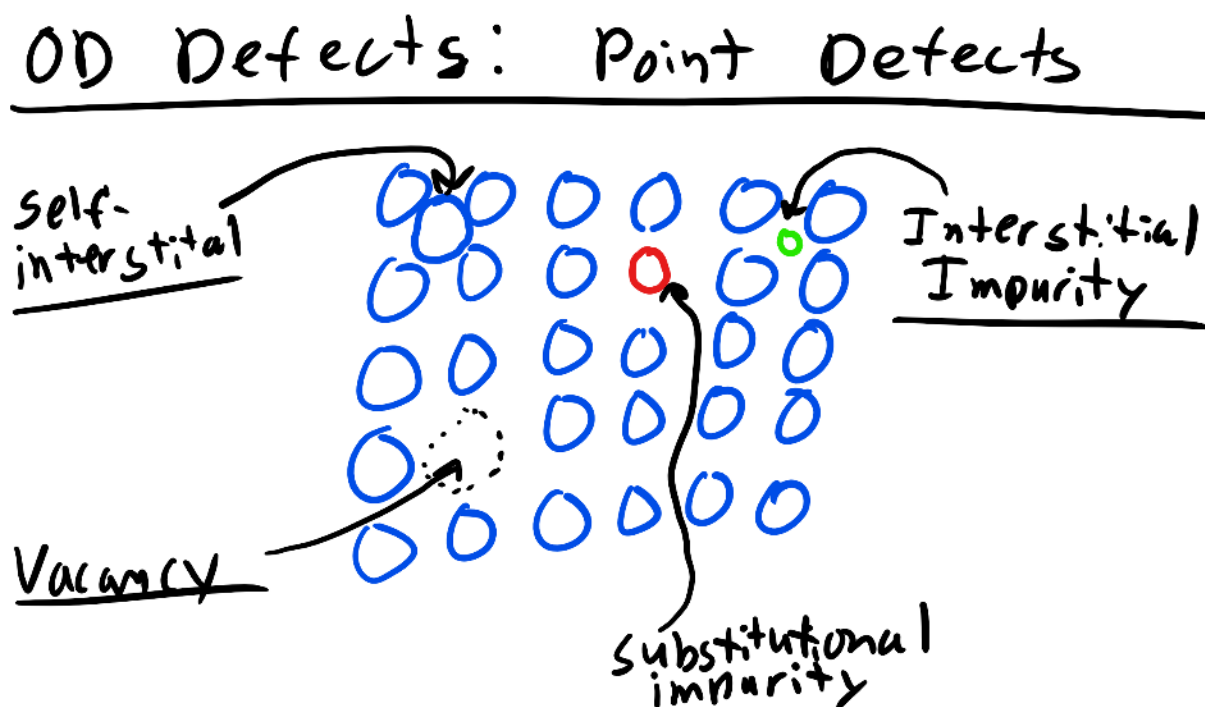


Figure Chapter2.1: 0D Point Defects

We can actually calculate the equilibrium concentration of vacancies, n ! Consider a reference state of a perfect crystal of N atoms and a continuous set of vacancies, n . The new state is a crystal containing a mixture of N atoms and vacancies. The total enthalpy change is then

$$\Delta H_f = n \Delta h_f \quad (\text{Chapter 2.1})$$

where Δh_f is the enthalpy of formation of a single vacancy. We can also get an idea about the change in configurational entropy from creating vacancies if we remember Boltzmann's entropy equation (he had it carved on his tombstone...show off)

$$S = k \ln \Omega_m \quad (\text{Chapter 2.2})$$

where k is the Boltzmann constant and Ω_m is the number of distinguishable ways you can arrange the system. The configurational entropy ΔS_c is then given by

$$\Delta S_c = S_{mix} - S_{ref} = k \ln \left(\frac{\Omega_m}{\Omega_{ref}} \right) = k \ln \Omega_m = k \ln \frac{(N+n)!}{N!n!} \quad (\text{Chapter 2.3})$$

where Ω_m is the number of distinguishable ways of arranging N atoms and n vacancies on $N+n$ sites and Ω_{ref} is the number of configurations in the ideal reference state, which is 1 since there are no defects. So the total Gibbs energy change is

$$\begin{aligned} \Delta G &= \Delta H - T\Delta S \\ &= n(\Delta h_f - T\Delta S_v) - kT[(N+n) \ln(N+n) - N \ln N - n \ln n] \end{aligned} \quad (\text{Chapter 2.4})$$

where ΔS_v is the vibrational entropy of the atoms surrounding the vacancy and we used Stirling's approximation $\ln X! \approx X \ln X - X$. Now how do we minimize Gibbs? We take the derivative and set it equal to zero:

$$\frac{\partial \Delta G}{\partial n} = \Delta h_f - T\Delta S_v + kT \ln \frac{n}{n+N} = 0 \quad (\text{Chapter 2.5})$$

We can now solve for the equilibrium fraction of vacant sites x_v

$$x_v = \frac{n}{n+N} = \exp\left(\frac{\Delta S_v}{k}\right) \exp\left(-\frac{\Delta h_f}{kT}\right) \quad (\text{Chapter 2.6})$$

You should notice in this equation that there is an exponential temperature dependence, known as Arrhenius dependence or Arrhenius's law. This is critical because there are many behaviors in Materials Science which are Arrhenius (project idea??). Let's take a look at how strongly the concentration of vacancies varies with temperature by looking an example Arrhenius plot below:

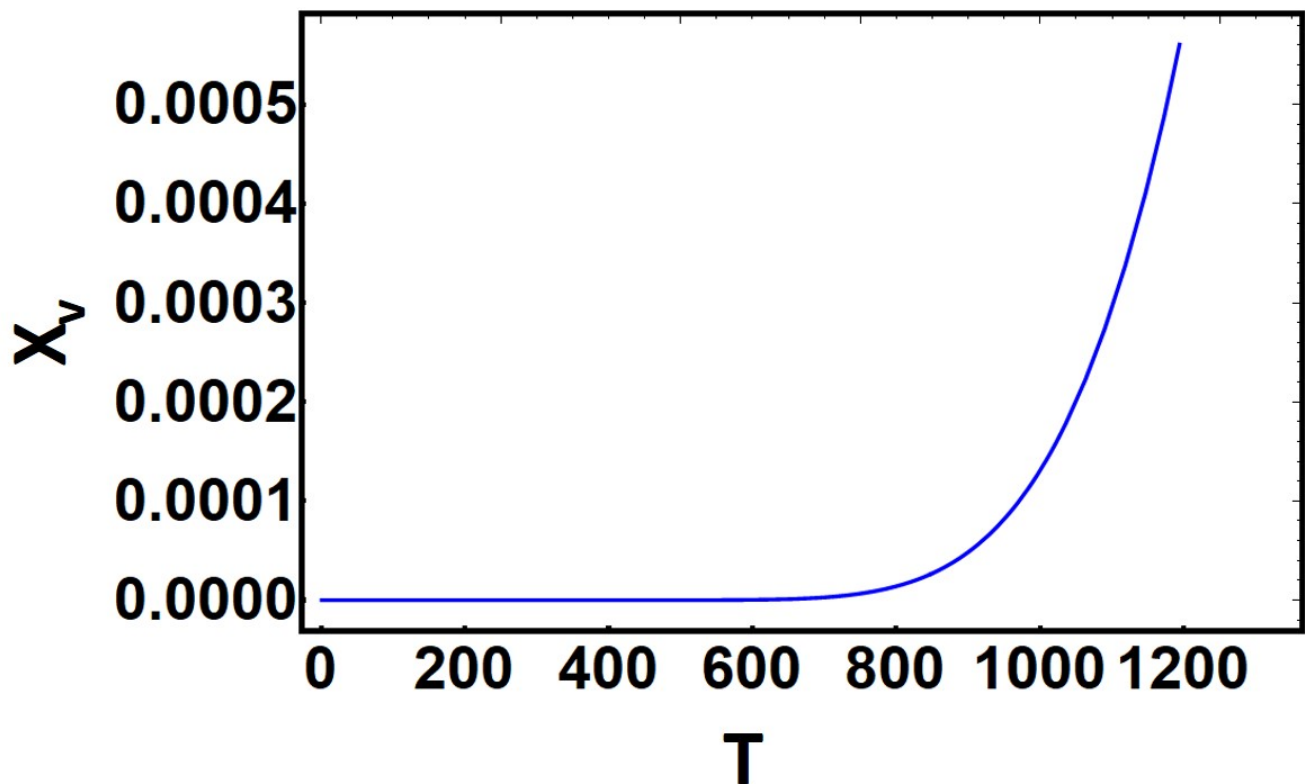


Figure Chapter2.2: Equilibrium Vacancy Concentration in Gold

Now typically we can assume that $\exp\left(\frac{\Delta S_v}{k}\right) \approx 1$. The enthalpy of formation of vacancies for metals is typically on the order of 15–150 kT (where $kT = 0.026$ eV). So we can clearly see that at room temperature the probability of forming vacancies will be pretty low already. Is this supported by the graph?

This method is not the typical way Arrhenius graphs are presented. It is actually better to plot the log of the equilibrium concentration of vacancies as a function of the reciprocal temperature $\frac{1}{T}$. That way we can extract the activation energy or energy of formation of the vacancy.

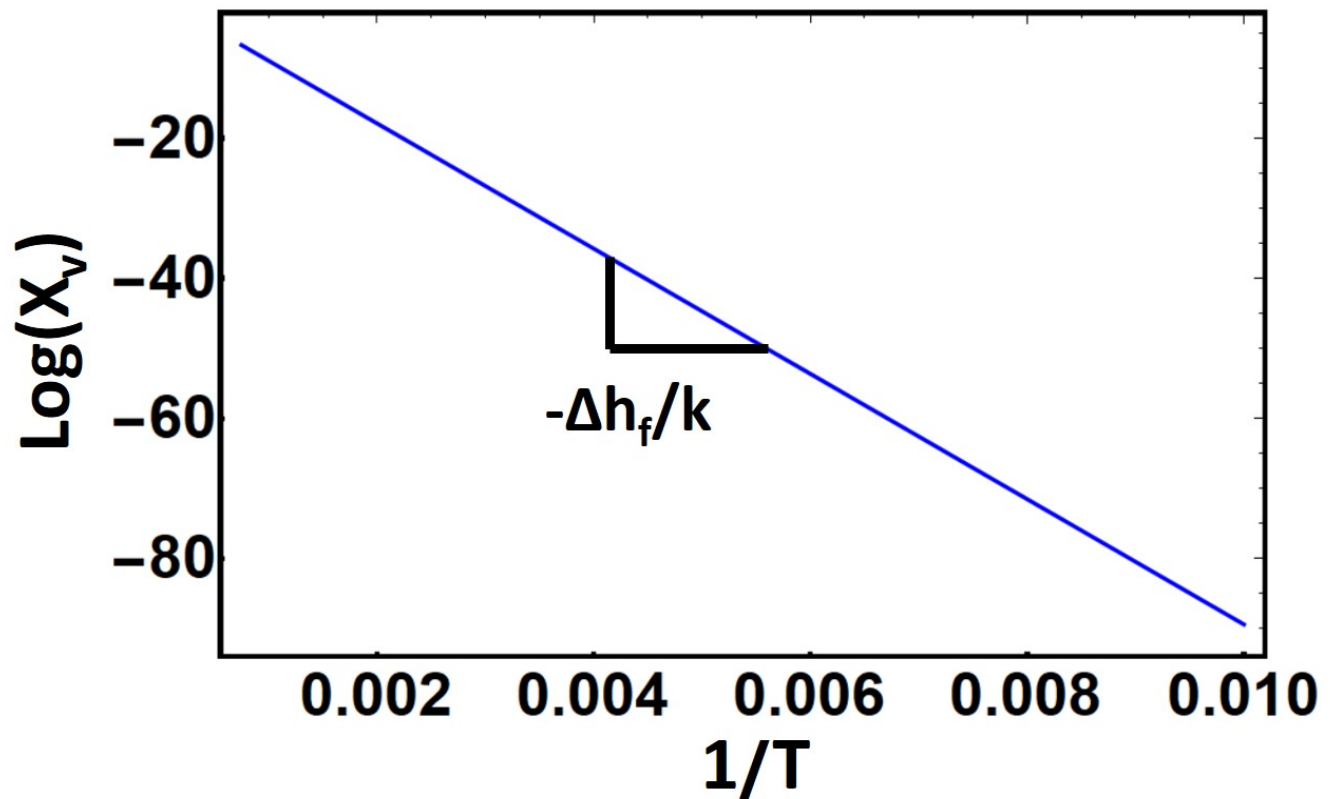


Figure Chapter2.3: Arrhenius Plot of Equilibrium Vacancy Concentration in Gold

Interstitials

An interstitial defect occurs when an atom occupies an interior site which is not normally occupied. If the interstitial is of the same species in a single component crystal it is a self-interstitial and we have the following equation for the equilibrium number of self-interstitials

$$x_i = \frac{n}{n + N} = \exp\left(\frac{\Delta s_v}{k}\right) \exp\left(-\frac{\Delta h_f}{kT}\right) \quad (\text{Chapter 2.7})$$

however now the Δs_v and Δh_f represent the enthalpy of formation and vibrational entropy for interstitial formation. As you might imagine the energy of formation for interstitials is lower for more open and less densely packed structures. Obviously there are also higher numbers of these 0D defects for nonequilibrium processes like quenching, irradiation, ion implantation, or cold working.

Self interstitials are classified as intrinsic interstitials but the more common and useful type of interstitial for our purposes as material scientists and for determining the mechanical behavior of materials are extrinsic interstitials. These are typically impurity defects of different size than the host or solvent lattice. Imagine C in Fe.

Often interstitials will occupy tetrahedral or octahedral sites. Tetrahedral sites are positions in the lattice such that the interstitial atom would fit between 4 lattice atoms that would form a tetrahedron around said atom. The same can be said for the octahedral sites but the only difference being there are 6 atoms.

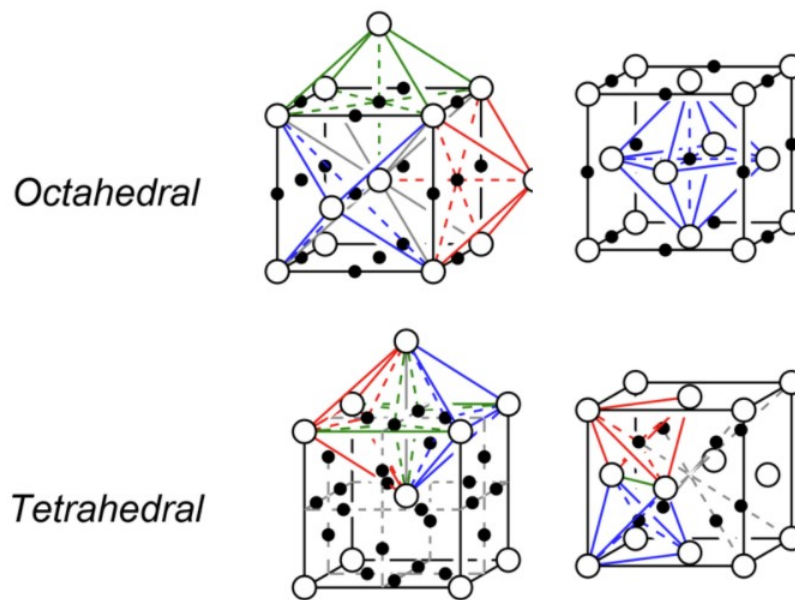


Figure Chapter2.4: Octahedral and Tetrahedral sites in BCC and FCC

Schottky and Frenkel Defects

In addition to vacancies and interstitials there are certain defects unique to ionic crystals which are Schottky and Frenkel defects. A Schottky defect is when there is the formation of a pair of vacancies in both the anion and cation of the ionic crystal. A Frenkel defect is formed by the creation of either an anion or cation vacancy and corresponding creation of an anion or cation interstitial.

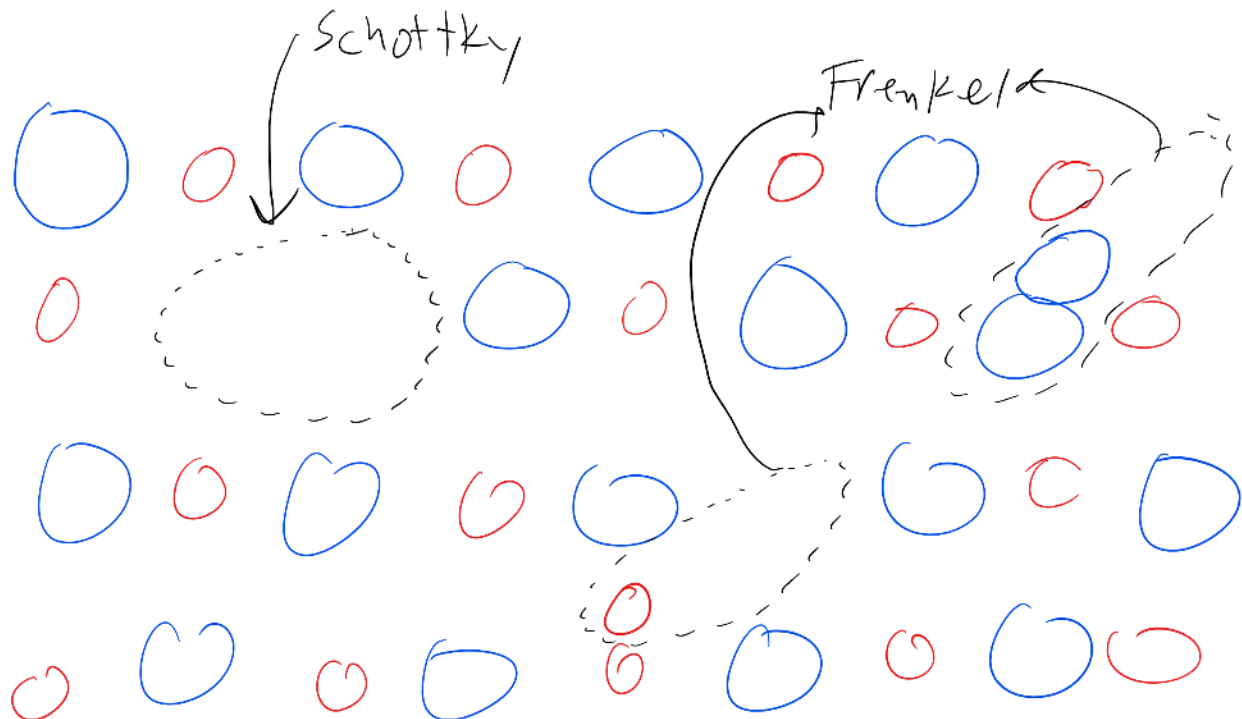


Figure Chapter2.5: Schottky and Frenkel Defects

Dislocation Defects (1D)

Imperfections that are localized along a space curve passing through an ordered medium are line imperfections. A dislocation is one such defect. A dislocation is a linear or one-dimensional line defect which involves translation of one part of a crystal with respect

to another part. A disclination involves rotation of one part with respect to another. We will deal with two types of dislocation in this class: edge and screw dislocations.

An edge dislocation is essentially an extra half plane of atoms that is inserted into the perfect crystal and it terminates within the crystal. You can see this below

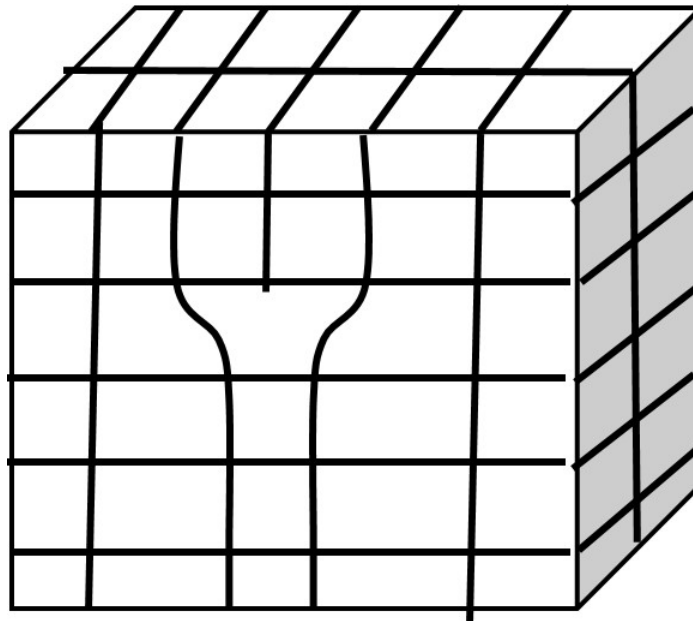


Figure Chapter2.6: Edge Dislocation

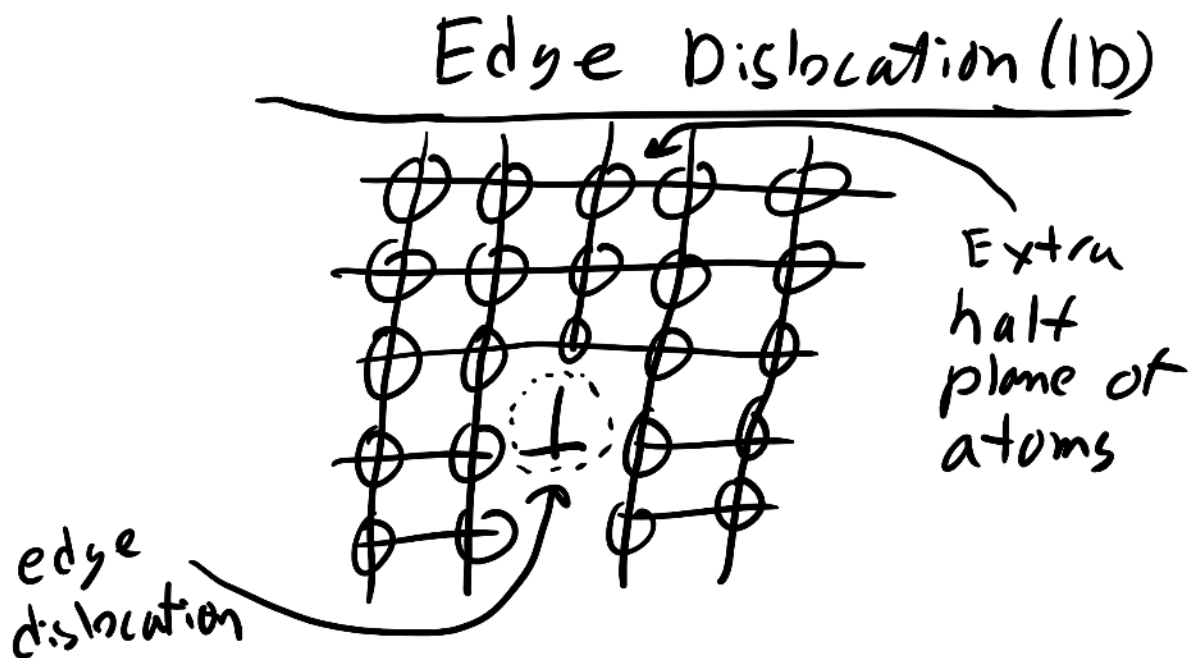


Figure Chapter2.7: Edge Dislocation 2

A screw dislocation is a bit harder to visualize but you can imagine that a screw dislocation can be formed by an applied shear stress, seen below:

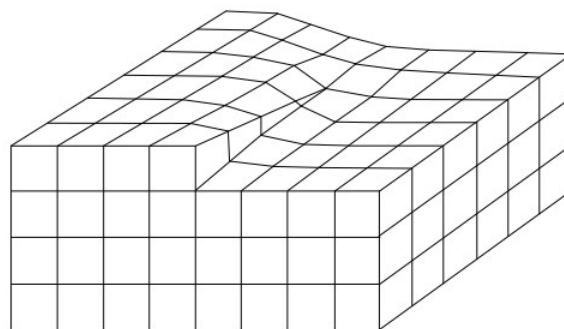


Figure Chapter2.8: Screw Dislocation

You can see that in this example some of the differences between edge and screw dislocations—one being that the screw dislocation motion will be perpendicular to the applied force but more on that in a little bit. There are also wedge and twist disclinations as well.

Associated with each dislocation is a dislocation core which is where the largest displacements of atoms from the ideal sites occur and they are concentrated along a dislocation line. We describe dislocations via a unit tangent vector t , and the Burgers vector b . The tangent vector is a unit vector that is tangential to the dislocation line at any given point. The Burgers vector b is defined in reference to the Burgers circuit. Now in this class we will use the SF/RH (start to finish, right-hand) convention to define the Burgers vector.

To define the Burgers vector:

1. Choose the positive sense of the unit tangent vector of the dislocation line.
2. By traveling along rows of lattice points make a right-hand circuit in the crystal containing the dislocation. Define a Start Point (S) and Finish Point (F).
3. This circuit would be a closed circuit in the perfect crystal but in this instance the circuit is only closed by the Burgers vector which connects your Start and Finish points.

A couple of other quick notes about some of the properties of dislocations:

- The Burgers vector will be conserved and that for a given dislocation there is one constant Burgers vector, even as the tangent vector changes.
- A dislocation cannot end inside a crystal.
- A pure edge dislocation has b perpendicular to t everywhere along the dislocation curve and $t \times b$ points toward the extra half plane of atoms.
- A pure screw dislocation is either parallel or antiparallel to t everywhere along the dislocation curve. A right-hand screw is parallel and a left-hand screw is anti-parallel.
- A dislocation that is neither pure edge or pure screw is a mixed dislocation and the vector component that is parallel to t is the screw component and the component that is perpendicular to t is called the edge component.
- Reversing the sense of t also reverses the sense of b .

Edge dislocation:

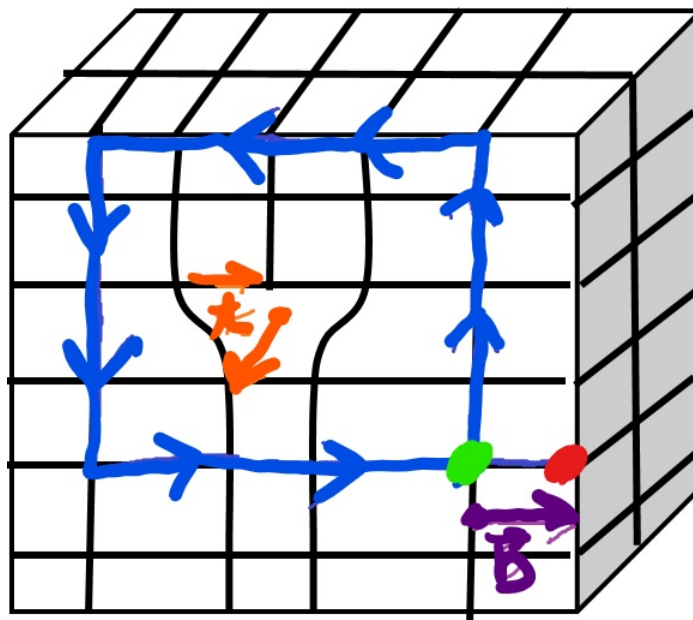


Figure Chapter2.9: Edge Dislocation Burgers Circuit

Right-hand screw dislocation:

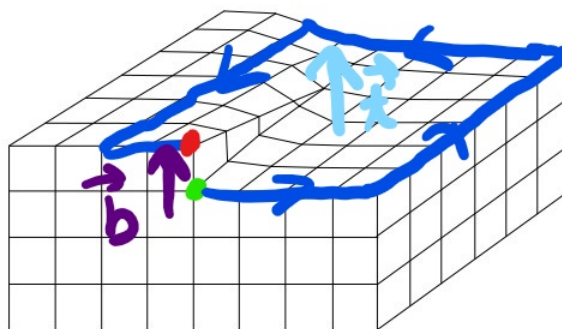


Figure Chapter2.10: Right Handed Screw Dislocation Burgers Circuit

Left-hand screw dislocation:

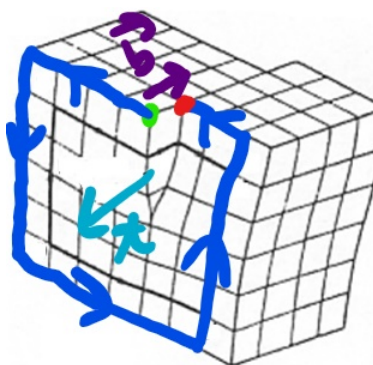


Figure Chapter2.11: Left Handed Screw Dislocation Burgers Circuit

While we are speaking of dislocations one of the key material properties that you will come across is the dislocation density ρ , which has units of m^{-2} . A highly cold worked material may have a dislocation density of 10^{12} cm^{-2} whereas a highly annealed material can be as low as 10^5 cm^{-2} . Dislocations are motile and they can move via slip and climb.

It is often the case that a dislocation will not be either pure edge, left, or right hand screw. Instead a dislocation will be mixed having some component that is edge or screw.

Grain Boundaries, External Surfaces, Phase Boundaries, Twin Boundaries, and Stacking Faults (2D)

Perhaps the most obvious 2D defect is just an external surface where the bonds at the surface are not satisfied which gives rise to an increase in surface energy or surface tension.

Grain Boundaries are interfaces at which crystals of different orientations abut. There are special types of grain boundaries like low-angle tilt and twist boundaries when the angle of misorientation of grains is not too large. In fact they are considered simple periodic arrays of dislocations.

2D Defects: Grain Boundaries(GB)

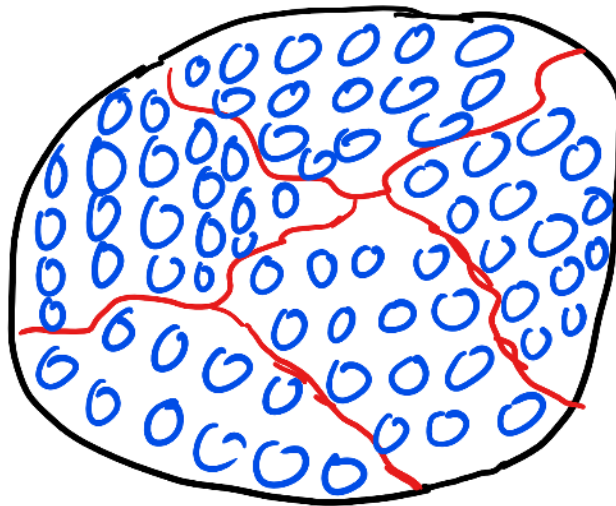


Figure Chapter2.12: Grain Boundaries

A twin boundary is a special type of grain boundary across which there is a specific mirror lattice symmetry. The region of material between these boundaries is a twin. Twins typically appear due to shear stresses or during annealing heat treatments after deformation. Annealing twins are more common in FCC crystals while mechanical twins are more common in BCC and HCP crystals.

Stacking faults are interfaces in crystals across which one part of the crystal is displaced relative to the other part by a displacement vector that is not a translational symmetry operation for that crystal. Remember that for FCC we had this ABCABC stacking and HCP we had ABABAB. A stacking fault in FCC would be ABCBCABCABC. If the fault is missing a layer that is an intrinsic stacking fault but if there is an extra layer that is an extrinsic stacking fault. Stacking fault energy has severe implications on the strain hardening behavior of materials.

There are also antiphase/interphase boundaries which are separate regions of the crystal by a relative translation that is not a symmetry operation of the crystal. It is a special type of stacking fault, one that connects the crystallographically nonequivalent occupied sites in a perfect crystal. They can be coherent, semi-coherent, or incoherent.

Bulk or Volume Defects (3D)

Finally there are also bulk or volume defects which include pores, cracks, foreign inclusions, and other phases.

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Chapter 3: Stress and Strain Curves

Lecture 3: Stress Strain Curves

Are you ready! We have talked enough about the atomistic length scale so now let's break some materials and look at stress strain curves right! Hold your horses for a second and let's cover some of the basics before we get started. Also as you can see from the title we will be going even further into the atomistic basis of elasticity, you will be glad we reviewed some material structure and bonding.

We are getting into the heart of this course which is the mechanical behavior of material which specifically refers to the material response to an applied load. This material response will depend on several factors including

- Internal forces and moments generated by external forces and moments
- Material properties: stiffness, strength, ductility, toughness, etc
- Component geometry

Specifically the mechanical behavior of materials and the mechanical properties of material will depend on the atomistic length scale we previously discussed. For example we will see today that stiffness will depend on binding energy, yield strength will depend on the presence of defects, etc.

But before we get into all this great material behavior let's do a quick review of internal and external forces. In previous classes we have discussed quite a bit about external forces but will also get into internal force more in-depth in this course.

We will also discuss quite a bit about moments which is the tendency of a force to cause rotation about a point or line and a moment can be defined as the cross product of a vector, $\vec{r}$, from a point or line to the point where a force $\vec{F}$ and note that this notation denotes a 1st rank tensor or a vector quantity as seen below

$$\vec{M}_A = \vec{r} \times \vec{F} \quad (\text{Chapter 3.1})$$

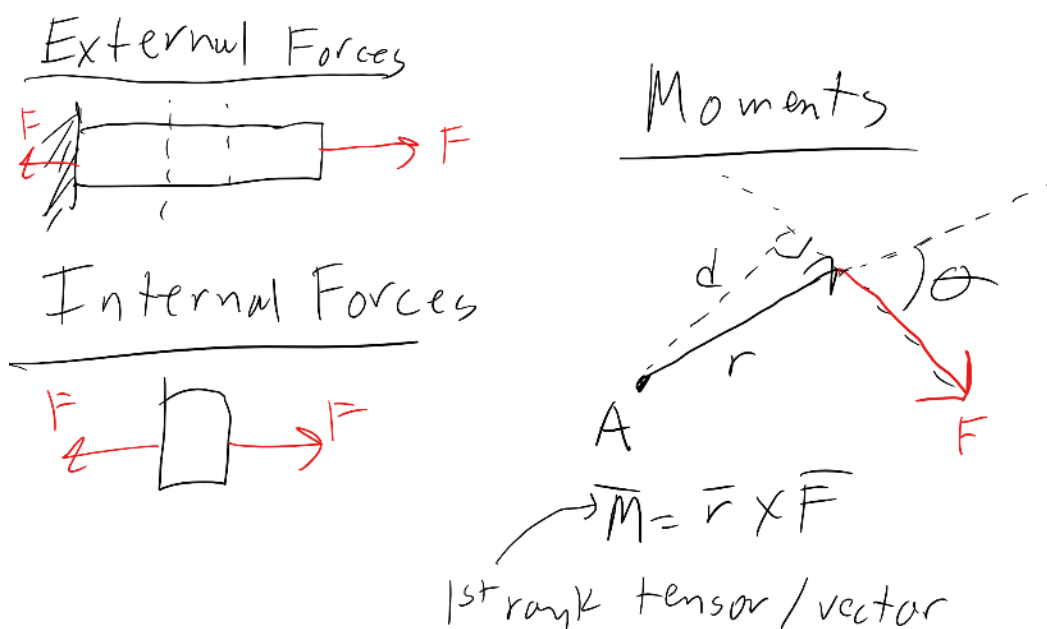


Figure Chapter3.1: Internal and External Forces as well as moments

Also in 2D we can find the magnitude of the moment by multiplying the magnitude of the force by the perpendicular distance between a point A and the line of action of force

$$|M_A| = |F \cdot d| = rF \sin \theta \quad (\text{Chapter 3.2})$$

In this class we will always define CCW as positive and CW as negative. Also if a material extends we will consider that force and displacement positive and if it compresses then that is negative.

Additionally when we assume that we are in static equilibrium, we will set the sum of all the forces and all the moments to zero and that will eliminate both translation and rotation as seen below

\$\$

$$\begin{aligned} \Sigma F &= 0 = ma \\ \Sigma M &= 0 = m\alpha r \end{aligned} \quad (\text{Chapter 3.3})$$

\]

Normal Stresses

We will define normal stresses as those applied perpendicular to the area. We will define any forces, stresses, or strain in tension as positive and any forces, stresses, or strain under compression will be considered negative. It should be noted that to have uniform normal stress in a bar the load must act through the centroid of the bars' cross section as seen below

$$(\bar{x}, \bar{y}) = \left(\frac{\int x dA}{\int dA}, \frac{\int y dA}{\int dA} \right) \quad (\text{Chapter 3.4})$$

At the end of a bar near the application of the load the stress will not be uniform unless the load is applied evenly over the area but becomes uniform at some distance, as stipulated by St. Venant's Principle.

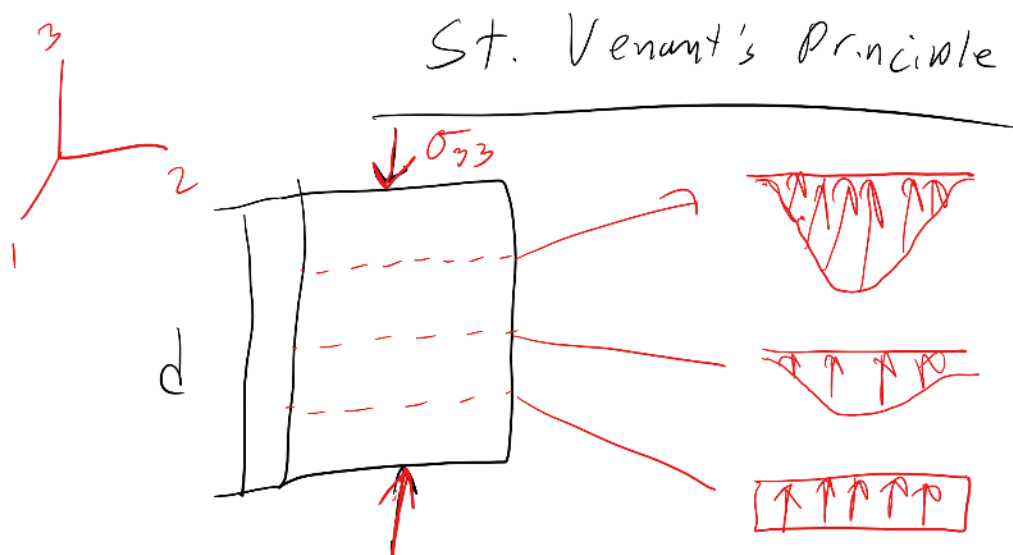


Figure Chapter3.2: St. Venant's principle

Normal Stress, σ , is a force normalized by the area over which it acts and critically the force is normal to the cross sectional area over which it acts

$$\sigma = \frac{F}{A} \quad (\text{Chapter 3.5})$$

where F is force (in Newtons) and A is the original cross-sectional area. This is the definition of the engineering stress. The true stress would be normalized by the instantaneous area, more on this a little bit later. We will use the engineering stress primarily in this class.

Now when a force is applied to a material that material will deform and displacement will occur and this displacement is described by strain. Specifically here normal strain, ϵ , is defined as

$$\epsilon = \frac{l_f - l_o}{l_o} = \frac{\Delta l}{l_o} \quad (\text{Chapter 3.6})$$

where l_f is the final length after deformation and l_o is the initial length.

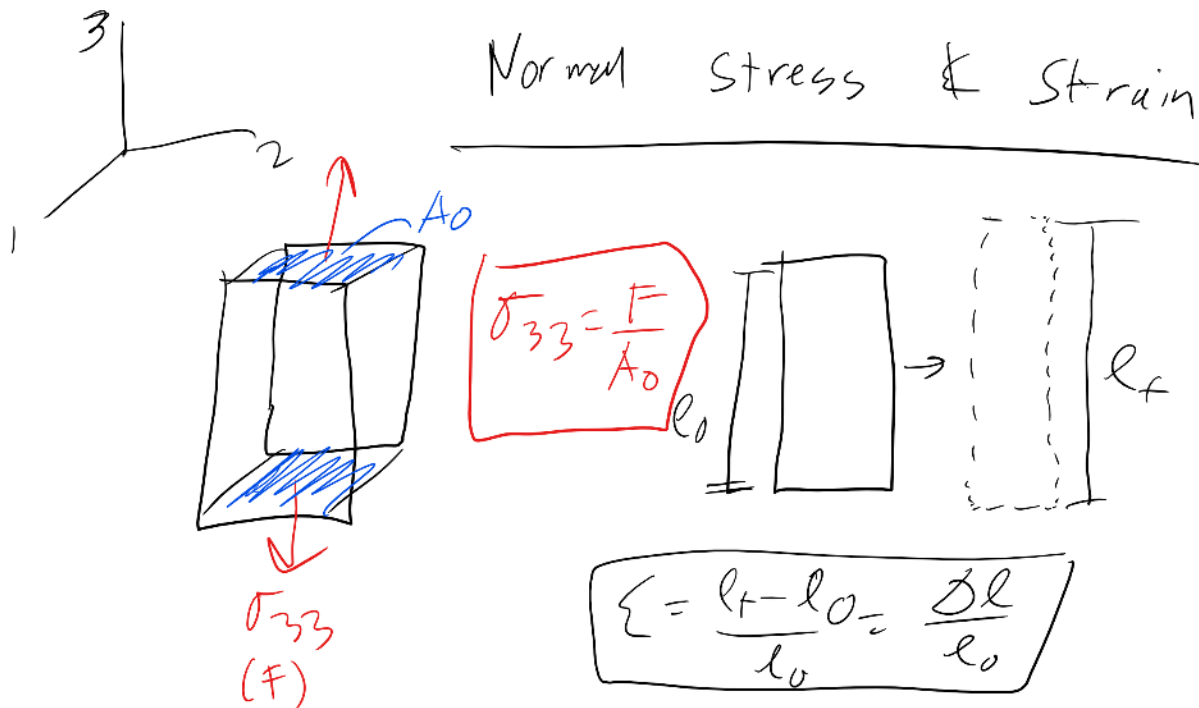


Figure Chapter3.3: Normal Stress and Strain

Hooke's Law for Isotropic Elastic Continuous Media

As we are all mechanical, civil, bio, computer science or really any engineers I am sure that Hooke's law is near and dear to your heart

$$F_s = -k\Delta x \quad (\text{Chapter 3.7})$$

Now you are all the experts with this expression but let me introduce you to another equation that is near and dear to the hearts of every material scientist and solid mechanics experts but can be very dangerous for students, so now I hate this equation

$$\sigma = E\epsilon \quad (\text{Chapter 3.8})$$

where E is the Young's modulus (sometimes you may see Y). Now, as you will see next lecture this equation is only applicable in the simple uniaxial stress state that you see here. This equation DOES NOT HOLD FOR OTHER COMPLEX STRESS STATES.

However, this equation is very relevant because when one produces a stress-strain curve the stress state is typically uniaxial tension using an instrument like our Instron machine in the laboratory. If there is nothing else that you take away from this course (and I know that you all will take much much much much more from this course) it is to master how to analyze a stress-strain curve. Whatever, engineering discipline that you eventually enter whether in academia or in industry you will be asked to work with a stress-strain curve, typically to select a material or to assess the material's performance.

Stress-Strain Curve:

When a material is placed under a stress state we will typically plot a stress-strain curve and that curve typically will have 3 distinct regions: I) Elastic, II) Plastic, III) Fracture.

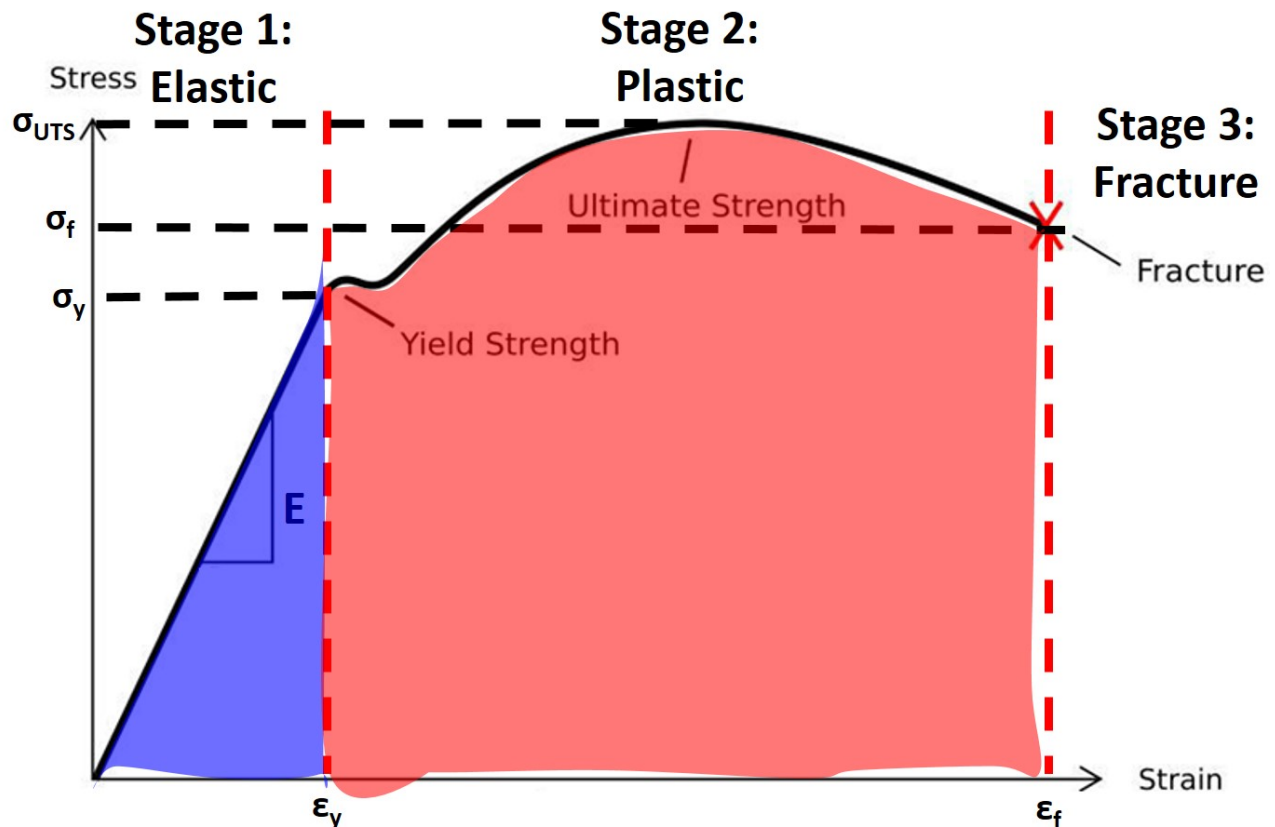


Figure Chapter3.4: Stress Strain Curve

I) Elastic Regime:

In the elastic regime the stress strain response is linear and the stress/strain is reversible, there is no hysteresis. This means you can recover the deformation upon unloading, i.e. the material will pop-back into place and the final length will be the same as the initial length upon unloading.

That describes the macroscopic mechanical response of the and if you look at what happens atomistically the bonds are being pulled but not broken and while dislocations are present they are not moving. This explains why there is no permanent or plastic deformation. You are just pulling on the bonds not breaking any bonds. Most materials behave linear and elastically at small strains, $\epsilon < 0.002$.

Many materials will behave mechanically as isotropic materials, and again isotropic means that the properties are all the same in all directions, one example is a poly-crystalline metal with randomly orientated grains.

Now there are many other materials that will behave anisotropically, meaning that the properties are different along different directions, some of the most common examples would be wood, titanium, composites, etc.

In this regime we see that stress is linear and proportional to strain. More importantly, in this stress regime we have constitutive equations that relate stress to strain and we will introduce these equations in lectures to come. This is the only regime of the stress-strain curve where this is the case. In other regions, there is no fundamental equation that allows us to do so and instead we must rely on empirical equations and in this class we will focus more on trends and scaling parameters.

Typical values of Young's modulus for some materials can be seen below

- Diamond 1000 GPa
- Alumina 390 GPa

- Tungsten 340 GPa
- Steel 200 GPa
- Copper 110 GPa
- Concrete 30 GPa
- Al 6061 and Glass 69GPa
- Polyethylene 0.2-0.7 GPa
- Rubbers 0.01-0.1 GPa

This is not a memorization class but it is always nice to have a couple of these material properties ready to impress at an interview. However, in this class a good rule of thumb is that if you are dealing with a ceramic you can approximate a Young's Modulus of 300 GPa, a metal to be 100GPa, and a polymer/biomaterial can vary between 100s of kPa to 10GPa so approximate it as 1GPa.

II) Plastic Regime:

Here you are plastically deforming the material. Macroscopically, once the material is stressed or strain such that the material enters the plasticity regime the deformation is irreversible. This means that the material will recover the elastic strain but the plastic deformation is irreversible so that the final length will be different than the initial length (it will be longer). There will be hysteresis upon unloading once the material enters this regime of the stress strain curve.

Atomistically, the plastic regime is distinct in that here the dislocation that are present in the elastic regime begin to become motile due to the stretching and breaking of bonds and resultant rearrangement of atoms. Additionally, in this regime dislocations and other defects can be created due to the rearrangement of atoms locally.

This regime initiates once the stress reaches σ_y which is the yield stress and the yield stress reaches ϵ_y the yield strain. This is the point where the stress-strain curve is no longer linear. Often times you will find in industry and sometimes in academia the yield stress is found using the 0.02% offset yield stress method in which a line with the same slope as the Young's modulus is drawn and the yield stress is determined at the point where the lines intersect. I personally have issues with this method so we will do a visual check and tack on some uncertainty to our measurement or justify with statistical methods. We can also see several other interesting points in this particular stress strain curve which does not represent all materials like the σ_{UTS} is the ultimate tensile strength. The ultimate tensile strength is defined as the largest stress value on the stress strain curve. In this particular curve it also indicates the onset of necking.

Necking is a type of plastic deformation that is denoted by a decrease locally in the cross-sectional area and forms a thin neck as it's namesake indicates. The neck is formed from instabilities and heterogeneities in the material and due to the inherent decrease in the cross-sectional area of the cross-section when under tensile stress/strain because of conservation of volume considerations (as well as local variations in strain hardening more on this in a second).

The stress-strain behavior again is not governed by constitutive relationships and instead many of the relationships and behavior in this regime that we will discuss in later lectures is empirical (evidence based) in nature. We will discuss much more of this regime in later lectures to come. Lots of cool behavior in this regime.

III) Fracture:

This last regime is the regime that everyone is most interested in and the most fun to explore when running a tensile testing experiment and that is the loud pop that follows Fracture.

In this regime, catastrophic fracture occurs in a material. This is denoted by σ_f which is the fracture stress and the ϵ_f is the fracture strain. Here macroscopically, the material cracks and new surfaces are created. Now this is very energetically unfavorable as we learned in our previous thermodynamics refresher, creating interfaces is typically very unfavorable. However, atomistically, the bonds are under immense strain near fracture and they are displaced far from their equilibrium distance so the elastic strain energy present in the bonds is incredible large and positive (very bad energetically). Even though, creating surfaces is unfavorable we can decrease the total free energy of the system by relieving this elastic strain energy by bond breaking and surface creation. This is the energy battle that determines when a material fractures, much more on this later. I know I know can we get to the end of the class so we can know everything about Mechanics yet, slow down but I appreciate the enthusiasm.

Fracture while the most fun practically is similar in nature to the plastic regime in that we do not have many fundamental equation that relate stress or strain here and inhomogeneities in the sample will cause fracture to be somewhat stochastic (random) in nature.

But nevertheless we will press on.

There are a couple of other material properties that we need to discuss at this point since we have reached the end of our stress-strain curve journey in terms of looking at the three regimes. We can also define the elastic strain energy you can define this value in terms of energy (Joule) or in terms of energy per unit volume. We can think about and calculate elastic strain energy in several ways, let's consider a representative volume element (RVE) a cube in this instance with a stress in the σ_{11} direction.

The force would simply be

$$F = \sigma_{11} \delta_2 \delta_3 \quad (\text{Chapter 3.9})$$

Assuming that initially the force is 0 then the average force would simply be

$$F_{avg} = \frac{\sigma_{11} \delta_2 \delta_3}{2} \quad (\text{Chapter 3.10})$$

Thus if we consider that the deformation or

$$\Delta_1 = \epsilon_{11} \delta_1 \quad (\text{Chapter 3.11})$$

The the work would be assuming linear elasticity,

$$W = F_{avg} \Delta_1 = \frac{\sigma_{11} \epsilon_{11} \delta_1 \delta_2 \delta_3}{2} \quad (\text{Chapter 3.12})$$

Or if we looked at the elastic strain energy per unit volume

$$\frac{dU_{ESE}}{dV} = \frac{\sigma_{11} \epsilon_{11}}{2} \quad (\text{Chapter 3.13})$$

Now this is one way to arrive at this expression, we can also simply look at the area under the curve which is

$$U_{ESE} = \int_0^{\epsilon_y} \sigma_{11} d\epsilon_{11} = \frac{\sigma_{11} \epsilon_{11}}{2} \quad (\text{Chapter 3.14})$$

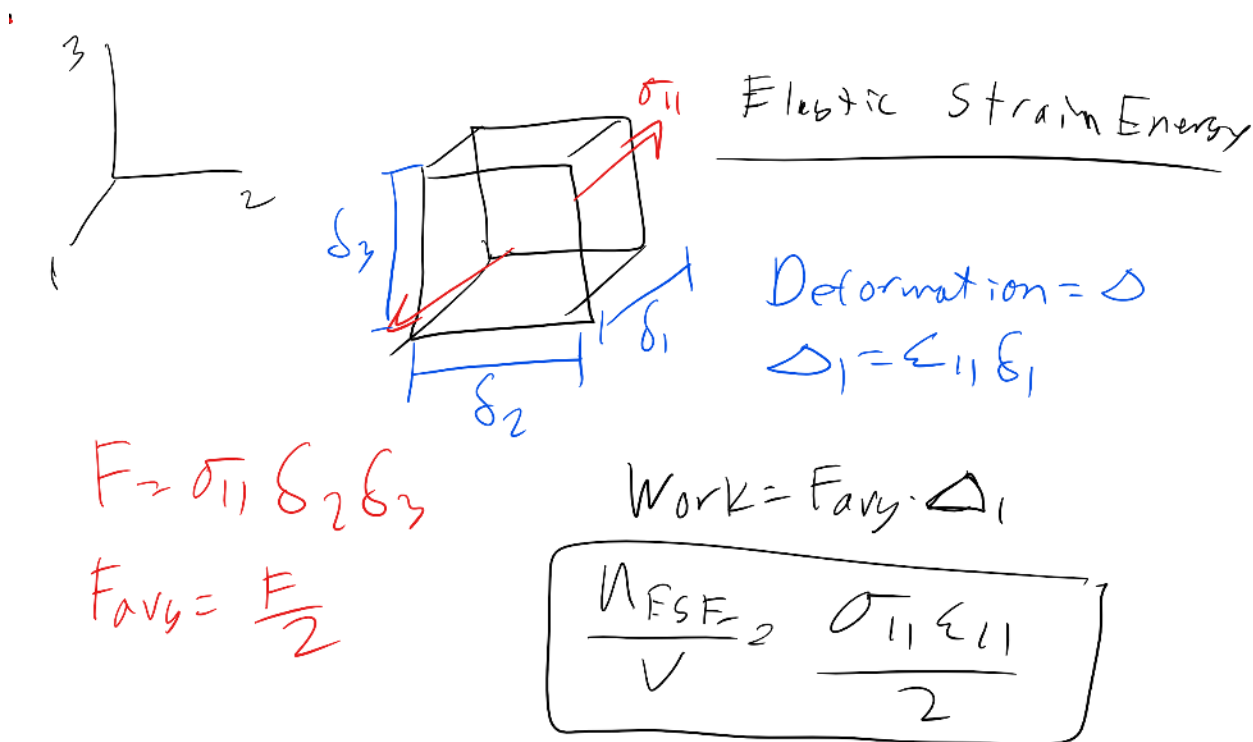


Figure Chapter3.5: Elastic Strain Energy

[Figure: Elastic Strain Energy — file: ese.jpg]

Now that is a little bit easier and as you can see the expression matches with your previous expression. Also you can check for yourself that the units are indeed energy per volume, maybe a problem set question....no way too easy.

We can do something very similar to shear stress for example the stress applied on the top plane here would be

$$F_{avg} = \sigma_{12} \delta_2 \delta_3 \quad (\text{Chapter 3.15})$$

The distance would then be

$$\Delta_{12} = \gamma_{12} \delta_3 \quad (\text{Chapter 3.16})$$

Then then the work would be

$$W = F_{avg} \Delta = \frac{\sigma_{12} \gamma_{12} \delta_1 \delta_2 \delta_3}{2} \quad (\text{Chapter 3.17})$$

and thus

$$\frac{dU_{ESE}}{dV} = \frac{\sigma_{12} \gamma_{12}}{2} \quad (\text{Chapter 3.18})$$

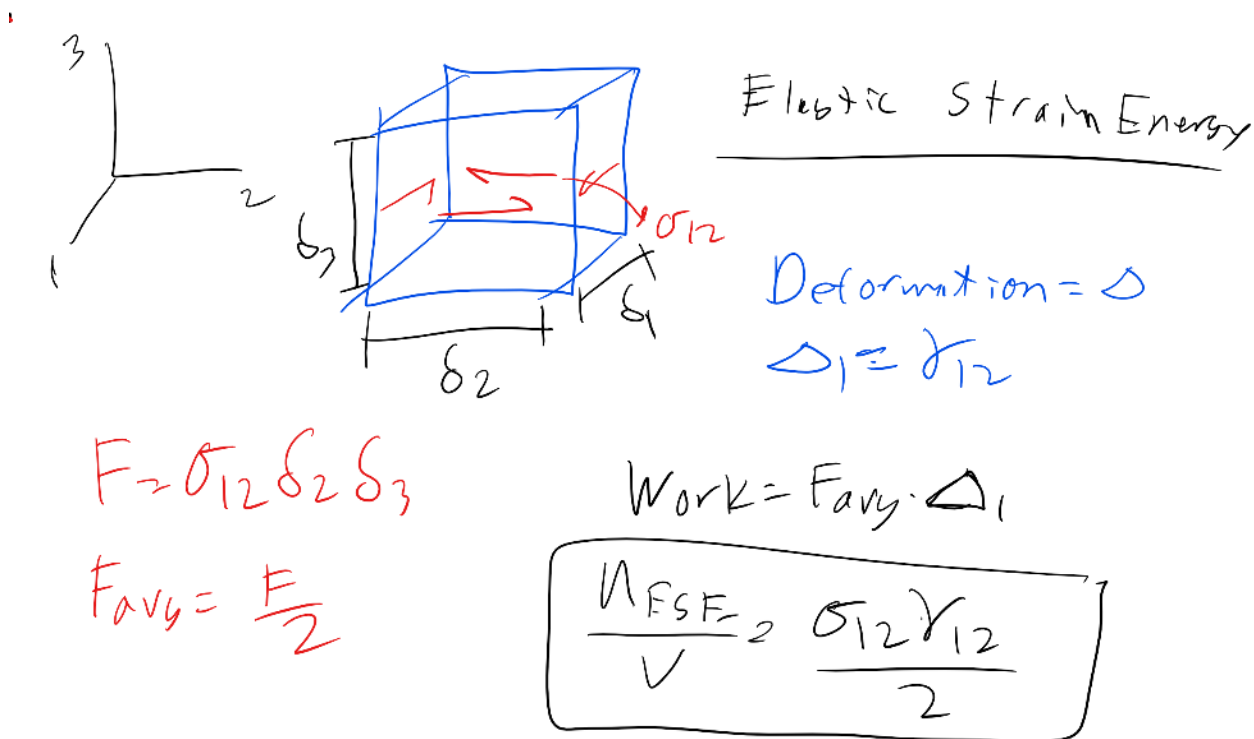


Figure Chapter3.6: Elastic Strain Energy for Shear Stress

In terms of strain energy we will also talk about how strain energy created a stress field in the crystal lattice around dislocations and we will explicitly calculate the strain energy associated.

One last value we should be aware of is toughness which is defined as

$$U_T = \int_0^{\epsilon_f} \sigma_{11} d\epsilon_{11} \quad (\text{Chapter 3.19})$$

This essentially the energy required to fracture a material, energy per volume to be precise. As you will soon see it is the total area under the curve both stress and the ability of a material to strain will determine toughness. Why is Kevlar a better body armour than steel? Let's discuss that right now but at this point we need to stop and make a clear point about the language that we have to use when discussing the material properties of materials. Word choice is critical here because they mean very different things. When we talk about the stiffness of materials we are talking about the Young's modulus of the material. The higher the Young's modulus the stiffer the material. When we talk about strength we are talking about the yield strength, the ultimate tensile strength, or the fracture

stress or strength. We are talking about how ductile a material is we are talking about the strain at failure. We also often talk about material resilience and toughness as well.

If a material is not as stiff it is called compliant, if a material is not strong it is weak, and if a material is not tough it is termed brittle.

Let's look at a few more stress-strain curves and talk about some differences that we can see just so that we can get a bit more acquainted. We will be going much much much more in-depth soon about some of these topics so don't worry, enjoy the overview while we can.

First let's break down some stress strain curves for different materials, specifically metals, ceramics, and polymers/biomaterials.

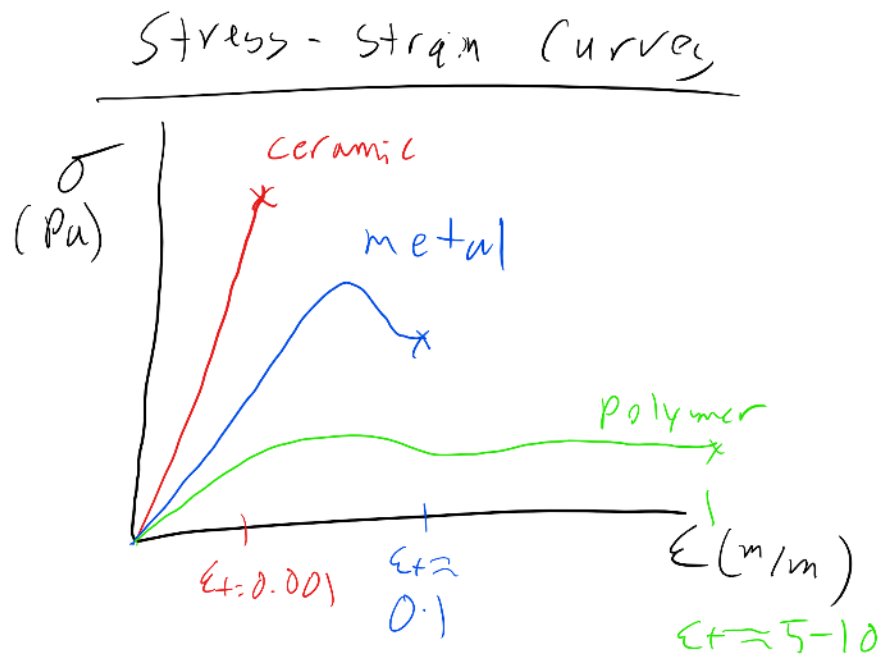


Figure Chapter3.7: Engineering Stress Strain Curves for Ceramic, Metal, and Polymers

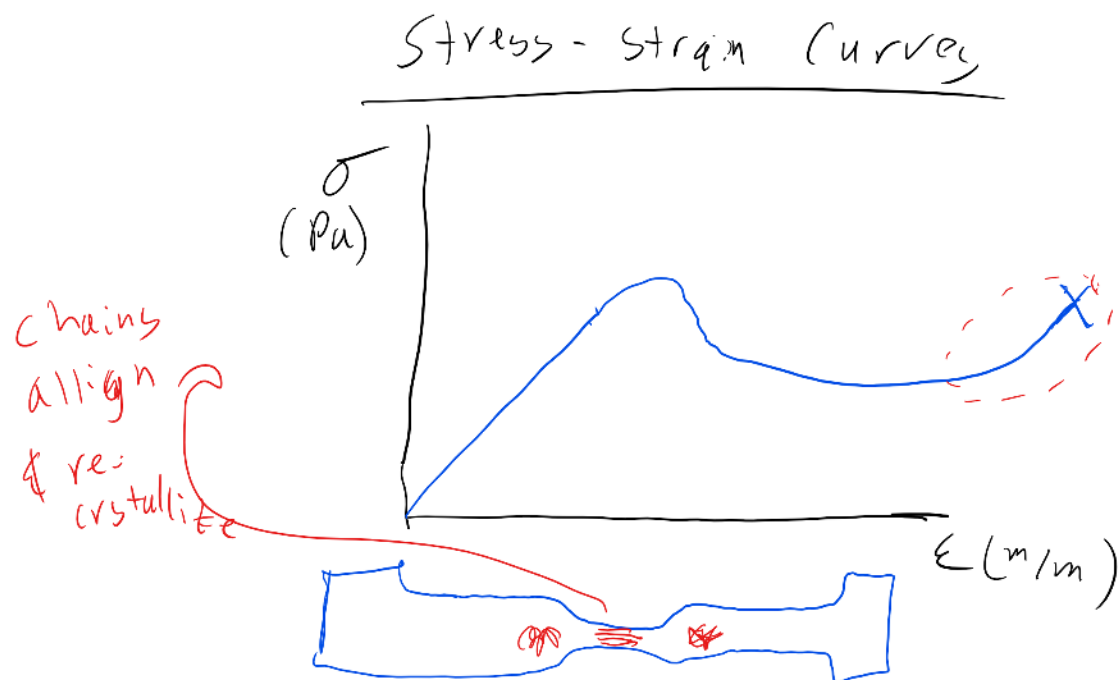


Figure Chapter3.8: Polymer chain alignment

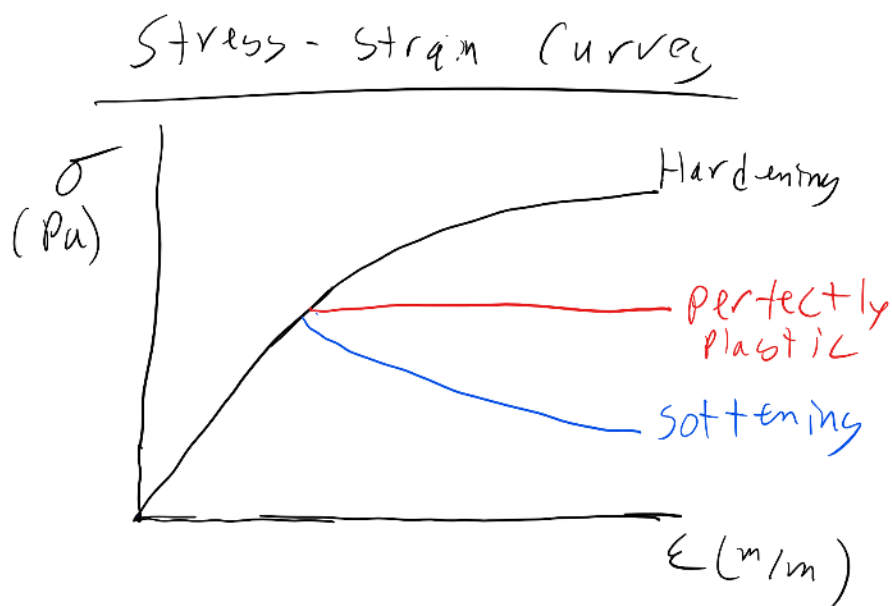


Figure Chapter3.9: Strain hardening, softening, and perfectly plastic

Now one thing you should have learned in materials science and what you will in fact learn here is that there are always counter-examples in materials science. But in general you will find that ceramics (glasses, tungsten, oxides, etc.) are typically very stiff but brittle. Many will exhibit little to no plastic deformation and many will fail suddenly at strains as small as $\epsilon_f = 0.001$. Metals will be less stiff but can be more ductile and fail at much larger strains on the order of $\epsilon_f = 0.1$. The ductility, stiffness, and strength depends on the bonding and the potential interaction as we will dive into more soon, so many soon. Polymers and biomaterials in

general are much more compliant but are extremely ductile some polymers or more accurately elastomers can fail at strains as large as $\epsilon_f = 5 - 10$ look at this that is approximately 4 orders of magnitude larger than for ceramics. This tells us a great deal about toughness as well, we can potential overcome a 3 order of magnitude differences in Young's modulus if we have such a discrepancy in the strain at failure.

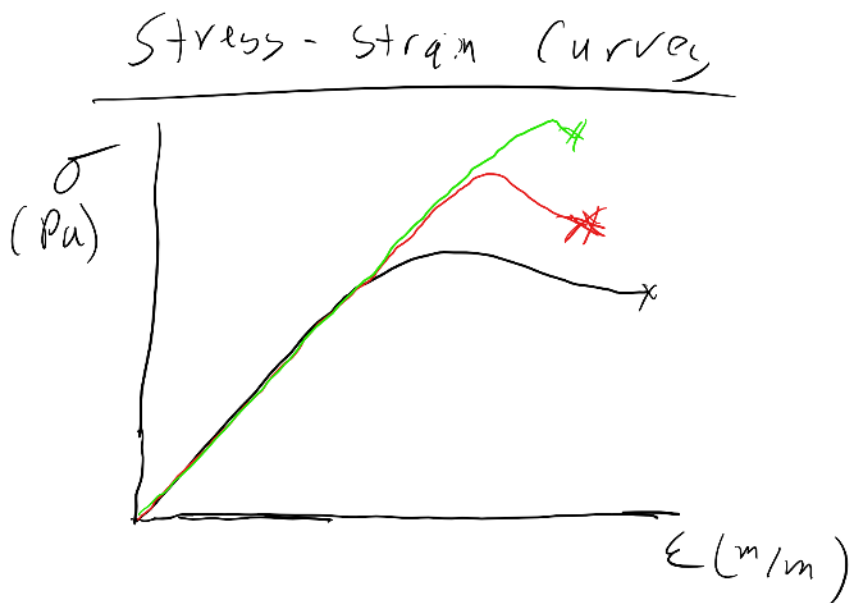


Figure Chapter3.10: Difference between stress strain curves

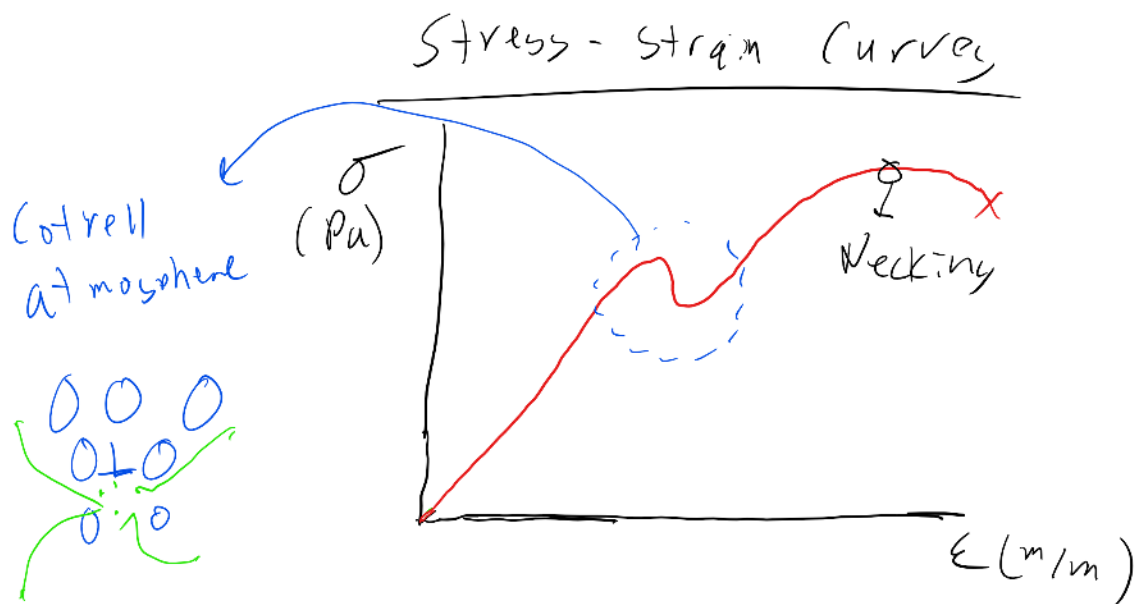


Figure Chapter3.11: Cottrell atmosphere

True Stress-Strain curves

Now so far we have been dealing with engineering stress and strain curves and often this will be the more common stress-strain curve you will encounter. However, sometimes you may see a true stress-strain curve. This will not be too common but sometimes these curves are useful to describe material response at large deformations or they are utilized in plasticity studies because once the material plastically deforms the area is no longer constant.

Previously our engineering definition of stress and strain were as follows

\$\$

$$\begin{aligned}\sigma_{eng} &= \frac{F}{A_o} \\ \epsilon_{eng} &= \frac{\Delta l}{l_o}\end{aligned}\quad (\text{Chapter 3.20})$$

\]

However to describe true stress we can no longer use these definitions as beyond the elastic limit the specimen dimensions can be significantly different from their original values.

Thus we have to introduce new definitions of stress and strain, true stress and true strain. Here we find

$$\sigma_{true} = \frac{F}{A} \quad (\text{Chapter 3.21})$$

where A is the instantaneous area. We can relate the true stress to engineering stress by invoking a conservation of volume argument such that the following condition must hold true

$$A_o l_o = A l \quad (\text{Chapter 3.22})$$

Additionally we, we can re-write our engineering strain using this relationship such at

$$\epsilon_{eng} = \frac{l - l_o}{l_o} = \frac{A_o}{A} - 1 \quad (\text{Chapter 3.23})$$

And thus we can also write

$$\frac{\sigma_{true}}{\sigma_{eng}} = \frac{F}{A} \frac{A_o}{F} = \epsilon_{eng} + 1 \quad (\text{Chapter 3.24})$$

and finally we get the relationship for the plasticity regime that

$$\sigma_{true} = \sigma_{eng}(1 + \epsilon_{eng}) \quad (\text{Chapter 3.25})$$

We can also write an expression to relate true strain to engineering strain in the plastic regime

$$d\epsilon_{true} = \frac{dl}{l} \quad (\text{Chapter 3.26})$$

Taking the integral

$$\epsilon_{true} = \int_{l_o}^{l_f} \frac{1}{l} dl = \ln \frac{l_f}{l_o} \quad (\text{Chapter 3.27})$$

Now to relate this expression to engineering strain we have to utilize the volume conservation expression we previously utilized and we can write the expression here

\$\$

$$\begin{aligned}\frac{l}{l_o} &= e^{\epsilon_{true}} = \frac{A_o}{A} = 1 + \epsilon_{eng} \\ \epsilon_{true} &= \ln(1 + \epsilon_{eng})\end{aligned}\quad (\text{Chapter 3.28})$$

\]

Another parameter that we will introduce here that you will often see in literature and particularly in polymers is the extension ratio $\lambda = \frac{l}{l_o}$ and this will allow us to re-write true stress and strain quite simply

\$\$

$$\begin{aligned}\sigma_{true} &= \sigma_{eng} \lambda \\ \epsilon_{true} &= \ln \lambda\end{aligned}\quad (\text{Chapter 3.29})$$

\]

Now this expression holds true up to necking. After which the strain is non-uniform and computing the true stress-strain curve is no longer meaningful after necking. However, if we were able to instantaneously measure the necked area we could generate an entire stress-strain curve as our relationship for true strain would be

$$\epsilon_{true} = \ln \frac{L}{L_o} = \ln \frac{A}{A_o} \quad (\text{Chapter 3.30})$$

Often for ductile metals you will typically see a power-law relationship for the expression for true stress and true strain

$$\sigma_{true} = A \epsilon_{true}^n = \log \sigma_{true} = \log A + n \log \epsilon_{true} \quad (\text{Chapter 3.31})$$

The parameter n is referred to as the strain hardening parameter, more on this a bit later but many ductile metals vary from $n = 0.02 - 0.5$. But speaking of strain hardening and strain softening....

Strain Hardening, Strain Softening, or Elastic-Perfectly Plastic

Some materials can strain harden, strain soften, or behave elastic-perfectly plastic for example we can describe the true stress beyond the yield stress as

$$\sigma_y = \sigma_y^o (1 + \epsilon_{true})^n \quad (\text{Chapter 3.32})$$

The materials will behave as follows depending on the strain hardening exponent n

- Strain Hardening $n > 0$
- Elastic-Perfectly Plastic $n = 0$
- Strain Softening $n < 0$

We can actually see how the true stress and strain curves compares the engineering stress and strain curve below

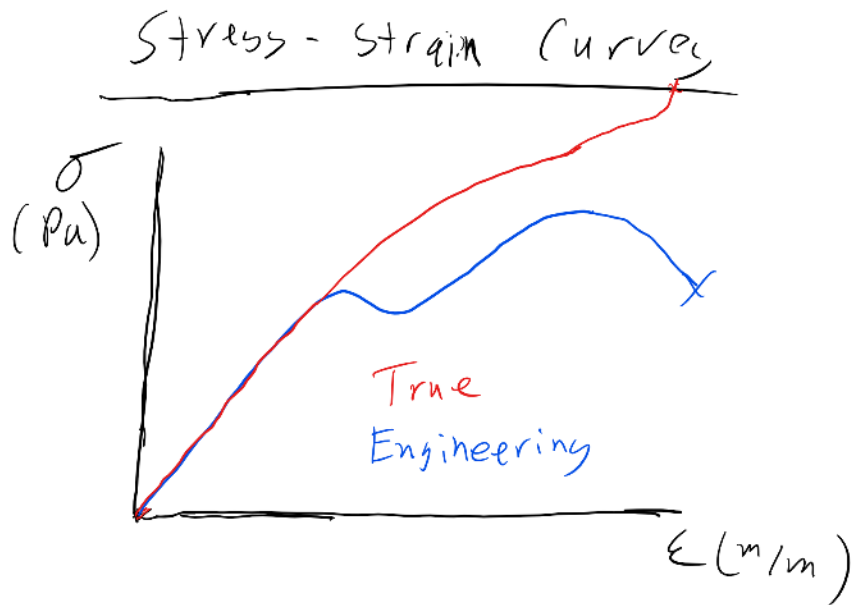


Figure Chapter3.6: Difference between engineering and true stress strain curves

Now you are all experts in everything stress-strain curves so we can end the class.....not so fast all of this that we have discussed is for a very very specific stress-state uniaxial tension. Unfortunately this is not a common stress state so we need to go much deeper and dive into the tensorial definition of stress and strain.

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Chapter 4: Tensor Notation of Stress and Strain

We have introduced some general notions of stress and strain definitions and you have likely encountered them in past courses; however, at this point in this class we have been focusing on relatively simple stress states, uniaxial tension. However, there are many other complex stress states that are more commonly found in real life applications both in industry and academia. The other important thing to clarify is that all the expressions that we will work with here only apply to the first regime of our stress-strain curve, i.e. linear elastic, and we will also assume the materials we work with are cubic and behave isotropically.

Tensorial Definition of Stress

We have previously defined normal stress as

$$\sigma = \frac{F}{A} \quad (\text{Chapter 4.1})$$

and we define positive stress if the material is under tension (material extends) or negative if the material compresses.

In addition to normal stress one will often encounter shear stresses as well. Shear stress occurs when the force is applied parallel to the area. For shear stresses we will define positive faces of elements as those with normal in positive 1, 2, or 3 directions. Positive shear will act in the positive direction on positive faces or act in the negative direction on the negative faces.

Shear stresses are also defined as force per unit area as seen below

$$\tau = \frac{F}{A} \quad (\text{Chapter 4.2})$$

where τ is shear stress. In this class we will instead utilize the tensorial definition of both stress and strain, but it should be noted that both are equivalent (unlike engineering and tensorial shear strain... more on this later).

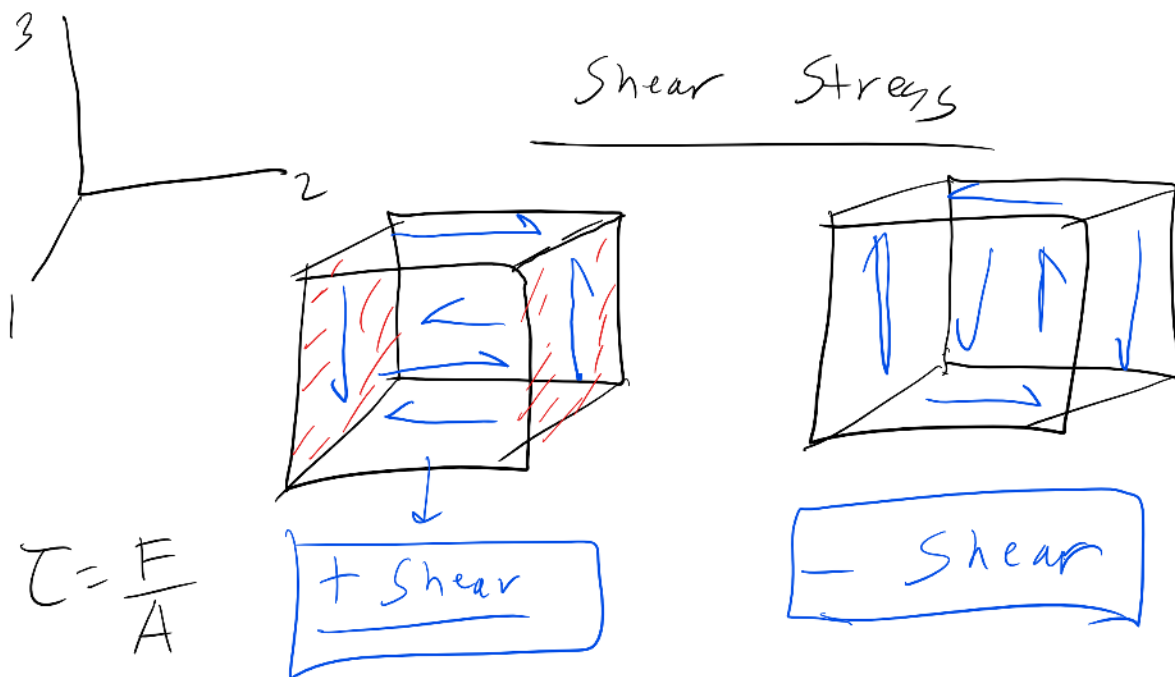


Figure Chapter4.1: Shear Stress

Stress is a second rank tensor property. You have most likely encountered several first rank tensor properties, i.e. vector quantities. The difference between a matrix and a tensor is that a tensor indicates a coordinate system while a matrix is just a matrix of numbers. The second rank nature of stress $\bar{\sigma}$ or σ_{ij} , has indices i and j that indicate directions in our coordinate system. In this class

we will use a 1–2–3 coordinate system. For stress, i denotes the normal to the plane on which the force is acting, and j is the direction of the force:

$$\sigma_{ij} = \frac{F_j}{A_i} \quad (\text{Chapter 4.3})$$

So our full stress tensor or our most generic stress state would be:

$$\sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \quad (\text{Chapter 4.4})$$

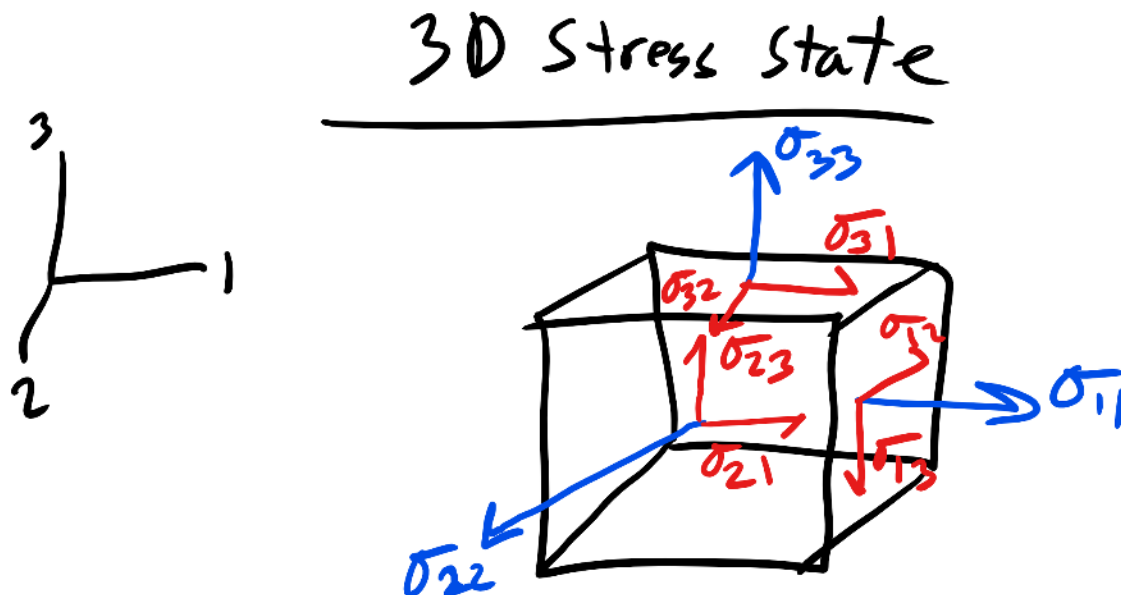


Figure Chapter4.2: 3D Stress State

Now this looks like a complex matrix with 9 independent components; however, they are not completely independent. We need to ensure that our representative volume element (RVE) is in equilibrium, i.e. $\Sigma F = 0$ and $\Sigma M = 0$.

To ensure that we are at equilibrium, let's look at the sum of the forces in the 2 direction:

$$\Sigma F_2 = \sigma_{32}\delta_1\delta_2 - \sigma_{23}\delta_1\delta_2 = 0 \quad (\text{Chapter 4.5})$$

This is a somewhat trivial result but the cool finding comes when we set the moments about the 1 axis to be equal to zero

$$\Sigma M_1 = \sigma_{23}\delta_3\delta_1\delta_2 - \sigma_{32}\delta_1\delta_2\delta_3 = 0 \quad (\text{Chapter 4.6})$$

We then find the following relationships that

$$\sigma_{23} = \sigma_{32} \quad (\text{Chapter 4.7})$$

Moreover we can extend this proof and then we will find that

$$\sigma_{12} = \sigma_{21} \quad (\text{Chapter 4.8})$$

$$\sigma_{13} = \sigma_{31} \quad (\text{Chapter 4.9})$$

$$\sigma_{31} = \sigma_{13}$$

(Chapter 4.10)

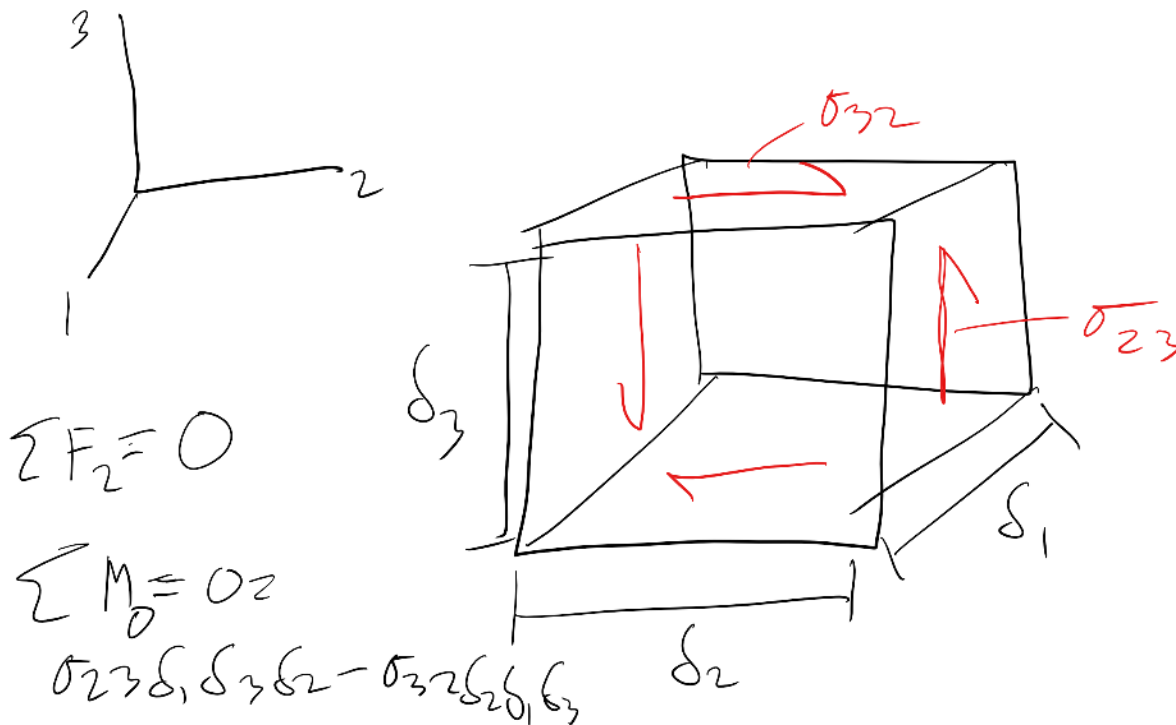


Figure Chapter4.3: Static Equilibrium Proof

Our second rank tensor reduces from 9 independent components to 6 independent components as seen below.

$$\sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{bmatrix}$$

(Chapter 4.11)

Now this ends our initial discussion of the tensorial definition of stress.

How about an inverse problem, draw the following RVE:

$$\sigma = \begin{bmatrix} 86 & 0 & -8 \\ 0 & -37 & 3 \\ -8 & 3 & 14 \end{bmatrix}$$

(Chapter 4.12)

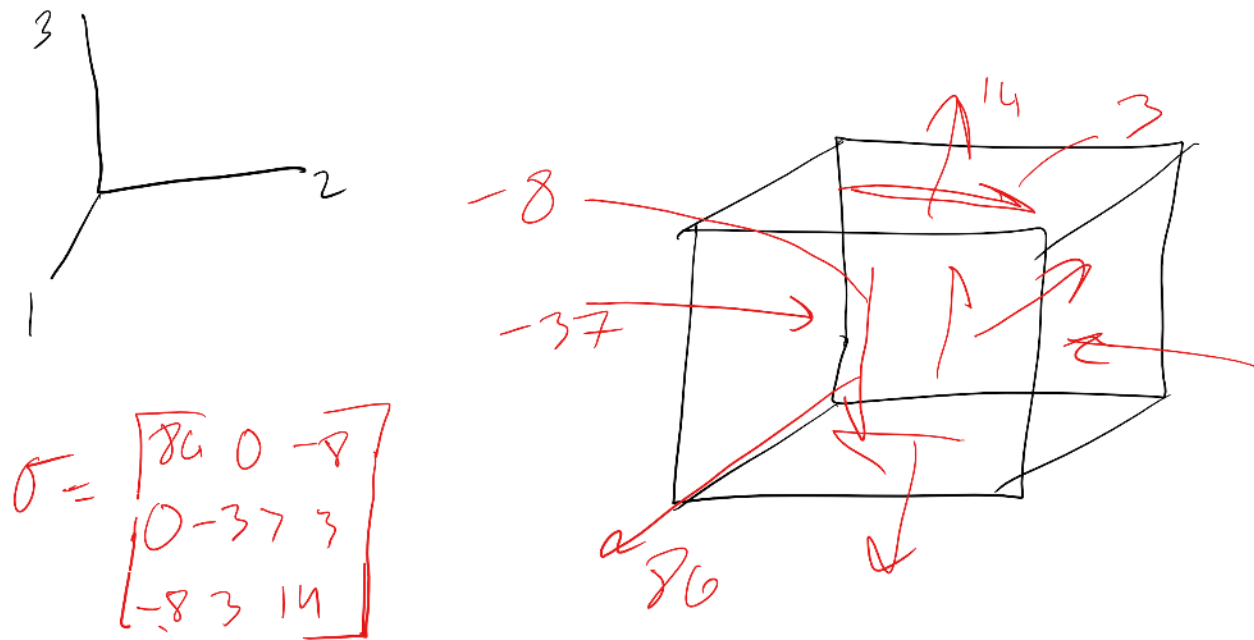


Figure Chapter4.4: Complex Stress State 2

Now you are experts but are you ready for strain? Of course you are—let's go.

Engineering Definition of Strain

We have previously defined normal strain as well as true strain but forget about true stress and strain for a little bit. Normal strain was defined as

$$\epsilon = \frac{\Delta l}{l_o} \quad (\text{Chapter 4.13})$$

and this was engineering strain. We also have a definition of engineering shear strain as seen below.

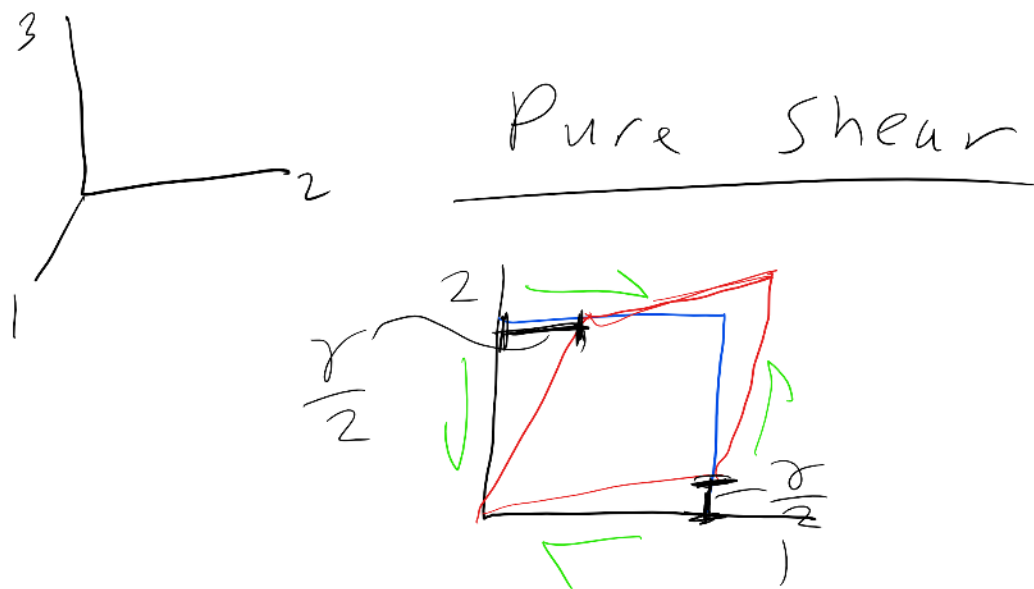


Figure Chapter4.5: Pure Shear State

$$\gamma = \frac{dL}{L} = \tan \theta$$

(Chapter 4.14)

Engineering Shear Strain

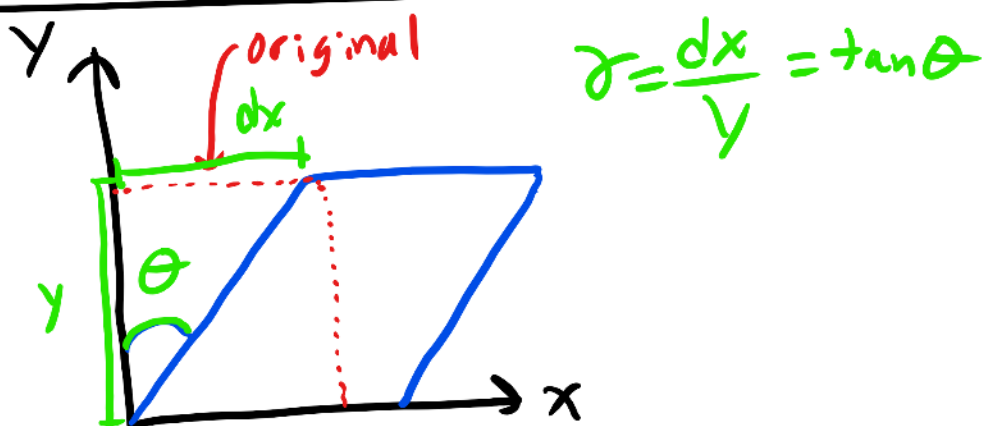


Figure Chapter4.6: Engineering Shear Strain]

This particular case is for simple shear and pure shear as well. Unfortunately, this definition is going to cause an issue in just a second. For a pure stress state we observe a proportional relationship between shear stress and shear strain in the elastic regime

which is defined as:

$$\tau = G\gamma \quad (\text{Chapter 4.15})$$

where G is the shear modulus. Remember this only holds for pure shear just like this $\sigma = E\epsilon$ holds for uniaxial tension only.

Now I mentioned a hiccup previously. When we talked about the engineering definition of normal and shear stress those definitions map directly to the tensorial definition of stress for both normal and shear stresses. For strain, engineering normal strain is the exact same as the tensorial definition but there is a difference for the shear strain. Thus we must introduce infinitesimal strain theory to reconcile this so we can move on to some very fun and complex problems.

Infinitesimal Strain Theory

Now more formally we can define strain using infinitesimal strain theory (if you are interested please read in Chapter 5 of Young and Lovell Introduction to Polymers). The essential idea is that you take an infinitesimally small representative volume element and displace the points. So the definition of strain becomes as follows:

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (\text{Chapter 4.16})$$

where x is an axis dimension and u is the displacement. We also have from this theory that:

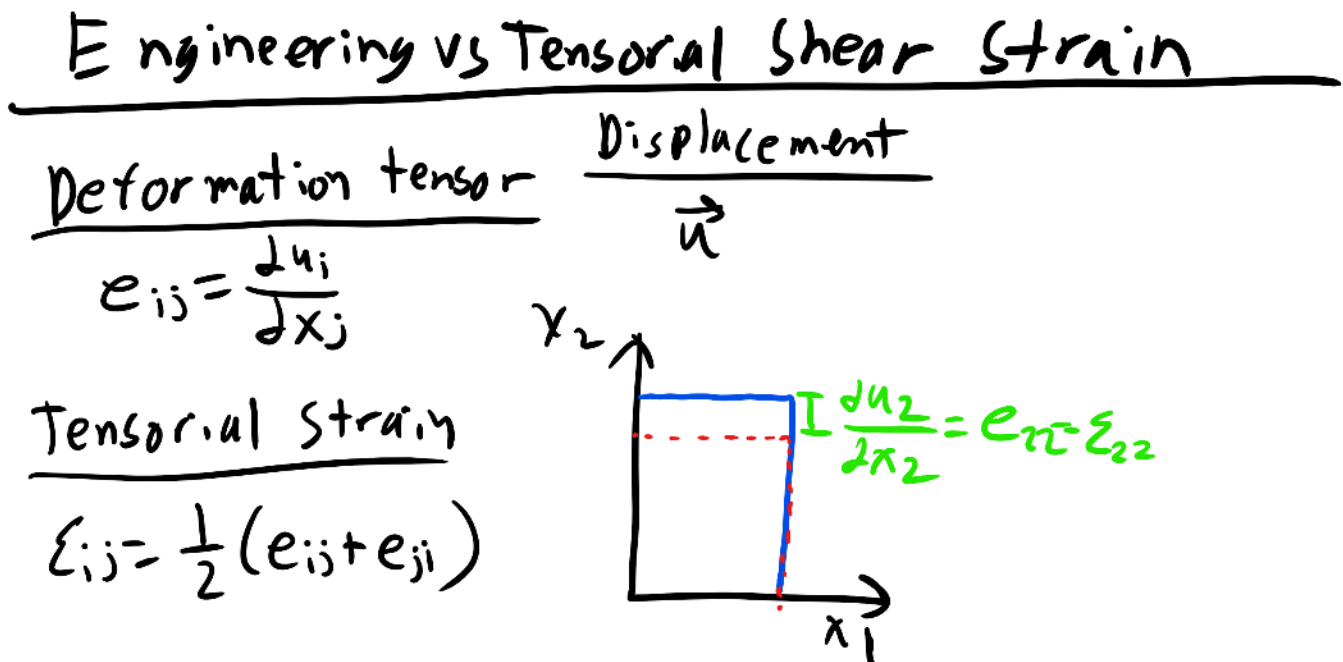


Figure Chapter4.7: Infinitesimal Strain Theory Diagram 1

Again, here we can see that our engineering definition of strain and our tensorial definition match perfectly. However, looking below for the case of strain we have an issue.

Engineering vs Tensorial Shear Strain

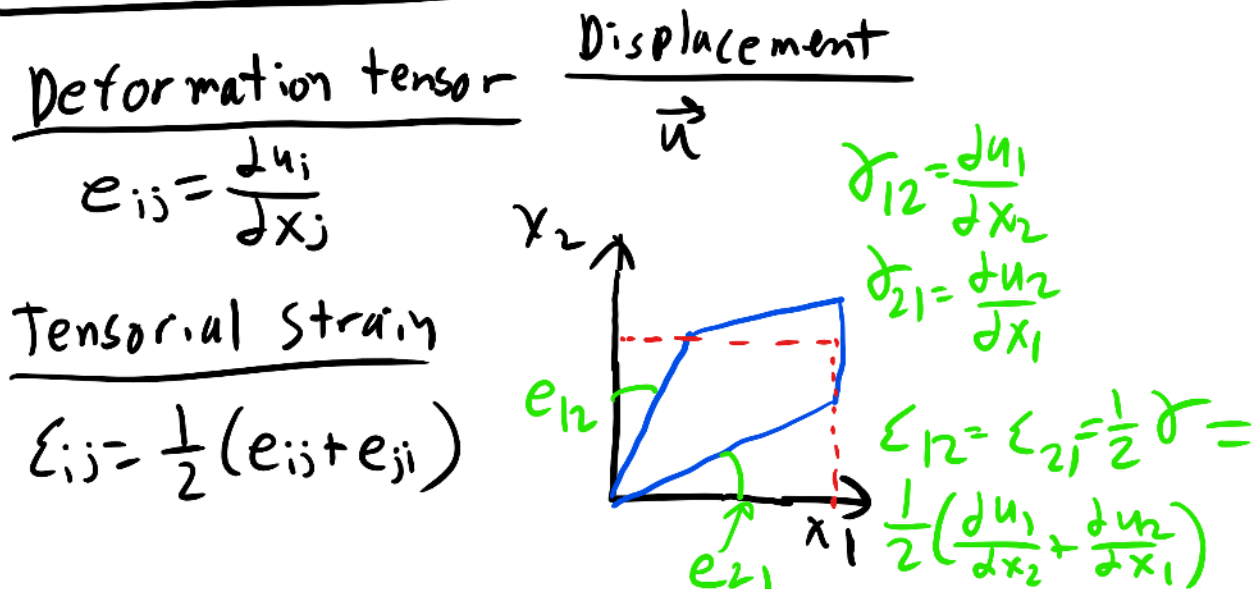


Figure Chapter4.8: Infinitesimal Strain Theory Diagram 2

We can see here that when applying the infinitesimal strain theory definition of tensorial strain we do not see this equivalence for engineering shear strain and tensorial shear strain. In fact, we see that the tensorial definition of shear strain is half the engineering shear strain. Thus, we must account for this and be careful when working with problems, i.e. is this the tensorial or engineering definition of shear strain.

$$\epsilon_{11} = \frac{\partial u_1}{\partial x_1} \quad (\text{Chapter 4.17})$$

$$\epsilon_{22} = \frac{\partial u_2}{\partial x_2} \quad (\text{Chapter 4.18})$$

$$\epsilon_{33} = \frac{\partial u_3}{\partial x_3} \quad (\text{Chapter 4.19})$$

$$\epsilon_{12} = \epsilon_{21} = \frac{1}{2} \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) \quad (\text{Chapter 4.20})$$

$$\epsilon_{23} = \epsilon_{32} = \frac{1}{2} \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right) \quad (\text{Chapter 4.21})$$

$$\epsilon_{31} = \epsilon_{13} = \frac{1}{2} \left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3} \right) \quad (\text{Chapter 4.22})$$

$$\gamma_{12} = \gamma_{21} = \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) \quad (\text{Chapter 4.23})$$

$$\gamma_{23} = \gamma_{32} = \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right) \quad (\text{Chapter 4.24})$$

$$\gamma_{31} = \gamma_{13} = \left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3} \right) \quad (\text{Chapter 4.25})$$

With all this we can now create our strain matrix, and seeing from the definitions above we know that $\epsilon_{12} = \epsilon_{21}$, $\epsilon_{23} = \epsilon_{32}$, and $\epsilon_{13} = \epsilon_{31}$, so that now our strain matrix has 6 independent components and can be written as:

$$\epsilon = \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{12} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{13} & \epsilon_{23} & \epsilon_{33} \end{bmatrix} \quad (\text{Chapter 4.26})$$

or equivalently:

$$\epsilon = \begin{bmatrix} \epsilon_{11} & \frac{\gamma_{12}}{2} & \frac{\gamma_{13}}{2} \\ \frac{\gamma_{12}}{2} & \epsilon_{22} & \frac{\gamma_{23}}{2} \\ \frac{\gamma_{13}}{2} & \frac{\gamma_{23}}{2} & \epsilon_{33} \end{bmatrix} \quad (\text{Chapter 4.27})$$

This will become increasingly important when we begin to rotate our coordinate systems in problems to come.

Now at this point we want to start to use these expressions to relate stress and strain using our series of constitutive equations, but one question at this point you may be asking is what is the origin of linear elasticity at the atomistic level. Well, I'm so glad you asked...

Atomistic Basis of Linear Elasticity and the Young's Modulus

In the previous lecture we learned about the Young's modulus and σ_f , but these aren't just values that we only find on a stress-strain curve. These are values that have an atomistic origin in nature. To understand these properties we have to remember that in the elastic regime we are simply stretching bonds and that the distance between bonds and the equilibrium distance between bonds is governed by an interatomic potential. Also, whenever you have a potential or a distribution you can relate the width of the distribution or any potential to the stiffness of that potential or distribution—see my paper about quantum harmonic oscillators and chemotactic traps, riveting read...

But we can relate the chemical bonding to how stiff a material will be or how compliant they are. This is very, very unique and something that we cannot do in the plasticity regime or fracture due to the fact that we have to deal with inhomogeneities in the system and other atomistic details, i.e. energy of dislocations, defects, etc. We will also see soon that for certain materials the stiffness is derived from entropic considerations.

Let's approach this from a thermodynamic perspective and consider a system under uniaxial tension in the 1 direction. Now the key thing to remember is that when you stretch bonds this changes the internal energy of the system. Looking at the Lennard-Jones (LJ) potential, if we increase the distance between atoms the internal energy of the system increases.

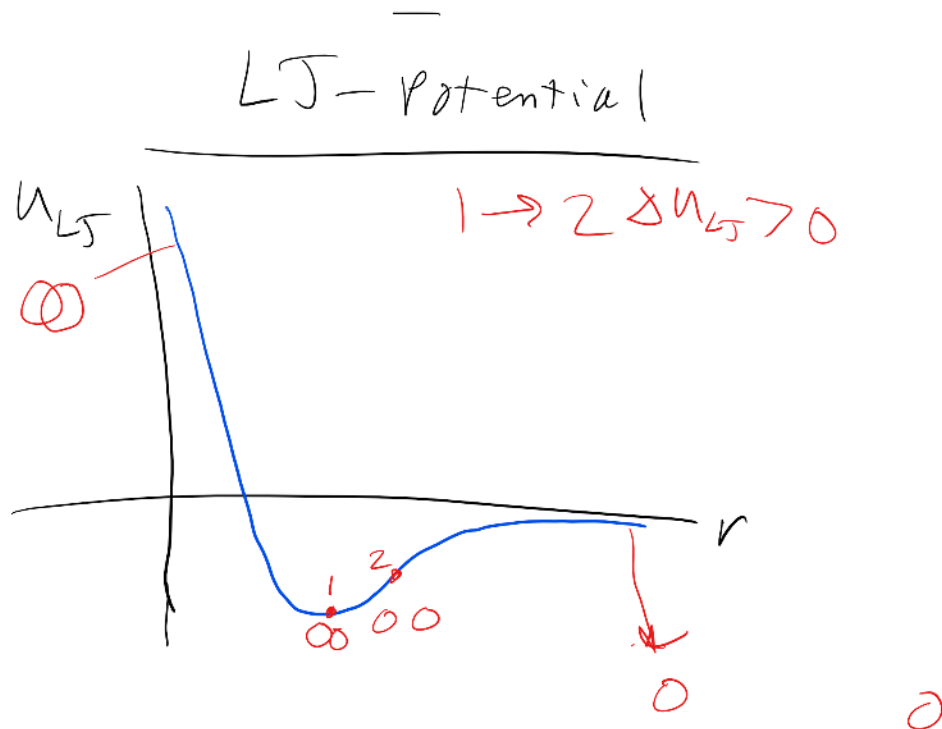


Figure Chapter 4.9: Energy of system increases as atoms displaced from equilibrium position

Now we know that the change in the internal energy of the system is equal to the sum of the work done on the material by the applied stress and the heat absorbed by the material (aren't you glad we had that reminder lecture for thermodynamics!!!)

$$dU = dW + dq \quad (\text{Chapter 4.28})$$

where work will simply be

$$dW = \sigma_{11} \delta_2 \delta_3 d\epsilon_{11} \delta_1 = \sigma_{11} d\epsilon_{11} V \quad (\text{Chapter 4.29})$$

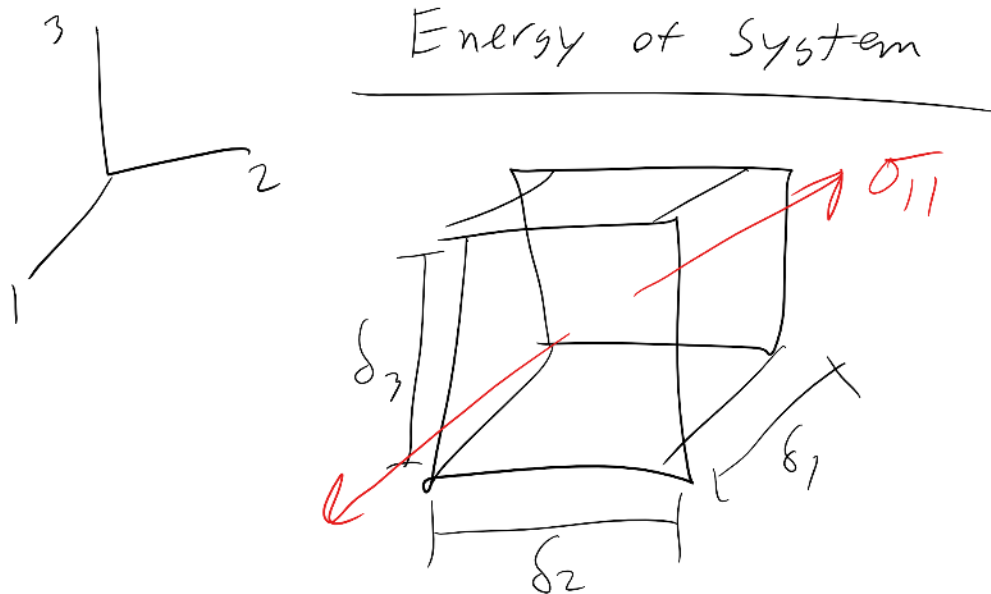


Figure Chapter4.10: Energy of system uniaxial tension

We also know from thermodynamics that:

$$dq = TdS \quad (\text{Chapter 4.30})$$

and thus:

$$dU = V\sigma d\epsilon + TdS \quad (\text{Chapter 4.31})$$

and rearranging in terms of stress:

$$\sigma = \frac{1}{V} \frac{dU}{d\epsilon} - \frac{TdS}{Vd\epsilon} \quad (\text{Chapter 4.32})$$

Right here it is important to note that for most crystalline materials (metals and ceramics) as well as amorphous materials that are well below the T_g , the value of $\frac{dS}{d\epsilon}$ will be very small to the point where the values may be negligible.

Now for polymers above the T_g and for rubbers or other elastomers we will see very soon that $\frac{dS}{d\epsilon}$ is very significant—a fantastic derivation of rubber elasticity is coming soon, don't worry it is riveting!

So for crystalline materials and for amorphous glassy materials we can simplify the expression and look at the internal energy per atom and instead at the atomic volume Ω , so our previous expression becomes:

$$\sigma = \frac{1}{\Omega} \frac{dU}{d\epsilon} \quad (\text{Chapter 4.33})$$

and thus for our Young's modulus:

$$E = \frac{d\sigma}{d\epsilon} = \frac{1}{\Omega} \frac{d^2U}{d\epsilon^2} \quad (\text{Chapter 4.34})$$

In general many potentials will have the following form:

$$U(r) = -\frac{A}{r^m} + \frac{B}{r^n} \quad (\text{Chapter 4.35})$$

where the first term is the attractive term and A is a constant while the m exponent is typically 1 for ionic crystals, and for covalent or metallic bonding it can vary between 4–6, whereas the repulsive term is the second term, B is a constant, and the n exponent can

vary between 9–12.

We can then start to write some components of the previous equation in terms of our potential. For example, we see that:

$$\epsilon = \frac{r - r_o}{r_o} = \frac{r}{r_o} - 1 \quad (\text{Chapter 4.36})$$

And if you plot the force you will also see that it is linear or Hookean near the equilibrium distance, and finally if you also plot the Young's modulus you will see that as r increases the Young's modulus decreases. This is important a little later but let's do some more math quickly...

So back to our derivation, now we know that:

$$E = \left(\frac{d\sigma}{d\epsilon} \right)_{\epsilon=0} \quad (\text{Chapter 4.37})$$

Also we know that:

$$d\sigma = \frac{dF}{r_o^2} \quad (\text{Chapter 4.38})$$

And we have that:

$$\frac{d\epsilon}{dr} = \frac{1}{r_o} \quad (\text{Chapter 4.39})$$

And now finally we can write:

$$E = \left(\frac{d\sigma}{dr} \frac{dr}{d\epsilon} \right)_{\epsilon=0} = \frac{1}{r_o} \left(\frac{d^2U}{dr^2} \right)_{\epsilon=0} \quad (\text{Chapter 4.40})$$

You can arrive at a similar expression to find an estimate of the Young's modulus using the elastic strain energy which we previously defined:

$$U_{ESE} = \frac{E\epsilon^2}{2} \quad (\text{Chapter 4.41})$$

And remember the elastic strain energy is simply a potential energy of our system so we can write:

$$E = \frac{d^2U_{ESE}}{d\epsilon^2} \quad (\text{Chapter 4.42})$$

and again we can relate the change in the distance to strain via this relationship $r = r_o(1 + \epsilon)$ and then:

$$\begin{aligned} E &= \frac{d}{d\epsilon} \left(\frac{dU_{ESE}}{dr} \frac{dr}{d\epsilon} \right) \\ &= \frac{d^2U_{ESE}}{dr^2} \left(\frac{dr}{d\epsilon} \right)^2 + \frac{dU_{ESE}}{dr} \frac{d^2r}{d\epsilon^2} = \frac{d^2U_{ESE}}{dr^2} r_o^2 \end{aligned} \quad (\text{Chapter 4.43})$$

Since r is linear in strain. We also know that the atomic volume $V = V_o = r_o^3$, so our strain energy per unit volume will simply be the energy per atom divided by the volume, and here the energy per atom will simply be:

$$E_{atom} = \frac{ZU(r)}{2} \quad (\text{Chapter 4.44})$$

where Z is the number of nearest neighbors. So we find:

$$U_{ESE} = \frac{E_{atom}(r) - E_{atom}(r_o)}{V} \quad (\text{Chapter 4.45})$$

And finally we arrive at the expression that:

$$E = \frac{Z}{r_o} \frac{d^2U}{dr^2} \quad (\text{Chapter 4.46})$$

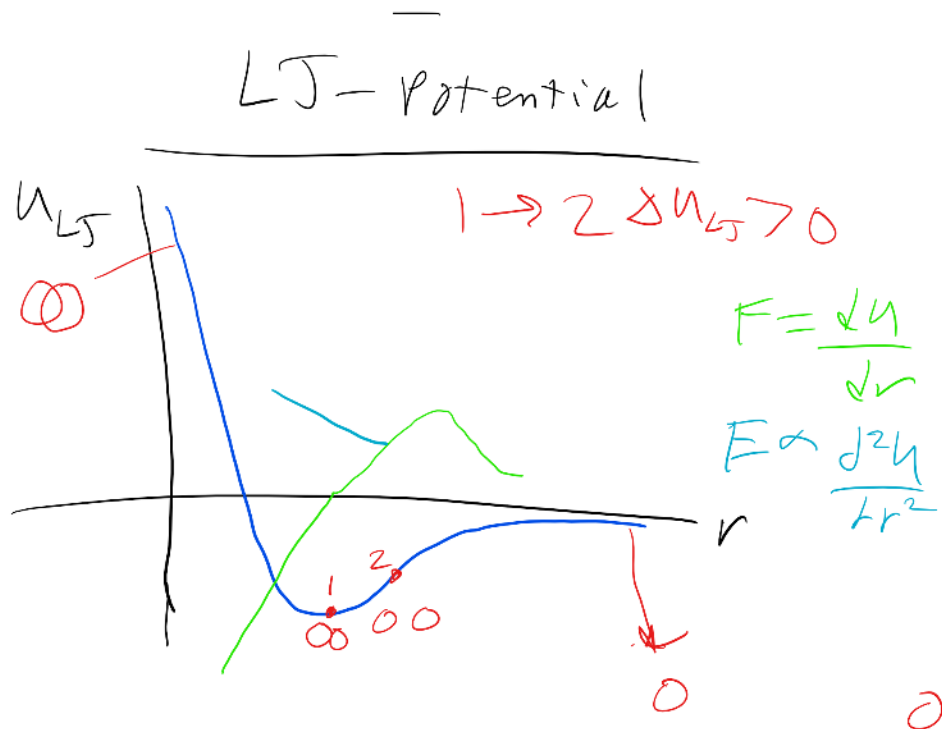


Figure Chapter4.11: Potential, Force, and Stiffness

Now you may find that this calculation may be very different from known values; however, it is important to note that there are much more complex potentials that are typically used, in particular embedded atom potentials (EAM), which take into account more complex and long-range next-neighbor interactions.

Now one question that we hinted at is what happens when temperature changes? Right now we have been assuming we are working at essentially 0 K. Well, let's figure this out together.

Thermal Expansion Coefficient

Let's go back once again to our good old friend the Lennard-Jones potential. When temperature increases, we know that the thermal energy increases, causing the atoms to vibrate and oscillate around their equilibrium distance r_0 . Now if the potential was symmetric or harmonic (like at the minimum of a quadratic function), then the atoms would be equally distributed at distances less than or greater than the equilibrium distance. However, as you can see, the Lennard-Jones and most atomic potentials are asymmetric or anharmonic, and thus when the atoms fluctuate they will tend to occupy positions with the lowest energy. One can see that as temperature increases and as the molecules deviate further and further from their equilibrium position, they will tend to adopt positions with lower energies. Thus, as you can see, on average the molecules will tend to expand because the larger interatomic distances have lower energies, and thus the materials will tend to expand.

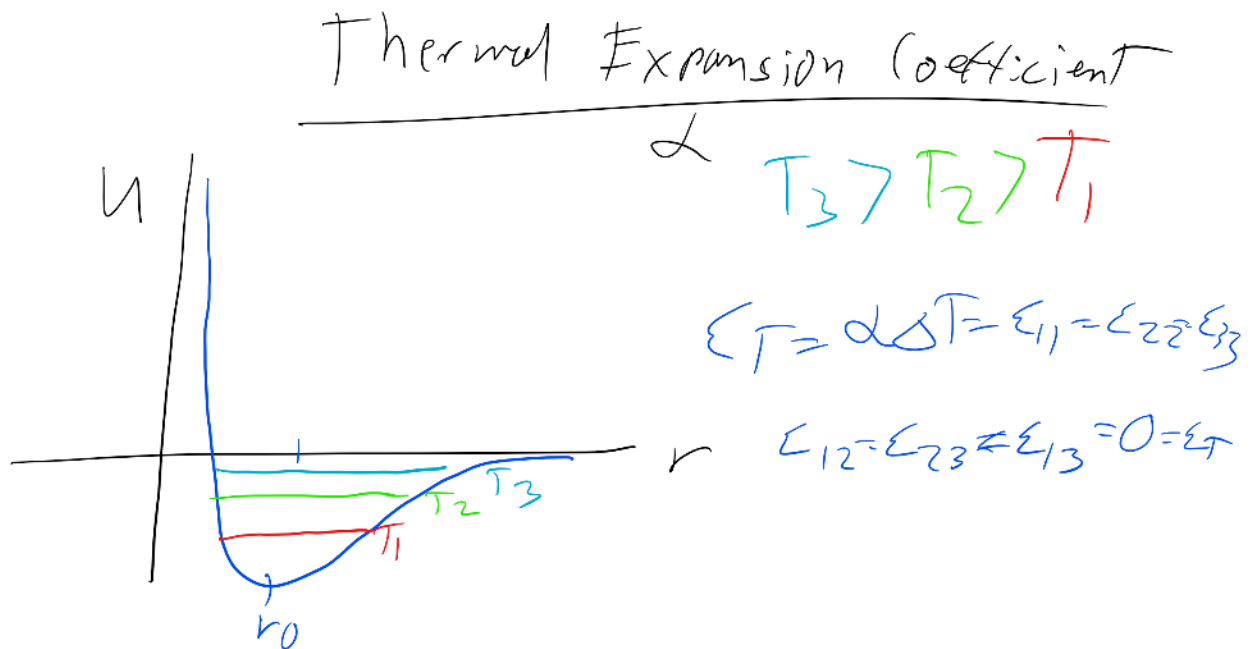


Figure Chapter4.12: Origin of Thermal Expansion Coefficient

So to put it simply, at $T = 0 \text{ K}$ the atoms will be at their equilibrium distance r_0 , and then as temperature increases, the atoms will essentially move up the anharmonic potential to lower their energy. The equilibrium distance thus shifts to the right depending on the thermal expansion coefficient α , and thus we can write this thermally induced strain as:

$$\epsilon_T = \alpha \Delta T \quad (\text{Chapter 4.47})$$

Now for linear elastic isotropic materials, the material will expand uniformly in all directions and there will be no shear strain from thermal expansion. Some typical thermal expansion coefficients for some materials can be seen below, all multiplied by 10^{-6} K^{-1} :

- Polymers: 50–500
- Metals: 5–50
- Ceramics: 1–10
- Glasses: 1–2

Taking into account thermal strain is incredibly important in many materials processes. When you heat a material that is a composite and cool it, this can induce residual stresses due to the incompatible thermal strains.

Rubber Elasticity

In previous courses you have hopefully come across the notion that for polymers there is a characteristic relaxation time where, when a mechanical load is applied, the polymer can behave like a viscous liquid or an elastic solid. We will talk more about this in this class as well. Many polymers are also viscoelastic in mechanical nature and we will discuss this as well, but there are also even other polymers (this is why polymers are the best) that exhibit elastic behavior for very long timescales, and these polymers are elastomers, and this property is rubber elasticity. We will describe the molecular characteristics that give rise to rubber elasticity, the physical model used to describe the rubbery response, and finally how we can use this model to find the stress-strain behavior of an elastomeric polymer.

Rubber Elasticity:

Typically when we discuss rubbers and the mechanics of rubbers or elastomers we will talk about networks. And when we deform those networks we describe this behavior as rubber elasticity. Microscopically, we envision a rubber network as a large, entwined set of polymer chains that are attached together by crosslinks, referring to points that join otherwise distinct chains. Crosslinks can

be chemical or physical in nature — chemical crosslinks refer to actual covalent bonds between chains (vulcanization), while physical crosslinks refer to non-specific interactions between chains. Examples of physical crosslinks include entanglements in polymer melts, glassy phase-separated regions in a rubbery matrix (as in high-impact polystyrene or HIPS), block copolymers, or possibly hydrogen bonding or other types of strong non-covalent bonds between groups that are highly separated along a chain.

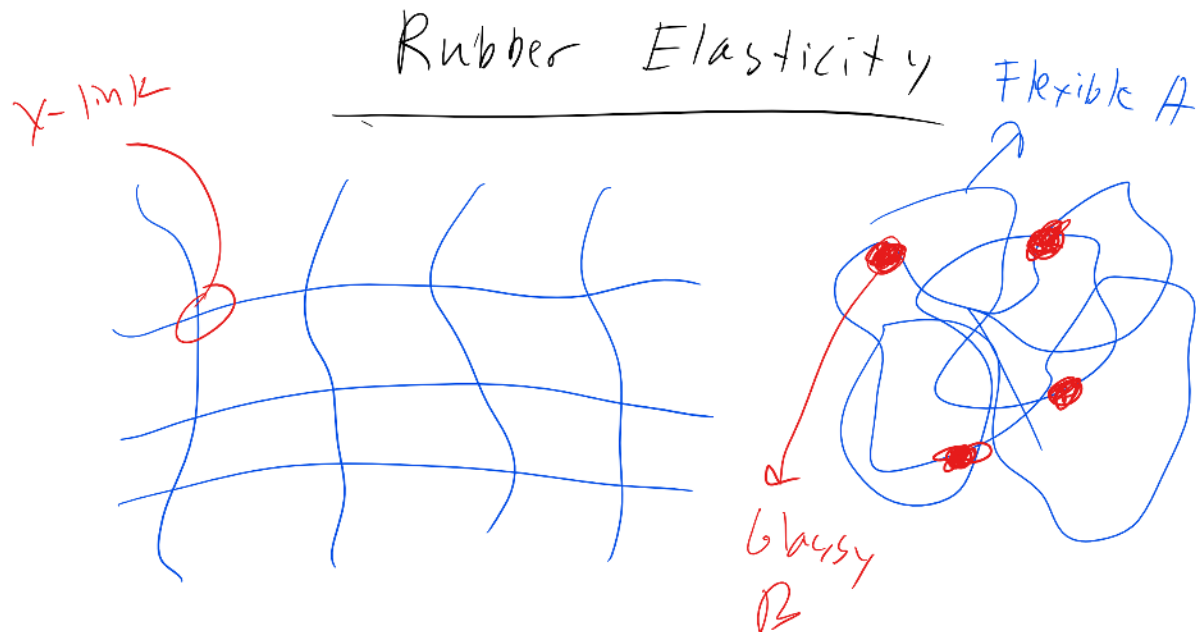


Figure Chapter4.13: Physical and chemical cross-links

The presence of crosslinks joins otherwise disparate chains together such that the entire rubber is connected and individual chains are no longer capable of diffusing completely independently in response to a perturbation. As a result, stressing a crosslinked network leads to a mechanical response that is partially characteristic of an elastic material and partially characteristic of a viscous material, with the important caveat that under a mechanical stress the overall network maintains mechanical robustness.

We will quantitatively describe how rubbery networks respond to stress using basic principles of mechanics and a thermodynamic description as well. It is critical to keep in mind the molecular structure that gives rise to rubbery behavior. The key concept to recognize is that a rubber is still composed of flexible polymer chains that can easily rearrange in the presence of a stress, allowing large amounts of strain when stressed. However, the presence of crosslinks prevents the chains from completely flowing, and as a result some solid-like mechanical behavior is observed. In the context of the discussion of relaxation time scales we could say that the rubber exhibits a longest relaxation time characteristic of a solid (the relaxation time associated with removing crosslinks) while having shorter relaxation times characteristic of liquids (the relaxation time associated with diffusing the polymer chains between crosslinks). We will have multiple relaxation times and see behaviors characteristic of both liquid and solid behavior.

Before describing this behavior and creating a theoretical framework we will be making several key assumptions:

1. Gaussian subchains between permanent crosslinks — that is, you can envision the part of a chain between two crosslinked points as a chain itself, which can be described by a Gaussian distribution. This assumption breaks down if the distance between crosslinks is very small.
2. Temperature well above T_g , so that the system has sufficient thermal energy for chains to rearrange.
3. Flexible chains with relatively easy backbone bond rotation potentials, again reflecting the ability of chains to rearrange.
4. Chain deformation occurs by conformational changes.
5. No relaxation by chain slip — the network appears as fixed on the time scale of experiment, i.e. physical crosslinks can be assumed to be permanent. This means that as we pull the rubber, the chains are not able to slide past each other and thus fall apart.
6. Affine deformation — microscopic deformation by same amount as macroscopic deformation; that is, any given chain's

dimensions change by the same ratio as the change in dimensions of the overall network.

7. No crystallization of the chains at large strains.

8. No change in volume of the rubber upon deformation, i.e. incompressibility assumption.

Now there are two distinct types of behavior that are well described by our rubber elasticity framework:

- Mechanical Deformation: we apply some stress and measure the strain response for a fixed volume.

- Gel Swelling: a polymer network swells due to mixing a solvent and the volume increases.

We have hinted at energetic competition for mechanically deforming a rubber network previously in other courses, specifically that stretching polymer chains decreases the conformational entropy of the chain and we had an expression for the energy of a stretched chain based on the change in the number of microstates:

$$G(r)_{stretch} = \frac{3kT}{2} \frac{r^2}{r_0^2} \quad (\text{Chapter 4.48})$$

Here energy increases if the chain extends, and thus we have an entropic spring restoring force that opposes pulling.

Let's start with the mechanical deformation first.

Rubber Elasticity System

As usual we want to think about the energetics and thermodynamics associated with changing the state of our system when we apply mechanical stress to the crosslinked polymer network. The initial state is the unstressed, relaxed polymer network. We assume that we have a large number of subchains which are the chain segments between crosslinked points. We assume that these subchains can be defined as Gaussian with unperturbed end-to-end distance $\langle r_0^2 \rangle$. We also assume that the molecular weight of each subchain, M_x , is the same. Given an initial set of chains, the molecular weight of each subchain will thus decrease as the degree of crosslinking is increased.

Upon applying a force (stress) to the network, we assume that the dimensions extend to a new end-to-end distance $\langle r^2 \rangle$. Here, we can invoke the assumption of an affine deformation — the deformation experienced by each individual subchain is equivalent to the deformation experienced by the whole network. Using this assumption, we can relate the microscopic perturbed dimensions to unperturbed dimensions via an extension ratio in each direction 1, 2, and 3, which is defined as the ratio between the macroscopic deformed length l_i in that direction and the undeformed length l_0 (assuming a sample with the same l_0 in all 3 directions). These extension ratios are:

$$\alpha_1 = \frac{l_1}{l_0} \quad (\text{Chapter 4.49})$$

$$\alpha_2 = \frac{l_2}{l_0} \quad (\text{Chapter 4.50})$$

$$\alpha_3 = \frac{l_3}{l_0} \quad (\text{Chapter 4.51})$$

Because of the affine deformation assumption, we can also write coordinates of an individual subchain in terms of the extension ratios, if we imagine deforming a subchain between one crosslink fixed at (0, 0, 0) and one crosslink fixed at (1, 2, 3), with deformed coordinates (1', 2', 3'):

$$1' = \alpha_1(1), \quad 2' = \alpha_2(2), \quad 3' = \alpha_3(3) \quad (\text{Chapter 4.52})$$

We also then see that the end-to-end distances are defined as:

$$r^2 = 1'^2 + 2'^2 + 3'^2 \quad (\text{Chapter 4.53})$$

$$r_0^2 = 1^2 + 2^2 + 3^2 \quad (\text{Chapter 4.54})$$

Finally, since we assume that the network is incompressible, the total volume change has to be equal to 0, which means that the product of the deformed lengths has to be equal to the product of the undeformed lengths:

$$\alpha_1 \alpha_2 \alpha_3 = 1 \quad (\text{Chapter 4.55})$$

Thermodynamic Perspective of Rubber Elasticity

Now we need a thermodynamic relationship to derive an expression between force and extension for a general material, which we can then apply to our polymer network. As usual, let's start with Gibbs:

$$G = H - TS \quad (\text{Chapter 4.56})$$

Finding the differential form of G , and including a work term for extension in U , gives:

$$dG = -SdT + VdP + Fdl \quad (\text{Chapter 4.57})$$

where G is the Gibbs free energy, l is the extension of the chain, and F is the force. By rearranging this equation we can see that F is:

$$F = \left(\frac{\partial G}{\partial l} \right)_{T,P} \quad (\text{Chapter 4.58})$$

We can thus take the derivative of our first expression for G with respect to l at constant T and P to get:

$$F = \left(\frac{\partial H}{\partial l} \right)_{T,P} - T \left(\frac{\partial S}{\partial l} \right)_{T,P} \quad (\text{Chapter 4.59})$$

Remember the physical interpretation: the equation above tells us that the force associated with a change in chain extension is related to the derivative of the enthalpy, which measures bond interactions, and entropy. For ideal rubbers, we assume that the change in enthalpy is 0 as the rubber network is stretched. So then:

$$F = -T \left(\frac{\partial S}{\partial l} \right)_{T,P} \quad (\text{Chapter 4.60})$$

Here we see that the restoring force of rubber elasticity is driven by entropy. We assume there is no change in enthalpy when a rubber is stretched, in part because of the fixed volume assumption — since the volume is not changing, the net number of interactions is assumed to be the same on average, so there is no net enthalpy change. This assumption of no net enthalpy change is one of the unique characteristics of polymers — for example, we could not apply the same reasoning to metals because of strong enthalpic changes associated with stretching bonds, etc. Even if we relax the assumption of a zero enthalpy change, we would still find that for polymers the change in entropy is the dominant term, allowing us to refer to the corresponding force as an entropic spring force.

Since the elastic force that arises from stressing a rubber network is related to the derivative of the entropy, we need to calculate the entropy based on the extension ratios defined previously. Entropy is related to the number of microstates available to the polymer, which is related to the probability distribution of the Gaussian subchains. So we can define the entropy change for a single chain as:

$$S_2 - S_1 = \Delta S = k \ln \frac{\Omega_2}{\Omega_1} \quad (\text{Chapter 4.61})$$

$$\Omega_1 = \text{const} \times \exp \left(\frac{-3r_0^2}{2nl^2} \right) \quad (\text{Chapter 4.62})$$

$$\Omega_2 = \text{const} \times \exp \left(\frac{-3(\alpha_1^2 l^2 + \alpha_2^2 2^2 + \alpha_3^2 3^2)}{2nl^2} \right) \quad (\text{Chapter 4.63})$$

Here we assume that $\Omega_1 \propto P(r_0)$ and $\Omega_2 \propto P(r)$ where $P(r)$ is the Gaussian distribution, and r_0 and r are the relaxed and stressed dimensions defined above. This then gives:

$$\Delta S = k \ln \frac{\Omega_2}{\Omega_1} = \frac{-3k}{2nl^2} [(\alpha_1^2 - 1)1^2 + (\alpha_2^2 - 1)2^2 + (\alpha_3^2 - 1)3^2] \quad (\text{Chapter 4.64})$$

Again, we are able to state that the entropy of a single chain is related to the extension ratios associated with the macroscopic sample because of our assumption of affine/homogeneous deformation. Right now we have the entropy in terms of the relaxed coordinates 1, 2, 3. In this state, where the overall chain dimensions can be described by the Gaussian distribution, then we can expect that there is no distinction between a random walk in either of the 3 directions, so the average contribution to $\langle r_0^2 \rangle$ from 1^2 , 2^2 , and 3^2 is the same so:

$$\langle 1^2 \rangle = \langle 2^2 \rangle = \langle 3^2 \rangle = \frac{\langle r_0^2 \rangle}{3} \quad (\text{Chapter 4.65})$$

Substituting in these values and knowing that $nl^2 = r_0$ gives:

$$\Delta S = \frac{-k}{2} (\alpha_1^2 + \alpha_2^2 + \alpha_3^2 - 3) \quad (\text{Chapter 4.66})$$

Finally, F is:

$$\Delta F_i = -T \left(\frac{\partial \Delta S(\alpha_i)}{\partial l_i} \right)_{T,P} \quad (\text{Chapter 4.67})$$

where l_i denotes the force in a given direction $i = 1, 2, 3$.

Uniaxial Deformation of a Rubber Network

Now that we have an expression for the change in entropy of a chain given some deformation and have a thermodynamic relation that yields the force associated with that deformation, we can start analyzing different scenarios. Let's start simple with uniaxial deformation and find the resulting elastic force. Let's take deformation along the x -axis so that:

$$\alpha_1 = \frac{l_1}{l_0} \quad (\text{Chapter 4.68})$$

$$\alpha_2 = \frac{1}{\sqrt{\alpha_1}} \quad (\text{Chapter 4.69})$$

$$\alpha_3 = \frac{1}{\sqrt{\alpha_1}} \quad (\text{Chapter 4.70})$$

Here, we calculate α_2 and α_3 from the incompressibility condition $\alpha_1 \alpha_2 \alpha_3 = 1$. We can then write ΔS in terms of just α_1 :

$$\Delta S(\alpha_1) = -\frac{k}{2} \left(\alpha_1^2 + \frac{2}{\alpha_1} - 3 \right) \quad (\text{Chapter 4.71})$$

The 3-dimensional problem has now broken down into only knowing the extension in a single dimension. We can take the derivative with respect to l_1 to find F , using the chain rule:

$$F_1 = -T \frac{\partial}{\partial l_1} \Delta S(\alpha_1) \quad (\text{Chapter 4.72})$$

$$= -T \frac{\partial}{\partial \alpha_1} \left(\frac{\partial \alpha_1}{\partial l_1} \right) \Delta S(\alpha_1) \quad (\text{Chapter 4.73})$$

$$= \frac{kT}{2l_0} \frac{\partial}{\partial \alpha_1} \left(\alpha_1^2 + \frac{2}{\alpha_1} - 3 \right) \quad (\text{Chapter 4.74})$$

$$F_1 = \frac{kT}{l_0} \left(\alpha_1 - \frac{1}{\alpha_1^2} \right) \quad (\text{Chapter 4.75})$$

To put this in more familiar terms, we can find the stress by dividing by the cross-sectional area (in the 2–3 plane), which we'll call A_0 . So far we've derived F_1 for a single chain only, and would ideally like to know the stress required to deform a network of z total subchains per volume V :

$$\sigma_1 = \frac{zF_1}{A_0} = \frac{zkT}{A_0 l_0} \left(\alpha_1 - \frac{1}{\alpha_1^2} \right) = N_{xlinks} kT \left(\alpha_1 - \frac{1}{\alpha_1^2} \right) \quad (\text{Chapter 4.76})$$

Here, we simplify by letting $A_0 l_0 = V$ and $\frac{z}{V} = N_{xlinks}$, where N_{xlinks} is the number of crosslinks per unit volume. Typically the restoring force is written in terms of the molecular mass of crosslinks instead of their number, so we can rearrange to find the crosslink molecular mass in terms of the density as:

$$M_x = \frac{\text{mass of polymer/volume}}{\text{number of subchains per volume}} = \frac{\rho}{N_{xlinks}/N_A} \quad (\text{Chapter 4.77})$$

$$\sigma_x = \frac{\rho N_A kT}{M_x} \left(\alpha_1 - \frac{1}{\alpha_1^2} \right) \quad (\text{Chapter 4.78})$$

where N_A is Avogadro's number. We can write the stress as a function of strain (the typical measurement of material deformation) using the relation:

$$\alpha_1 = \frac{l_1}{l_0} = \frac{l_0 + \Delta l}{l_0} = 1 + \frac{\Delta l}{l_0} = 1 + \epsilon_1 \quad (\text{Chapter 4.79})$$

$$\sigma_1 = \frac{\rho N_A kT}{M_x} \left(1 + \epsilon_1 - \frac{1}{(1 + \epsilon_1)^2} \right) \quad (\text{Chapter 4.80})$$

In the limit of small strains, we see that the stress scales linearly with the strain, and hence we can define the Young's modulus:

$$E = \frac{\rho N_A kT}{M_x} \quad (\text{Chapter 4.81})$$

Let's stop here for a moment and appreciate this result. We see here that for a rubber network the Young's modulus increases with temperature and decreases with the molecular weight of crosslinks. This implies that if we increase the density of crosslinks, then the molecular weight of the crosslinks decreases and the Young's modulus goes up, leading to a greater elastic restoring force. However, do recall that if the density gets too high, the assumption of Gaussian subchains will eventually break down, and the derivation will no longer be valid.

Since we have shown that the Young's modulus depends on crosslink molecular mass (and hence crosslink density), and we have stated that entanglements can act as physical crosslinks at short times (since at longer times the entanglements will eventually diffuse away), then we can measure the elastic response of an entangled melt at some known temperature to approximate the number of statistical segments between entanglements N_E . In principle, this type of experiment would also allow us to identify the critical molecular weight for crossing over between the Rouse and reptation regimes, since the onset of the reptation regime would be associated with the onset of elastic behavior at small timescales.

Limits of Rubber Elasticity Model

This model works very well at applied strains that are relatively low; however, in regimes where the chain extension is high, the model begins to break down.

- Strain-induced Crystallization: at large extensions the polymer chains can pack tightly and form crystalline regions (shish-kebob spherulites), and thus the Young's modulus will be larger than predicted by theory.
- Subchain Length Reaches Contour Length: at this point we are pulling on covalent bonds and the Young's modulus will approach that of metals.

- Bond Rotation Away from Trans State at High Extension: (see discussion below).
- Dangling Ends: experimental Young's modulus is lower than theory because there are regions between the end of the chain and crosslink that can form entanglements. This increases the crosslink density of the network somewhat artificially, as the physical crosslinks disappear when deformation occurs.
- System Temperature Drops Below T_g : recall that we are implicitly assuming that the rubbery network is above its glass transition temperature, and thus chains are freely able to deform and hence explore a full conformational space. If the network is cooled below the glass transition temperature, the entropic spring arguments will fail because the network no longer acts like a Gaussian chain, but instead will give an elastic response consistent with the kinetic barriers to chain rearrangement.
- Too Many Crosslinks: a major assumption of this model is that every subchain in the rubbery network can be treated as a Gaussian chain, and thus loses a significant amount of conformational entropy upon stretching. If the crosslink density is high, however, the number of segments between crosslinks will correspondingly become very low and the subchains may no longer be considered Gaussian.
- Too Few Crosslinks: if the chains are too long, entanglements can occur between subchains and the entanglements can act like crosslinks on short timescales, so we could imagine the effective crosslink density being much higher than anticipated due to the presence of crosslinks. Note that even in the case of moderate crosslinking density, there will typically be chain ends which are capable of forming crosslinks and may result in spurious results.

Now that was quite a deviation from where we were headed in terms of relating stress to strain via constitutive equations for linear elastic isotropic cubic materials. So let's get back on track, and before we get into some really nice linear algebra we have to define one more very important material property, and that is the Poisson ratio.

Poisson's Ratio

Now what happens to the dimensions perpendicular to the direction of applied force when the material is subjected to uniaxial tension? We know from experience that a body being pulled in tension will contract laterally. This lateral strain is described by the Poisson's Ratio:

$$\nu = -\frac{\epsilon_L}{\epsilon_A} \quad (\text{Chapter 4.82})$$

[Figure: General Poisson's Ratio]

where ϵ_L is the lateral strain and ϵ_A is the axial strain. Note the negative sign which signifies a decrease in length. Some typical examples for Poisson's ratio are:

- Metals: 0.3
- Ceramics: 0.2
- Polymers/Biomaterials: 0.4
- Regular Hexagonal Honeycomb: 1
- Cork: 0
- Isotropic solids: $-1 < \nu < 0.5$

Now that we know the Poisson ratio, we can start to develop our constitutive equations for complex stress states.

Biaxial and Complex Stress States

What happens when we have a more complex stress state and we are interested in the stress state of a particular plane of orientation angle θ ? Well, we do this the same way we resolve force vectors onto a new axis of interest. Let's look at a case of plane stress, which is a case when all the stress is contained in one plane.

So far we have been dealing with simple uniaxial stress along the principal testing direction; however, often materials can also be subjected to shear stress or strain.

With this information let us move on to more complex stress states, specifically one that typically exists on a free, not constrained, surface of a stressed material.

Consider the element which is initially stressed in the 1 direction by applying σ_{11} . There will be a resultant strain:

$$\epsilon_{11} = \frac{\sigma_{11}}{E} \quad (\text{Chapter 4.83})$$

$$\epsilon_{22} = \frac{-\nu\sigma_{11}}{E} \quad (\text{Chapter 4.84})$$

The element is then stressed in the 2 direction by applying σ_{22} . The resultant strain will be:

$$\epsilon_{22} = \frac{\sigma_{22}}{E} \quad (\text{Chapter 4.85})$$

$$\epsilon_{11} = \frac{-\nu\sigma_{22}}{E} \quad (\text{Chapter 4.86})$$

Therefore, the total strain in the x and y directions will be:

$$\epsilon_{11} = \frac{\sigma_{11} - \nu\sigma_{22}}{E} \quad (\text{Chapter 4.87})$$

$$\epsilon_{22} = \frac{\sigma_{22} - \nu\sigma_{11}}{E} \quad (\text{Chapter 4.88})$$

We can solve these two equations (two unknowns and two equations) to find the total stress in the x and y directions:

$$\sigma_{11} = \frac{E(\epsilon_{11} + \nu\epsilon_{22})}{1 - \nu^2} \quad (\text{Chapter 4.89})$$

$$\sigma_{22} = \frac{E(\epsilon_{22} + \nu\epsilon_{11})}{1 - \nu^2} \quad (\text{Chapter 4.90})$$

3D Stress State

We can extend this even further to find the total strain if there is another stress applied, σ_z , in the z direction:

$$\epsilon_{11} = \frac{1}{E}[\sigma_{11} - \nu(\sigma_{22} + \sigma_{33})] \quad (\text{Chapter 4.91})$$

$$\epsilon_{22} = \frac{1}{E}[\sigma_{22} - \nu(\sigma_{33} + \sigma_{11})] \quad (\text{Chapter 4.92})$$

$$\epsilon_{33} = \frac{1}{E}[\sigma_{33} - \nu(\sigma_{11} + \sigma_{22})] \quad (\text{Chapter 4.93})$$

We can similarly write the stress as well:

$$\sigma_{11} = \frac{E}{(1 + \nu)(1 - 2\nu)} \left[(1 - \nu)\epsilon_{11} + \nu(\epsilon_{22} + \epsilon_{33}) \right] \quad (\text{Chapter 4.94})$$

$$\sigma_{22} = \frac{E}{(1 + \nu)(1 - 2\nu)} \left[(1 - \nu)\epsilon_{22} + \nu(\epsilon_{33} + \epsilon_{11}) \right] \quad (\text{Chapter 4.95})$$

$$\sigma_{33} = \frac{E}{(1 + \nu)(1 - 2\nu)} \left[(1 - \nu)\epsilon_{33} + \nu(\epsilon_{11} + \epsilon_{22}) \right] \quad (\text{Chapter 4.96})$$

General Expression for Strain in Complex Stress-State

We can also introduce here a more general way to write strain where:

$$\epsilon_{ij} = \frac{1}{E} \left[(1 + \nu) \sigma_{ij} - \nu \sigma_{kk} \delta_{ij} \right] \quad (\text{Chapter 4.97})$$

where δ_{ij} is the Kronecker Delta, which will be 1 when $i = j$ and 0 when $i \neq j$.

Or we can describe this in linear algebra form as follows, where that large matrix relating our strain and stress tensors is known as our compliance matrix S . If you flip and relate stress to strain you will work with a stiffness matrix C .

$$\begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \epsilon_{23} \\ \epsilon_{13} \\ \epsilon_{12} \end{bmatrix} = \begin{bmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1+\nu}{E} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1+\nu}{E} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1+\nu}{E} \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} \quad (\text{Chapter 4.98})$$

We can also relate this to engineering shear strain and the shear modulus G :

$$\begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \gamma_{23} \\ \gamma_{13} \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G} \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} \quad (\text{Chapter 4.99})$$

Where we can write the shear modulus in terms of the Young's modulus as:

$$G = \frac{E}{2(1 + \nu)} \quad (\text{Chapter 4.100})$$

We can also define the bulk modulus, κ , in the case of hydrostatic stress, i.e. all shear stresses are 0 and all normal stresses are equal, i.e. $\sigma_{11} = \sigma_{22} = \sigma_{33} = \sigma_{hydro}$:

$$\kappa = \frac{\sigma_{hydro}}{\frac{\Delta V}{V_0}} = \frac{E}{3(1 - 2\nu)} \quad (\text{Chapter 4.101})$$

Example: Jewelry Maker — Strain Without Stress?

A jewelry maker creates a die to form a new cufflink made of steel. We need to know how much stress to apply to the metal slab to reduce the thickness to 3 mm. The die is a simple channel that does not constrain the metal in the 1-direction, and the channel is well lubricated so that all frictional forces and stresses along the channel walls can be ignored.

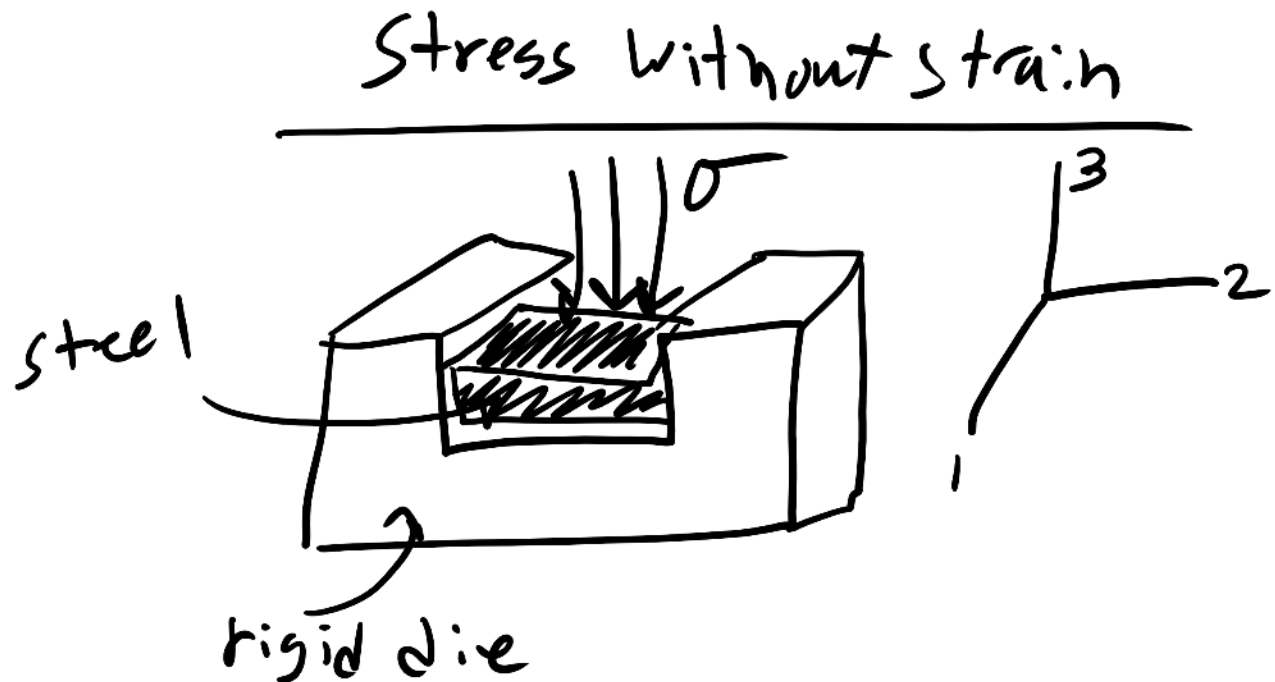


Figure Chapter4.14: Die in which steel of initial thickness 6 mm will be subjected to normal stress σ_{33}

a.) State all the components of the stress tensor under the applied stress.

Well, there is clearly a stress in the 3 direction. What about 1 and 2?

b.) Which normal strain components are zero and why?

c.) Use your answers in part a) and b) to express the relationship between the non-zero stresses in this system.

Finally, I won't leave until we complete thin-walled pressure vessels!

Pressure Vessels: A Special Stress State

Finally, let's consider a very common scenario, a thin-walled pressure vessel. The thin-walled vessel has an applied pressure difference ΔP between the internal pressure and the environment. The wall thickness is sufficiently small where we can say $t \ll R$ or that $\frac{R}{t} \geq 10$.

What is the stress state? It is a plane stress state due to symmetry considerations. Therefore, we need to find σ_1 and σ_2 , which we will accomplish by drawing free body diagrams.

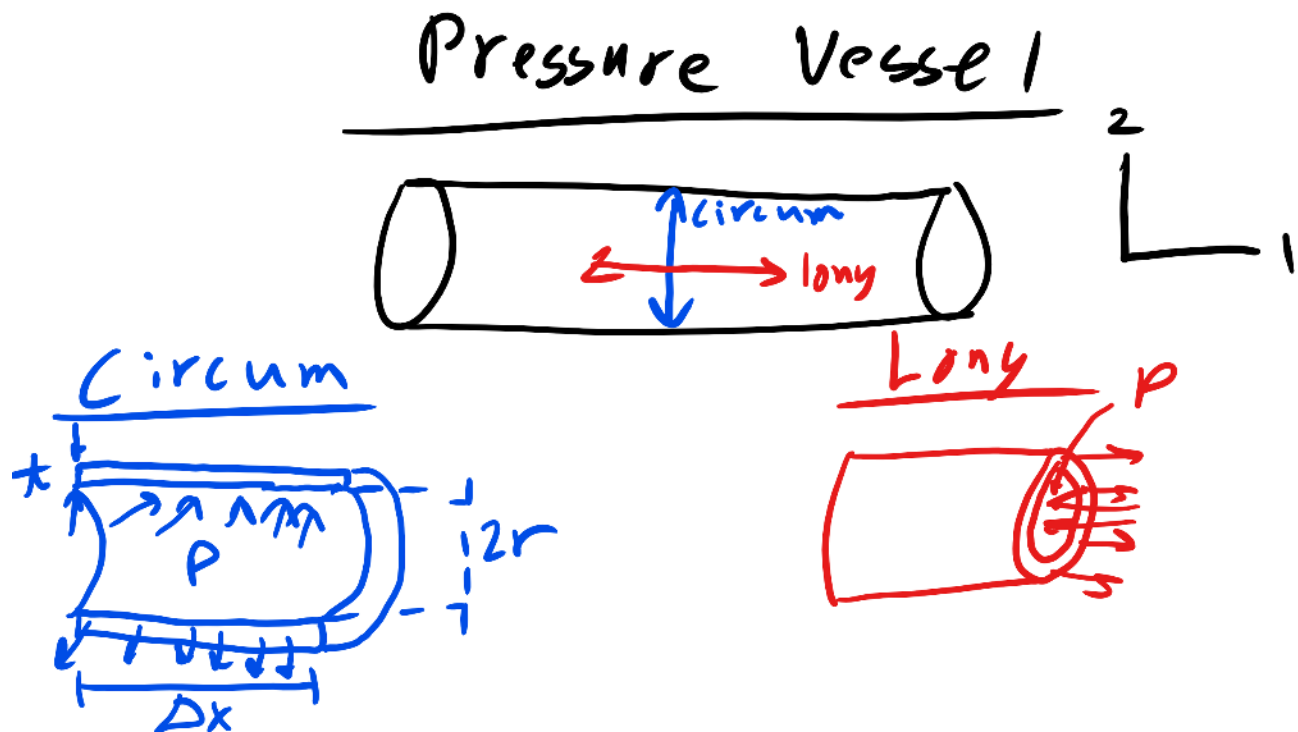


Figure Chapter4.15: Pressure Vessel

Let us first consider the longitudinal direction. Remember that the forces must sum to zero.

$$\sum F_1 = 0 = \Delta P \pi r^2 - \sigma_{11} 2 \pi r t \quad (\text{Chapter 4.102})$$

$$\sigma_{11} = \sigma_{\text{Longitudinal}} = \frac{\Delta P r}{2t} \quad (\text{Chapter 4.103})$$

We have the longitudinal stress, so now let us look at the other direction, circumferential or hoop, and again the forces must sum to equal zero:

$$\sum F_2 = 0 = -\Delta P \Delta x 2R + \sigma_{22} \Delta x t 2 \quad (\text{Chapter 4.104})$$

$$\sigma_{22} = \sigma_{\text{Hoop}} = \frac{\Delta P R}{t} \quad (\text{Chapter 4.105})$$

As you can see, the hoop stress is twice as large as the longitudinal stress, so you should expect the material to fail in such a manner, unless there are extenuating conditions, i.e. defects, corrosion, different processing, etc. The strain ratio for hoop to longitudinal strain is nearly 4:1.

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Chapter 5: Stress Transformations

We have introduced our critical constitutive equations for relating stress and strain for linear elastic isotropic cubic materials. This is great and it was a lot of work to reach out to these expressions; however, in all of the stress states that we worked with, the stresses were applied parallel to our coordinate system axes.

This was very fortuitous, but there are a myriad of applications where this will not be the case and in that instance it will be important that we are able to resolve or determine the stress state at arbitrary rotations or other coordinate systems. This will be particularly pertinent and relevant when we get into yield and plasticity, as certain materials will tend to fail when shear stresses are maximized or when normal stresses are maximized. So the toolkit that we will develop will be multipronged and we will take several approaches, many of which will require a little bit of linear algebra—so I hope that you are ready.

Resolving Stress on Plane of Interest

Now I know that all of you are statics experts, so one way that we can resolve the stresses in a new coordinate system is by first applying our static equilibrium conditions for the forces in our new coordinate system. First, we must define a new coordinate system that aligns with the plane of interest, i.e. we must rotate our old coordinate axes (x, y) to align with our new coordinate axes (x', y').

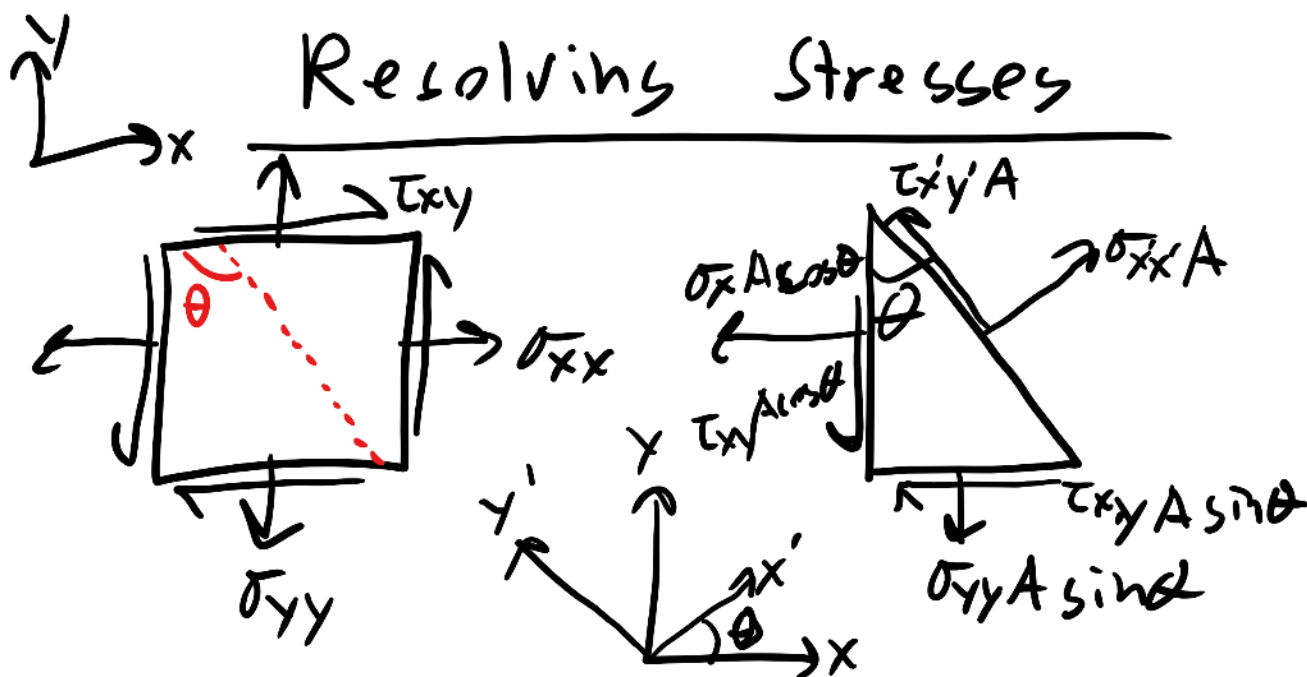


Figure Chapter5.1: Biaxial stress condition and investigating stress state in an arbitrary plane

Then we balance out the forces assuming static equilibrium:

$$\sum F_{x'} = 0 = \sigma_{x'x'} A' - (\tau_{xy} A' \sin \theta) \cos \theta - (\sigma_{yy} A' \sin \theta) \sin \theta - (\tau_{xy} A' \cos \theta) \sin \theta - (\sigma_{xx} A' \cos \theta) \cos \theta \quad (\text{Chapter 5.1})$$

After some rearranging and trigonometric transformations:

$$\sigma_{x'x'}(\theta) = \frac{\sigma_{xx} + \sigma_{yy}}{2} + \frac{\sigma_{xx} - \sigma_{yy}}{2} \cos 2\theta + \tau_{xy} \sin 2\theta \quad (\text{Chapter 5.2})$$

$$\sigma_{y'y'}(\theta) = \frac{\sigma_{xx} + \sigma_{yy}}{2} - \frac{\sigma_{xx} - \sigma_{yy}}{2} \cos 2\theta - \tau_{xy} \sin 2\theta \quad (\text{Chapter 5.3})$$

$$\tau_{x'y'}(\theta) = -\left(\frac{\sigma_{xx} - \sigma_{yy}}{2}\right) \sin 2\theta + \tau_{xy} \cos 2\theta \quad (\text{Chapter 5.4})$$

We have successfully transformed the stress state to our new coordinate system!

Now, in addition to finding the stress state in a new coordinate system, it is also helpful to find the principal stress state, which is the stress state where there exist only normal stresses and all shear stresses are equal to zero. To do this we can simply solve for when the normal stresses are maximized or when the shear stress values are zero, and we will find that the principal stress angle will be simply:

$$\tan 2\theta = \frac{\tau_{xy}}{\frac{\sigma_{xx} - \sigma_{yy}}{2}} \quad (\text{Chapter 5.5})$$

We can then substitute this back into the above equations and get:

$$\sigma_1 = \frac{\sigma_{xx} + \sigma_{yy}}{2} + \sqrt{\left(\frac{\sigma_{xx} - \sigma_{yy}}{2}\right)^2 + \tau_{xy}^2} \quad (\text{Chapter 5.6})$$

$$\sigma_2 = \frac{\sigma_{xx} + \sigma_{yy}}{2} - \sqrt{\left(\frac{\sigma_{xx} - \sigma_{yy}}{2}\right)^2 + \tau_{xy}^2} \quad (\text{Chapter 5.7})$$

σ_1 and σ_2 are the principal normal stresses, and you can see by definition that $\sigma_1 > \sigma_2$. We can do the same for the maximum shear stress and find that:

$$\tau_{xy,\max} = \sqrt{\left(\frac{\sigma_{xx} - \sigma_{yy}}{2}\right)^2 + \tau_{xy}^2} \quad (\text{Chapter 5.8})$$

Now, how many of you can do this upon request at a job interview or memorize these equations for 30+ years? My guess is probably not many of you can do so. Additionally, I like to refer to this as the plug-and-chug method as it does not leave much intuition or thought—students tend to just plug and chug into the equations. Plus I will tend to not ask questions that you can solve easily using these expressions, so I would not utilize this method. Additionally, it is not general for the 3D stress state, but let's hold off on that for a while.

Mohr's Circle: A Graphical Approach

Another approach that is often the bane of many mechanics students is Mohr's Circle. But today we will demystify Mohr's Circle and, more importantly, learn when it is useful to utilize this technique and when it is better and perhaps more appropriate to use our linear algebra approach.

Let's take the following example. I have the following stress tensor, all in MPa, as seen below:

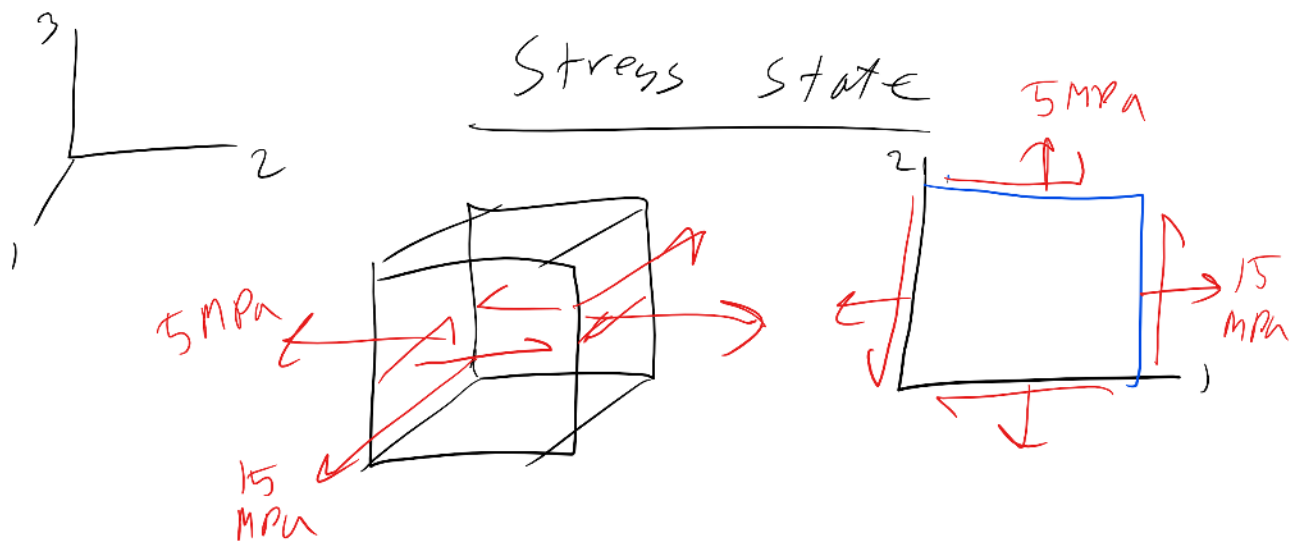


Figure Chapter5.2: Stress-State

$$\sigma = \begin{bmatrix} 15 & 4 & 0 \\ 4 & 5 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (\text{Chapter 5.9})$$

Now what is the principal stress state and the values of principal stress? What about the stress state for a 15° clockwise rotation around the 3-axis?

Now we can find this by plugging and chugging it into our equations, and we will find the values as seen below...

However, this is not physical and we don't really gain any intuition and, most importantly, it is a pain to do, and when I ask harder questions this will be very difficult to do.

Now I would suggest instead to utilize another more graphical, visual, and helpful tool, which is Mohr's Circle construction. Otto Mohr, a German engineer in the 1800s, recognized that we can represent the principal stress state graphically. We can re-write the equations above and sum the square of Eq. $(\sigma_{x'x'})$ and Eq. $(\tau_{x'y'})$ to give us:

$$\left[\sigma_1 - \left(\frac{\sigma_{xx} + \sigma_{yy}}{2} \right) \right]^2 + \tau_{xy, \max}^2 = \left(\frac{\sigma_{xx} - \sigma_{yy}}{2} \right)^2 + \tau_{xy}^2 \quad (\text{Chapter 5.10})$$

You should notice that this form has a similar structure to the equation of a circle:

$$(x - c)^2 + y^2 = r^2 \quad (\text{Chapter 5.11})$$

where the center of the circle is $\frac{\sigma_{xx} + \sigma_{yy}}{2}$ and the radius of the circle is $\sqrt{\left(\frac{\sigma_{xx} - \sigma_{yy}}{2} \right)^2 + \tau_{xy}^2}$. We can plot Mohr's Circle for an arbitrary initial stress state.

The way that we will practically utilize Mohr's Circle is as follows (note that this works when considering plane stress states only):

1. Draw a plot with normal stress on the x-axis and shear stress τ on the y-axis.
2. Treat the stress tensor as a coordinate system with x-axis values for normal stress and y-axis values for shear stress. Plot the coordinates on the graph.
3. The 4 coordinates that you may possibly have (or 2 coordinates) are points that will lie on your Mohr's Circle. Draw a line connecting two of the points.

- When drawing the line, pick the line such that the smaller normal stress has a positive shear stress value and the larger stress has the negative value—i.e. draw the top part of the line on the left and bottom on the right.
- Determine the length of this line as this will determine the diameter of your circle and thus the radius as well.
- Determine where the line crosses the x-axis; this is the center of your Mohr's Circle.
- Determine the angle between your line and the x-axis; this angle is 2θ . It is 2θ due to the equations and transformations described above.
- Once you have the center, radius, and 2θ values, you can find the principal stress state, principal stress angle, maximum shear stress value and angle, and then you can use geometry to get other stress states.

This is best illustrated by doing an example below for the previous stress state.

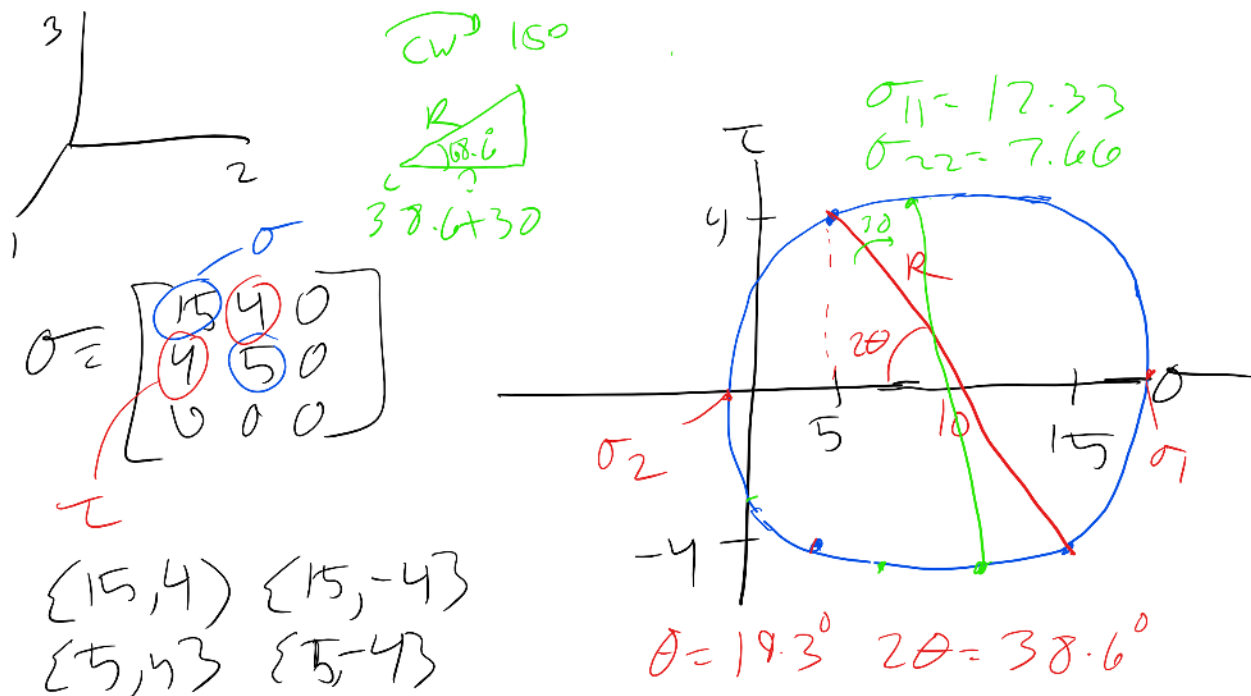


Figure Chapter5.3: Mohr's Circle drawn

Now if you are still unsure about Mohr's Circle you are in luck—I have about 5 hours of videos of worked examples posted on my YouTube channel, so go nuts!

Plane Stress Linear Algebra Transformations

Now as we see above, Mohr's Circle can be very useful for the geometrically gifted or inclined—but I am not one of those people. Also, I find that when trying to determine the stress state at an arbitrary rotation, Mohr's Circle can become a bit cumbersome, and I always fear that I may possibly forget the 2θ caveat.

So I would suggest instead—or better yet, to supplement Mohr's Circle—we can use a linear algebra approach and a rotation matrix to convert stresses in one coordinate system to another coordinate system. Again, remember that we are still only working with plane stress states here, not 3D stress state transformations. So let's get started.

Let's start by first defining our transformation matrix T where:

$$[T] = \begin{bmatrix} c^2 & s^2 & 2sc \\ s^2 & c^2 & -2sc \\ -sc & sc & c^2 - s^2 \end{bmatrix} \quad (\text{Chapter 5.12})$$

where $c = \cos \theta$ and $s = \sin \theta$.

So we now write that:

$$\sigma' = T\sigma \quad (\text{Chapter 5.13})$$

or similarly:

$$\begin{bmatrix} \sigma_{11'} \\ \sigma_{22'} \\ \sigma_{12'} \end{bmatrix} = \begin{bmatrix} c^2 & s^2 & 2sc \\ s^2 & c^2 & -2sc \\ -sc & sc & c^2 - s^2 \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{bmatrix} \quad (\text{Chapter 5.14})$$

So we can utilize this linear algebra approach and solve the same question. As you can see, it is a very elegant way to solve these problems and requires minimal coding, but you still have a clear intuition for how to solve these problems. However, often I will still draw the circle to keep the rotations clear.

Mohr's Circle and Linear Algebra for Strain

Now before we move on to dealing with some complex 3D stress states and rotations of our representative volume element (RVE), you often see Mohr's Circle and transformations of stress only, but I was never personally taught how to deal with strain transformations. But no worries—let's learn how to do this together right now.

We can follow a very similar procedure for Mohr's Circle. If we do some transformations, you will see the equations look very similar in form to those for our stress equations:

$$\epsilon_{x'x'}(\theta) = \frac{\epsilon_{xx} + \epsilon_{yy}}{2} + \frac{\epsilon_{xx} - \epsilon_{yy}}{2} \cos 2\theta + \frac{\gamma_{xy}}{2} \sin 2\theta \quad (\text{Chapter 5.15})$$

$$\epsilon_{y'y'}(\theta) = \frac{\epsilon_{xx} + \epsilon_{yy}}{2} - \frac{\epsilon_{xx} - \epsilon_{yy}}{2} \cos 2\theta - \frac{\gamma_{xy}}{2} \sin 2\theta \quad (\text{Chapter 5.16})$$

$$\frac{\gamma_{xy}}{2}(\theta) = -\left(\frac{\epsilon_{xx} - \epsilon_{yy}}{2}\right) \sin 2\theta + \frac{\gamma_{xy}}{2} \cos 2\theta \quad (\text{Chapter 5.17})$$

So for Mohr's Circle we can simply follow very similar steps as we did for stress, but we just have to make the following adjustments:

1. Draw a plot with normal strain on the x-axis and shear strain $\frac{\gamma}{2}$ on the y-axis.
2. Treat the strain tensor as a coordinate system with x-axis values for normal strain and y-axis values for shear strain. Plot the coordinates.
3. The 4 coordinates that you may possibly have (or 2 coordinates) are points that will lie on your Mohr's Circle. Draw a line connecting two of the points.
4. Determine the length of this line; this will determine the diameter of your circle and thus the radius as well.
5. Determine where the line crosses the x-axis; this is the center of your Mohr's Circle.
6. Determine the angle between your line and the x-axis; this angle is 2θ . IT IS 2θ DUE TO THE EQUATIONS AND TRANSFORMATIONS DESCRIBED ABOVE.
7. Once you have the center, radius, and 2θ values, you can find the principal strain state, principal strain state angle, maximum shear strain value and angle, and then you can use geometry to get other stress states.

One question you may be asking as we get started is: why do we plot $\frac{\gamma}{2}$ and not γ ? Well, that goes back to infinitesimal strain theory, and we said that the tensorial definition of shear strain and engineering shear strain had the following relationship $\epsilon_{12} = \frac{\gamma_{12}}{2}$. Aren't you glad we covered that in lecture?

Let's get to work and use the following strain tensor, all in microstrain:

$$\epsilon = \begin{bmatrix} 340 & 90 & 0 \\ 90 & 110 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (\text{Chapter 5.18})$$

We can also do a similar linear algebra transformation for strain as well, but we have to account for the following complication: we have the definition that $\epsilon_{xy} = \frac{1}{2}\gamma_{xy}$, so we have to account for this in our transformation specifically via the introduction of the Reuter's Matrix.

$$[R] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} \quad (\text{Chapter 5.19})$$

So to transform to new coordinate systems for strain we have to do the following:

$$\epsilon' = RTR^{-1}\epsilon \quad (\text{Chapter 5.20})$$

This is assuming that we are writing our strain tensor ϵ in the following form, working with engineering shear strain values:

$$\epsilon = \begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \gamma_{12} \end{bmatrix} \quad (\text{Chapter 5.21})$$

If you have already converted to the tensorial definition of stress and strain you are good and can skip the Reuter's matrix and use our usual transformation:

$$\epsilon' = T\epsilon \quad (\text{Chapter 5.22})$$

Isotropic Stress-Strain Transformations for Plane Stress-Strain States

Now if we want to relate or transform stress and strain tensors in one coordinate system to another, we can do the following transformation:

$$\begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \gamma_{23} \\ \gamma_{13} \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G} \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} \quad (\text{Chapter 5.23})$$

$$\begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ 0 \\ 0 \\ 0 \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G} \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} \quad (\text{Chapter 5.24})$$

or more visually appealing:

$$\begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} \frac{1}{E} & -\frac{\nu}{E} & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & 0 \\ 0 & 0 & \frac{1}{G} \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{bmatrix} \quad (\text{Chapter 5.25})$$

Obviously, this can be written differently if you were to use the tensorial definition of shear strain, but often you will be given the engineering shear strain. However, we know previously how we can change coordinate systems for both stress and strain independently. We can now combine the two and change coordinate systems for both strain and stress as follows:

$$\begin{bmatrix} \epsilon_{11'} \\ \epsilon_{22'} \\ \gamma_{12'} \end{bmatrix} = RTR^{-1}ST^{-1} \begin{bmatrix} \sigma_{11'} \\ \sigma_{22'} \\ \sigma_{12'} \end{bmatrix} \quad (\text{Chapter 5.26})$$

A good exercise is to write out each transformation to see if this indeed makes sense, as you will get several problems where you will have to work out the correct transformation—i.e. no plug and chug in this class, so we will develop some linear algebra intuition.

3D Stress Transformations

Now we have up to this point only been working with stress transformations for plane stress states. But what happens if we have a complex 3D stress state? How do we rotate this and obtain our new stress tensor? What about finding principal stress states? How

about the rotation to obtain principal strain or maximum shear stress? Wow, what great questions—let's get into it right now.

We have to introduce a new transformation matrix in order to deal with complex 3D stress state rotations, which we call Q :

$$Q = \begin{bmatrix} \cos(a) & \cos(b) & \cos(c) \\ \cos(d) & \cos(e) & \cos(f) \\ \cos(g) & \cos(h) & \cos(i) \end{bmatrix} \quad (\text{Chapter 5.27})$$

where a is the angle between 1 and $1'$, b is the angle between 1 and $2'$, c is the angle between 1 and $3'$, d is the angle between 2 and $1'$, e is the angle between 2 and $2'$, f is the angle between 2 and $3'$, g is the angle between 3 and $1'$, h is the angle between 3 and $2'$, and i is the angle between 3 and $3'$.

So in general we can transform to our new stress tensor in the new coordinate system as follows:

$$\sigma' = Q^T \sigma Q \quad (\text{Chapter 5.28})$$

where Q^T is the transpose of this transformation matrix.

Now you have all the tools to transform stress and strain for virtually every scenario, so I am excited to see what I write for your problem set...

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Chapter 6: Anisotropic Linear Elasticity

Anisotropic Linear Elasticity

Thus far we have been working with a very specific subset of materials—those being isotropic, linear, elastic, cubic materials. Whew... that is a lot of caveats! And as you know, many materials that we work with do not fall under this category, most notably composite materials, which are becoming increasingly critical and ubiquitous in both the aerospace and automotive industries due to the push toward materials with a high stiffness or strength-to-density ratio, which saves on fuel costs.

But before we get into cool composite mechanics, let's start and look at some very general expressions for how to still utilize our elastic constitutive relationships to determine stress from strain or vice versa. This is a critical point: we are still in the linear elastic regime. We have not left this regime and will not do so until our plasticity lecture.

Now we have hinted at a very complex relationship and have introduced it in a slightly different form previously, but again I want to introduce our simple version of Hooke's Law for uniaxial tension:

$$\sigma = E\epsilon \quad (\text{Chapter 6.1})$$

But now, for complex stress states, we treat stress and strain as second rank tensor properties, $\bar{\sigma}$ and $\bar{\epsilon}$. And if we want a relationship between two second rank tensors we have to introduce another tensor to be consistent with linear algebra to relate the two, and that tensor essentially stands in for our Young's modulus. It is referred to as our stiffness tensor C and our compliance tensor S , and we have the relationship that $S = C^{-1}$.

We can see our general relationships below:

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl} \quad (\text{Chapter 6.2})$$

$$\epsilon_{ij} = S_{ijkl}\sigma_{kl} \quad (\text{Chapter 6.3})$$

As you can see, this will get very messy quickly. Instead of our nice and simple stress tensor that we were working with previously that we assumed to be isotropic and cubic and having only 6 independent components, the full anisotropic fourth rank stiffness and compliance tensors have 81 independent elastic components. Now, typically for almost every material this will not be the case—there will be symmetries that reduce this number drastically.

We can also reduce it further right now by remembering the convenient relationships that reduced the number of independent components in our stress and strain second rank tensors to 6. Remembering this, we can make a quick change in notation where we have:

We can make a quick change in notation where we have:

$$\sigma_{11} = \sigma_1 \quad (\text{Chapter 6.4})$$

$$\sigma_{22} = \sigma_2 \quad (\text{Chapter 6.5})$$

$$\sigma_{33} = \sigma_3 \quad (\text{Chapter 6.6})$$

$$\sigma_{23} = \sigma_4 \quad (\text{Chapter 6.7})$$

$$\sigma_{13} = \sigma_5 \quad (\text{Chapter 6.8})$$

$$\sigma_{12} = \sigma_6 \quad (\text{Chapter 6.9})$$

Before we move on to strain, it is critical at this point that we stop and say that here σ_1 is not the maximum principal stress—it is literally just σ_{11} . So again, be very careful with notation here, develop an intuition and understanding for why we are using these equations, and do not plug and chug. That will be critical for your future success as an engineer well beyond this course.

We can also do something similar for strain as well:

$$\epsilon_{11} = \epsilon_1 \quad (\text{Chapter 6.10})$$

$$\epsilon_{22} = \epsilon_2 \quad (\text{Chapter 6.11})$$

$$\epsilon_{33} = \epsilon_3 \quad (\text{Chapter 6.12})$$

$$\gamma_{23} = 2\epsilon_{23} = \epsilon_4 \quad (\text{Chapter 6.13})$$

$$\gamma_{13} = 2\epsilon_{13} = \epsilon_5 \quad (\text{Chapter 6.14})$$

$$\gamma_{12} = 2\epsilon_{12} = \epsilon_6 \quad (\text{Chapter 6.15})$$

With this we can now write out the most general relationship, and it should be noted that once we make this change we are no longer working with a tensor but a matrix, since we changed our directional notation. So now our relationship becomes:

$$\epsilon_i = S_{ij}\sigma_j \quad (\text{Chapter 6.16})$$

or equivalently:

$$[\epsilon] = [S][\sigma] \quad (\text{Chapter 6.17})$$

Now, just by making this change from tensor to matrix we have gone from 81 components in our compliance tensor to a 36-component matrix, so our math has become much simpler.

Now if we expand this expression for the most general anisotropic material, we would have:

$$\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{21} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{31} & S_{32} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{41} & S_{42} & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & S_{53} & S_{54} & S_{55} & S_{56} \\ S_{61} & S_{62} & S_{63} & S_{64} & S_{65} & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} \quad (\text{Chapter 6.18})$$

However, we must remember that we had previously shown that our stress and strain tensors were symmetric due to our static equilibrium conditions (i.e., the sum of forces and moments must equal zero). With this symmetry in our stress and strain tensors—and the fact that we can have no hysteresis in our strain energy density (see full proof in Roylance, *Constitutive Equations*)—we can write that $S_{ij} = S_{ji}$.

$$\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{12} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{13} & S_{23} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{14} & S_{24} & S_{34} & S_{44} & S_{45} & S_{46} \\ S_{15} & S_{25} & S_{35} & S_{45} & S_{55} & S_{56} \\ S_{16} & S_{26} & S_{36} & S_{46} & S_{56} & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} \quad (\text{Chapter 6.19})$$

So we have reduced from 81 to 21 independent components, and this is the compliance matrix that will hold true for the most anisotropic material possible—i.e., a triclinic structure.

But we can reduce this even more by invoking Onsager's theorem, which states that materials cannot exhibit properties of higher symmetry than that of the material itself. In other words, depending on the symmetry of the material, some of these constants could disappear. Note: for a more complete discussion of Onsager, read Sam Allen's **Kinetics of Materials**—the best description that I have come across.

For example:

- Triclinic materials: have all 21 independent coefficients
- Monoclinic materials: have 13 independent coefficients
- Orthorhombic/orthotropic materials: have 9 independent coefficients (examples include wood, composite laminate, and semi-crystalline polyethylene)
- Tetragonal materials: have 7 independent coefficients
- Cubic materials: have 3 independent coefficients, which can be reduced to 2 if the material is isotropic

Before going into this let's prove that we will only have 2 independent components for isotropic cubic linear elastic materials. Remember for cubic materials ($a=b=c$ and $\alpha = \beta = \gamma = 90^\circ$ for cubic) you will find that there are only \textbf{2} independent elastic constants E and ν as we have worked with previously.

But let's break this down piece by piece to determine what each of these compliance components are. Let's start with assuming that we only apply σ_1 then we know that we should obtain the following expression our Hooke's Law

$$\epsilon_1 = S_{11}\sigma_1 \quad (\text{Chapter 6.20})$$

thus we find that

$$S_{11} = \frac{1}{E_1} \quad (\text{Chapter 6.21})$$

You can do a similar proof to find that

$$S_{22} = \frac{1}{E_2}, \quad S_{33} = \frac{1}{E_3} \quad (\text{Chapter 6.22})$$

If we were also to apply pure shear for example only σ_4 then we would get the following expression

$$\epsilon_4 = S_{44}\sigma_4 \quad (\text{Chapter 6.23})$$

and thus

$$S_{44} = \frac{1}{G_{23}} \quad (\text{Chapter 6.24})$$

and similarly

$$S_{55} = \frac{1}{G_{13}}, \quad S_{66} = \frac{1}{G_{12}} \quad (\text{Chapter 6.25})$$

However we also know previously that if we apply a tension stress in one direction the material will contract in transverse directions due to volume conservation and Poisson's ratio thus we also know that if we only apply σ_1 then for the strain in the 2 direction

$$\epsilon_2 = S_{21}\sigma_1 \quad (\text{Chapter 6.26})$$

and in general to define Poisson's ratio we have

$$\nu_{ij} = -\frac{\epsilon_j}{\epsilon_i} \quad (\text{Chapter 6.27})$$

where ϵ_j is the transverse strain and ϵ_i is the direction of the applied stress so with this we have that

$$S_{21} = -\frac{\nu_{12}}{E_1} \quad (\text{Chapter 6.28})$$

and similarly we will find that

$$S_{31} = -\frac{\nu_{13}}{E_1}, \quad S_{32} = -\frac{\nu_{23}}{E_2} \quad (\text{Chapter 6.29})$$

and we also know that $S_{ij} = S_{ji}$ so we know that

$$S_{12} = S_{21}, \quad -\frac{\nu_{12}}{E_1} = \frac{\nu_{21}}{E_2} \quad (\text{Chapter 6.30})$$

and you can derive the others similarly. Now the question becomes what about S_{14} , S_{15} , and S_{16} ? These components attempt to relate normal strain to shear stress and we know previously that all such stresses should be zero, but note that there are times for woven fabrics they may have non-zero values so it can depend on the material but typically these will be zero as shear stresses shouldn't generate normal strains.

Additionally for components like S_{45} , S_{46} , and S_{56} which attempt to relate shear strain in one plain to shear stress in another plain these will also typically be zero. So in general we should expect a matrix to look as follows

$$\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{bmatrix} = \begin{bmatrix} \frac{1}{E_1} & -\frac{\nu_{21}}{E_2} & -\frac{\nu_{31}}{E_3} & 0 & 0 & 0 \\ -\frac{\nu_{12}}{E_1} & \frac{1}{E_2} & -\frac{\nu_{32}}{E_3} & 0 & 0 & 0 \\ -\frac{\nu_{13}}{E_1} & -\frac{\nu_{23}}{E_2} & \frac{1}{E_3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G_{23}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G_{13}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G_{12}} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} \quad (\text{Chapter 6.31})$$

Now for cubic materials the Young's modulus does not vary as a function of direction and the same holds for the shear modulus, as well as the Poisson's ratio so we get for cubic materials that

$$\begin{bmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{12} & S_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{44} \end{bmatrix} \quad (\text{Chapter 6.32})$$

and for isotropic materials we remember that we have the following relationship between Young's Modulus and the shear modulus which is

$$G = \frac{E}{2(1 + \nu)} = \frac{1}{2(S_{11} - S_{12})} \quad (\text{Chapter 6.33})$$

So we can re-write the matrix to be a function of two constant for linear elastic isotropic cubic materials

$$\begin{bmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{12} & S_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(S_{11} - S_{12}) & 0 & 0 \\ 0 & 0 & 0 & 0 & 2(S_{11} - S_{12}) & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(S_{11} - S_{12}) \end{bmatrix} \quad (\text{Chapter 6.34})$$

Well that is great but what about for materials with lower symmetries? Let's dive into how our compliance matrix looks like for orthorhombic/orthotropic materials, just a reminder you can look up orthorhombic crystal structure or you can see that orthotropic materials will have 9 independent elastic constants as seen below

$$\begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ S_{12} & S_{22} & S_{23} & 0 & 0 & 0 \\ S_{13} & S_{23} & S_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{66} \end{bmatrix} \quad (\text{Chapter 6.35})$$

There is also an interesting subset of materials that also exhibit transversely isotropic symmetry, i.e. the material will be isotropic in one plane (for this example assume the 1-2 plane is isotropic) and will have \textbf{5 independent elastic constants}, one such of example of these materials are extruded materials.

$$\begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{13} & 0 & 0 & 0 \\ S_{13} & S_{13} & S_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(S_{11} - S_{12}) \end{bmatrix} \quad (\text{Chapter 6.36})$$

We can re-write this here because we know that

$$\frac{1}{G_{12}} = \frac{2(1 + \nu_{12})}{E_1} = 2(S_{11} - S_{12}) \quad (\text{Chapter 6.37})$$

We have been very general thus far but one of the most common anisotropic materials that you will encounter are biomaterials and more importantly composites. Let's take a quick detour to discuss these increasingly important materials.

Rotation of Compliance Tensor

We can also develop some rotation matrices to rotate our compliance matrix as well as follows for rotations around the 1 axis for stress and strain respectively to be T_1^σ and T_1^ϵ

$$T_1^\sigma = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & c^2 & s^2 & 2sc & 0 & 0 \\ 0 & s^2 & c^2 & -2sc & 0 & 0 \\ 0 & -sc & sc & c^2 - s^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & c & -s \\ 0 & 0 & 0 & 0 & s & c \end{bmatrix} \quad (\text{Chapter 6.38})$$

and

$$T_1^\epsilon = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & c^2 & s^2 & sc & 0 & 0 \\ 0 & s^2 & c^2 & -sc & 0 & 0 \\ 0 & -2sc & 2sc & c^2 - s^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & c & -s \\ 0 & 0 & 0 & 0 & s & c \end{bmatrix} \quad (\text{Chapter 6.39})$$

Also we now that to transform to a new coordinate system

$$\sigma' = T_1^\sigma \sigma^o \quad (\text{Chapter 6.40})$$

and

$$\epsilon' = T_1^\epsilon \epsilon^o \quad (\text{Chapter 6.41})$$

so we get that

$$\epsilon^o = S^o \sigma^o \quad (\text{Chapter 6.42})$$

and

$$\epsilon' = S' \sigma' \quad (\text{Chapter 6.43})$$

Now we get that

$$S' = T_1^\epsilon S^o (T_1^\sigma)^{-1} \quad (\text{Chapter 6.44})$$

And for the 2 axis:

$$T_2^\sigma = \begin{bmatrix} c^2 & 0 & s^2 & 0 & -2sc & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ s^2 & 0 & c^2 & 0 & 2sc & 0 \\ 0 & 0 & 0 & c & 0 & s \\ sc & 0 & -sc & 0 & c^2 - s^2 & 0 \\ 0 & 0 & 0 & -s & 0 & c \end{bmatrix} \quad (\text{Chapter 6.45})$$

and

$$T_2^\epsilon = \begin{bmatrix} c^2 & 0 & s^2 & 0 & -sc & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ s^2 & 0 & c^2 & 0 & sc & 0 \\ 0 & 0 & 0 & c & 0 & s \\ 2sc & 0 & -2sc & 0 & c^2 - s^2 & 0 \\ 0 & 0 & 0 & -s & 0 & c \end{bmatrix} \quad (\text{Chapter 6.46})$$

And for the 3 axis:

$$T_3^\sigma = \begin{bmatrix} c^2 & s^2 & 0 & 0 & 0 & 2sc \\ s^2 & c^2 & 0 & 0 & 0 & -2sc \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & c & -s & 0 \\ 0 & 0 & 0 & s & c & 0 \\ -sc & sc & 0 & 0 & 0 & c^2 - s^2 \end{bmatrix} \quad (\text{Chapter 6.47})$$

and

$$T_3^\epsilon = \begin{bmatrix} c^2 & s^2 & 0 & 0 & 0 & sc \\ s^2 & c^2 & 0 & 0 & 0 & -sc \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & c & -s & 0 \\ 0 & 0 & 0 & s & c & 0 \\ -2sc & 2sc & 0 & 0 & 0 & c^2 - s^2 \end{bmatrix} \quad (\text{Chapter 6.48})$$

Composite Mechanics

Composite materials are materials that contain typically more than one type of material combined. This typically involves a material matrix which is the major component in terms of volume fraction. This matrix material is reinforced by an additional material typically one that is stiffer or tougher than the matrix material. The material that reinforces the matrix can be in particle form, fibers, or precipitates. A composite can also be a porous material like metal foams, concrete, ECM, etc.

Let's take a look at a particle reinforced composite that is composed of a matrix which has some elastic modulus, E_m , and volume fraction, f_m . There is also the particle reinforcement in this case which again has an associated elastic modulus, E_p , and volume fraction f_p . Thus the total composite modulus, $E_{\text{composite}}$, is:

$$E_{\text{composite}} = E_m f_m + E_p f_p \quad (\text{Chapter 6.49})$$

Empirically, there is typically a constant that is less than 1 for the particle reinforcement contribution, but again that constant can only be found empirically.

[Figure: Composites pulled in the transverse or longitudinal/axial direction.]

Let's now look at a fiber reinforced composite that is pulled or stressed in the transverse direction with respect to the longitudinal or axial direction of the fibers. The stresses are the same on the matrix and the fibers. However, the strains of the fiber and matrix will be different. With these constraints:

$$\sigma_m = \sigma_f = \sigma \quad (\text{Chapter 6.50})$$

$$\epsilon_c = \epsilon_m f_m + \epsilon_f f_f \quad (\text{Chapter 6.51})$$

$$\epsilon_c = \sigma \left(\frac{f_m}{E_m} + \frac{f_f}{E_f} \right) \quad (\text{Chapter 6.52})$$

$$\frac{1}{E_c} = \frac{f_f}{E_f} + \frac{f_m}{E_m} \quad (\text{Chapter 6.53})$$

If we instead pull parallel to the fiber longitudinal or axial direction, the strain is the same but now the stresses will be different for the fibers and the matrix. With those constraints we get:

$$\sigma_c = \sigma_f f_f + \sigma_m f_m \quad (\text{Chapter 6.54})$$

$$\epsilon_c = \epsilon_m = \epsilon_f \quad (\text{Chapter 6.55})$$

$$\sigma_c = E_f \epsilon_f + E_m \epsilon_m \quad (\text{Chapter 6.56})$$

$$E_c = E_f f_f + E_m f_m \quad (\text{Chapter 6.57})$$

We can see the difference in the Young's modulus in both of these directions as a function of volume fraction in the plot below:

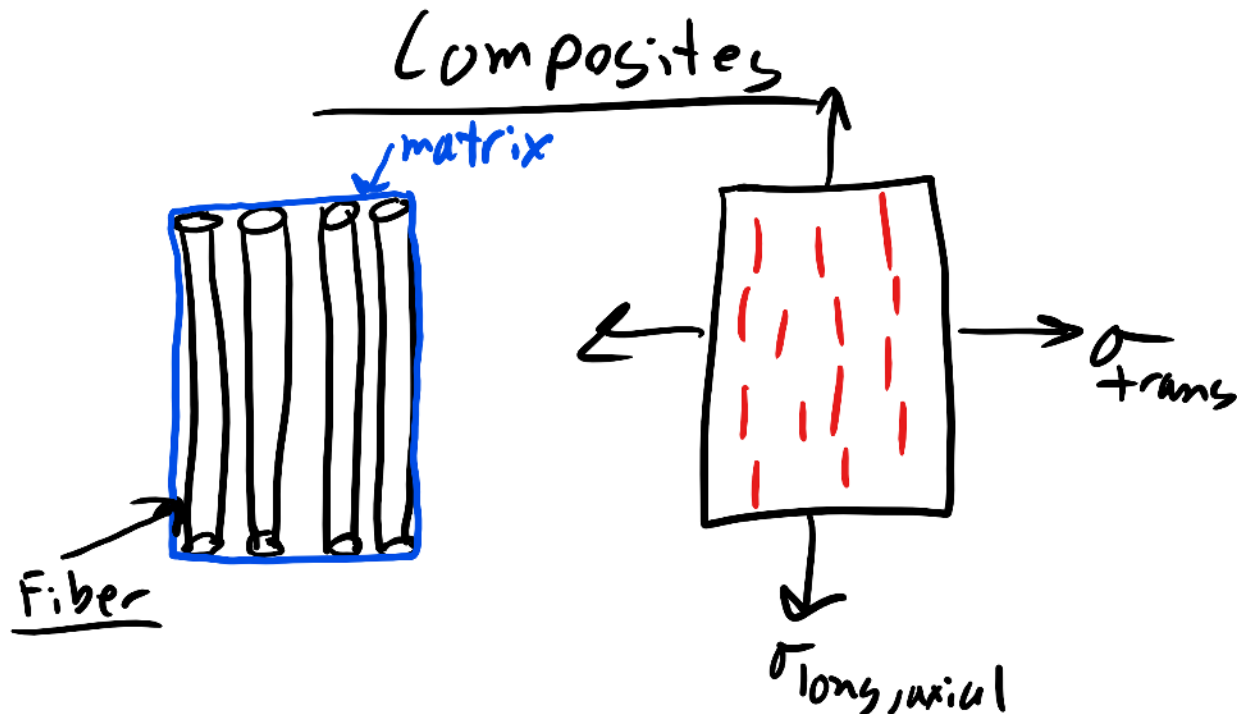


Figure Chapter6.1: Composite modulus as a function of fiber fraction.

Transversely Isotropic Composite

Let's go a bit further and do an example of a composite or laminate that is transversely isotropic (i.e. $E_{33} = E_{22} \neq E_{11}$).

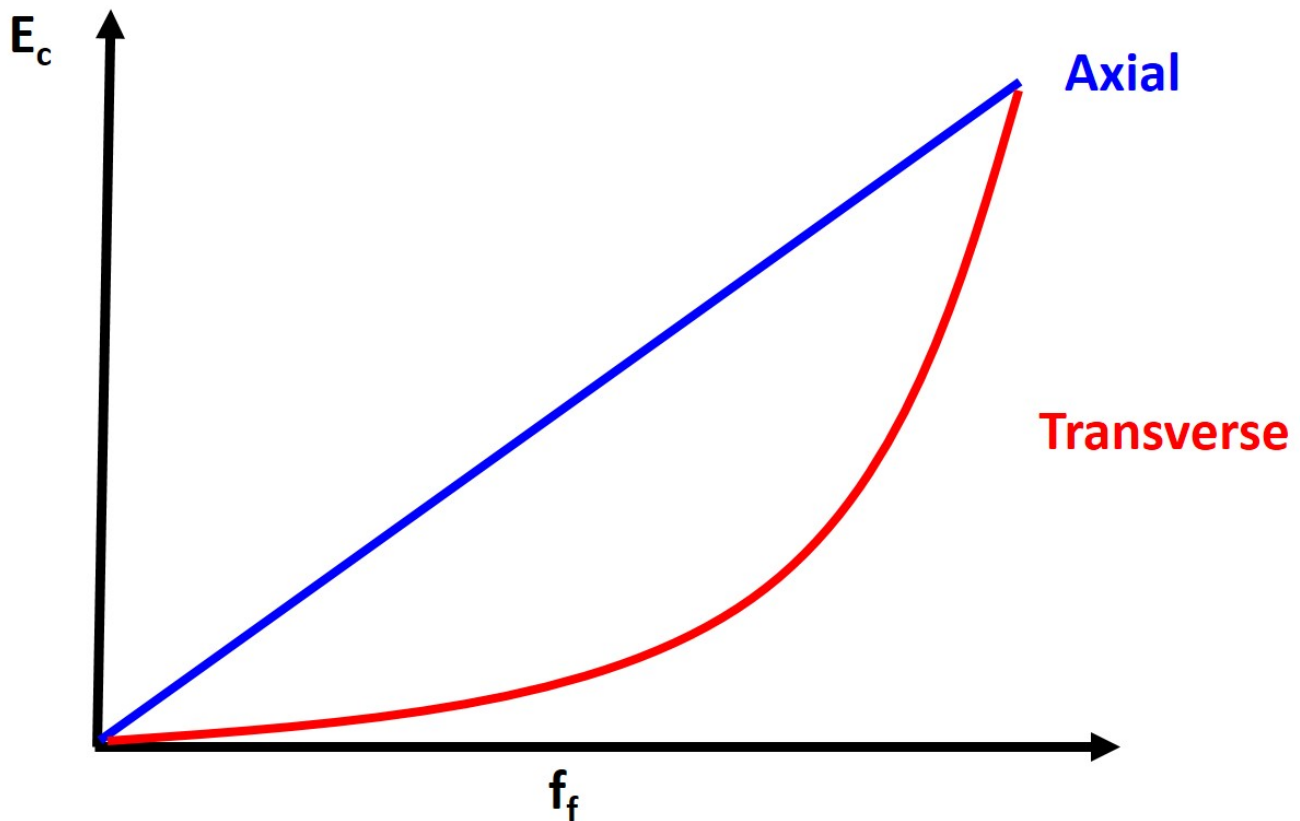


Figure Chapter6.2: Schematic of a fiber composite.

In this scenario our compliance and stiffness matrices would look like this:

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{C_{11}-C_{12}}{2} \end{bmatrix} \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{bmatrix} \quad (\text{Chapter 6.58})$$

or equivalently:

$$\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{bmatrix} = \begin{bmatrix} \frac{1}{E_1} & -\frac{\nu_{21}}{E_2} & -\frac{\nu_{31}}{E_2} & 0 & 0 & 0 \\ -\frac{\nu_{12}}{E_1} & \frac{1}{E_2} & -\frac{\nu_{32}}{E_2} & 0 & 0 & 0 \\ -\frac{\nu_{13}}{E_1} & -\frac{\nu_{23}}{E_2} & \frac{1}{E_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G_{12}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G_{23}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G_{13}} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} \quad (\text{Chapter 6.59})$$

We can see from this that as a result we will have that $\epsilon_4 = \epsilon_5 = 0$. We also know that from our conditions of tensor symmetry:

$$\frac{\nu_{21}}{E_2} = \frac{\nu_{12}}{E_1} \quad (\text{Chapter 6.60})$$

$$\frac{\nu_{13}}{E_1} = \frac{\nu_{31}}{E_2} \quad (\text{Chapter 6.61})$$

$$\frac{\nu_{23}}{E_2} = \frac{\nu_{32}}{E_2}$$

(Chapter 6.62)

Now a typical scenario for composites will be when they are placed under plane stress conditions, and we can then simplify our matrix and only focus on the in-plane stress and strains where we now have:

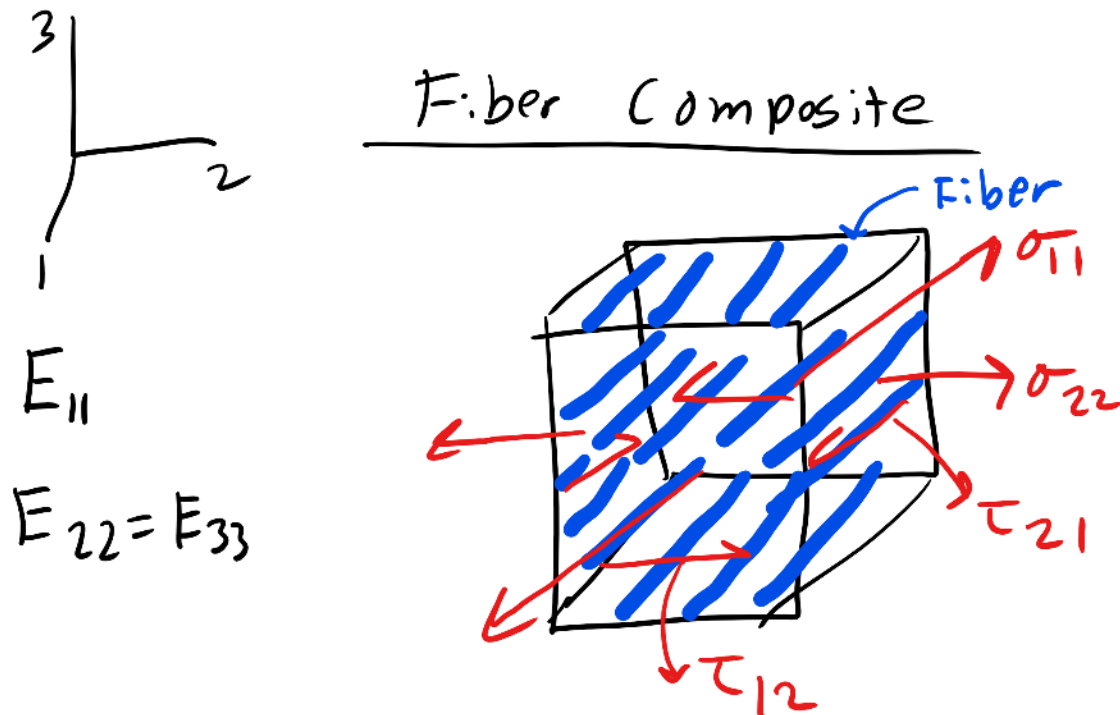


Figure Chapter6.3: Plane Stress Conditions of Composite.

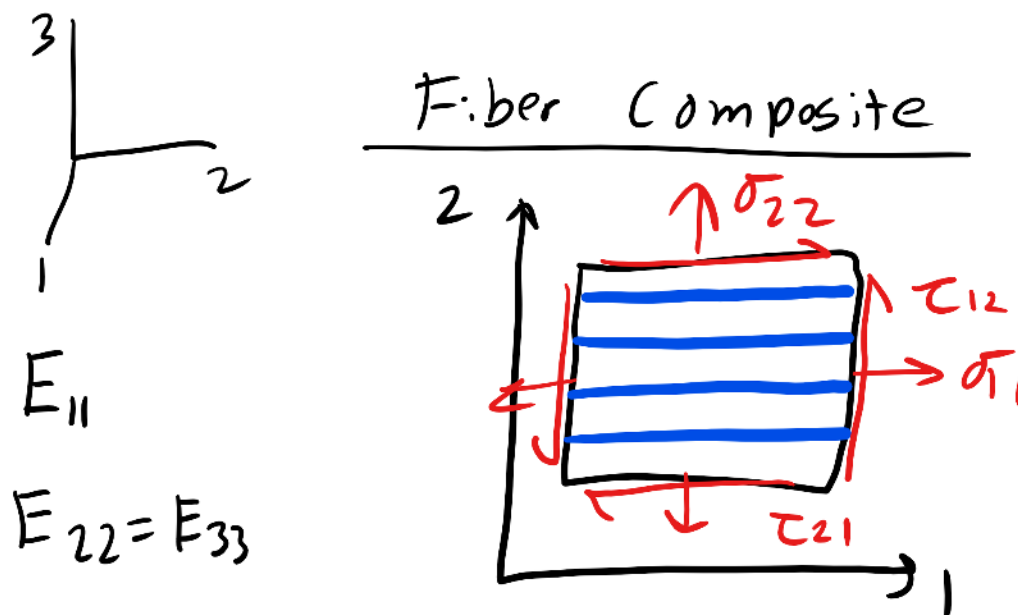


Figure Chapter6.4: Plane Stress Conditions of Composite (alternate view).

$$\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ 0 \\ 0 \\ 0 \\ \epsilon_6 \end{bmatrix} = \begin{bmatrix} \frac{1}{E_1} & -\frac{\nu_{21}}{E_2} & -\frac{\nu_{31}}{E_2} & 0 & 0 & 0 \\ -\frac{\nu_{12}}{E_1} & \frac{1}{E_2} & -\frac{\nu_{32}}{E_2} & 0 & 0 & 0 \\ -\frac{\nu_{13}}{E_1} & -\frac{\nu_{23}}{E_2} & \frac{1}{E_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G_{12}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G_{23}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G_{13}} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} \quad (\text{Chapter 6.63})$$

or more visually appealing:

$$\begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \gamma_{12} \end{bmatrix} = \begin{bmatrix} \frac{1}{E_1} & -\frac{\nu_{21}}{E_2} & 0 \\ -\frac{\nu_{12}}{E_1} & \frac{1}{E_2} & 0 \\ 0 & 0 & \frac{1}{G_{12}} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_{12} \end{bmatrix} \quad (\text{Chapter 6.64})$$

This is great, but this only applies if we are pulling along the principal axes. How can we express the properties of this material when stressed along arbitrary directions with respect to the principal axes? Well, we will use linear algebra!

We have previously seen in the elasticity lecture how to rotate stresses and strains in relation to Mohr's circle, and we can do the same thing here. We will use our same rotation matrices, transformation matrix T , as previously defined, and we can obtain stress after an arbitrary rotation:

$$\begin{bmatrix} \sigma_{x'} \\ \sigma_{y'} \\ \sigma_{xy'} \end{bmatrix} = [T] \begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_{xy} \end{bmatrix} \quad (\text{Chapter 6.65})$$

For strain, again we have to deal with this factor of 2 in relating shear strain, so first we have to account for $\epsilon_{12} = \frac{\gamma_{12}}{2}$. Therefore, we have to introduce another matrix, the Reuter Matrix (R) as previously defined. So to convert to a rotated coordinate system:

$$\begin{bmatrix} \epsilon_{x'} \\ \epsilon_{y'} \\ \gamma_{xy'} \end{bmatrix} = RTR^{-1} \begin{bmatrix} \epsilon_x \\ \epsilon_y \\ \gamma_{xy} \end{bmatrix} \quad (\text{Chapter 6.66})$$

Now we can finally determine the strain at an arbitrary rotation for a transverse isotropic polymer composite or laminate, which can be seen below when we combine these expressions:

$$\begin{bmatrix} \epsilon_{x'} \\ \epsilon_{y'} \\ \gamma_{xy'} \end{bmatrix} = RTR^{-1}ST^{-1} \begin{bmatrix} \sigma_{x'} \\ \sigma_{y'} \\ \sigma_{xy'} \end{bmatrix} \quad (\text{Chapter 6.67})$$

You can take this composite mechanics a bit further and discuss layered composites. A great discussion—but one that involves a considerable amount of linear algebra knowledge—is given by Roylance, so please feel free to look this up and perhaps it may inspire a unique project... Mathematica anyone?

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Chapter 7: Linear Viscoelasticity

Linear Viscoelasticity (LVE)

So far we have dealt with continuum isotropic linear elasticity and anisotropic linear elasticity. All these modes of deformation are independent of time, rate, and temperature. However, today we will discuss linear viscoelasticity whose deformation is governed by time, rate, and temperature. Linear viscoelasticity is the deformation between that of an elastic solid and a viscous fluid. We can actually see this in the name linear viscoelasticity. There is still a linear relationship between stress and strain for a given time and temperature. The "visco" term denotes a time component and "elasticity" denotes reversibility. The elastic solid will again behave Hookean with the relationship:

$$\sigma = E\epsilon \quad (\text{Chapter 7.1})$$

and the viscous fluid will be governed by this new equation:

$$\sigma = \eta \dot{\epsilon} \quad (\text{Chapter 7.2})$$

Most of you are likely familiar with the concept of viscosity (peanut butter is more viscous than water) and have likely encountered this in a fluid mechanics or heat transfer class. And while you might not have been familiar with the equation above, you may be more familiar with the following equation:

$$\tau = \eta \frac{d\gamma}{dt} \quad (\text{Chapter 7.3})$$

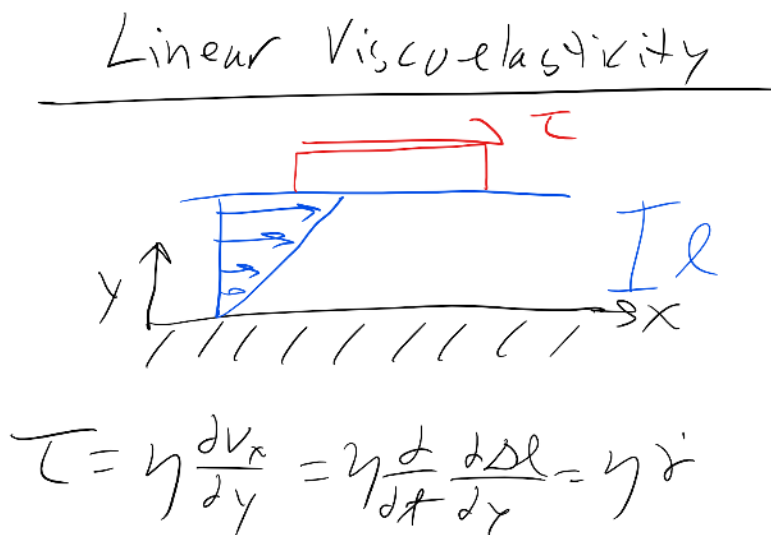


Figure Chapter7.1: Fluid under shear.

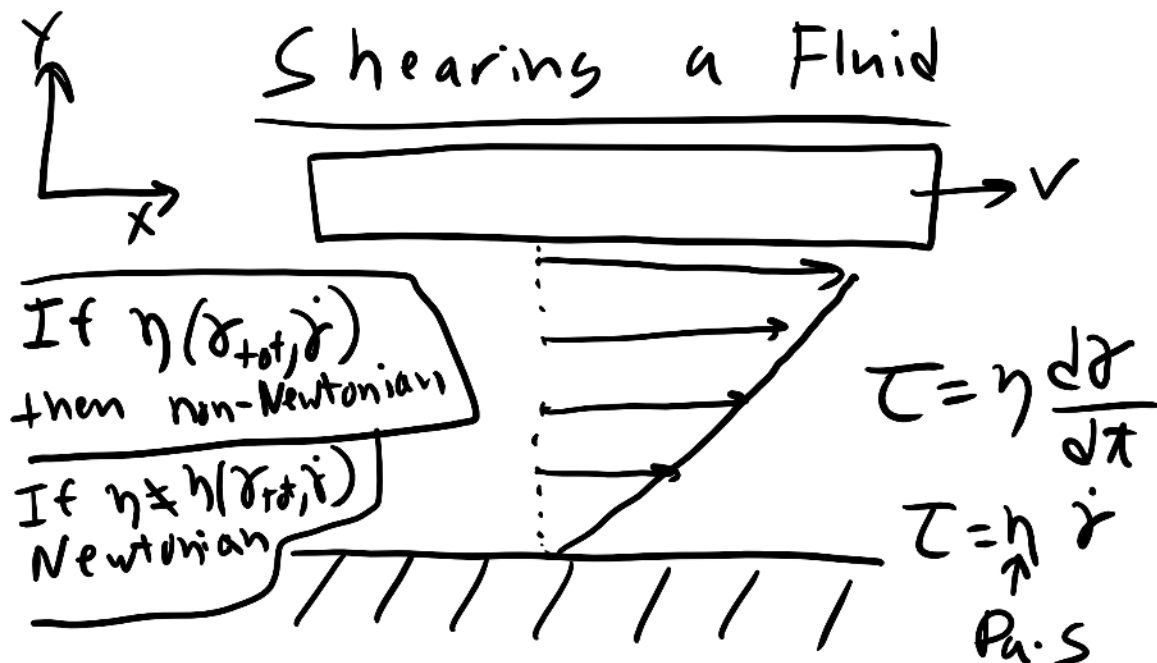


Figure Chapter7.2: Shearing a Fluid.

where τ is shear force, η is viscosity, and $\frac{d\gamma}{dt}$ is strain rate. Note that you can write this expression and re-derive it by considering the velocity profile as a function of y for a channel of length l , and you would obtain:

$$\tau = \eta \frac{\partial v_x}{\partial y} = \eta \frac{\partial}{\partial t} \frac{\partial \Delta l}{\partial y} = \eta \frac{\partial \epsilon}{\partial t} \quad (\text{Chapter 7.4})$$

You can think of this equation in the context of a channel filled with some fluid. When you apply a shear force to one plate, the plate will apply a shear force to the liquid. You'll notice that this equation has a very similar form to Hooke's law, but we replace strain with strain rate and Young's modulus with viscosity. We see that the faster the strain rate, the larger the resistive shear force, and the larger the viscosity, the larger the shear force. This makes sense, as pulling a plate through water is easier than pulling it through peanut butter. At very slow strain rates the shear force goes to zero, which is a property of liquids, whereas solids can be approximated as having infinite viscosity so they will not flow.

Thus if this were a liquid deformed under an applied shear stress there is no recovery when the shear stress is removed. But here this is linear because there is a proportional increase in σ and $\frac{d\gamma}{dt}$ for some time or temperature. You can see this scenario schematically shown here.

When the viscosity is independent of strain rate or total strain, as is the case above, that material is Newtonian. Polymers, however, are typically non-Newtonian, i.e. viscosity is not a constant quantity but is dependent on strain rate or total strain. We can see an example in one of my favorite YouTube videos in the lecture slides. However, linear viscoelasticity is typically used to describe the mechanical response for polymers, glasses, tissues, and cells.

There are other types of interesting materials where the viscosity changes. For example, thixotropic materials will exhibit a decrease in viscosity as fluid flows—paints and fluidized granular beds are such examples. Rheopectic materials are those where viscosity will increase as the fluid flows, i.e. blood or printer ink.

Additionally, viscosity is yet another example of a material property that exhibits an Arrhenius temperature dependence:

$$\eta = \eta_0 e^{\frac{Q}{RT}} \quad (\text{Chapter 7.5})$$

So we can clearly see here how the mechanical behavior of linear viscoelastic (LVE) materials is governed by both time and temperature, a common theme which will reappear over and over again.

Actually, let's take a step back and explore this concept a little bit by looking at one of the most common types of materials that behaves viscoelastically—those being polymers and other soft matter.

Time-Temperature Equivalence of Polymeric Materials

There is a well-defined difference in the Young's modulus between glassy, amorphous polymers and rubbery elastic polymers. Furthermore, we know that there is a temperature dependence for the Young's modulus. Below the T_g the modulus is very high, while at higher temperatures the modulus falls to that of a rubber. This relationship is typically drawn on a $\log(E)$ vs. $\log(T)$ plot where the several order of magnitude difference between the glassy and rubbery moduli is clear.

Polymer Mechanical Behavior vs Temp

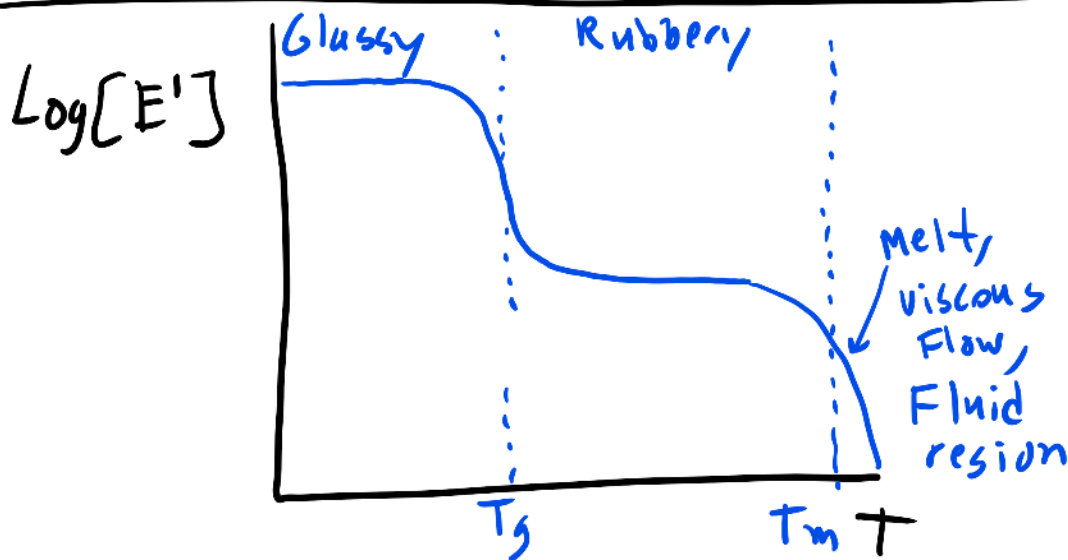


Figure Chapter7.3: Polymer Stiffness vs. Temperature.

Time - Temp - Equivalence

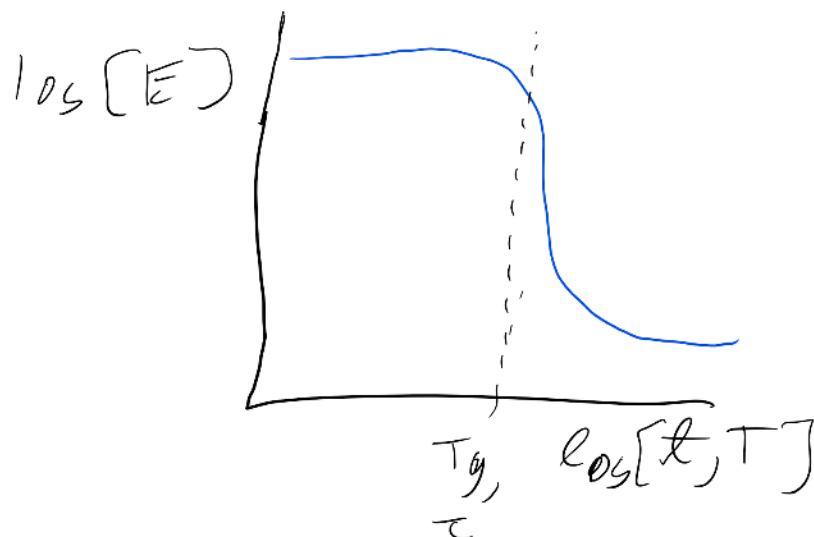


Figure Chapter7.4: Time-temperature equivalence.

One other thing that must be noted is that at high temperatures, strictly amorphous polymers will have moduli that fall to zero; only crosslinked rubbers will maintain a non-zero modulus at high temperatures that is relatively invariant compared to the change between the amorphous and rubbery moduli. If there are no crosslinks, the polymer will simply flow irreversibly.

Polymer Mechanical Behavior vs Temp

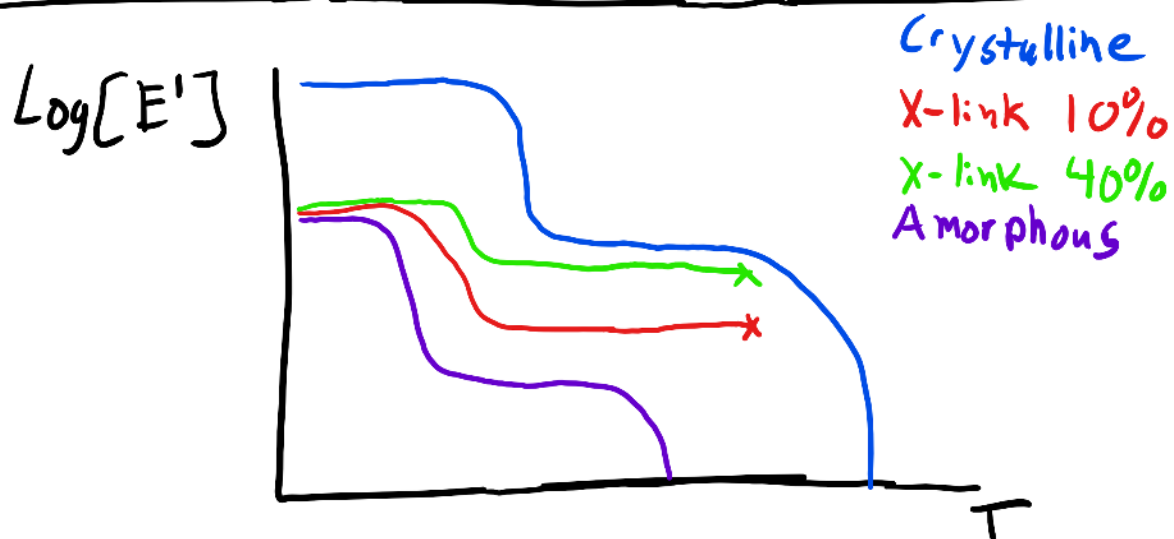


Figure Chapter7.5: Crystalline, Amorphous, and Cross-Linked Polymeric Stiffness vs. Temperature.

Now, if we remember back to the discussion of the glass transition, we said that the onset of glassy behavior is really due to the change in the characteristic relaxation time of a polymer, and how that relaxation time compares to the experimental time associated with a given stress effect. The glass transition would then be interpreted as changing the relaxation time with temperature, which molecularly could be understood as providing more (or less) thermal energy to overcome barriers to flow. However, we also said that if you change the timescale of the perturbation (e.g. deform a polymer really fast) you could obtain glassy behavior even without changing the temperature. This information leads us to believe that the modulus of a polymer is also time dependent, a fact that is borne out empirically. In fact, the graph of $\log(E)$ vs $\log(T)$ is qualitatively the same as the plot of $\log(E)$ vs. $\log(\text{time})$, reflecting the origin of the glass transition.

In addition to changing the value of the Young's modulus, changing the timescale or temperature of an experiment can qualitatively change the shape of a stress-strain curve as well. For example, heating up a brittle, glassy polymer sample will decrease the Young's modulus but also increase the ductility of the sample, allowing longer elongations and more plastic deformation. There is thus a ductile-to-brittle transition where the polymer switches from undergoing stable plastic deformation (necking) to brittle failure; the exact temperature depends on the rate of testing and vice versa.

Finally, note that semi-crystalline polymers are characterized by a degree of crystallinity, which reflects the relative proportion of amorphous to crystalline regions. We would imagine that these regions could have very different moduli, especially above the glass transition temperature, and thus would expect the modulus to depend highly on the degree of crystallinity. This is indeed the case, and the modulus of semi-crystalline polymers has been observed to increase by a factor of over 100 as the degree of crystallinity increases. At low degrees of crystallinity, this change can be regarded as an increase in an effective crosslinking density for the amorphous regions, as the crystalline regions will likely bear very little load themselves. However, as the degree of crystallinity gets higher, the material can be more accurately regarded as a composite of a low modulus material and a high modulus material, a problem that is often treated in materials science.

Glass Transition Temperature

We have just discussed how non-crystalline amorphous polymers can be distinguished from semi-crystalline polymers based on the presence of long-range order. However, another critical parameter that is utilized to describe amorphous polymers is the glass transition temperature (T_g). Typically, non-crystalline polymers can be broadly classified as either rubbery or glassy, both of which exist as highly interpenetrated/entangled Gaussian coils at relatively high temperatures above the glass transition temperature.

When we say interpenetrated, the physical picture is of polymer coils that overlap with each other such that separate coils intertwine with each other. In this highly interpenetrated state, without solvent, the polymer acts as if it is unperturbed—that is, in the melt state the polymer is at the θ condition, and can be treated as an ideal chain. You can think of melt polymers as essentially feeling some pressure due to surrounding polymers that overcomes excluded volume effects, yielding an ideal state. The ideal nature of polymers in the melt make them much easier to think about theoretically.

The glass transition temperature is the temperature at which a polymer transitions from its fluid-like state to a glassy state. When we say a glass, we mean a material with only short-range order but lacking the translational fluctuations associated with liquids. Hence it is like a solid, but with randomly positioned atoms rather than ordered ones as we expect in a crystal. We can identify the physical origin of the glass transition temperature in two different ways—first, you can think of increasing the temperature from below the glass transition, or you can think of decreasing the temperature from above the glass transition temperature. In either case, the glass transition is a competition between the available thermal energy kT and the strength of intermolecular bonds ϵ_{ij} .

If we think of increasing temperature, then the glass transition temperature is the point at which thermal energy is sufficient to break local intermolecular bonds, enabling fluid-like motions—that is, the point where $kT > \epsilon_{ij}$. If we think of decreasing temperature, then the glass transition temperature is the point at which the viscosity of the polymer essentially becomes infinite, eliminating molecular motion. In either case, the key property of a glass is that the rearrangement of atoms is hindered, limiting the ability of the system to relax to equilibrium when a stress or perturbation is applied. This is intimately related to the concept of a characteristic relaxation time, which we will now discuss.

Relaxation Time τ^*

The physical properties of amorphous polymers (and materials in general) are influenced by τ^* , the characteristic relaxation time of the polymer, and how large this relaxation time is relative to a relevant experimental time (or interaction time) t . The relaxation

time is essentially a measure of how long it takes for a material to return to equilibrium after the application of some perturbation. The ratio between the relaxation time and experimental time is called the Deborah number, $De = \frac{\tau^*}{t}$. It is easiest to think of the importance of the relaxation time in terms of known material behavior.

Let's consider as an example a system consisting of some material in a container such that the material is attached to the container walls. We impose a perturbation on the system consisting of moving the walls of the container apart such that the material in the container is deformed or stretched.

First, consider the case that the relaxation time of a material is much smaller than the experimental time, such that $\tau^* \ll t$ and $De \ll 1$. Because the relaxation time is so much lower than the experimental time, the material effectively relaxes instantaneously to the new system dimensions as the perturbation is applied; in other words, the system adjusts to the new constraint by relaxing to equilibrium immediately. Physically, we could imagine this as the material rearranging its constituent molecules to instantaneously fill the new volume of the container—we would say that the material flows, and call the material in the container a liquid.

Now consider the opposite case, where the relaxation time is much greater than the experimental time such that $\tau^* \gg t$ and $De \gg 1$. Now when we adjust the walls of the container, the material effectively never relaxes to equilibrium as the perturbation occurs, instead being driven very far from equilibrium into a high-energy state. In our physical example, we would imagine the material in the container being stretched but being unable to adjust the positions of its atoms because the relaxation time is so long, so that the material instead builds up a large amount of strain energy; we would consider this an elastic response and call the material an elastic solid.

Note that the only distinction we are drawing here between the liquid and solid case is the experimental time—this implies that if we apply a stress or strain to a solid and wait long enough, it would appear to flow like a liquid. In the case of crystalline solids this would be due to the gradual movement of defects throughout the material to change the solid dimensions. In an intermediate regime where the relaxation time is roughly the same as the experimental time, the material will exhibit behavior consistent with both viscous liquids and elastic solids; we call these materials viscoelastic.

We can gain some understanding of relaxation times from the molecular structure of a given material. For example, for small molecules like water, the relatively free motion of water due to its small size would lead to a small relaxation time, and hence water is only solid at low temperatures. Polymers tend to exhibit a longer relaxation time due to the connectivity of monomers, requiring collective motion to adjust to a perturbation. As we will discuss shortly, at lower temperatures the energetic cost for this motion is too great to allow the polymer to flow, leading to glassy behavior. We might also imagine, then, that polymers with more rigid backbones have longer relaxation times due to the lessened flexibility of the chain.

Characterizing a polymer as a rubber, liquid, or solid (glass) is impossible without further information on the overall environment, as the response of the polymer depends on the time scales involved. We will also see that the relaxation time in polymers is a function of temperature, yielding many of the characteristic mechanical properties which we will discuss in future lectures. To wrap up: if the molecular motion is slow or hindered, the relaxation time of the polymer is very long and thus the polymer exhibits solid-like behavior.

Back to Glass Transition Temperature

A key point about the glass transition temperature is that it is not strictly a thermodynamic transition. The melting temperature, for example, results because there is some specific temperature for materials where the free energy of the liquid phase becomes lower than the free energy of the solid phase, leading to melting behavior (and more specifically there is an abrupt change in thermodynamic quantities reflecting a first-order phase transition). Hence, the melting point is thermodynamic in nature, resulting from the competition between the higher entropy liquid phase and lower enthalpy solid phase.

The glass transition, however, is not strictly thermodynamic, as a glass is not a stable thermodynamic phase but rather a kinetically trapped phase resulting from the large energy barriers faced by a glass when it must adjust to a perturbation. The glass transition thus reflects the kinetics and time scales of a system, and as such the transition temperature is not easily defined—in fact, the exact measurement depends on cooling rate, and typically a range of glass transition temperatures are reported for specific samples.

Free Volume Theory of T_g

An explanation for the origin of the glass transition temperature comes from free volume theory. Free volume (not to be confused with excluded volume) is the space in a polymer sample in excess of the volume present in a random, densely packed glass. Free

volume is the volume that monomers in a particular sample are able to access via thermal fluctuations. In a liquid state, we would imagine that the free volume is high, allowing large fluctuations and easy response to perturbations due to the availability of free volume through which monomers can move. By contrast, in the glassy state the free volume is very low and as a result molecular motion is hindered by steric or excluded volume considerations. The free volume is thus:

$$V_F(T) = V(T) - V_0(T) \quad (\text{Chapter 7.6})$$

where V_0 is the volume of a close-packed random glass (0.63), V is the actual volume of the sample, and V_F is the free volume. Note the temperature dependence of each term, which comes from thermal expansion governed by the thermal expansion coefficient:

$$\alpha = \frac{1}{V} \frac{\partial V}{\partial T} \quad (\text{Chapter 7.7})$$

As we gradually increase the temperature the volume available to the system will increase, reflecting increased fluctuations in monomer positions due to more available thermal energy.

Since the thermal expansion coefficient will be different between the glass and fluid states, V_F will increase with increasing temperature because the thermal expansion coefficient in the liquid state α_l is greater than the thermal expansion coefficient α_g in the glassy state (this controls the increase in V_0 with T). We can now write:

$$V_F(T) = V_F(T_g) + (T - T_g) \frac{dV_F}{dT} \text{ for } T > T_g \quad (\text{Chapter 7.8})$$

Dividing by V puts the right side in terms of the difference in thermal expansion coefficients and reduces all volumes to fractions of the total volume:

$$f_F(T) = f_F(T_g) + (T - T_g)(\alpha_l - \alpha_g) \quad (\text{Chapter 7.9})$$

T_g is then defined as the point where this fractional free volume falls below some critical value, and practically speaking can be found by looking at where the slope of the sample volume changes as a function of temperature (reflecting the change in expansion coefficient). Below the critical value, we can imagine the positions of the monomers are frozen due to the low volume available for monomer movements.

By this definition, polymers with greater free volume in the fluid state will experience a lower glass transition temperature, since you will have to decrease the temperature more to reduce the free volume fraction to the critical threshold. Qualitatively, this makes sense since if there is more free volume originally, it requires less thermal energy to access that volume, and so the glass transition temperature will be lower. This observation implies that the glass transition temperature will depend significantly on the molecular structure of the polymer. Finally, it has been shown experimentally that the critical fraction for the glass transition is fairly constant across many different molecules, making this analysis appropriate.

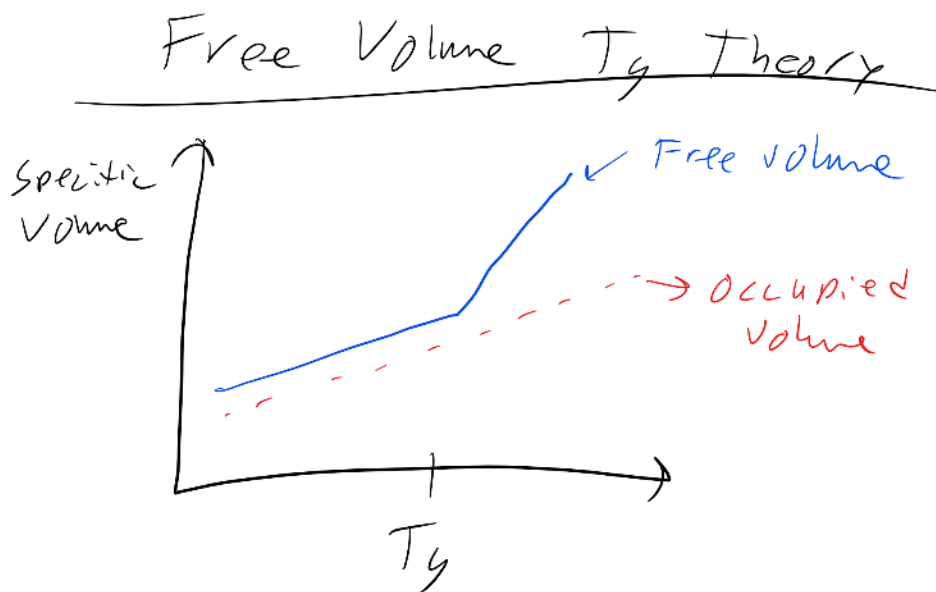


Figure Chapter7.6: Free Volume and T_g .

The glass transition temperature is also dependent on the rate of cooling of the sample. The cooling rate dependence of the glass transition temperature can be explained by what's called percolation. If we imagine the polymer sample superimposed on a lattice, and each lattice point can be thought of as either in the glassy state or fluid state, then the network is percolated when a connected network of glassy points spans the entire lattice. In other words, it is not necessary for the entire polymer sample to be glassy; it is only necessary for connected regions that cross the network to be glassy, since these connections essentially cut off the fluid parts from each other, leading to glassy behavior on the macroscale.

We can think of each lattice point as transitioning between fluid and glassy with some characteristic probability, and can also imagine some other characteristic probability for the point to transition from glassy back to fluid. Physically, this reflects the ability of monomers to move through the available free volume, and hence at lower temperatures we expect the probability of a fluid-to-glass transition to increase, and the probability for a glass-to-fluid transition to decrease as the decreasing free volume favors the glassy state.

As we cool the sample, then, the probability of forming a glass progressively becomes higher, and the time taken for glass points to transition back to fluid takes progressively longer. If we cool at a very fast rate, lattice points will have sufficient time to transition from fluid to glass but not back (since as we cool it takes longer and longer for the glass-to-fluid transition), leading quickly to a percolated network at a high temperature since glassy behavior will be observed as soon as connected glassy regions span the sample. If we cool at a slower rate, a percolated network is more difficult to form because at higher temperatures the relatively short time associated with the glass-to-fluid transition will disrupt the network as it forms. This means that the glass transition will be observed at a lower overall temperature.

T_g and Chemical Structure of Monomers

Trends in T_g can be explained by looking at the chemical structure of monomers due to the influence of monomer structure on both chain flexibility and free volume. Recall that T_g is determined by the onset of long-range cooperative molecular motion, meaning the motion of 10–30 connected chain monomers at once. The cooperative motion requires both sufficient thermal energy to induce the movement of these monomers and sufficient free volume for the monomers to move into. Both of these requirements are influenced by monomer structure. There are essentially three elements of monomer structure that can influence these motions:

1. Chain interactions – energetic interactions between monomers
2. Ease of rotation about main chain bonds – whether there is significant steric hindrance to rotation
3. Amount of free volume available – how densely the monomers pack

We can think of polymers as essentially divided into their backbone and sidechains coming from that backbone. In polymers with flexible backbones, like polyethylene (lots of C–C single bonds) and PDMS (Si–O bonds, which are flexible due to the 4 electrons on the oxygen atoms in place of hydrogens), the hindrance to rotation is low and hence less thermal energy is necessary to induce molecular motion, leading to a low T_g .

On the other hand, polymers with phenyl molecules along the backbone (e.g. polycarbonate) tend to have a much higher T_g , since the bulky phenyl constituent greatly increases the amount of energy necessary for rotation (i.e. the rigidity). Note that we can generally relate C_∞ to the rigidity of a backbone, and hence expect T_g to increase with C_∞ .

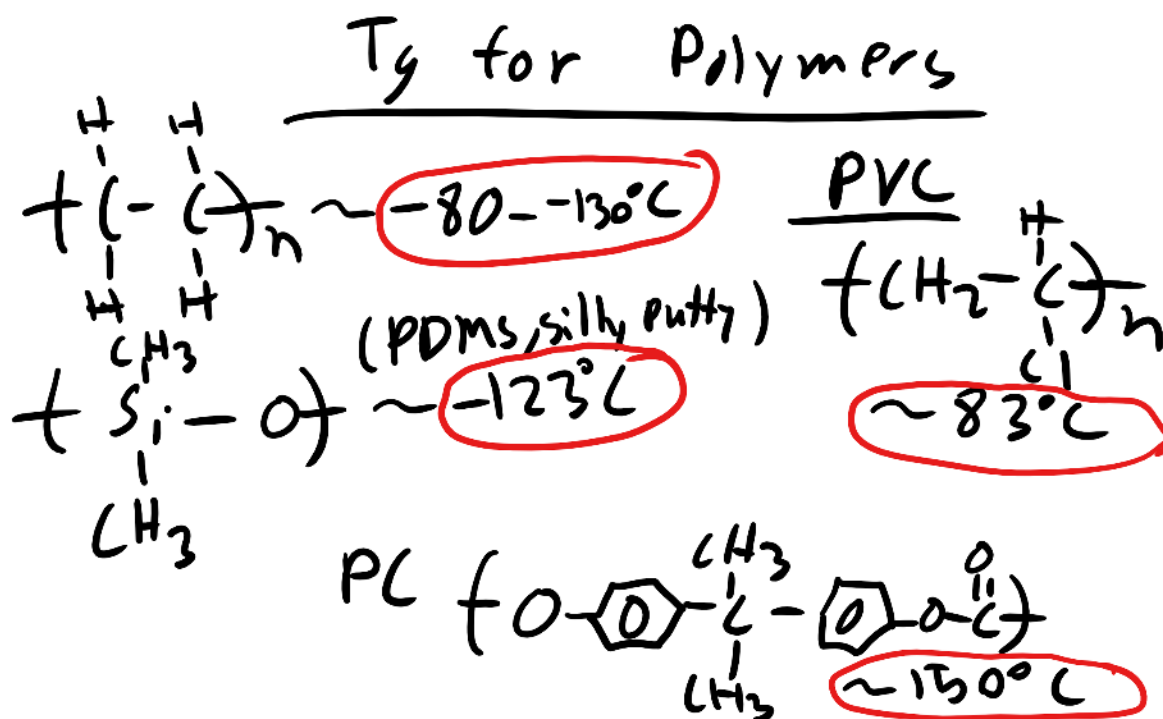


Figure Chapter 7.7: T_g for Various Polymers and Influence of Chain Structure.

Similarly, large bulky sidechains, such as phenyl groups, also oppose rotation due to steric hindrance, and in addition decrease the amount of free volume available since they occupy a greater excluded volume, leading to a higher glass transition temperature. Finally, intermolecular interactions, such as hydrogen bonds or ionic interactions, which are typically seen between sidechains, will tend to greatly increase the glass transition temperature since thermal energy will also have to break these bonds to induce rotation.

The lecture notes provide some examples of polymers, sidechains, and the related T_g values. The main principles to keep in mind are that chain flexibility allows easier cooperative movement of monomers, decreasing the T_g , and increased free volume around the chain backbone lowers the barrier to cooperative movement and hence decreases the T_g .

We can also relate these observations back to the idea of crystallinity, as well, as the factors that influence the glass transition temperature will also influence the ability of polymers to crystallize. In fact, there is a correlation between T_g and T_m for semi-crystalline polymers — typically T_g is about 0.5 to 0.8 T_m in Kelvin.

Spring and Dashpot Models

One of the most common ways to model and conceptualize the idea of linear viscoelasticity and to recreate the mechanical behavior that we just saw is to build spring–dashpot models. The time-dependent mechanical behavior can be represented by a spring–dashpot model. The dashpot is essentially just a plunger in a cylinder of fluid while the spring is essentially a spring.

The mechanical response of the spring is Hookean and represents an elastic response. The spring is described by the following equation:

$$\sigma_s = E_s \epsilon_s \quad (\text{Chapter 7.10})$$

where σ_s is the stress in the spring, E_s is the stiffness of the spring, and ϵ_s is the strain in the spring.

The mechanical response of the dashpot is a viscous, time-dependent response (we are at a constant temperature) and we can describe it as:

$$\sigma_d = \eta_d \dot{\epsilon}_d \quad (\text{Chapter 7.11})$$

where σ_d is the stress in the dashpot, η_d is the viscosity of the dashpot, and $\dot{\epsilon}_d$ is the strain rate of the dashpot.

Now, when we connect these components in series, parallel, or some other combination we can model certain LVE material mechanical behaviors phenomenologically. Let's take a look at one such model, the Maxwell Model.

Maxwell Model

Let's take a look at the Maxwell model, which is a combination of a spring in series with a dashpot that contains a Newtonian fluid.

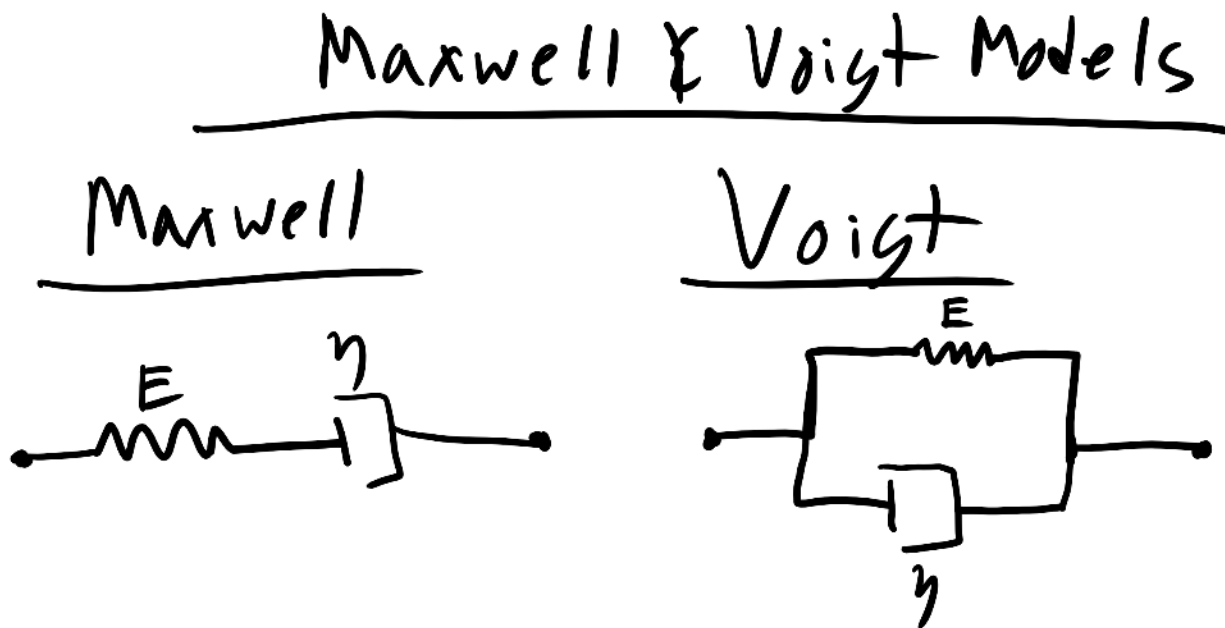


Figure Chapter7.8: Maxwell and Kelvin-Voigt Models for Viscoelasticity.

Now let's say that we stress the system with some applied stress σ_M . In this configuration, the stresses will be the same for the spring and the dashpot as they are arranged in series; however, the strains in the dashpot and the spring will be different, which gives us the following relationships:

$$\sigma_M = \sigma_s = \sigma_d \quad (\text{Chapter 7.12})$$

$$\epsilon_M = \epsilon_s + \epsilon_d \quad (\text{Chapter 7.13})$$

$$\dot{\epsilon}_M = \dot{\epsilon}_s + \dot{\epsilon}_d \quad (\text{Chapter 7.14})$$

$$\dot{\epsilon}_M = \frac{\dot{\sigma}_M}{E} + \frac{\sigma_M}{\eta} \quad (\text{Chapter 7.15})$$

This last expression is the constitutive equation for the Maxwell Model.

With this system we can do two types of experiments: stress relaxation ($\epsilon = \epsilon_0$, i.e. constant strain) and creep ($\sigma = \sigma_0$, i.e. constant stress).

For stress relaxation we can plug into our equation and solve for how the stress in our Maxwell model should vary over time:

$$0 = \frac{1}{E} \frac{d\sigma}{dt} + \frac{\sigma}{\eta} \quad (\text{Chapter 7.16})$$

$$\int_{\sigma_0}^{\sigma} \frac{d\sigma}{\sigma} = \int_0^t \frac{-E}{\eta} dt \quad (\text{Chapter 7.17})$$

$$\sigma(t) = \sigma_0 \exp\left(\frac{-Et}{\eta}\right) \quad (\text{Chapter 7.18})$$

$$\sigma(t) = \sigma_0 \exp\left(\frac{-t}{\tau}\right) \quad (\text{Chapter 7.19})$$

where $\tau = \frac{\eta}{E}$ is the relaxation time. Here we predict that the stress will decay to zero, which is in disagreement with the way many viscoelastic materials behave—they must retain some stress.

Similarly for creep:

$$\frac{d\epsilon}{dt} = 0 + \frac{\sigma_0}{\eta} \quad (\text{Chapter 7.20})$$

$$\int_{\epsilon_0}^{\epsilon} d\epsilon = \int_0^t \frac{\sigma_0}{\eta} dt \quad (\text{Chapter 7.21})$$

$$\epsilon(t) = \epsilon_0 + \frac{\sigma_0 t}{\eta} \quad (\text{Chapter 7.22})$$

This result does not give us the glassy–viscoelastic–rubbery transition we expected to see.

Kelvin-Voigt Model

There is also the Kelvin-Voigt (KV) model, which has the spring and dashpot arranged in parallel.

In this case, the strain is the same, because they are in parallel, but now the stresses are different, so we get:

$$\epsilon_{KV} = \epsilon_s = \epsilon_d \quad (\text{Chapter 7.23})$$

$$\sigma_{KV} = \sigma_s + \sigma_d \quad (\text{Chapter 7.24})$$

$$\sigma_{KV} = E_s \epsilon_s + \eta_d \dot{\epsilon}_d \quad (\text{Chapter 7.25})$$

$$\dot{\epsilon}_{KV} = \frac{\sigma_{KV}}{\eta_d} - \frac{E_s}{\eta_d} \epsilon_{KV} \quad (\text{Chapter 7.26})$$

Again, this last expression is the constitutive equation for the KV model.

Now for stress relaxation we get the final equation for stress versus time as:

$$\sigma(t) = E\epsilon_0 \quad (\text{Chapter 7.27})$$

The KV model is particularly bad here, where the model predicts an infinite spike in stress and then a time-independent stress afterwards.

For creep we get:

$$\epsilon(t) = \frac{\sigma_0}{E} \left[1 - \exp\left(-\frac{t}{\tau}\right) \right] \quad (\text{Chapter 7.28})$$

Here again the KV model does not give a transition from glassy to viscoelastic, and then again to rubbery.

Now, as you can see, the Maxwell and KV models are not very realistic, in particular the stress relaxation for the KV and the creep expression for Maxwell. A better model would be the Standard Linear Solid Model.

Standard Linear Solid Model

You can now build even more complex combinations to model viscoelastic properties, like the Standard Linear Solid Model or Maxwell-Zener Model, which combines both models to better capture the behavior of viscous materials—and there are many more complex models as well to represent the behavior of materials.

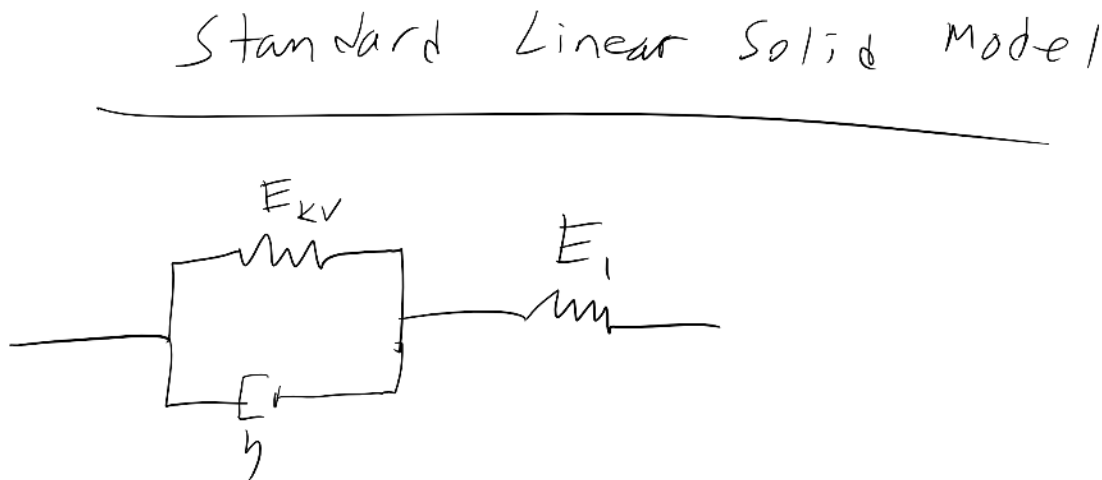


Figure Chapter7.9: Standard Linear Solid Model.

Here we can see that we have a spring in series with our KV model. We know that for parallel components we will add stress and the strains will be equivalent, whereas for series components we will add strains and stresses will be equivalent. So for the total system we will find that:

$$\epsilon_{SLS} = \epsilon_{KV} + \epsilon_1 \quad (\text{Chapter 7.29})$$

$$\sigma_{SLS} = \sigma_{KV} = \sigma_1 \quad (\text{Chapter 7.30})$$

where SLS indicates the entire model, KV indicates the KV arm, and 1 indicates the spring.

Now we can start to write some expressions below:

$$\epsilon_{SLS} = \epsilon_{KV} + \epsilon_1 \quad (\text{Chapter 7.31})$$

$$\epsilon_{SLS} + \epsilon_{SLS} \frac{E_2}{\eta} = \frac{\sigma_{SLS}}{\eta} \left(1 + \frac{E_2}{E_1} \right) + \frac{\sigma_{SLS}}{E_1} \quad (\text{Chapter 7.32})$$

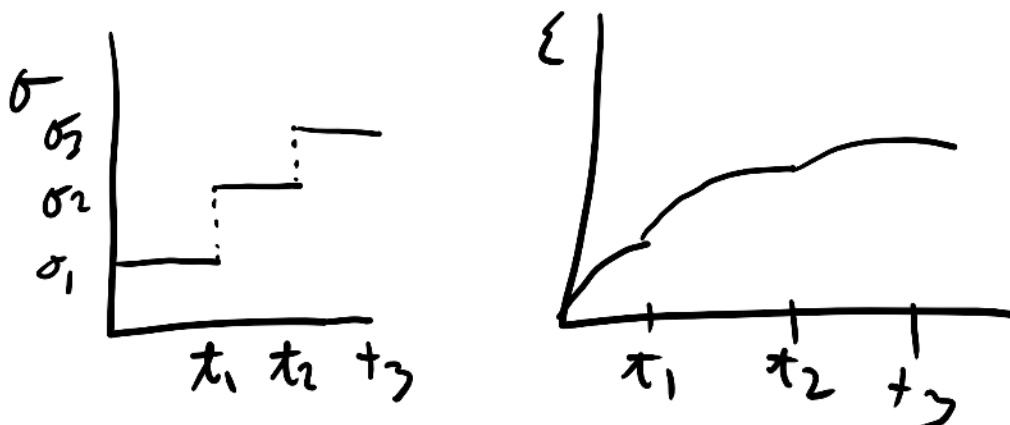
This model is much better, as we obtain an exponential response for both creep and stress relaxation. However, these are just models and give poor numerical results, but the general trends are very consistent. There are infinite models that can be built with increasing complexity, as seen below.

Boltzmann Superposition Principle and Creep Compliance

Another approach that can be taken to modeling creep and stress relaxation is by leveraging the fact that stress and strain are linearly related at a given time and temperature. As this is true, we can use the Boltzmann superposition principle to determine the stress by summing the strain during multiple deformation steps and defining a parameter called the creep compliance $J(t)$, which relates strain to stress as a function of time:

$$\epsilon(t) = J(t)\sigma \quad (\text{Chapter 7.33})$$

Creep Compliance & Boltzmann Superposition



$$\epsilon(t) = \sigma_1 J_1(t-t_1) + (\sigma_2 - \sigma_1) J_2(t-t_2) \dots$$

Figure Chapter7.10: Modeling Strain Using Boltzmann Superposition Principle and the Creep Compliance.

You essentially treat each loading step as making an individual contribution to the final deformation, and you can obtain the final deformation by simply summing each contribution, i.e.:

$$\epsilon(t = t_n) = \Delta\sigma_1(t_n - t_1) + \Delta\sigma_2(t_n - t_2) + \Delta\sigma_3(t_n - t_3) \quad (\text{Chapter 7.34})$$

You can do the same procedure for stress relaxation, but you have to define the stress relaxation modulus $G(t)$.

Dynamic Mechanical Testing

The more utilized characterization technique is instead dynamic mechanical testing to probe the viscoelastic behavior of materials. In this experiment the polymer is subjected to a sinusoidal loading at variable frequencies which can be described as:

$$\sigma_{\text{applied}} = \sigma_0 \sin \omega t \quad (\text{Chapter 7.35})$$

This is the applied stress, but remember we are dealing with a viscoelastic material so there will be a phase lag, δ , in the strain behavior which will also be sinusoidal:

$$\epsilon = \epsilon_0 \sin \omega t \quad (\text{Chapter 7.36})$$

So what we will end up with is that the material will actually experience a stress that contains the phase lag as shown below:

$$\sigma = \sigma_0 \sin(\omega t + \delta) \quad (\text{Chapter 7.37})$$

$$\sigma = \sigma_0 \sin \omega t \cos \delta + \sigma_0 \cos \omega t \sin \delta \quad (\text{Chapter 7.38})$$

Dynamic Mechanical Testing

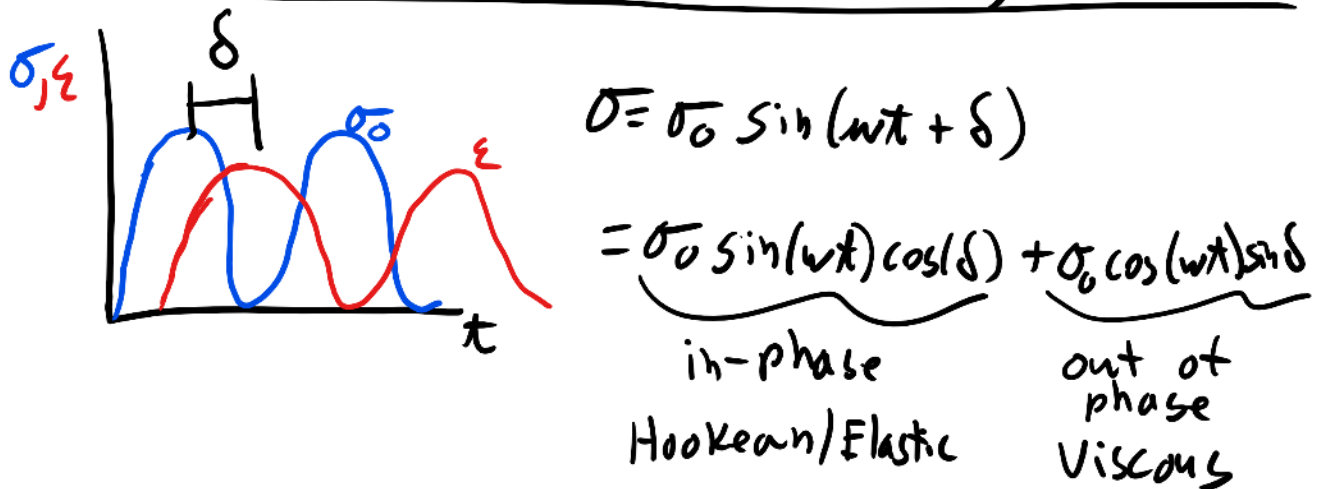


Figure Chapter7.11: Dynamic Mechanical Testing.

In the equation above, the first term represents the component that is in phase with the strain or the elastic response, while the second term represents the out-of-phase behavior or the viscous response. We can then define two elastic moduli to describe the in-phase and out-of-phase behavior. The storage or elastic modulus is the in-phase contribution and is defined as:

$$E' = \frac{\sigma_0 \cos \delta}{\epsilon_0} \quad (\text{Chapter 7.39})$$

and the loss modulus is the out-of-phase component and is defined as:

$$E'' = \frac{\sigma_0 \sin \delta}{\epsilon_0} \quad (\text{Chapter 7.40})$$

We can now re-write our expression for the stress in the material as:

$$\sigma = E' \sin \omega t + E'' \cos \omega t \quad (\text{Chapter 7.41})$$

then by definition we have that:

$$\tan \delta = \frac{E''}{E'} \quad (\text{Chapter 7.42})$$

This is sometimes called the loss tangent and essentially represents the amount of energy lost over the energy stored. You might also see these expressions written using complex variables like so:

$$\epsilon = \epsilon_0 e^{i\omega t} \quad (\text{Chapter 7.43})$$

$$\sigma = \sigma_0 e^{i(\omega t + \delta)} \quad (\text{Chapter 7.44})$$

$$E = \frac{\sigma_0}{\epsilon_0} e^{i\delta} = \frac{\sigma_0}{\epsilon_0} (\cos \delta + i \sin \delta) = E' + iE'' \quad (\text{Chapter 7.45})$$

Analysis of Dynamic Mechanical Testing Experiments

Typically you will find, at a fixed temperature, that the loss tangent and the loss modulus are very small at both very low and very high frequencies and they will typically peak at intermediate frequencies. The storage modulus is high at high frequencies (short times), which should make sense intuitively as polymers will typically behave glassy or elastic at high frequencies and short times (strain rate is faster than the relaxation time of the polymer). At low frequencies (long times, longer than the relaxation time), the polymer will behave more like a viscous fluid.

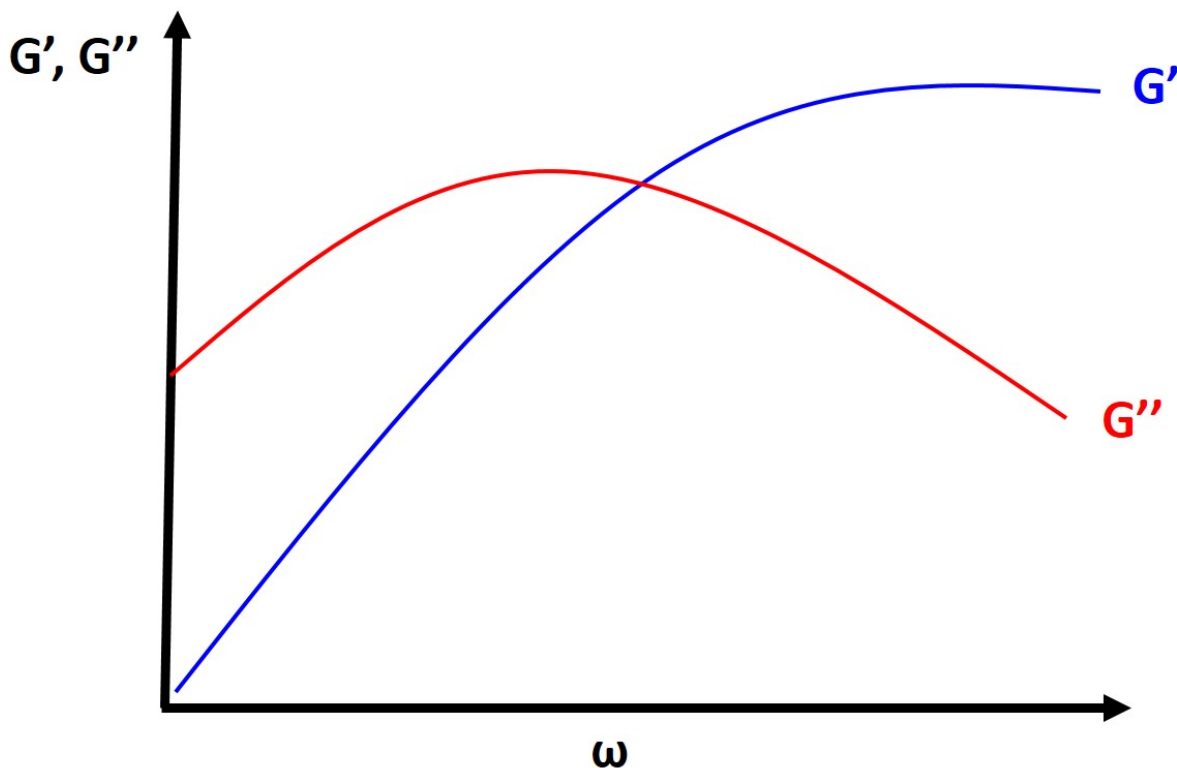


Figure Chapter7.12: Viscoelastic Behavior of Polymers.

More importantly, from this analysis we can determine experimentally the characteristic relaxation time from the point where G' and G'' intersect.

More often we will find that typical DMA experiments plot G' , G'' , and $\tan \delta$ as a function of temperature. Here you will typically see larger peaks and changes in these parameters, as we have already seen that the modulus of polymers is temperature dependent. Alternatively, as we have already discussed at length, the temperature will affect the amount of molecular motion and free volume, which will increase and affect these properties, particularly the loss tangent. So you will expect to see large changes at the glass transition temperature and melting temperature, but you might also expect to see other small peaks associated with secondary transitions (note this is not referring to second-order thermodynamic transitions like T_g , this is just referring to the magnitude of the

peaks) associated with molecular motion of the polymer, such as the temperature at which backbone side group rotation is accessible.

As you can see in the figure, the primary observable and measurable change in the storage modulus occurs when you pass through T_g . However, the more subtle difference in behavior can be found in the variation of the loss tangent as a function of temperature. Here we can see multiple different peaks at different temperatures with varying amplitudes. In these plots each peak is typically labeled α, β, γ , etc., in order of descending temperature. In this graph the α peak or relaxation corresponds to the T_g in an amorphous polymer or it could be T_m for a semi-crystalline polymer. The β peak here corresponds to cooperative motion of segments of the main chain. The γ peak is due to phenyl group rotation around the backbone, and the δ peak has been linked to some wiggling of the phenyl group most likely due to defects or tacticity differences.

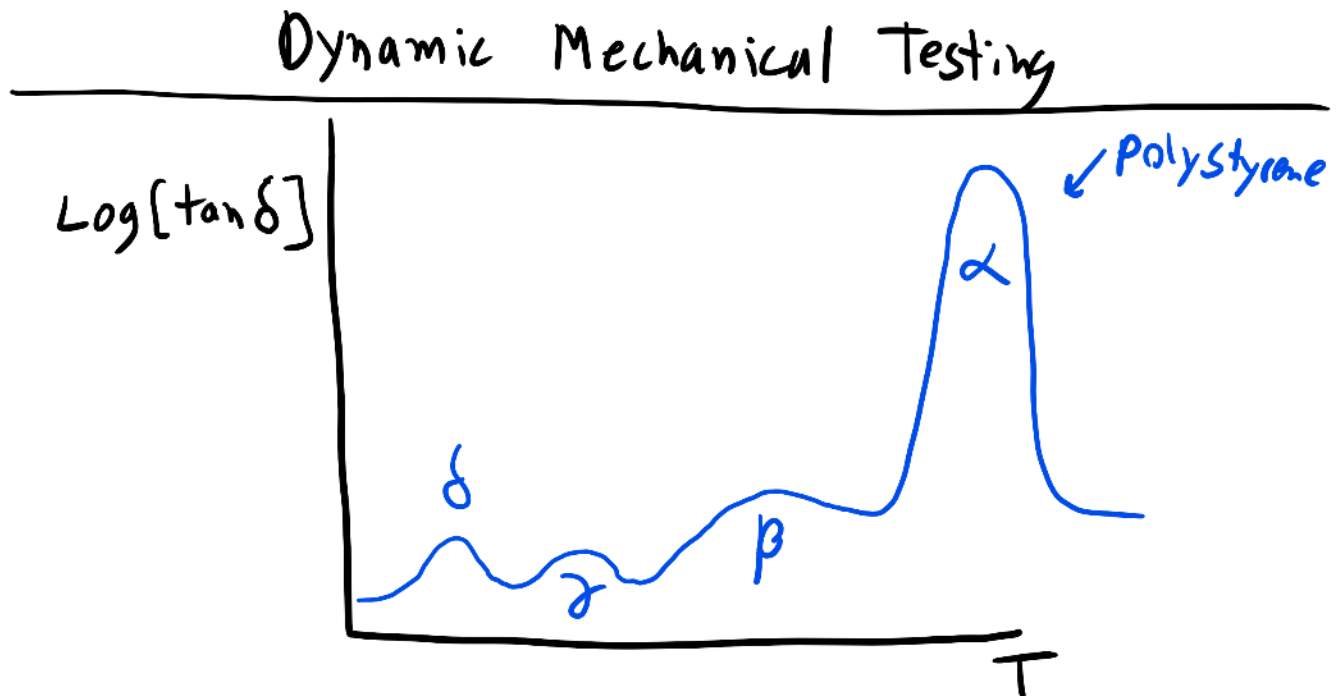


Figure Chapter7.13: DMT Transition Analysis in Polystyrene.

For semi-crystalline polymers this analysis can become even more difficult because of the microstructure of spherulites. This makes it very difficult to separate the amorphous and crystalline behavior. One example of this can be seen for LDPE and HDPE. You can see some similar transitions (i.e. γ) but also stark differences. The primary difference between LDPE and HDPE is the amount of branching, which is much larger in LDPE than in HDPE. Here the α and α' peaks are associated with motion in the crystalline regions, while the γ peak is associated with the amorphous region. Finally, the β relaxation is associated with the motion of the branches.

Now, the analysis of these peaks in polymers is a great source of debate, but when analyzing them just make a reasoned argument thinking about the thermal energy required for a particular type of motion.

Dynamic Mechanical Testing

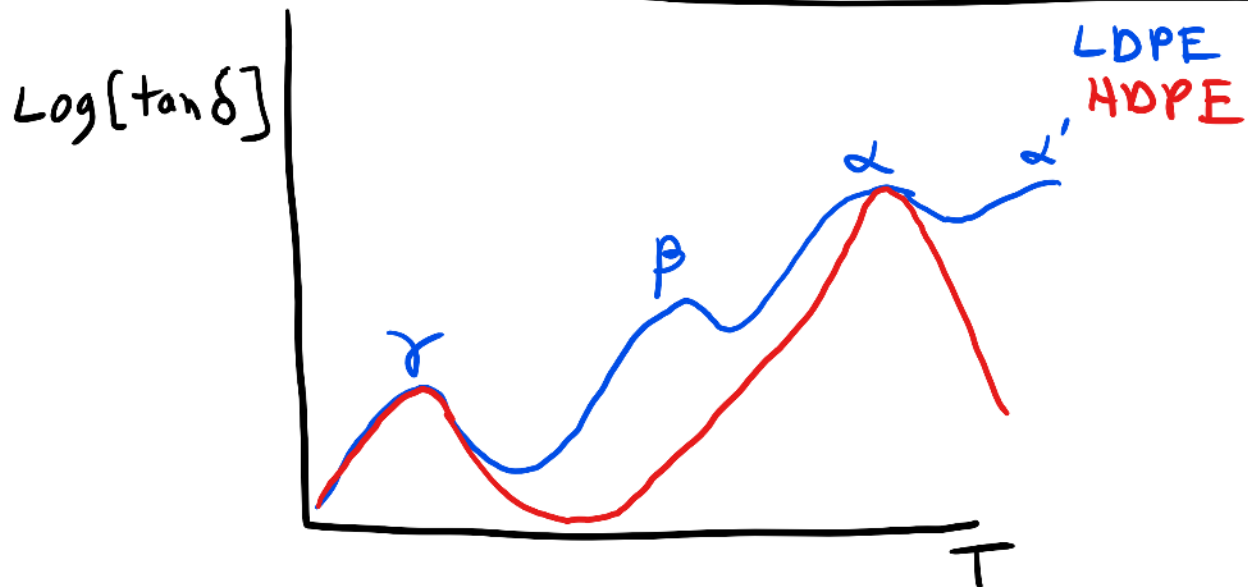


Figure Chapter7.14: DMT Transition Analysis in HDPE and LDPE.

Time-Temperature Equivalence

For viscoelastic polymers there is a theoretical equivalence of time and temperature. We have seen previously that a polymer can exhibit glassy or rubbery behavior by changing either the temperature or the strain rate, i.e. time. So we can establish the principle of time-temperature superposition, or the theoretical equivalence between changing the timescale or temperature of an experiment.

An experimentally derived equation relating these two quantities, known as the WLF equation, was found by noticing that you can superpose curves by keeping one curve fixed and shifting all the others by different amounts horizontally parallel to the logarithmic time axis. We can take a reference temperature point, T_s , and a temperature point, τ_s , in order to fix one curve. We then have to find the τ for a new curve with the same compliance as our reference curve at T_s . The amount of shift will then simply be $\log \tau_s - \log \tau$, which we will define as our shift factor:

$$\log a_T = \log \tau_s - \log \tau = \log \frac{\omega_s}{\omega} \quad (\text{Chapter 7.46})$$

Time Temperature Superposition

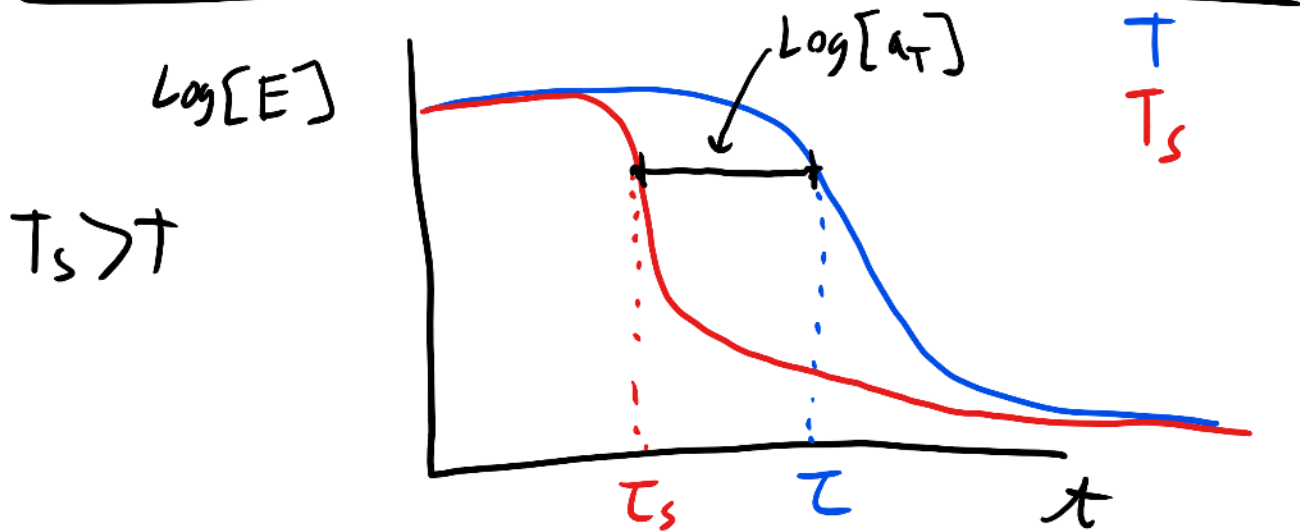


Figure Chapter7.15: WLF Time-Temperature Superposition.

[Figure: WLF Time-Temperature Superposition.]

With this, Williams, Landel, and Ferry (WLF) empirically fit these polymer curves and found the following empirical equation:

$$\log a_T = \frac{-C_1(T - T_s)}{C_2 + (T - T_s)} \quad (\text{Chapter 7.47})$$

where C_1 and C_2 are empirical fitting constants, 17.44 and 51.6 K respectively, if one chooses $T_s = T_g$. This equation was later re-derived using theory based on free volume, akin to the theory for the glass transition, reflecting similar physical origins. The derivation is beyond the scope of this lecture (and you are probably sick of derivations at this point), but you can read it in Young and Lovell, Chapter 5. The resulting equation is:

$$\log a_T = \frac{-(B/2.303f_g)(T - T_g)}{f_g/\alpha + (T - T_g)} \quad (\text{Chapter 7.48})$$

where f_g is the fractional free volume at the glass transition temperature and α is the volumetric thermal expansion coefficient. Typically for polymers, $f_g = 0.025$ and $\alpha = 4.8 \times 10^{-4} \text{ K}^{-1}$. B is another fitting constant.

Limitations of WLF

The WLF equation is applicable to homogeneous, linear viscoelastic materials that are isotropic and amorphous. They must be in the temperature range T_g to $T_g + 100^\circ\text{C}$.

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Chapter 8: Beam Bending, Buckling, and Torsion

Elastic Loading Topics: Bending, Buckling, and Torsion

Before we move into plasticity, we have three elastic loading topics to discuss, and these are still very important and relevant loading states and phenomena: bending, buckling, and torsion respectively.

You have probably already encountered beam bending in other courses and perhaps buckling, but we again are going to take a slightly different approach—specifically approaching this from the materials perspective.

We can define a beam as anything that can carry transverse loads. This can range from typical civil engineering structural applications (bridges, trusses, pool diving boards, etc.) to more exotic applications like Atomic Force Microscopy (AFM), which utilizes a cantilever beam, or thin-film substrates that have thermal mismatch resulting in bending. Other examples include cellular solids like foams, honeycomb structures, tissues, and even sporting equipment like ski poles.

When dealing with beam bending problems, we must consider several things before we start to approach the problem. Specifically, we must consider:

- Support Reactions
- Internal Forces
- Internal Moments
- Internal Stresses
- Deflections
- Support Type: roller, pin, or fixed end

Additionally, different supports will have different reaction forces and moments. For example:

- Roller: Reaction force in the y-direction
- Pin: Reaction force in the x and y directions
- Simple Frictionless Surface: Reaction force in the y-direction
- Fixed Support: Reaction forces in x, y, and a reaction moment

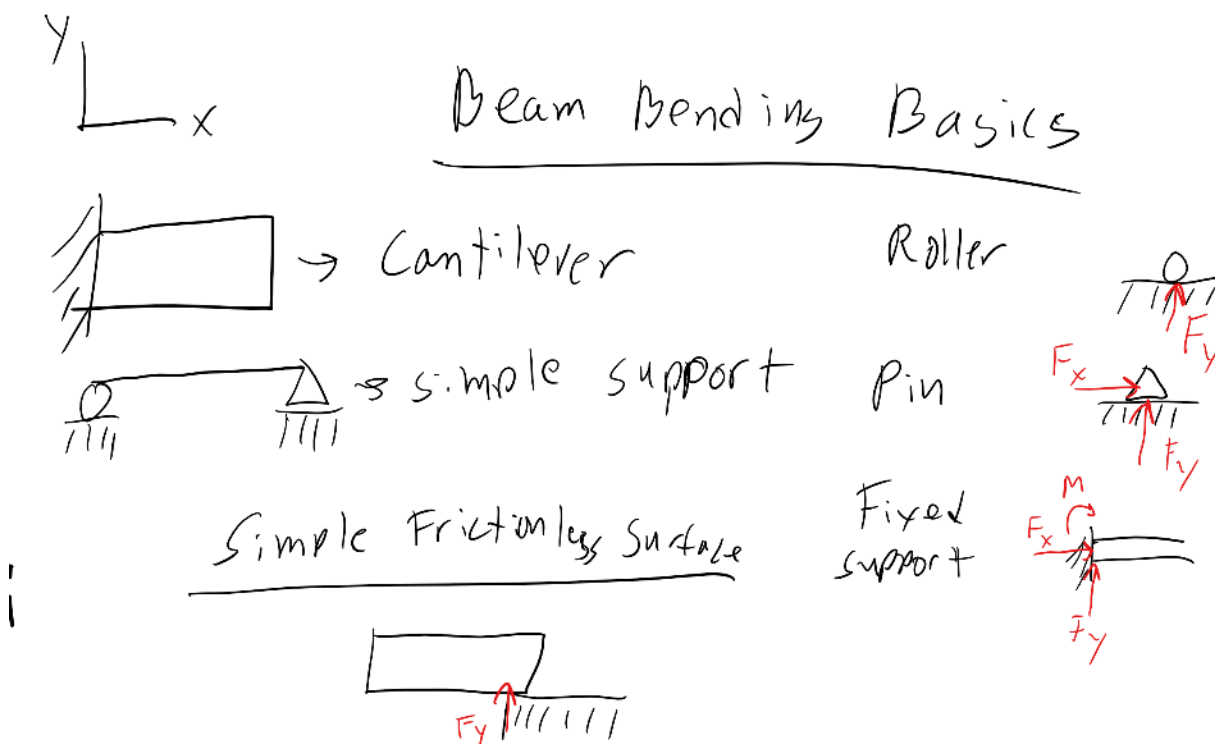


Figure Chapter8.1: Beam bending basics.

Soon we will be working with free body diagrams as well as shear force and moment distributions within structures. Why do we want to do this? We need to find the locations of maximum shear forces and bending moments because material failure will often occur at regions of maximum shear forces (denoted as V) and bending moments (M). These shear forces and bending moments can vary along the length of the beam. Moreover, shear stress depends on the shear forces, whereas normal stresses depend on the bending moment. Finally, the amount of deflection will also depend on the bending moment.

Let's start off with some background on how we will work with beams and support reaction diagrams. This should have been covered in other courses, but let's give ourselves a quick reminder.

Sign Convention and Coordinate System Reminder

Before we get started, let's do one more reminder of our coordinate system and what we will determine as positive and negative forces, shears, and moments.

- Tension will be defined as positive.
- Compression as negative.
- Shear is positive if the force is acting on a face with a normal in the positive direction and also has a force pointed in the positive direction.

For forces, any force which points in the positive direction relative to our coordinate system will be defined as positive. Counterclockwise (CCW) moments are positive, and clockwise (CW) moments are negative.

For beams:

- A positive internal shear force V acts downward on the right-hand face of a beam or upward on the left-hand face of a beam.
- A positive internal bending moment M acts CCW on the right-hand face of the beam and CW on the left-hand face of a beam.

You can also consider a bending moment as positive if tension is on the bottom of the beam and negative if tension is at the top.

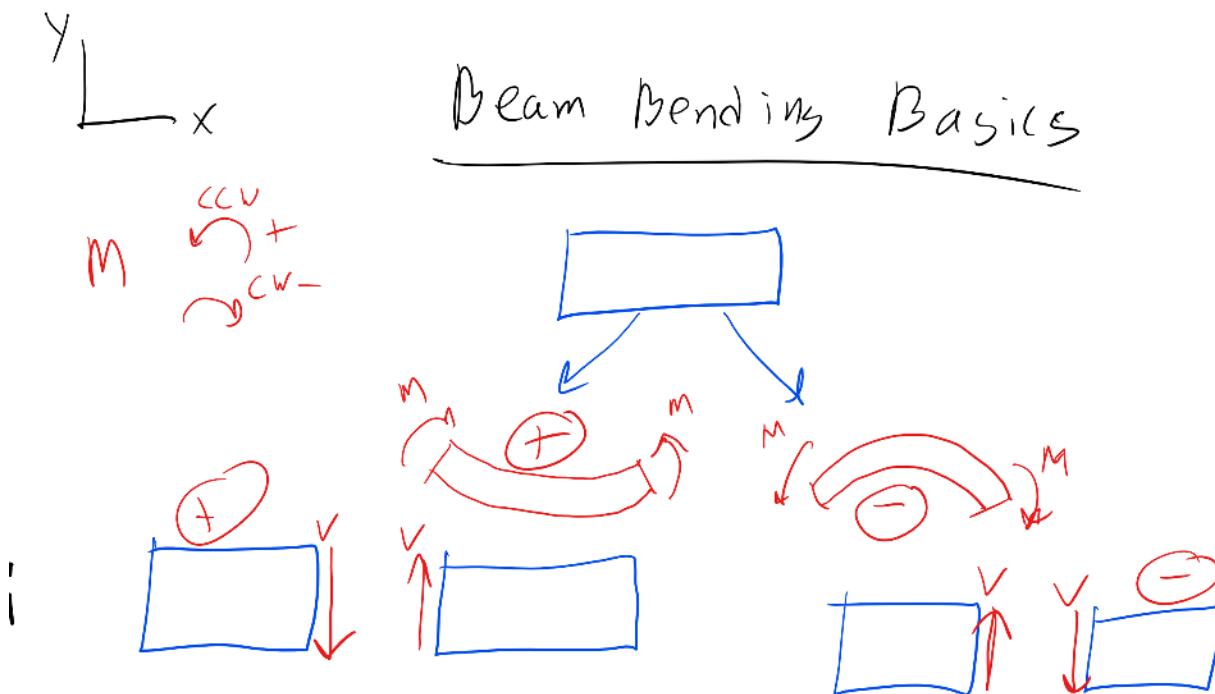


Figure Chapter8.2: Beam bending positive and negative shear forces and moments.

The key point to this entire discussion is that before you approach any mechanics problem, if there is not a coordinate system defined, you must define one before you start anything. Keep this in mind—it will be very important that you double-check this as you approach problems.

Support Reactions in Beams

Let's first consider a fixed-end supported cantilever beam of length l with a load P applied at the end. At the fixed end we will have one reaction force F_y and a reaction moment M_0 .

For virtually all of our beam bending problems we will start as follows to develop our problem-solving framework:

1. Coordinate System
2. Free Body Diagram
3. Equilibrium Expressions
4. Solve for Unknowns

As you can see below we have defined our coordinate system and we have drawn our free body diagram. Now we can apply our equilibrium conditions, remembering that we have:

$$\Sigma F = 0 \quad (\text{Chapter 8.1})$$

$$\Sigma M = 0 \quad (\text{Chapter 8.2})$$

Let's start as we always will and draw the Free Body Diagram (FBD).

So for this scenario we will have the following equilibrium conditions:

$$\Sigma F_y = 0 = -P + F_y \quad (\text{Chapter 8.3})$$

$$\Sigma M_0 = 0 = M_0 - Pl \quad (\text{Chapter 8.4})$$

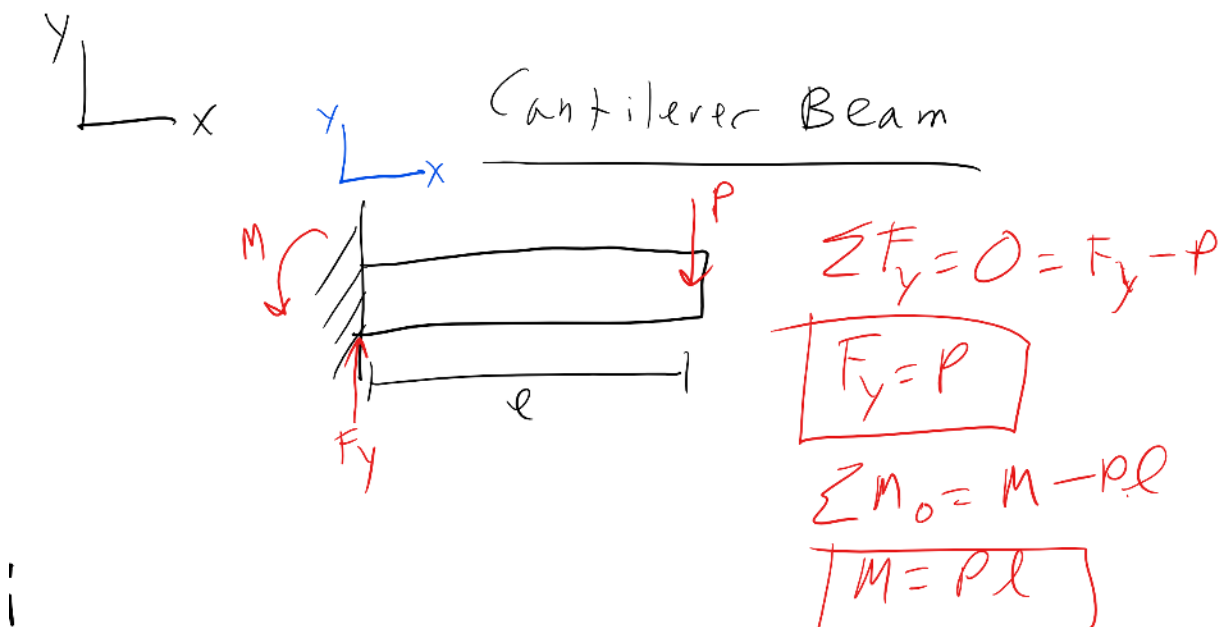


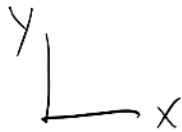
Figure Chapter8.3: Cantilever beam bending reaction forces.

Hopefully that has jogged some memories! Let's do another one of these types of reminder problems with a distributed load on a beam that has a roller support at A and a pin at B. You can see the distributed load as well as a directly applied load. Let's do our static equilibrium problem:

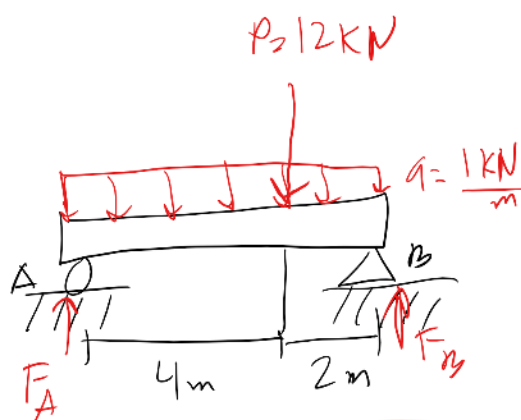
$$\Sigma F_y = 0 = F_A - P - 1 + F_B \quad (\text{Chapter 8.5})$$

$$\Sigma M_A = 0 = F_B(6\text{ m}) - 1 \frac{\text{kN}}{\text{m}} (6\text{ m})(3\text{ m}) - 12 \frac{\text{kN}}{\text{m}} (4\text{ m})$$

(Chapter 8.6)



Simple Supported beam



$$\begin{aligned} \Sigma F_y = 0 &= -1 \frac{\text{kN}}{\text{m}} \cdot 6\text{ m} - 12 \text{ kN} + F_B + F_A \\ \Sigma M_A = 0 &= -12 \text{ kN} \cdot 4\text{ m} + F_B \cdot 6\text{ m} - 1 \frac{\text{kN}}{\text{m}} \cdot 6\text{ m} \cdot 3\text{ m} \end{aligned}$$

$$F_A = 7 \text{ kN} \quad F_B = 11 \text{ kN}$$

Figure Chapter8.4: Simple support beam reaction forces under distributed load.

Fixed-End Support Cantilever Beam with Point Load Applied

Now that we have some of the fundamentals down and we remember them, let's actually go ahead and start with our first shear force diagram $V(x)$ and our bending moment diagram $M(x)$ for an end-loaded cantilever beam that has a fixed-end support.

Let's start as always with our free body diagram (FBD), but we also have some additional steps to our algorithm:

1. Coordinate System
2. Free Body Diagram
3. Equilibrium Expressions
4. Solve for Unknowns
5. Cut beam starting at $x = 0$ right before the first applied load
6. Write equilibrium equations again and then solve for the internal shear moment and bending moment of the beam

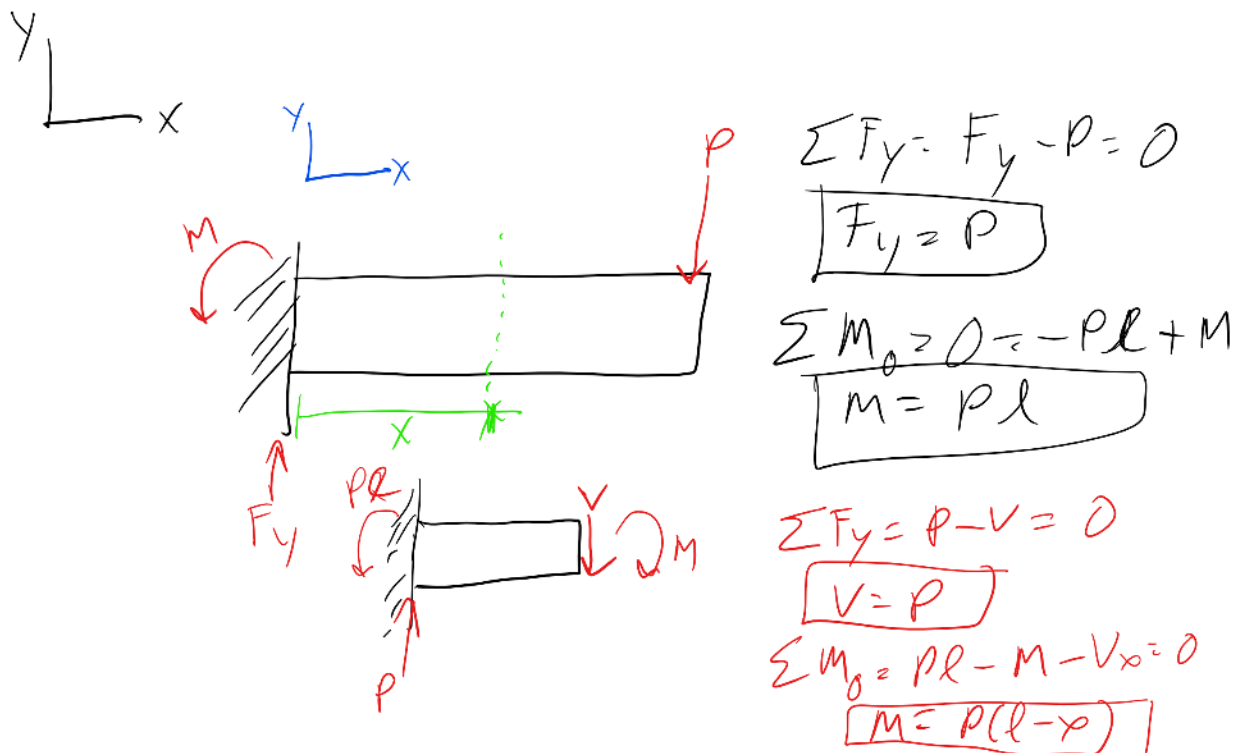


Figure Chapter8.5: Fixed-end supported cantilever beam point load applied.

We have to make a cut along some point x from the fixed-end support of our beam and draw a free body diagram to determine our static equilibrium equations. When we cut our beam, it is often easiest to start with the shear forces before we get into moments.

We know that for a fixed-support beam we will have a reaction force that opposes the load applied at the end, and this will be positive in this system. Additionally, once we make our cut, the internal shear will be negative relative to this applied force.

In terms of moments, we know that we will have a positive moment at our fixed support, and at the end of our cut component/free body diagram we will have a negative internal moment. With this conceptual understanding we can work on our equilibrium expressions and obtain:

$$\sum F_y = 0 = P - V \quad (\text{Chapter 8.7})$$

$$\sum M_x = 0 = Pl - Px - M \quad (\text{Chapter 8.8})$$

and thus we get the equations for our internal shear force and bending moment as a function of x :

$$V(x) = P \quad (\text{Chapter 8.9})$$

$$M(x) = P(l - x) \quad (\text{Chapter 8.10})$$

We can see in our diagram that the shear force is independent of distance along the beam, but the maximum bending moment occurs at the fixed end—as we might have intuitively predicted before this problem. Note that due to our convention, we will state that we have a negative bending moment due to the fact that there is tension at the top of our beam.

Four-Point Bending

Let's do another problem for a very common mechanical test: four-point bending.

Consider the four-point bending scenario below where two loads are applied on a roller and pin support.

As always, let's start with our FBD.

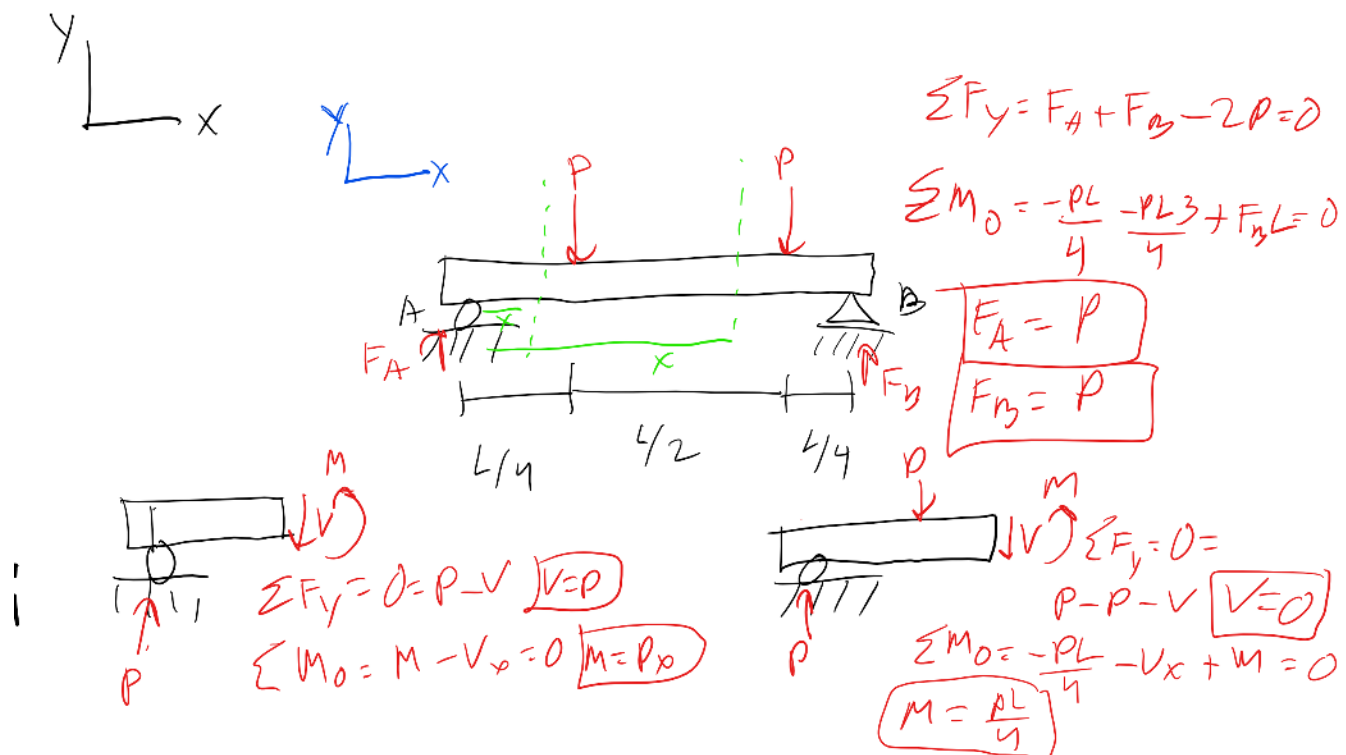


Figure Chapter8.6: Four-point bending test.

Here we are going to have to take two cuts in order to solve this problem. If we look at our first cut near position 1, we will have the following equilibrium conditions:

$$\sum F_y = 0 = P - V \quad (\text{Chapter 8.11})$$

$$\sum M_{x1} = 0 = M - Px \quad (\text{Chapter 8.12})$$

and thus we get the equations for our internal shear force and bending moment as a function of x :

$$V(x) = P \quad (\text{Chapter 8.13})$$

$$M(x) = Px \quad (\text{Chapter 8.14})$$

Note that we do not have a reaction moment at either support. Also, we should recognize the symmetry in this problem, so we only have to make two cuts because everything else is exactly the same.

For our second cut we can see:

$$\sum F_y = 0 = -V + P - P \quad (\text{Chapter 8.15})$$

$$\sum M_{x2} = 0 = M - Px - P\left(x - \frac{l}{4}\right) \quad (\text{Chapter 8.16})$$

and thus we get the equations for our internal shear force and bending moment as a function of x :

$$V(x) = 0 \quad (\text{Chapter 8.17})$$

$$M(x) = \frac{Pl}{4} \quad (\text{Chapter 8.18})$$

Distributed Load on a Beam with Roller and Pin Supports at the Ends

Let's analyze a simply supported beam (roller at A, pin at B) under a uniformly distributed load (UDL) of intensity q over the full span l .

We can replace the distributed load by an equivalent concentrated load:

$$dF = q dx \Rightarrow F = \int_0^l q dx = ql \quad (\text{Chapter 8.19})$$

The line of action of the equivalent force passes through the centroid of the loaded region:

$$x_F = \frac{\int_0^l x dF}{F} = \frac{\int_0^l x q dx}{ql} = \frac{ql^2/2}{ql} = \frac{l}{2} \quad (\text{Chapter 8.20})$$

Support Reactions

By symmetry (or equilibrium equations):

$$\Sigma F_y = 0 = F_A + F_B - ql \quad (\text{Chapter 8.21})$$

$$\Sigma M_A = 0 = F_B l - ql \frac{l}{2} \quad (\text{Chapter 8.22})$$

$$F_A = F_B = \frac{ql}{2} \quad (\text{Chapter 8.23})$$

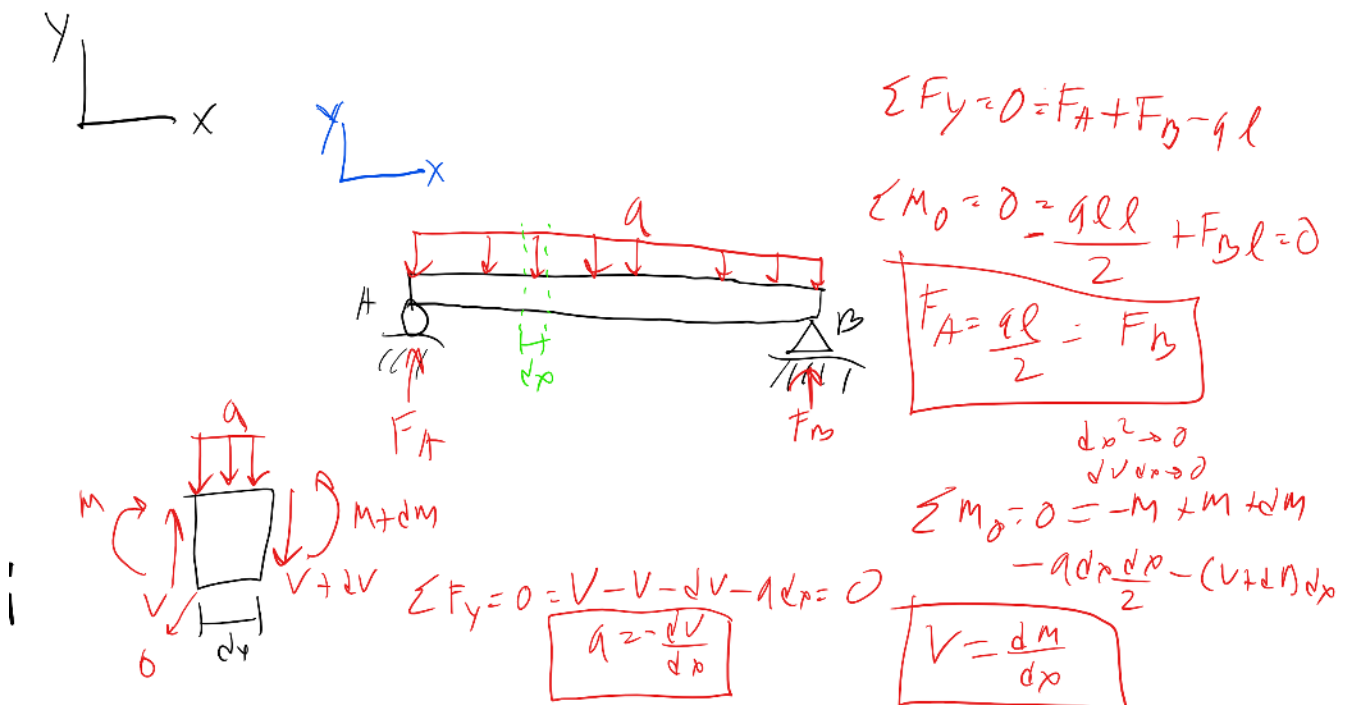


Figure Chapter8.7: Distributed load on simply supported beam.

Shear and Moment Equations

Now make a cut at a distance x from A ($0 \leq x \leq l$) and write the equilibrium equations for the left segment.

Shear equilibrium:

$$\Sigma F_y = 0 = -V - qx + F_A \quad (\text{Chapter 8.24})$$

$$V(x) = -qx + \frac{ql}{2} = q \left(\frac{l}{2} - x \right) \quad (\text{Chapter 8.25})$$

Moment equilibrium about the cut:

$$\Sigma M_x = 0 = M - F_A x + (qx) \frac{x}{2} \quad (\text{Chapter 8.26})$$

$$M(x) = F_A x - \frac{qx^2}{2} = \frac{qlx}{2} - \frac{qx^2}{2} \quad (\text{Chapter 8.27})$$

Differential Relationships (useful checks)

$$q(x) = -\frac{dV}{dx}, \quad V(x) = \frac{dM}{dx} \quad (\text{Chapter 8.28})$$

Check with our equations:

$$V(x) = q \left(\frac{l}{2} - x \right) \Rightarrow \frac{dV}{dx} = -q \Rightarrow q = -\frac{dV}{dx} \quad (\text{Chapter 8.29})$$

$$M(x) = \frac{qlx}{2} - \frac{qx^2}{2} \Rightarrow \frac{dM}{dx} = \frac{ql}{2} - qx = V(x) \quad (\text{Chapter 8.30})$$

Everything checks perfectly.

Key Takeaways

- Under a uniform load q , the shear force $V(x)$ varies linearly and the bending moment $M(x)$ varies quadratically.
- Maximum shear occurs at the supports, and maximum bending moment occurs at midspan.
- The identities $q = -\frac{dV}{dx}$ and $V = \frac{dM}{dx}$ are excellent tools for checking your diagrams.

Stresses in Beams

Beam Bending Assumptions

So far we have demonstrated that when we apply a load on a beam, internal shear and bending moments are created. This gives rise to both shear and normal stresses, and typically as we will show, the normal stresses are much greater than shear stresses, in particular when the length-to-height ratio of the beam is large, i.e. $\frac{l}{h} > 10$. Again, our entire purpose of learning about this topic is to avoid material failure, so we will focus on regions of maximum stress.

Now in doing so we will make several critical assumptions:

- The beam is straight.
- The material is linear elastic, isotropic, and cubic.
- The cross-section is symmetric.
- The beam is stable (no lateral buckling).

Thus, as the schematic below indicates, we will typically be dealing with scenarios as we have done previously, where one face is in tension and the other is in compression. There is also a plane along the longitudinal axis called the neutral axis that experiences no stress.

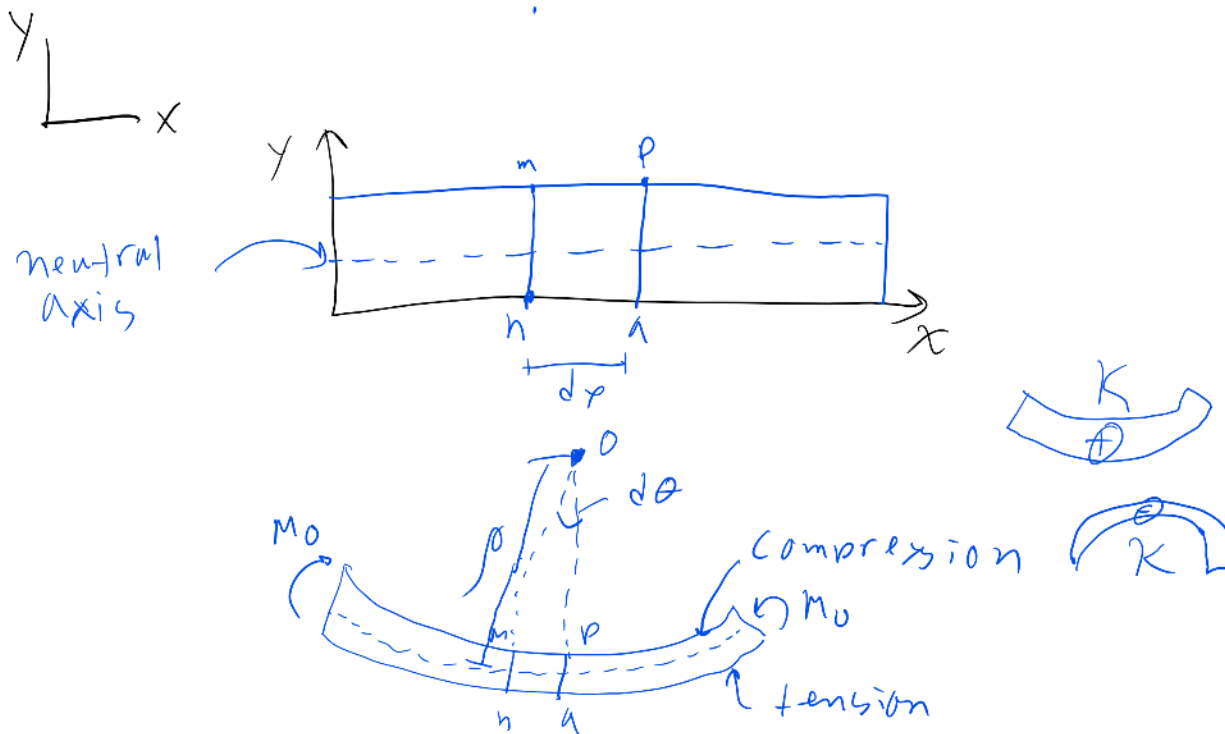


Figure Chapter 8.8: Bending schematic.

We must also distinguish between pure bending, which exhibits a constant bending moment, and non-uniform bending, where the bending moment is not constant.

Typically when we bend a beam such that it experiences positive bending near the top, the beam will be in compression, and as we move toward the bottom of the beam (height-wise), we transition from compression to no stress at the neutral axis, and then tension at the bottom of the beam.

If the material is brittle, failure will occur via crack propagation in the tensile region, whereas if a material is weak under compression, failure will occur via buckling at the top surface. We have a good idea conceptually of what is going on, but now we need to develop an expression that will tell us how this stress is distributed in a beam.

We will derive this relationship in three steps:

1. Geometric Statement
2. Constitutive Equation
3. Equilibrium Conditions

Geometric Statement

Looking at the schematic of the beam, we can clearly see that sections $\overline{mn}$ and $\overline{pq}$ will rotate with respect to one another, and if we extrapolate these lines, they intersect at a point O , the center of curvature. The distance from O to the neutral axis is given by the radius of curvature ρ . We assume that the distance between $\overline{mn}$ and $\overline{pq}$ at the neutral axis is constant dx , so we can develop the following relationship for curvature:

$$\kappa = \frac{1}{\rho} = \frac{d\theta}{dx} \quad (\text{Chapter 8.31})$$

If we have pure bending, ρ is constant; it will not be if we have non-uniform bending. Additionally, curvature has the same sense of positive and negative as the bending moment.

Constitutive Equation

We can now obtain the normal strain in the x-direction, because we know that longitudinal planes other than the neutral axis will change length and produce strain in this direction. Consider a segment $\overline{ef}$ at a distance y from the neutral axis.

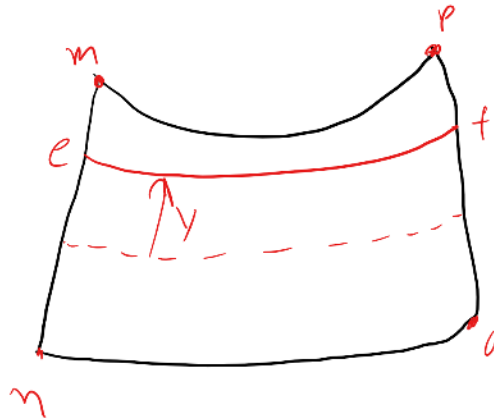
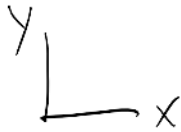


Figure Chapter8.9: Bending constitutive equation.

We find that:

$$l_o = dx = \rho d\theta \quad (\text{Chapter 8.32})$$

$$l_i = (\rho - y)d\theta \quad (\text{Chapter 8.33})$$

$$\epsilon_{xx} = \frac{l_i - l_o}{l_o} = -\frac{y}{\rho} = -y\kappa \quad (\text{Chapter 8.34})$$

We see that when $y \rightarrow 0$, the strain also goes to 0 at the neutral axis. When y is positive, we have negative (compressive) strain at the top of the beam and vice versa for the bottom—all matching intuition.

Assuming linear elasticity, we can use Hooke's Law:

$$\sigma_{xx} = E\epsilon_{xx} = -Ey\kappa \quad (\text{Chapter 8.35})$$

The stress varies linearly from the neutral axis. Because we are dealing with uniaxial bending stress in the x-direction, we also have the following strain components:

$$\epsilon_{xx} = -y\kappa \quad (\text{Chapter 8.36})$$

$$\epsilon_{yy} = \nu y\kappa \quad (\text{Chapter 8.37})$$

$$\epsilon_{zz} = \nu y\kappa \quad (\text{Chapter 8.38})$$

We can also define transverse curvature (anelastic curvature):

$$\kappa_{xx} = -\frac{\epsilon_{xx}}{y}, \quad \kappa_{yy} = -\frac{\epsilon_{yy}}{y}, \quad \kappa_{zz} = -\frac{\epsilon_{zz}}{y} \quad (\text{Chapter 8.39})$$

Equilibrium Conditions

Now we apply equilibrium conditions to relate stress to the bending moment. For a differential element dA :

$$\Sigma F_x = 0 = \int_A \sigma_{xx} dA = \int_A -yE\kappa dA \quad (\text{Chapter 8.40})$$

Since neither E nor κ is zero, the only way for the total force to be zero is if:

$$\int_A y dA = 0 \quad (\text{Chapter 8.41})$$

which means the centroid $\bar{y} = 0$. Thus, the neutral axis passes through the centroid of the cross-section.

Next, consider the bending moment at the centroid (origin). The total moment must balance the distributed stress:

$$\Sigma M_o = 0 = -M - \int_A \sigma_{xx} y dA \quad (\text{Chapter 8.42})$$

$$M = - \int_A \sigma_{xx} y dA = E\kappa \int_A y^2 dA \quad (\text{Chapter 8.43})$$

Define the second moment of area (moment of inertia):

$$I = \int_A y^2 dA \quad (\text{Chapter 8.44})$$

For common cross-sections:

- Rectangular beam: $I_z = \frac{bh^3}{12}$
- Circular beam: $J = \int_A r^2 dA = \int_A (z^2 + y^2) dA = 2I_z = \frac{\pi r^4}{4}$

Now we can write the bending moment as:

$$M = E\kappa I \quad (\text{Chapter 8.45})$$

and the bending stress as:

$$\sigma_{xx} = -E\kappa y = -\frac{My}{I} \quad (\text{Chapter 8.46})$$

When the bending moment is positive and y is positive, we have compression at the top and tension at the bottom.

We can also derive the strain energy due to bending per unit volume U_b :

$$U_b = \int_V U_{ESE} dV = \int_l \int_A \frac{\sigma_{xx}^2}{2E} dA dl = \int_l \frac{M^2}{2EI} dl \quad (\text{Chapter 8.47})$$

A very useful relationship in beam design, as it links strain energy to the moment and stiffness.

Beam Deflection

Thus far we have been focused almost exclusively on the forces, bending, and the stresses that develop in a beam when a load is applied. However, it is often extremely important to know how far a beam will deflect from the neutral axis. This is critical because certain materials or applications will have limitations on the amount of deflection that can occur. Additionally, we can also easily measure the amount of deflection and then back out the load or material properties as well.

Let's take a look at a beam bending scenario below where we have some given amount of deflection v and an angle θ that describes the angle between the x-axis and the tangent to the deflection curve. The question becomes: what is the deflection at m_2 ?

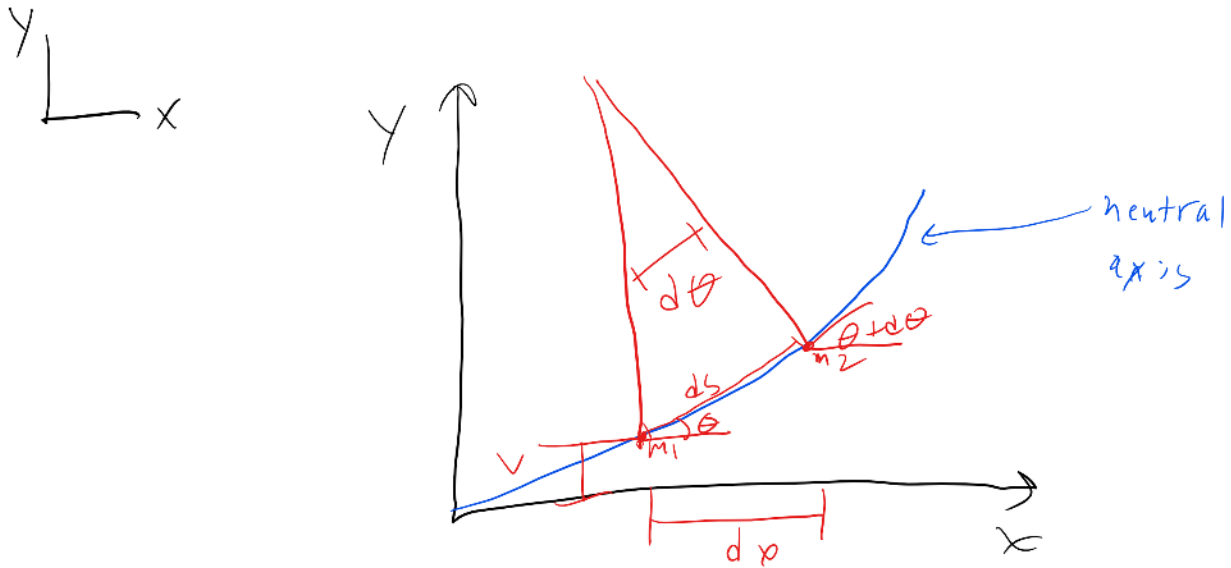


Figure Chapter8.10: Deflection for cantilever beam.

We know that:

$$\rho d\theta = ds \quad (\text{Chapter 8.48})$$

$$\kappa = \frac{1}{\rho} = \frac{d\theta}{ds} \quad (\text{Chapter 8.49})$$

Using the small angle approximation:

$$\cos \theta = \frac{dx}{ds} \approx 1 \quad (\text{Chapter 8.50})$$

therefore $ds \approx dx$, so we can obtain another expression for curvature:

$$\kappa = \frac{d\theta}{ds} = \frac{d\theta}{dx} = \frac{d^2v}{dx^2} \quad (\text{Chapter 8.51})$$

and we can also write:

$$\frac{d\theta}{dx} = \frac{d^2v}{dx^2} = \frac{M}{EI} \quad (\text{Chapter 8.52})$$

This is a very useful relationship because we can integrate $M(x)$ twice to get the deflection $v(x)$, and obtain constants of integration by establishing boundary conditions. Additionally, this term EI is referred to as the flexural rigidity, a key quantity for deflection.

The Euler–Bernoulli Equation

We can develop a more general equation for beam bending using the Euler–Bernoulli beam equation, which rearranges the above in terms of a general distributed load $q(x)$:

$$\frac{d^2}{dx^2} \left(EI \frac{d^2v}{dx^2} \right) = q(x) \quad (\text{Chapter 8.53})$$

If the flexural rigidity EI is constant, we can simplify this to:

$$EI \frac{d^4 v}{dx^4} = q(x) \quad (\text{Chapter 8.54})$$

We can also relate this equation to bending moments and shear forces:

$$M = -EI \frac{d^2 v}{dx^2} \quad (\text{Chapter 8.55})$$

$$V = -\frac{d}{dx} \left(EI \frac{d^2 v}{dx^2} \right) \quad (\text{Chapter 8.56})$$

Thus, we have a 4th-order differential equation that we must solve to find the equation for beam deflection, requiring four boundary conditions.

Boundary Conditions for Beam Bending

It is critical to observe that the bending moment is related to the second derivative of the deflection, and the shear force is related to the third derivative of displacement. This will be important as we determine boundary conditions.

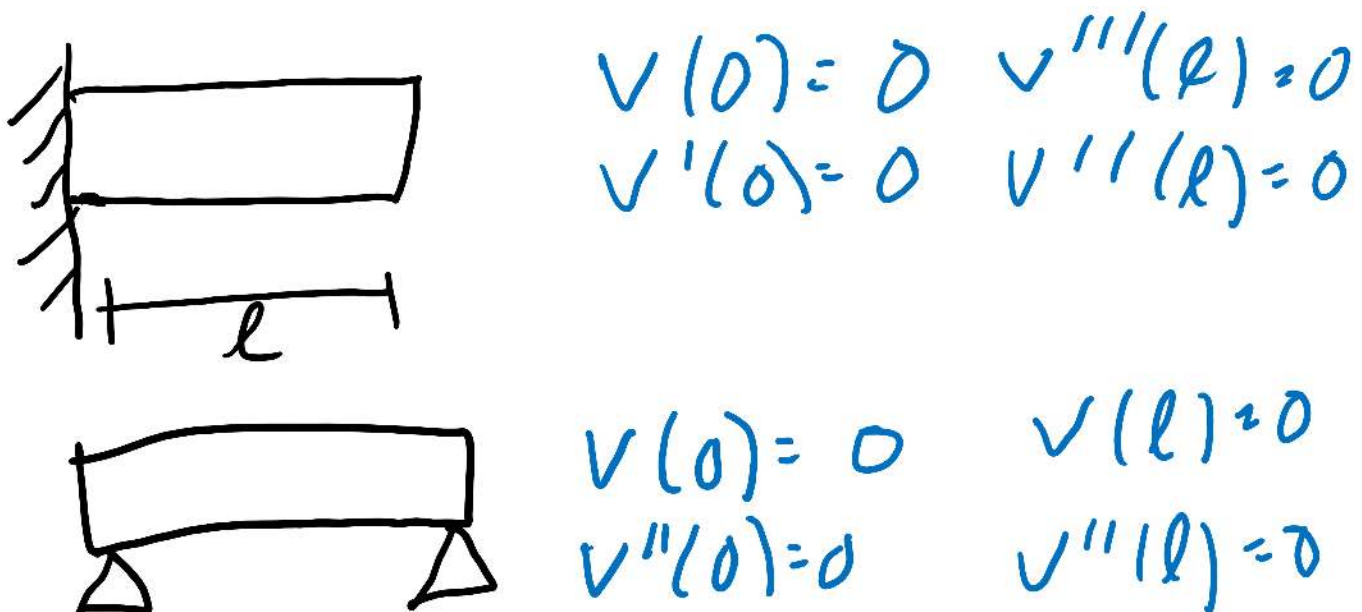


Figure Chapter8.11: Common beam bending scenarios.

Common boundary conditions:

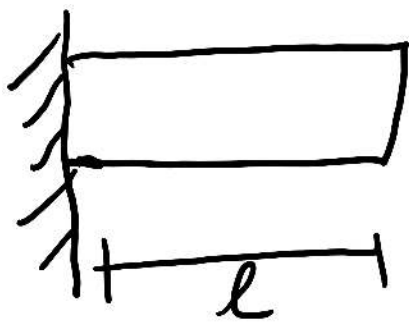
- For a cantilever beam, at the fixed support there can be no deflection or slope:

$$v(0) = 0, \quad v'(0) = 0 \quad (\text{Chapter 8.57})$$

At the free end (no external moment or shear):

$$v''(l) = 0, \quad EI v'''(l) = P \quad (\text{Chapter 8.58})$$

- For a simply supported beam, there is no deflection at the supports ($v = 0$), but the slope v' is not necessarily zero; the bending moment is zero at the supports.



$$\begin{array}{ll} V(0) \neq 0 & V(l) = 0 \\ M(0) \neq 0 & M(l) = 0 \end{array}$$



$$\begin{array}{ll} V(0) \neq 0 & V(l) \neq 0 \\ M(0) = 0 & M(l) = 0 \end{array}$$

Figure Chapter8.12: Common beam bending scenarios in terms of shear and bending moment values.

Deflection Examples: Cantilever, 3-Point, and Distributed Load

Deflection for Simple End-Loaded Cantilever Beam with Fixed Support

Let's look at the simple cantilever beam problem below. We can identify several boundary conditions.

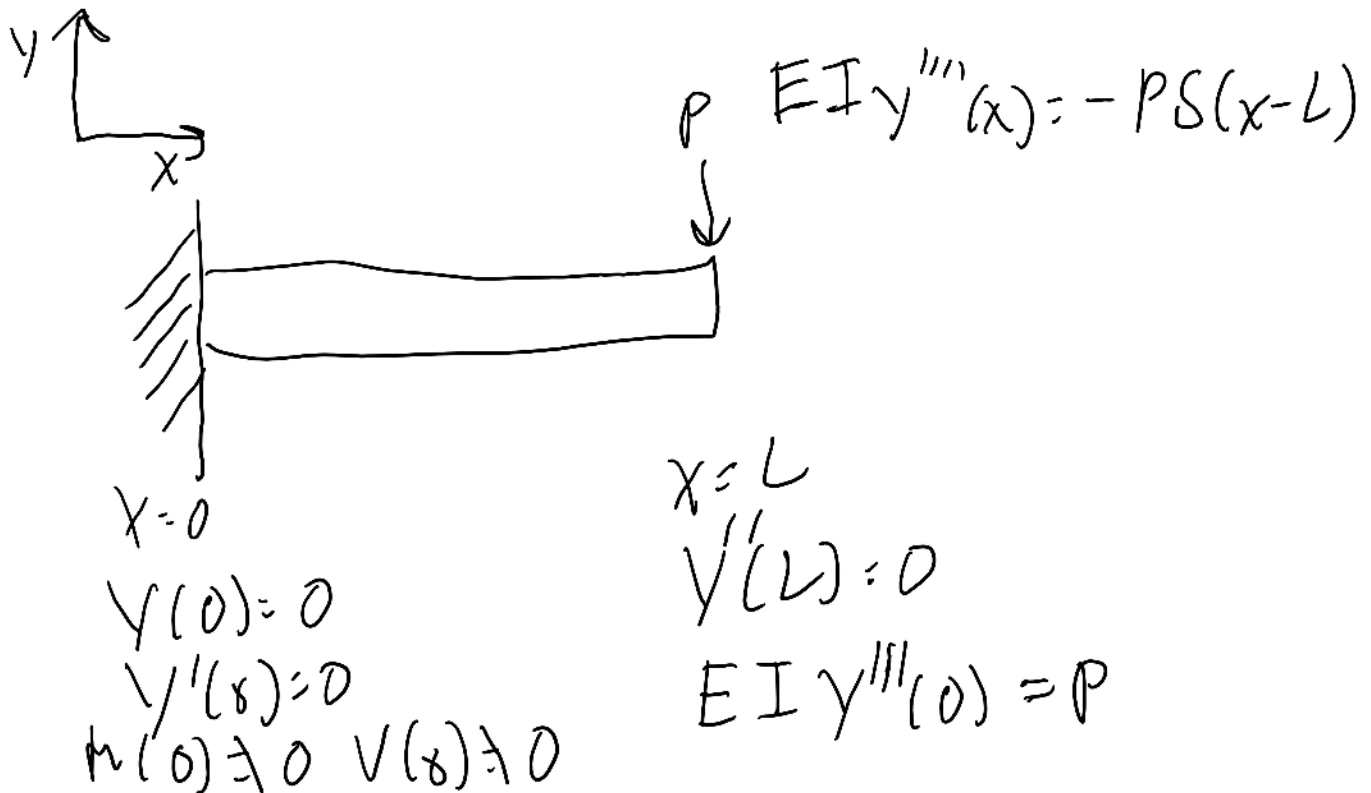


Figure Chapter8.13: Deflection for cantilever beam.

For a cantilever beam:

- At the wall (fixed end), the beam will not deflect, and the slope of deflection should also be zero.

$$v(0) = 0, \quad v'(0) = 0$$

(Chapter 8.59)

- At the free end, there will be no bending or shear moment:

$$v''(l) = 0, \quad EIv'''(l) = P \quad (\text{Chapter 8.60})$$

The differential equation for the deflection curve is given by the Euler-Bernoulli relation:

$$EI \frac{d^4 v}{dx^4} = 0 \quad (\text{Chapter 8.61})$$

Solving this equation with the given boundary conditions, we can find the expression for deflection using symbolic or numerical tools such as Mathematica.

Three-Point Bending Test

Now let's consider the very common three-point bending test.

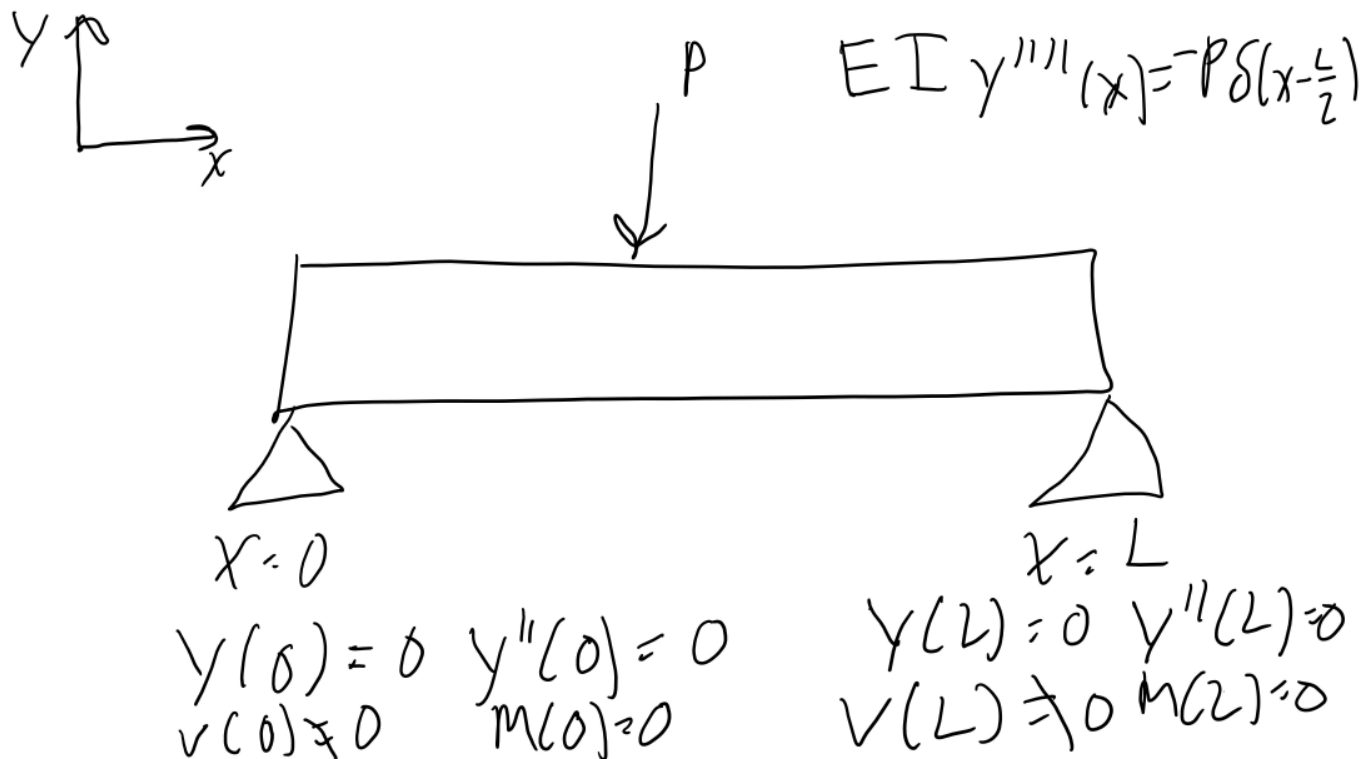


Figure Chapter8.14: 3-point bending test.

For this beam, the load P is applied at the midpoint of a simply supported beam of length l .

The governing equation is:

$$EI \frac{d^4 v}{dx^4} = 0 \quad (\text{Chapter 8.62})$$

and the boundary conditions are:

$$v(0) = 0, \quad v(l) = 0, \quad M(0) = M(l) = 0 \quad (\text{Chapter 8.63})$$

Solving this system yields the deflection profile, with the maximum deflection at midspan:

$$v_{max} = \frac{Pl^3}{48EI} \quad (\text{Chapter 8.64})$$

Distributed Load Example

We can also analyze a simply supported beam with a uniform distributed load q .

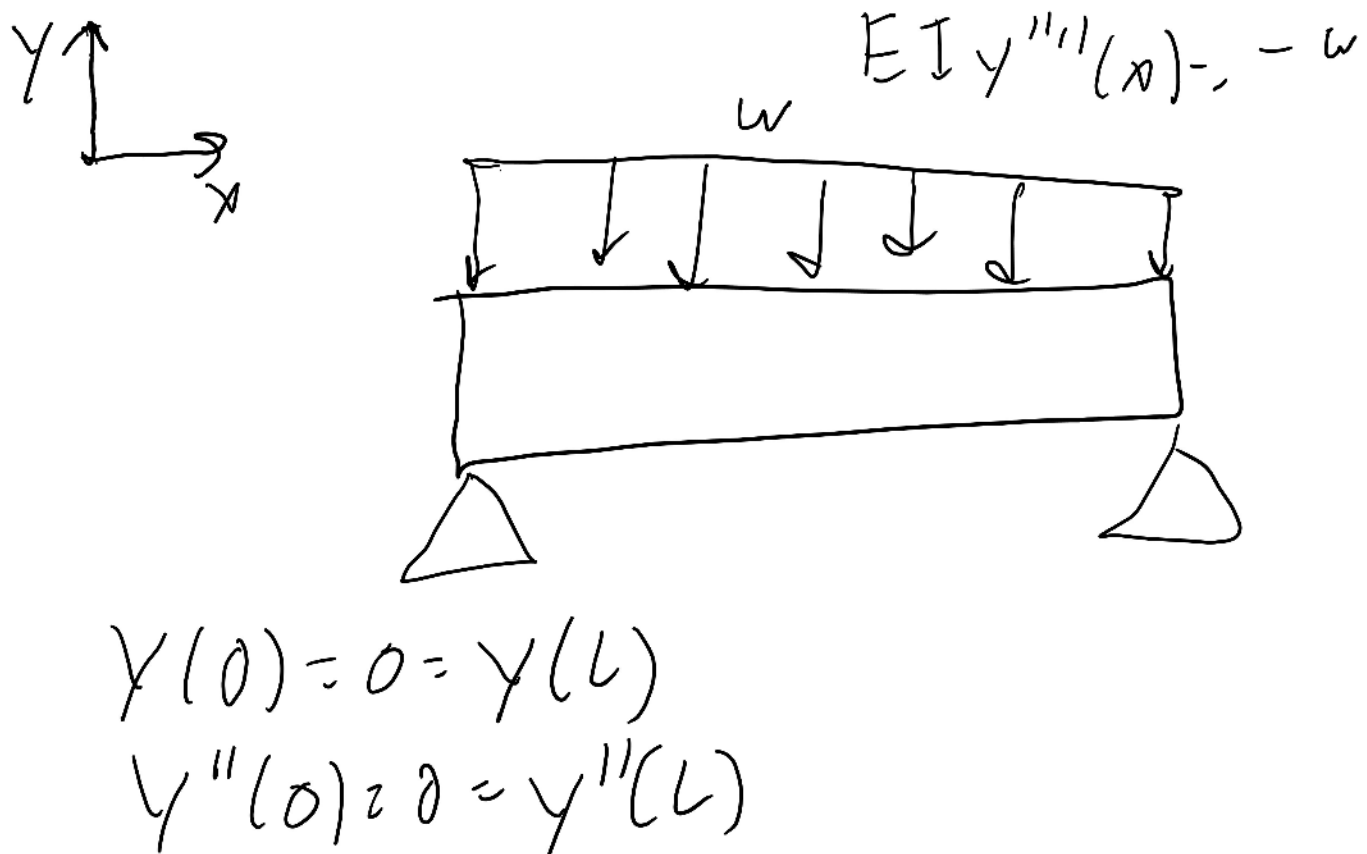


Figure Chapter8.15: Distributed loads on simply supported beam.

The governing differential equation is now:

$$EI \frac{d^4 v}{dx^4} = q \quad (\text{Chapter 8.65})$$

Solving for $v(x)$ using the appropriate boundary conditions for a simply supported beam:

$$v(0) = 0, \quad v(l) = 0, \quad M(0) = M(l) = 0 \quad (\text{Chapter 8.66})$$

yields the maximum deflection:

$$v_{max} = \frac{5ql^4}{384EI} \quad (\text{Chapter 8.67})$$

All of these examples demonstrate how beam deflection can be predicted analytically by solving differential equations under the correct boundary conditions.

Buckling

When a material is placed under compression, the material will not typically fail via crack propagation, as compressive stress does not assist in crack propagation (typically). Instead, many materials under pure compressive stress will fail via buckling.

We will examine a particularly important and ubiquitous case: column buckling. A column is defined as a long, slender member that is loaded in compression, and buckling is an instability phenomenon. When we mention stability, we are referring to whether the system will return to its initial state when perturbed.

- A stable system will return to its initial state.
- An unstable system will not return to its initial state.

You have likely seen this illustrated in a physics course where a ball rolling down a hill is unstable, but one at the bottom of a well is stable. There are also neutral and metastable systems, but more on that in other courses.

Now, you may imagine that a longer column will buckle at lower applied loads, and if we increase the cross-sectional area, it will increase the applied load required for buckling. Buckling is associated with a change in shape—bending occurs. Let's develop a framework to describe buckling.

Ideal Column with Pinned Ends

Let's start with an ideal column with pinned ends. We will assume:

- The beam is straight.
- The material is linear elastic.
- The load is perfectly aligned with the column axis.

As the column is loaded, buckling will proceed through several stages:

1. Elastic shortening — the column is stable and compresses linearly.
2. At a critical load, instability begins — the column bends laterally.

What is this critical load, and how does it relate to the flexural modulus, beam length, and geometry?

We start by defining our coordinate system and drawing a free body diagram. The deflection at the top of the beam is v .

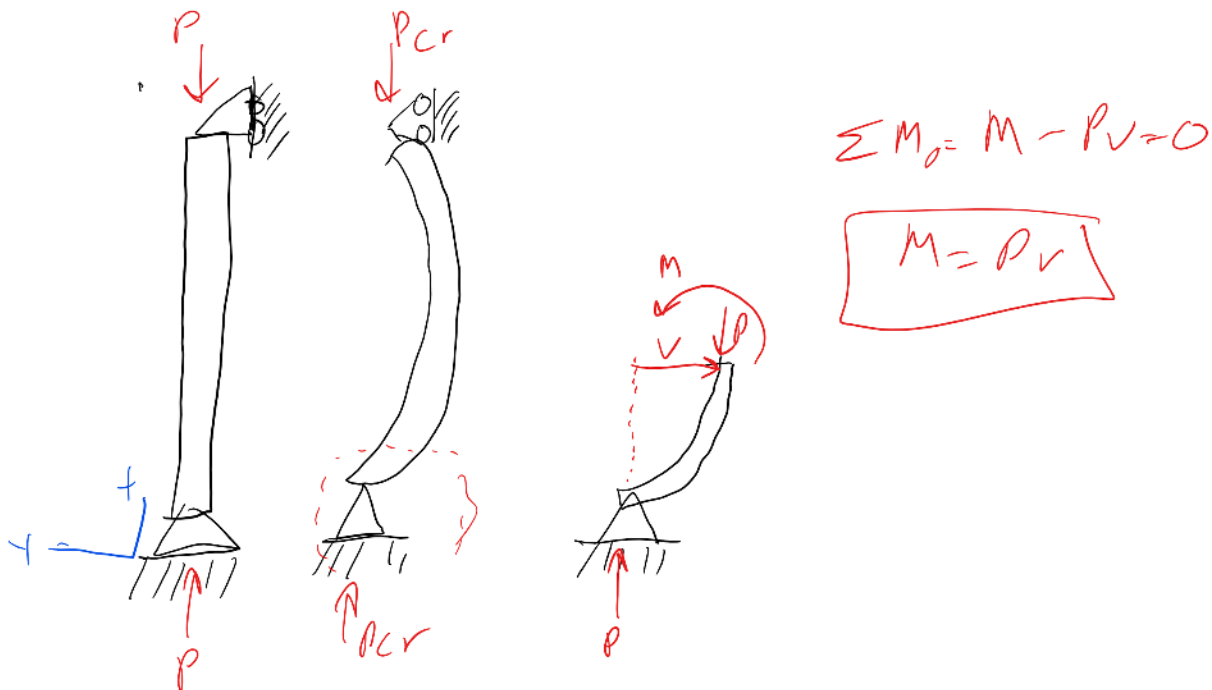


Figure Chapter8.16: Deflection beam buckling.

From the free body diagram, the material experiences a bending moment $M = Pv$, and we can relate this to our old friend, the Euler–Bernoulli relation:

$$\frac{d^2v}{dx^2} = \frac{M}{EI} = \frac{Pv}{EI} \quad (\text{Chapter 8.68})$$

The differential equation is:

$$EI \frac{d^2v}{dx^2} + Pv = 0 \quad (\text{Chapter 8.69})$$

The boundary conditions for a pinned–pinned column are:

$$v(0) = 0, \quad v(l) = 0 \quad (\text{Chapter 8.70})$$

The general solution is:

$$v = c_1 \sin \left(\sqrt{\frac{P}{EI}} x \right) + c_2 \cos \left(\sqrt{\frac{P}{EI}} x \right) \quad (\text{Chapter 8.71})$$

Applying the boundary conditions:

$$v(0) = 0 \Rightarrow c_2 = 0 \quad (\text{Chapter 8.72})$$

$$v(l) = 0 \Rightarrow \sin \left(\sqrt{\frac{Pl^2}{EI}} \right) = 0 \quad (\text{Chapter 8.73})$$

which implies:

$$\sqrt{\frac{Pl^2}{EI}} = n\pi \quad (\text{Chapter 8.74})$$

Thus, the lowest load that causes buckling (the critical load) is:

$$P_{cr} = \frac{\pi^2 EI}{l^2} \quad (\text{Chapter 8.75})$$

where $n = 1$ corresponds to the first buckling mode. Higher modes ($n = 2, 3, \dots$) correspond to higher loads and more half-wavelengths along the column.

We see that the critical load for buckling is linearly dependent on E and I , but scales inversely with l^2 . Hence, longer columns buckle under smaller loads. Ideally, we would also want a constant I about all cross-sectional axes for uniform buckling resistance.

Moment of Inertia Comparison: Solid vs. Thin-Walled Cylinder

Let's compare the moment of inertia for a solid cylinder and a thin-walled hollow cylinder.

[Figure: Moment of inertia for solid sphere and thin-walled section.]

$$I_s = \frac{\pi r^4}{4}, \quad m_s = \rho \pi r^2 \quad (\text{Chapter 8.76})$$

$$I_t = \pi R^3 t, \quad m_t = \rho 2\pi R t \quad (\text{Chapter 8.77})$$

For the same mass:

$$\rho \pi r^2 = \rho 2\pi R t \Rightarrow r = \sqrt{2Rt} \quad (\text{Chapter 8.78})$$

Thus:

$$\frac{I_t}{I_s} = \frac{R}{t} \quad (\text{Chapter 8.79})$$

So, for the same mass, a tube has a much larger moment of inertia than a solid cylinder by a factor of $\frac{R}{t}$, which explains why tubes and I-beams are common structural choices.

However, very thin-walled sections can fail by local buckling, where the stress to buckle locally is given by:

$$\sigma_{local \text{ buckling}} = \frac{Et}{R\sqrt{3(1-\nu^2)}} \quad (\text{Chapter 8.80})$$

Local buckling can be mitigated by adding longitudinal and circumferential stiffeners or by using honeycomb or foam cores—leading us to an important class of materials: open-cell foams.

Open-Cell Foams and Buckling Relationships

Open-cell foams form complex geometries composed of polyhedral cells, but we can do some simple first-order modeling using dimensional analysis and by assuming that the cell geometry of foams of different densities is similar.

Let's look at an open-cell structure under compressive load. We can make a simple approximation of how the open-cell foam will behave.

[Figure: Open-cell foam beam buckling.]

We start with the following proportional relationships:

$$\sigma \propto \frac{F}{l^2} \quad (\text{Chapter 8.81})$$

$$\epsilon \propto \frac{\delta}{l} \quad (\text{Chapter 8.82})$$

$$\delta \propto \frac{Fl^3}{E_s I} \quad (\text{Chapter 8.83})$$

$$I \propto t^4 \quad (\text{Chapter 8.84})$$

Combining these gives the apparent modulus of the foam:

$$E^* = \frac{\sigma}{\epsilon} \propto \frac{F/l^2}{\delta/l} \propto E_s \left(\frac{t}{l} \right)^4 \quad (\text{Chapter 8.85})$$

Additionally, we can show that the ratio of the density of the open-cell structure to the density of the solid material gives us the following relationship:

$$\frac{\rho^*}{\rho_s} \propto \frac{V_s}{M_s} \frac{M_s}{V_{total}} \propto \frac{t^2}{l^2} \quad (\text{Chapter 8.86})$$

Combining these two expressions gives the Young's modulus of the open-cell foam:

$$E^* = c_1 E_s \left(\frac{\rho^*}{\rho_s} \right)^2 \quad (\text{Chapter 8.87})$$

where c_1 is a constant, E_s is the Young's modulus of the solid material, ρ^* is the apparent density of the foam, and ρ_s is the density of the solid.

We can also get the critical buckling stress in an open-cell structure by recalling our earlier relationships:

$$\sigma_{ocb} \propto \frac{P_{cr}}{l^2} \propto E_s \left(\frac{t}{l} \right)^4 \quad (\text{Chapter 8.88})$$

Thus, combining this with the density relationship, we find:

$$\sigma_{ocb} = c_2 E_s \left(\frac{\rho^*}{\rho_s} \right)^2 \quad (\text{Chapter 8.89})$$

Typically, during compression, bands of cells buckle sequentially until all have collapsed at high strains (around $\epsilon \approx 0.8$), at which point the opposing cells contact and the stress rises sharply due to densification. These materials are particularly adept at absorbing energy—one reason cellular solids like foams and honeycombs are used extensively in energy absorption and impact mitigation applications.

Now that we've completed our discussion of bending and buckling, we'll move on to the third major elastic loading mode: torsion.

Torsion

Torsion is a critical loading state and is extremely ubiquitous in mechanical and structural systems, especially in the automotive industry. A twisting moment, or torque, consists of forces that act through a distance or a lever arm. The general definition of torque is:

$$T = r \times F \quad (\text{Chapter 8.90})$$

where r is the lever arm vector and F is the force vector.

When a material is under torsion, the material experiences shear stresses and angular displacements. We can determine these torsional stresses and displacements using a methodology very similar to what we did for normal stresses and deflection in bending. We will follow the same three-step framework:

1. Geometric Statement
2. Constitutive Equation
3. Equilibrium Conditions

Geometric Statement

Looking at the figure below, we define a differential element of length dz which rotates through an infinitesimal angle $d\theta$. The displacement δ at a radial distance r from the axis is:

$$\delta = rd\theta \quad (\text{Chapter 8.91})$$

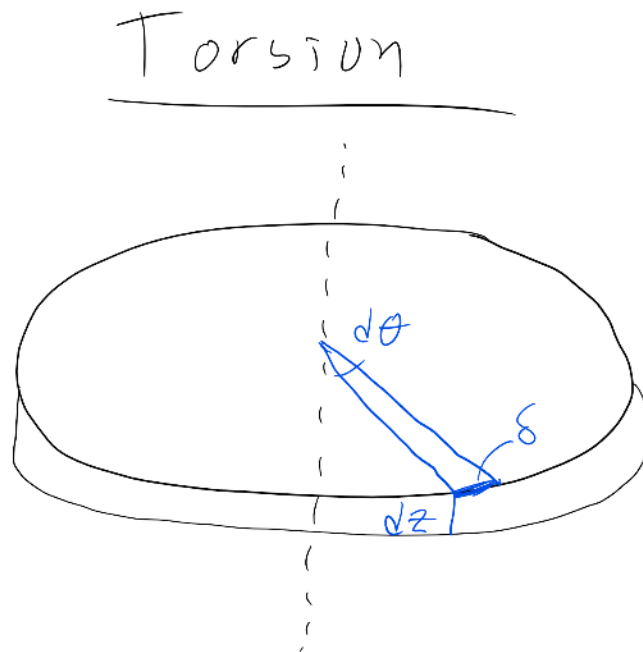


Figure Chapter8.17: Torsion geometrical statement.

Constitutive Equation

We know that this is similar to the expression for shear strain, so we can write:

$$\gamma_{z\theta} = \frac{\delta}{dz} = r \frac{d\theta}{dz} \quad (\text{Chapter 8.92})$$

Assuming that we are in the linear elastic regime, the shear stress is given by:

$$\sigma_{z\theta} = G\gamma_{z\theta} = Gr \frac{d\theta}{dz} \quad (\text{Chapter 8.93})$$

where G is the shear modulus of the material.

Equilibrium Equation

Now we can apply the equilibrium condition by summing the moments on a differential area dA . The total torque is then obtained by integrating over the entire cross-sectional area:

$$T = \int_A \sigma_{z\theta} r dA = G \frac{d\theta}{dz} \int_A r^2 dA \quad (\text{Chapter 8.94})$$

The term $\int_A r^2 dA$ is known as the **polar moment of inertia**, denoted J :

$$J = \int_A r^2 dA \quad (\text{Chapter 8.95})$$

For a circular or annular cross-section, this can be calculated as:

$$J = \int_{r_i}^{r_o} r^2 (2\pi r dr) = \frac{\pi(r_o^4 - r_i^4)}{2} \quad (\text{Chapter 8.96})$$

We can rearrange the torque relationship as follows:

$$\frac{d\theta}{dz} = \frac{T}{GJ} \quad (\text{Chapter 8.97})$$

Integrating along the length l :

$$\theta = \int_0^l \frac{T}{GJ} dz = \frac{Tl}{GJ} \quad (\text{Chapter 8.98})$$

where θ is the total angle of twist in radians.

Finally, substituting back into our stress relationship:

$$\sigma_{z\theta} = Gr \frac{d\theta}{dz} = \frac{Tr}{J} \quad (\text{Chapter 8.99})$$

This is a very useful and elegant result. We see that the torsional shear stress varies linearly with the radial position r , and the maximum shear stress occurs at the outer surface of the shaft ($r = r_o$):

$$\sigma_{max} = \frac{Tr_o}{J} \quad (\text{Chapter 8.100})$$

Interestingly, the expression for torsional stress does not explicitly depend on the material—only on geometry and applied torque—because the shear modulus G cancels out.

Elastic Strain Energy in Torsion

We can also derive this using strain energy. The elastic strain energy per unit volume is:

$$U_{ESE} = \frac{\sigma_{z\theta} \gamma_{z\theta}}{2} = \frac{1}{2G} \left(\frac{Tr}{J} \right)^2 \quad (\text{Chapter 8.101})$$

Integrating over the volume of the specimen:

$$U = \int_V U_{ESE} dV = \int_l \int_A \frac{1}{2G} \left(\frac{Tr}{J} \right)^2 dA dz \quad (\text{Chapter 8.102})$$

Assuming T , G , and J are constant along the length:

$$U = \frac{T^2 l}{2GJ} \quad (\text{Chapter 8.103})$$

The torque–twist relationship can also be derived from the energy expression:

$$\theta = \frac{\partial U}{\partial T} = \frac{Tl}{GJ} \quad (\text{Chapter 8.104})$$

Once again, we see perfect consistency among our geometric, constitutive, equilibrium, and energy approaches.

This concludes our exploration of elastic loading states: bending, buckling, and torsion. Next, we will move into the plastic deformation regime, where materials no longer behave linearly or elastically.

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Chapter 9: Plasticity Regime

Plasticity Regime

In the plastic regime, we have discussed previously that deformation is permanent and irreversible. Additionally, unlike in the elastic regime where we spend a considerable amount of time deriving and developing constitutive equations that relate stress to strain, in the plastic regime we will not have such relationships. Instead, we will develop our understanding of the mechanical behavior of materials from an empirical, evidence-based perspective.

Some materials, like ceramics, exhibit very little to no plasticity and tend to fracture before yielding occurs. Additionally, in this lecture we will only discuss low-temperature plasticity — i.e. at temperatures below those where creep can be activated. (Creep will be discussed in a subsequent lecture.) For metals, the temperature for creep to occur is typically $\frac{T}{T_m} > 0.3$ and for ceramics $\frac{T}{T_m} > 0.5$.

One of the critical parameters that defines plasticity and dominates our discussion is the yield strength. The yield strength can be measured in several different ways:

- Uniaxial Tension Testing
- Hardness Testing
- Nanoindentation

Before we get too deep into plasticity, let's start with a fun calculation of what should be the theoretical yield strength of a material to highlight a critical aspect of materials science — that defects are essential to determining mechanical behavior.

Theoretical Yield Strength of Materials

We have previously shown that by taking an atomistic perspective we were able to develop a good approximation of the stiffness of a material from first principles. Let's attempt a similar approach for yielding.

Consider a perfect crystal subjected to a shear stress. For yielding to occur, atoms must slide over one atomic spacing.

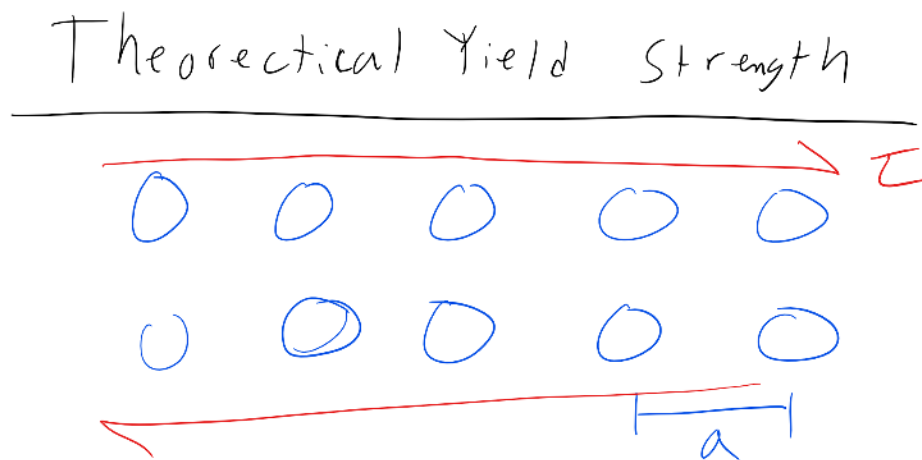


Figure Chapter9.1: Theoretical yield strength.

If we consider the forces required to do so, we must consider the bond energy function, as discussed previously when deriving the Young's modulus. We can approximate this force function using a harmonic expression:

$$\tau = \tau_{max} \sin\left(2\pi \frac{x}{a}\right) \quad (\text{Chapter 9.1})$$

where a is the interatomic spacing, typically $2R$. The engineering shear strain is then:

$$\gamma = \frac{x}{a} \quad (\text{Chapter 9.2})$$

We can relate τ_{max} to the shear modulus G as follows:

$$\frac{d\tau}{d\gamma} = \frac{d\tau}{dx} \frac{dx}{d\gamma} = a\tau_{max} \frac{2\pi}{a} \cos\left(\frac{2\pi}{a}\right) \quad (\text{Chapter 9.3})$$

$$G = \left(\frac{d\tau}{d\gamma}\right)_{\gamma \rightarrow 0} = 2\pi\tau_{max} \quad (\text{Chapter 9.4})$$

Thus, the material should yield at a stress of approximately:

$$\tau_{yield} = \frac{G}{2\pi} \approx \frac{G}{10} \quad (\text{Chapter 9.5})$$

For most materials, this would predict a yield strength of about 10 GPa, yet experimental yield stresses are typically only 10–100 MPa — about three orders of magnitude smaller. Why?

Even with more accurate potential models, the theoretical prediction still does not match experimental results. The answer lies in a subtle but profound realization that defects control plasticity. This realization led to one of the most significant theories in materials science: Dislocation Theory.

Dislocation Theory

Before we get deep into dislocation theory, let's recall some of our old friends: edge dislocations, screw dislocations, point defects, and grain boundaries. This is where all those concepts come together.

Historically, the question of why the theoretical yield strength was so much higher than the experimental value was answered independently by Taylor, Polanyi, and Orowan. They proposed that we do not have to slip entire planes of atoms simultaneously — which would require breaking all bonds in a plane — but instead, a few or even one bond at a time can move.

To visualize this, imagine an inchworm moving along a surface. In effect, a single extra half-plane of atoms moves incrementally from its equilibrium position to a new position halfway between atomic planes, creating an edge dislocation in the process.

A dislocation produces a local stress/strain field in the crystal lattice. Specifically, at the top of the dislocation, atoms are compressed relative to their equilibrium positions, while below the dislocation there is a tensile region where smaller atoms can diffuse. The amount of atomic displacement or distortion depends on bond stiffness. The interplanar spacing between close-packed planes is greater for FCC than for BCC structures, leading to larger distortions in FCC materials. The dislocation width is smaller in ionically bonded ceramics and even smaller in covalently bonded materials due to their higher bond stiffness.

Edge Dislocation

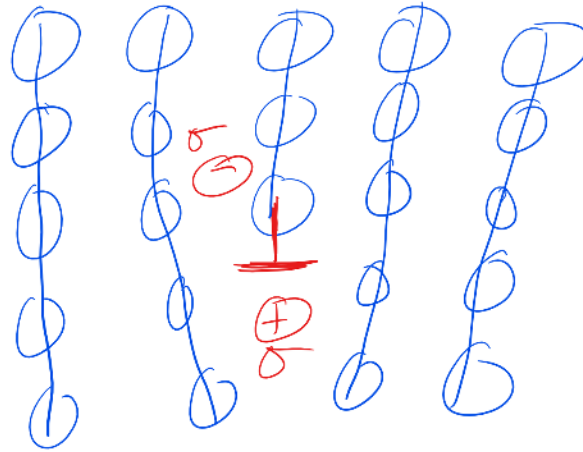


Figure Chapter9.2: Local stress field around dislocation.

Intuitively, a dislocation can move much more easily than an entire slip plane, since only a small number of bonds need to be broken sequentially. This motion of dislocations is referred to as slip, and whether a material can slip depends on several factors.

However, dislocations are not entirely free to move without resistance. When a dislocation moves, it drags along regions of compressive and tensile distortion, which create local strain fields that resist motion. This resistance is referred to as the Peierls force, and it depends on the crystal type, temperature, and other factors. Generally, materials with wide dislocations have a lower Peierls force. Hence, this force is smaller for FCC materials than BCC materials, and smaller for metals than ceramics. The Peierls force also decreases with temperature since dislocation motion becomes thermally activated.

Dislocation Stress Fields

We can describe the stress field associated with an edge or screw dislocation for isotropic, linear elastic materials. Consider an infinite edge dislocation along the z-axis with a Burgers vector along the x-axis. The stress field is given by:

$$\sigma_{xx} = -Dy \frac{3x^2 + y^2}{(x^2 + y^2)^2} \quad (\text{Chapter 9.6})$$

$$\sigma_{yy} = Dy \frac{x^2 - y^2}{(x^2 + y^2)^2} \quad (\text{Chapter 9.7})$$

$$\sigma_{xy} = Dx \frac{x^2 - y^2}{(x^2 + y^2)^2} \quad (\text{Chapter 9.8})$$

$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy}) \quad (\text{Chapter 9.9})$$

$$D = \frac{Gb}{2\pi(1 - \nu)} \quad (\text{Chapter 9.10})$$

All other stress components are zero.

For a screw dislocation, the displacement field can be described as follows. If we take a circular path around the dislocation, we find that $u_x = u_y = 0$ and $u_z = b$. The displacement can be expressed as:

Stress Field: Screw Dislocation

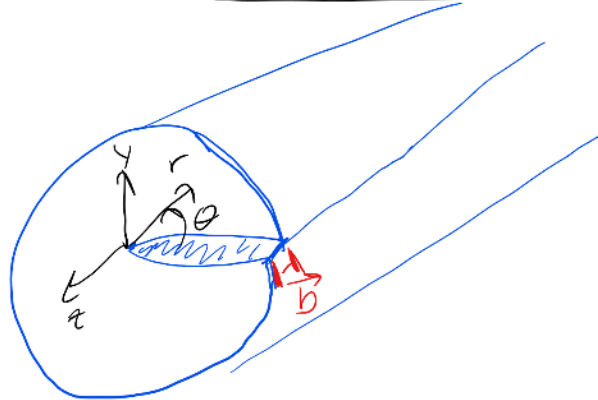


Figure Chapter9.3: Local stress field around screw dislocation.

$$u_z = \frac{b\theta}{2\pi} = \frac{b}{2\pi} \tan^{-1} \left(\frac{y}{x} \right) \quad (\text{Chapter 9.11})$$

The normal strains are all zero:

$$\epsilon_{xx} = \frac{\partial u_x}{\partial x} = \epsilon_{yy} = \frac{\partial u_y}{\partial y} = \epsilon_{zz} = \frac{\partial u_z}{\partial z} = 0 \quad (\text{Chapter 9.12})$$

The shear strains are:

$$\gamma_{xy} = \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} = 0 \quad (\text{Chapter 9.13})$$

$$\gamma_{yz} = \frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y} = \frac{bx}{2\pi(x^2 + y^2)} \quad (\text{Chapter 9.14})$$

$$\gamma_{xz} = \frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z} = \frac{-by}{2\pi(x^2 + y^2)} \quad (\text{Chapter 9.15})$$

The corresponding stresses are:

$$\sigma_{xz} = -\frac{Gby}{2\pi(x^2 + y^2)} \quad (\text{Chapter 9.16})$$

$$\sigma_{yz} = \frac{Gbx}{2\pi(x^2 + y^2)} \quad (\text{Chapter 9.17})$$

All other stress components are zero.

These equations were first derived in 1905, long before the modern understanding of dislocations and their stress fields. A few key observations can be made:

- The stress is proportional to the Burgers vector and the shear modulus.
- There is a singularity at the dislocation core where linear elasticity breaks down.
- Screw dislocations produce pure shear stress.
- Edge dislocations produce both normal and shear stresses, resulting in compression above and tension below the slip plane.

The presence of normal stresses in edge dislocations enables strong interactions with point defects, as we will discuss next.

Dislocation Energy

Now that we know the stress fields generated by edge and screw dislocations, we can calculate their corresponding elastic strain energy. Let's begin with a screw dislocation, using cylindrical coordinates for simplicity. For a screw dislocation, we can write the stress as:

$$\sigma_{\theta z} = \frac{Gb}{2\pi r} \quad (\text{Chapter 9.18})$$

The associated shear strain is:

$$\gamma_{\theta z} = \frac{b}{2\pi r} \quad (\text{Chapter 9.19})$$

The elastic strain energy per unit volume is then:

$$U_{screw} = \int_V \frac{1}{2} \sigma_{\theta z} \gamma_{\theta z} dV \quad (\text{Chapter 9.20})$$

Substituting, we find:

$$U_{screw} = \int_V \frac{Gb^2}{8\pi^2 r^2} dV = l \int_{r_0}^r \frac{Gb^2}{8\pi^2 r^2} 2\pi r dr \quad (\text{Chapter 9.21})$$

Since a dislocation is a one-dimensional defect, we usually express the energy per unit length:

$$\frac{U_{screw}}{l} = \frac{Gb^2}{4\pi} \ln \left(\frac{r}{r_0} \right) \quad (\text{Chapter 9.22})$$

A similar expression can be derived for an edge dislocation:

$$\frac{U_{edge}}{l} = \frac{Gb^2}{4\pi(1-\nu)} \ln \left(\frac{r}{r_0} \right) \quad (\text{Chapter 9.23})$$

Important observations:

- The energy scales with Gb^2 .
- The energy diverges logarithmically as the radius increases, indicating that isolated dislocations have very high energy.
- Dislocations tend to move toward free surfaces or combine destructively with other dislocations to reduce their strain energy.

Dislocation Interactions with Point Defects

Dislocations can also interact with point defects. When a vacancy forms in a crystal, the surrounding atoms relax inward, resulting in a negative relaxation volume Δv_v . For an interstitial atom, relaxation is outward, producing a positive relaxation volume Δv_i . These relaxation volumes interact with the hydrostatic pressure in the crystal, defined as:

$$p = -\sigma_{hydrostatic} = -\frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33}) \quad (\text{Chapter 9.24})$$

This interaction modifies the formation energy of the defect:

$$\Delta H_x^{f'} = \Delta H_x^f + p\Delta v_x$$

(Chapter 9.25)

If the internal pressure is positive, the formation energy of a vacancy decreases (making it easier to form), while the formation energy of an interstitial increases.

Screw dislocations, which are pure shear defects, do not have hydrostatic pressure components and thus do not significantly interact with point defects. Edge dislocations, however, have both tensile and compressive regions, leading to strong interactions.

At the top of an edge dislocation (compressive region, $p > 0$), vacancies are attracted. Below the dislocation (tensile region, $p < 0$), interstitials are attracted. Since interstitials produce larger volume changes than vacancies, their driving force for diffusion is correspondingly stronger. This explains the formation of defect atmospheres — such as Cottrell atmospheres — where solute atoms segregate to dislocations and pin them in place.

Mechanical Forces on Dislocations

Let's now consider the mechanical forces acting on dislocations. Imagine a solid under a shear stress σ_{31} and assume that the solid is a cube with dimensions l_1, l_2, l_3 .

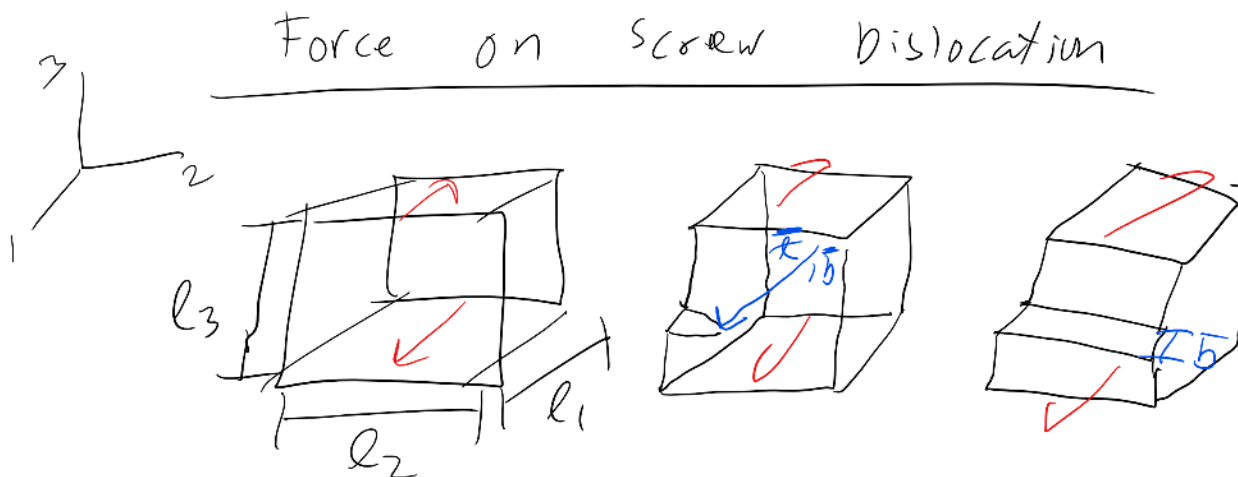


Figure Chapter9.4: Force on a screw dislocation.

As shown, a screw dislocation nucleates and moves, leaving behind a step one Burgers vector in height as it passes through the crystal. The Burgers vector is always parallel to the direction of slip motion — the direction in which the dislocation moves.

The work done on the body by the applied shear stress is:

$$\Delta W = \sigma_{31} l_1 l_2 b$$

(Chapter 9.26)

Alternatively, we can consider the work done as the product of force per unit length f and the distance moved by the dislocation over the area $l_1 l_2$:

$$\Delta W = f l_1 l_2$$

(Chapter 9.27)

Equating these expressions gives the force per unit length exerted by the applied stress on the dislocation:

$$f = \sigma_{31} b$$

(Chapter 9.28)

A similar expression can be derived for edge dislocations. This force can also be derived from the gradient of the strain energy per unit length:

$$f = -\frac{\partial(U/l)}{\partial d} \quad (\text{Chapter 9.29})$$

where d is the dislocation displacement. The strain energy decreases as the dislocation moves toward a free surface — a key driving force for recovery and annealing processes.

Peach–Koehler Force

To generalize the dislocation force, consider a dislocation with Burgers vector $\bar{b}$, line direction $\bar{t}$, and an external stress tensor σ . If the dislocation moves an infinitesimal distance ds in direction $\bar{e}$, the work done is:

$$dW = -\bar{b} \cdot [\sigma(\bar{t} \times \bar{e})] ds \quad (\text{Chapter 9.30})$$

The force per unit length on the dislocation is then:

$$\bar{f} = -\frac{dW}{ds} = \bar{e} [(\sigma\bar{b}) \times \bar{t}] \quad (\text{Chapter 9.31})$$

or equivalently,

$$\bar{f}_{PK} = (\sigma\bar{b}) \times \bar{t} \quad (\text{Chapter 9.32})$$

This is the Peach–Koehler force, which describes the mechanical force acting on a dislocation line in any stress field. It is important to emphasize that the force arises from the external stress field, not from the dislocation's own stress. The applied stress can come from other dislocations, grain boundaries, or external loading.

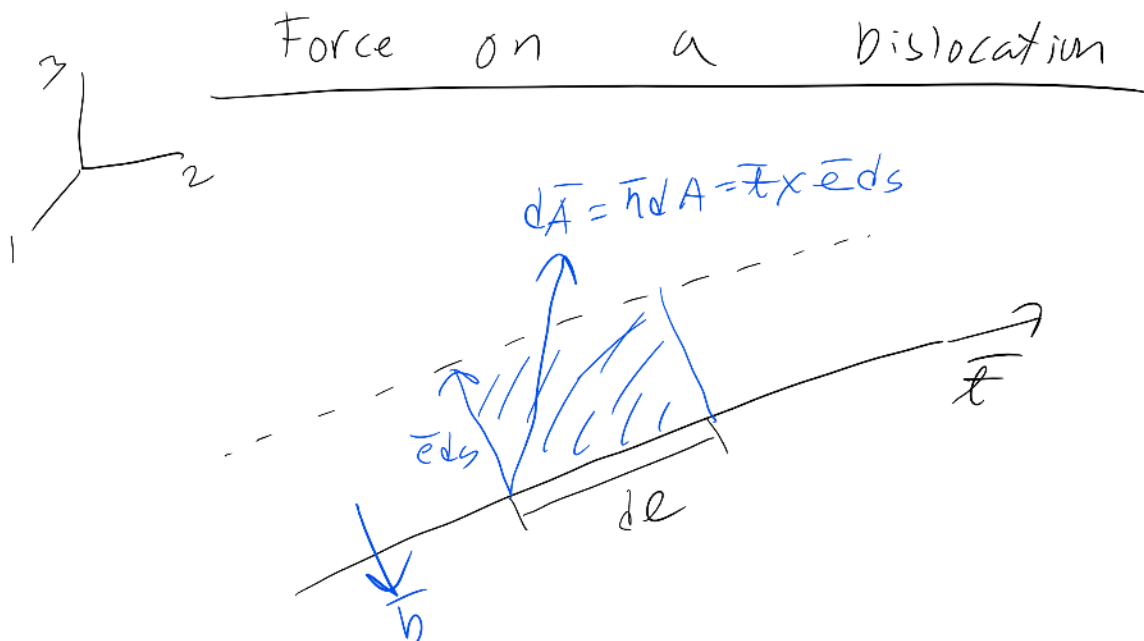


Figure Chapter9.5: Peach–Koehler force (PK).

This derivation is a remarkable result — we have derived a force at the defect level using continuum mechanics and energy concepts. This multiscale linkage between atomic and macroscopic behavior is a hallmark of materials science. Importantly, the Peach–Koehler force represents a thermodynamic driving force (derived from energy gradients), not a classical Newtonian force.

Dislocation Glide and Climb

The Peach–Koehler force provides the driving force for dislocation motion. When the force acts within the dislocation's slip plane, it causes glide. Glide occurs when shear stress is applied along the slip plane, allowing the dislocation to move through the crystal lattice and produce plastic deformation. The dislocation moves in the plane that contains both its line direction and Burgers vector.

Dislocation climb, on the other hand, involves motion perpendicular to the slip plane. Climb requires the diffusion of vacancies or atoms to or from the dislocation core and is therefore a thermally activated process. Climb is crucial for high-temperature deformation mechanisms such as creep.

Mixed dislocations, which have both edge and screw components, can experience both glide and climb, depending on local stress and temperature conditions.

Diffusion in Materials Refresher

Before continuing our discussion of dislocation motion, it is useful to review the fundamental principles of diffusion, as diffusion is essential for dislocation climb and other thermally activated processes.

Thermodynamics is the study of equilibrium states, where the state variables of a system do not change with time. Kinetics, in contrast, is the study of the rates at which systems that are out of equilibrium evolve toward equilibrium under the influence of various driving forces.

Diffusion and Fick's First Law

Diffusion is the phenomenon of material transport by atomic motion. It typically involves the flux of chemical components, which arises from gradients in driving forces such as electrostatic potential, stress, temperature, or chemical potential.

Fick's First Law expresses diffusion due to a concentration gradient:

$$\vec{J}_i = -D\nabla c_i = -D \frac{\partial c_i}{\partial x} \quad (\text{Chapter 9.33})$$

where:

- D is the diffusion coefficient (mass diffusivity),
- $\vec{J}_i$ is the flux of species i ,
- ∇c_i is the concentration gradient.

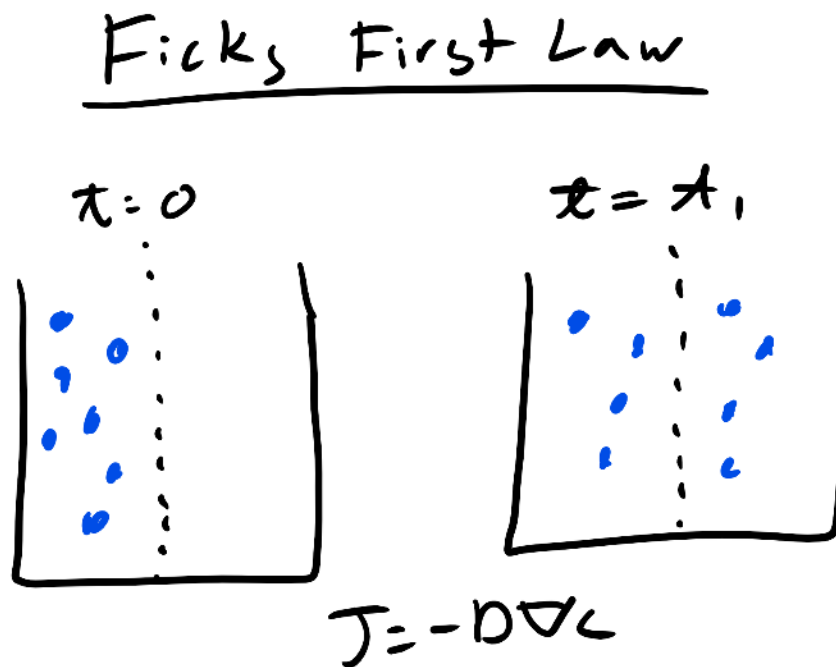


Figure Chapter9.6: Schematic of Fickian Flux.

This equation has the same mathematical form as other transport laws. For example, in heat transfer:

$$\vec{J}_Q = -k\nabla T \quad (\text{Chapter 9.34})$$

where $\vec{J}_Q$ is the heat flux, k is the thermal conductivity, and ∇T is the temperature gradient.

Similarly, for charge flow:

$$\vec{J}_q = -\nabla\phi \quad (\text{Chapter 9.35})$$

where $\vec{J}_q$ is the charge flux and $\nabla\phi$ is the gradient of electric potential.

In all cases, flux is proportional to the negative gradient of a potential — a general statement that a system tends to move toward equilibrium by dissipating gradients.

Charged Species

One example of diffusion involving charged species occurs in lithium-ion batteries, where both chemical and electric field gradients contribute to ionic flux. The total flux is the sum of these contributions. Depending on their relative magnitudes, the system may exhibit zero net flux (steady state) or even “uphill” diffusion if the electric field dominates.

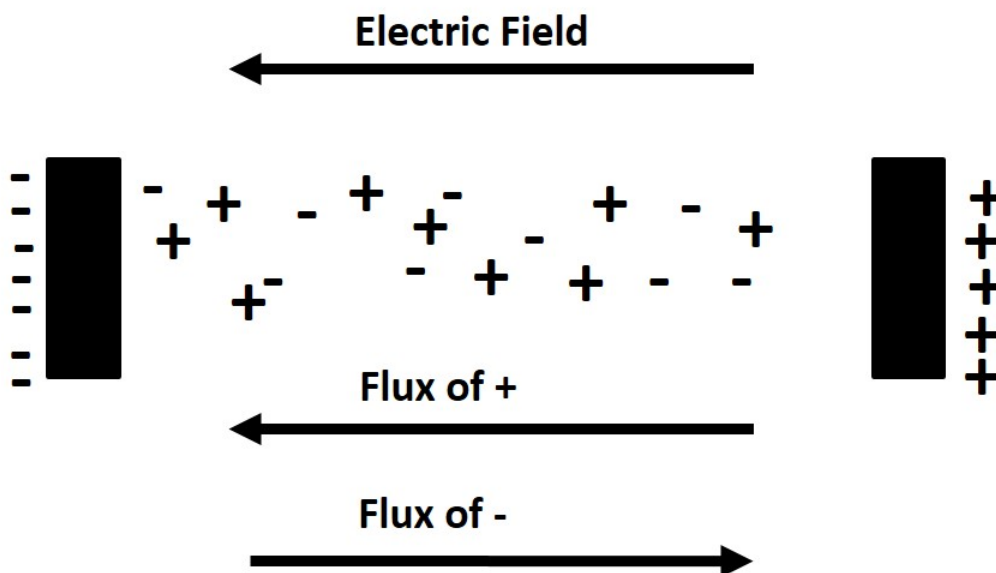


Figure Chapter9.7: Electric Driven Diffusion.

Temperature Gradients

Diffusion can also be driven by thermal gradients. Typically, atoms migrate toward regions of higher temperature because increased atomic vibration lowers activation barriers for diffusion.

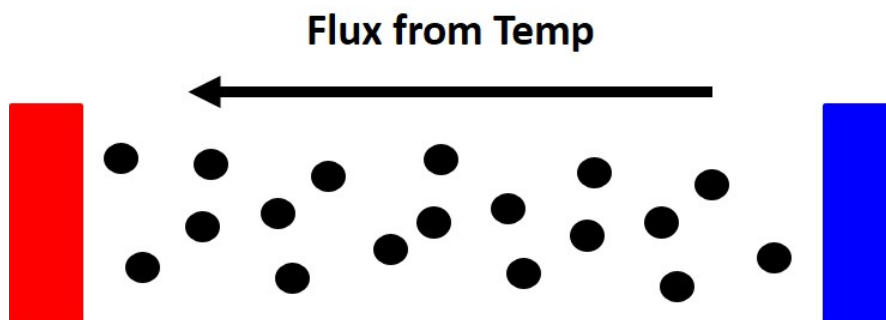


Figure Chapter9.8: Temperature Driven Diffusion.

Curvature Effects

Diffusion can also be driven by surface curvature. Material tends to diffuse from regions of positive curvature (convex) to regions of negative curvature (concave), smoothing the surface over time.

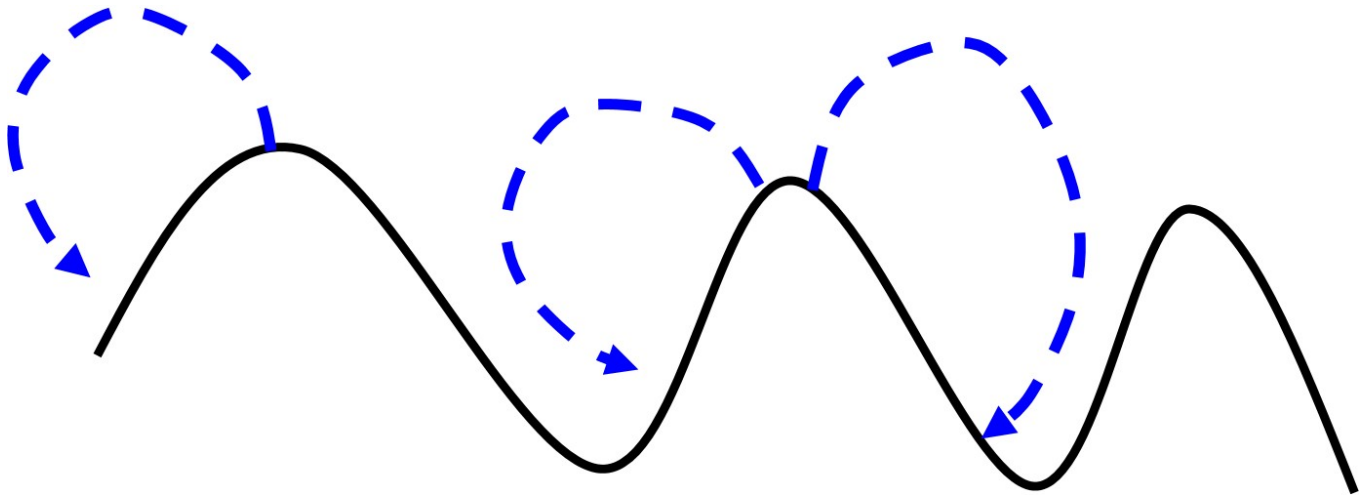


Figure Chapter9.9: Curvature Driven Gradient.

Stress-Driven Diffusion

Stress gradients can drive atomic motion as well. In regions of hydrostatic stress, atoms tend to diffuse from compressive regions to tensile regions. Around an edge dislocation, for example, solute atoms will diffuse toward the tensile region beneath the dislocation until a steady-state configuration is reached — this is known as a Cottrell atmosphere.

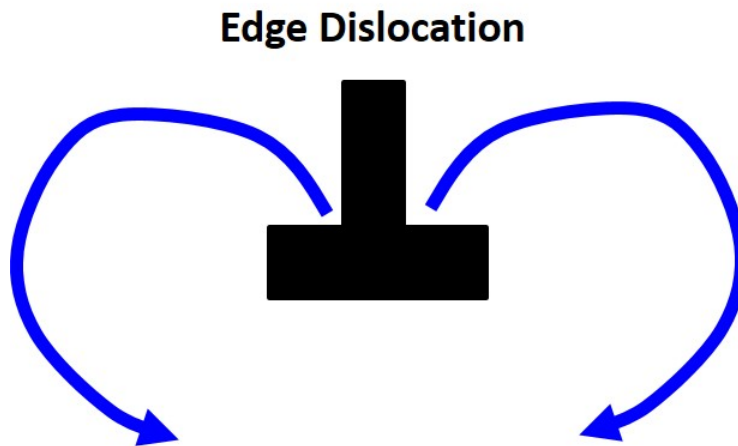


Figure Chapter9.10: Stress Driven Diffusion.

Fick's Second Law

So far, we have considered steady-state diffusion under constant gradients, but diffusion in most materials is time-dependent. To account for this, we use Fick's Second Law:

$$\frac{\partial c}{\partial t} = \dot{n} - \nabla \cdot \vec{J} \quad (\text{Chapter 9.36})$$

where $\dot{n}$ is the rate of creation of new species (often zero) and $\vec{J}$ is the flux. Substituting Fick's First Law ($\vec{J} = -D\nabla c$) gives:

$$\frac{\partial c}{\partial t} = D(c)\nabla^2 c + \frac{dD(c)}{dc}(\nabla c)^2 \quad (\text{Chapter 9.37})$$

This form applies when the diffusivity D depends on concentration. For most engineering cases, D is approximately constant, reducing the equation to the classical form:

$$\frac{\partial c}{\partial t} = D \nabla^2 c \quad (\text{Chapter 9.38})$$

This partial differential equation describes how the concentration field $c(x, t)$ evolves with time. We can solve it for specific boundary conditions, such as a diffusion couple.

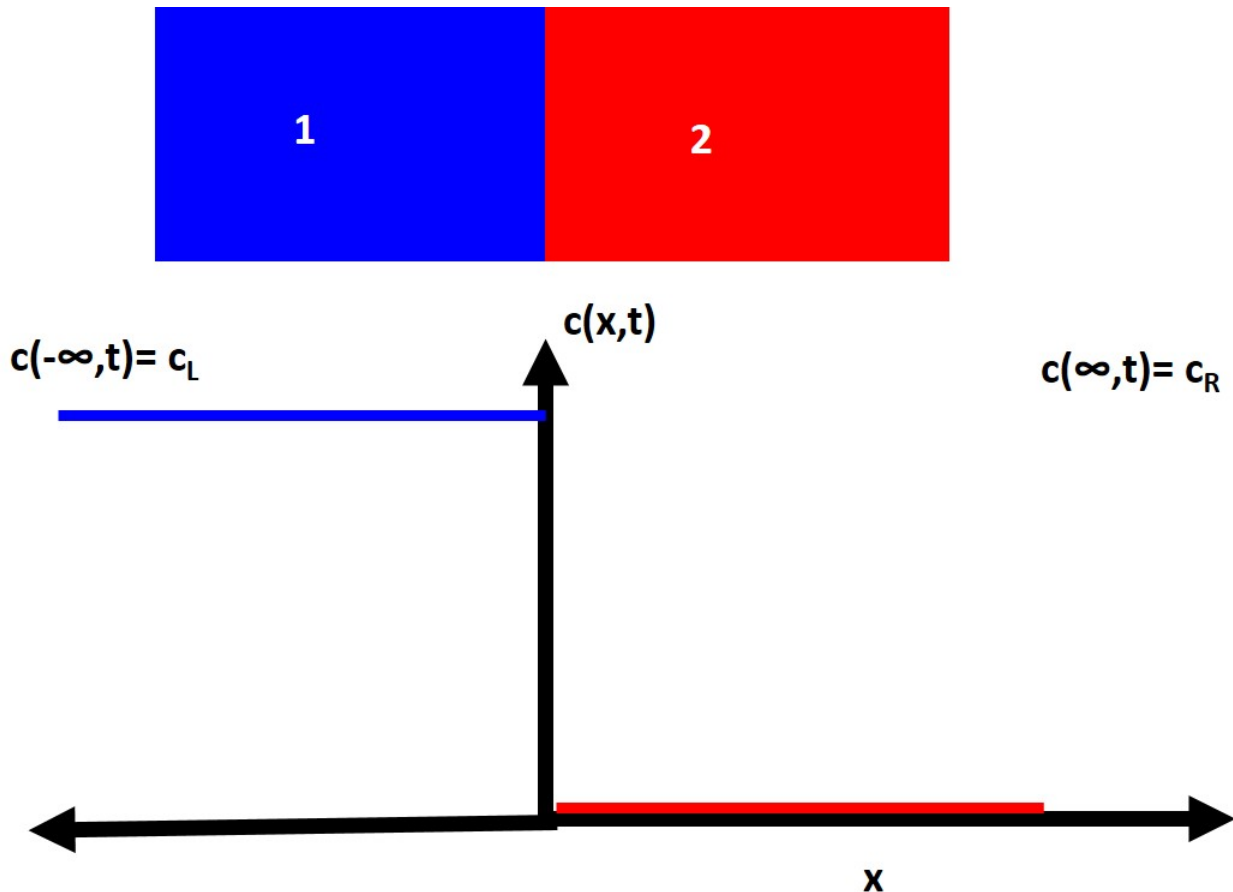


Figure Chapter9.11: Diffusion Couple Concentration Evolution.

To solve this, we introduce a dimensionless variable:

$$\eta = \frac{x}{\sqrt{4Dt}} \quad (\text{Chapter 9.39})$$

Using this substitution, Fick's Second Law (in one dimension) simplifies to an ordinary differential equation in η :

$$-2\eta \frac{\partial c}{\partial \eta} = \frac{\partial^2 c}{\partial \eta^2} \quad (\text{Chapter 9.40})$$

The boundary conditions are:

$$c(\eta = -\infty) = c^L, \quad c(\eta = \infty) = c^R \quad (\text{Chapter 9.41})$$

The solution is:

$$c(\eta) = c^L + \frac{a_1}{\sqrt{\pi}} \left(\int_0^{-\infty} e^{-\zeta^2} d\zeta + \int_0^{\eta} e^{-\zeta^2} d\zeta \right) \quad (\text{Chapter 9.42})$$

In practice, this is equivalent to the well-known error function solution for diffusion in a semi-infinite medium.

When can we make the semi-infinite approximation?

The semi-infinite approximation applies when the diffusion length is much smaller than the specimen size:

$$l > 10\sqrt{Dt} \quad (\text{Chapter 9.43})$$

Engineering Approximation for Diffusion Depth

Many diffusion problems can be solved analytically using the above substitution or numerically. However, there is also a simple engineering approximation for estimating diffusion depth. The solutions to diffusion problems often have an error function (erf) shape, which flattens out for $\text{erf}(x) \approx 1$. This occurs when $x \approx 2$, so we can estimate the diffusion depth x as:

$$1 = \frac{x}{2\sqrt{Dt}} \quad (\text{Chapter 9.44})$$

This provides a quick estimate for how far atoms or species have diffused in a given time.

Arrhenius Temperature Dependence of Diffusion and Anisotropy

So far, we have discussed the concentration dependence of diffusivity D , but D also depends strongly on temperature and crystal structure. The temperature dependence follows an Arrhenius relationship:

$$D = D_0 \exp\left(\frac{-Q_a}{kT}\right) \quad (\text{Chapter 9.45})$$

where D_0 is the pre-exponential factor and Q_a is the activation energy for diffusion.

Diffusion is also often anisotropic, especially in crystalline materials where the diffusion path length varies by direction. For example:

Cubic materials:

$$\begin{bmatrix} D_{11} & 0 & 0 \\ 0 & D_{11} & 0 \\ 0 & 0 & D_{11} \end{bmatrix} \quad (\text{Chapter 9.46})$$

Tetragonal or hexagonal materials:

$$\begin{bmatrix} D_{11} & 0 & 0 \\ 0 & D_{11} & 0 \\ 0 & 0 & D_{33} \end{bmatrix} \quad (\text{Chapter 9.47})$$

Orthorhombic materials:

$$\begin{bmatrix} D_{11} & 0 & 0 \\ 0 & D_{22} & 0 \\ 0 & 0 & D_{33} \end{bmatrix} \quad (\text{Chapter 9.48})$$

Monoclinic materials:

$$\begin{bmatrix} D_{11} & 0 & D_{13} \\ 0 & D_{22} & 0 \\ D_{31} & 0 & D_{33} \end{bmatrix} \quad (\text{Chapter 9.49})$$

Triclinic materials:

$$\begin{bmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix} \quad (\text{Chapter 9.50})$$

This shows how the crystal symmetry determines the number of independent diffusion coefficients.

Diffusion as a Random Walk

Another way to think about diffusion is as a series of discrete atomic jumps in a random walk. The diffusivity can be expressed as:

$$D = \frac{N\Gamma\langle r^2 \rangle f}{2d} \quad (\text{Chapter 9.51})$$

where:

- $\langle r^2 \rangle$ is the mean squared jump distance,
- d is the dimensionality of diffusion (1D, 2D, or 3D),
- f is the correlation factor that accounts for non-random motion,
- N is the number of available neighboring sites,
- Γ is the atomic jump frequency.

The jump frequency is itself thermally activated and follows an Arrhenius form:

$$\Gamma = \nu \exp\left(\frac{-G^m}{kT}\right) \quad (\text{Chapter 9.52})$$

where ν is the attempt frequency (on the order of atomic vibration frequencies) and G^m is the migration free energy for the atomic jump.

The correlation factor f quantifies how correlated successive atomic jumps are:

- For a perfect random walk, $f = 1$.
- For completely back-and-forth motion (each jump reversed by the next), $f = 0$.

Most diffusion processes in solids have $f \approx 1$.

Diffusion Mechanisms

We now apply this framework to the major diffusion mechanisms found in solids.

Vacancy Diffusion

The predominant mechanism for self-diffusion in metals (FCC, BCC, HCP) and many ionic crystals is vacancy diffusion. The atom moves by jumping into an adjacent vacant lattice site.

For an FCC crystal, the diffusivity can be expressed as:

$$D = a^2 \nu \exp\left(\frac{S_v^m + S_v^f}{k}\right) \exp\left(\frac{-H_v^m - H_v^f}{kT}\right) \quad (\text{Chapter 9.53})$$

where:

- a is the lattice constant,
- S_v^m and S_v^f are the migration and formation entropies of the vacancy,
- H_v^m and H_v^f are the migration and formation enthalpies,
- $N = 12$ for FCC (12 nearest neighbor sites),
- The jump distance is $r = \frac{a}{\sqrt{2}}$.

Interstitial Diffusion

Interstitial diffusion occurs for small solute atoms moving through the interstitial sites of a crystal lattice of much larger atoms. This mechanism is much faster than vacancy diffusion since it does not require vacancy formation.

For example, consider the interstitial diffusion of carbon in BCC iron (ferrite). Carbon atoms occupy octahedral interstitial sites. The diffusivity is:

$$D = \frac{a^2}{6} \nu \exp\left(\frac{S^m}{k}\right) \exp\left(\frac{-H^m}{kT}\right) \quad (\text{Chapter 9.54})$$

where:

- a is the lattice parameter,
- $N = 4$ for BCC (4 neighboring octahedral sites),
- The jump distance is $r = \frac{a}{2}$.

Other Diffusion Mechanisms

In addition to vacancy and interstitial diffusion, several other mechanisms can occur:

- Interstitialcy (kick-out) mechanism, where two atoms exchange positions cooperatively.

- Ring mechanism, common in ionic and covalent materials.
- Grain boundary diffusion and surface diffusion, which occur at higher rates due to more open atomic packing at interfaces.

Diffusion Depends on Local Environment

The diffusivity of a material also depends on its local microstructural environment — whether atoms are in the bulk lattice, near a dislocation core, along a grain boundary, or on a free surface. The relative magnitudes of diffusion coefficients are generally:

$$D^L > D^S > D^D \approx D^B > D^{XL} \quad (\text{Chapter 9.55})$$

where:

- D^L : diffusivity in a liquid
- D^S : diffusivity along a surface
- D^D : diffusivity along a dislocation
- D^B : diffusivity along a grain boundary
- D^{XL} : bulk (crystalline lattice) diffusivity

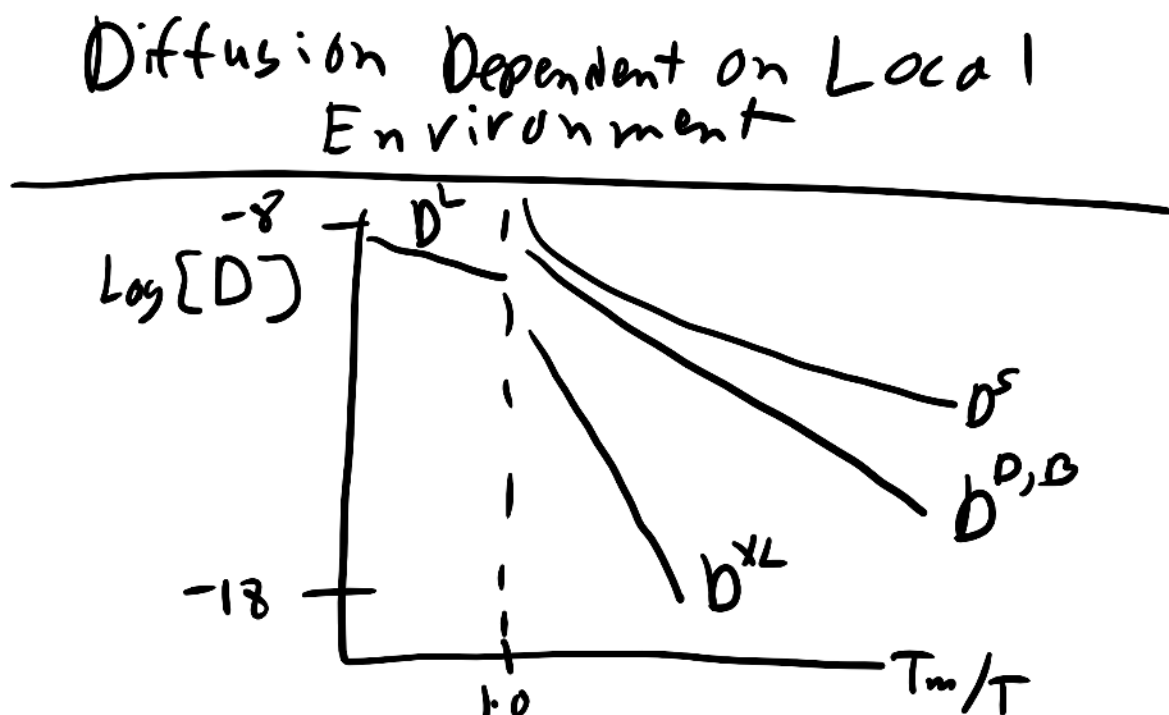


Figure Chapter9.12: Diffusion in different environments.

This ranking makes intuitive sense. Regions with more free volume, such as grain boundaries or surfaces, provide easier pathways for atomic migration, resulting in higher diffusivity. In contrast, atoms in a perfect crystal must rely solely on thermal vibrations to open space for diffusion, making bulk diffusion much slower.

Elastic Strain Energy of Edge Dislocation Dipoles

Let us now examine how two dislocations interact elastically. Consider two edge dislocations separated by a distance d , each with Burgers vectors b_1 and b_2 . The first dislocation is located at the origin. We can think of these dislocations analogously to electric dipoles — with opposite Burgers vectors, they attract; with the same Burgers vectors, they repel.

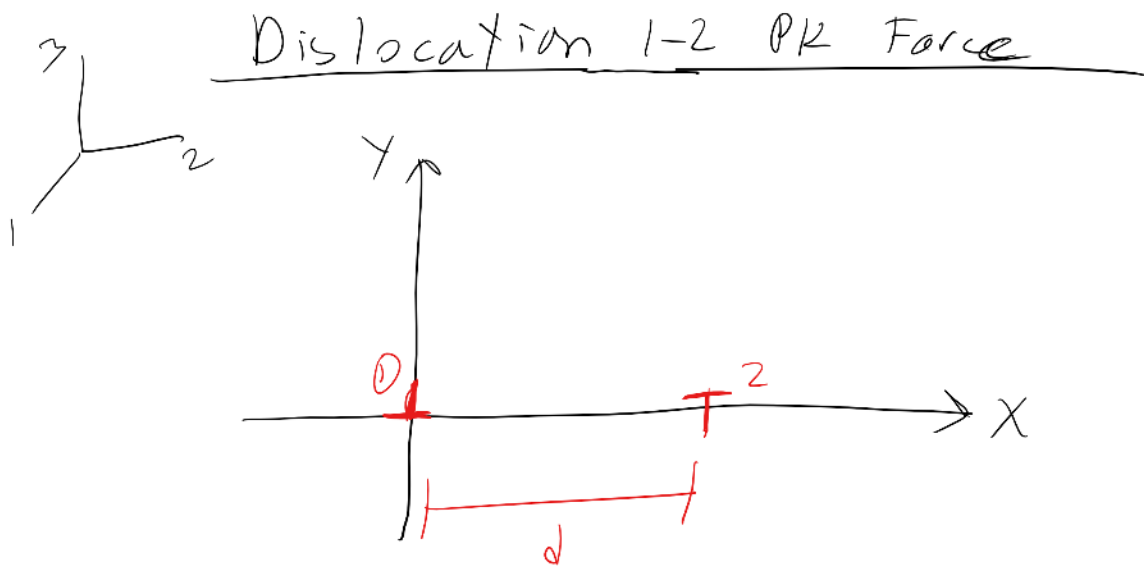


Figure Chapter9.13: Peach–Koehler force between two dislocations.

The stress field of the first dislocation produces a force on the second dislocation that can be calculated using the Peach–Koehler formalism:

$$\bar{b}_2 = b_2 i, \quad \bar{t}_2 = k \quad (\text{Chapter 9.56})$$

$$\bar{f}_{12} = (\sigma^1 \cdot \bar{b}_2) \times \bar{t}_2 = \sigma_{xy}^1 b_2 i - \sigma_{xx}^1 b_2 j \quad (\text{Chapter 9.57})$$

Focusing on motion along the x-axis, the force per unit length is:

$$f_{12} = \sigma_{xy}^1 b_2 = \frac{Gb_1 b_2}{2\pi(1-\nu)d} \quad (\text{Chapter 9.58})$$

This expression matches our intuition — dislocations with the same Burgers vector repel, while dislocations with opposite Burgers vectors attract and can annihilate each other.

We can also calculate the elastic strain energy associated with two dislocations by integrating the force required to move them apart from a state where they were annihilated (separation r_0) to a separation distance d :

$$\frac{\Delta U_{\text{edge-int}}}{l} = \int_{r_0}^d f_{12} dx = \frac{Gb^2}{2\pi(1-\nu)} \ln\left(\frac{d}{r_0}\right) \quad (\text{Chapter 9.59})$$

This equation shows that for two dislocations of opposite Burgers vectors, the free energy decreases as they move closer together — confirming that annihilation is energetically favorable.

Dislocation Motion

Returning to dislocation motion, recall that glide occurs within the slip plane of the dislocation, while climb involves motion perpendicular to the slip plane. Climb requires the absorption or emission of vacancies or interstitials, and is therefore thermally activated.

The normal to the glide plane is given by:

$$\bar{n} = \frac{\bar{t} \times \bar{b}}{|\bar{t} \times \bar{b}|} \quad (\text{Chapter 9.60})$$

Note that by this definition, a pure screw dislocation does not have a unique glide plane, enabling a special mechanism known as cross-slip. Cross-slip is important for plastic deformation in metals, particularly at low temperatures, and occurs when a screw dislocation moves from one slip plane to another.

Slip Systems

Each material has a specific set of crystallographic planes and directions on which dislocations preferentially glide, known as slip systems.

For FCC materials:

$$\begin{aligned} \text{Slip planes: } \{111\}, \quad \text{Slip directions: } \langle 110 \rangle, \\ \text{Slip system: } \{111\}\langle 110 \rangle \end{aligned} \quad (\text{Chapter 9.61})$$

For BCC materials:

$$\begin{aligned} \text{Slip planes: } \{110\}, \quad \text{Slip directions: } \langle 111 \rangle, \\ \text{Slip system: } \{110\}\langle 111 \rangle \end{aligned} \quad (\text{Chapter 9.62})$$

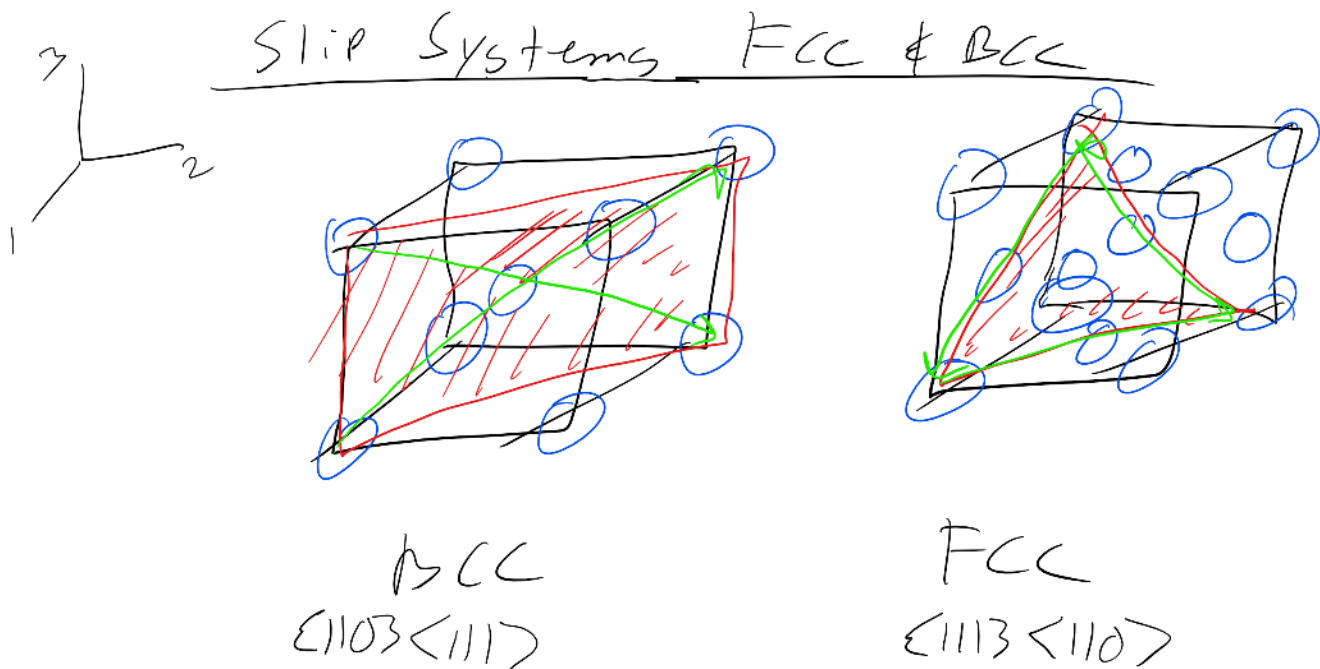


Figure Chapter9.14: Slip systems.

These directions and planes are the most densely packed in their respective lattices. Because they minimize the energy per unit length of the dislocation, they are the most energetically favorable slip systems. In materials with high stacking fault energies (such as aluminum), dislocations tend to remain undissociated, whereas in low stacking fault energy materials (such as copper), dislocations can split into partials.

Glissile and Sessile Dislocations

Dislocations that can move easily are called glissile, while those that are immobile under applied stress are sessile. Sessile dislocations can form when dislocation reactions produce new dislocations with Burgers vectors that are not aligned with any slip system, preventing glide. Sessile dislocations play an important role in strain hardening.

Dislocation Climb

Dislocation climb requires atomic transport perpendicular to the slip plane. This process is governed by the diffusion of vacancies or interstitials to and from the dislocation core. It is therefore slow at low temperatures and becomes significant during high-temperature creep.

The motion of dislocations under applied stress can be analyzed in terms of the resolved shear stress τ acting on the slip system. The resolved shear stress is given by:

$$\tau = \alpha_{ij} \sigma_{ij} \quad (\text{Chapter 9.63})$$

$$\alpha_{ij} = \frac{1}{2}(\bar{b}_i \bar{n}_j + \bar{b}_j \bar{n}_i) \quad (\text{Chapter 9.64})$$

Here, α_{ij} is the Schmid tensor, which projects the stress tensor onto the slip system.

A critical resolved shear stress (CRSS), denoted τ_{crss} , must be reached before a dislocation can move. This is sometimes referred to as the lattice resistance. For FCC metals, τ_{crss} is small, so dislocations glide easily. In contrast, for covalent or ionic solids (e.g., diamond or ceramics), τ_{crss} is extremely high, and fracture often occurs before any significant plastic deformation.

Kink Motion, Climb Kinetics, and Orowan's Equation

At low temperatures in certain materials, particularly BCC metals, dislocation motion can occur via the nucleation and migration of kinks. A kink is a step on a dislocation line within its glide plane, whereas a jog is a step that moves out of the glide plane.

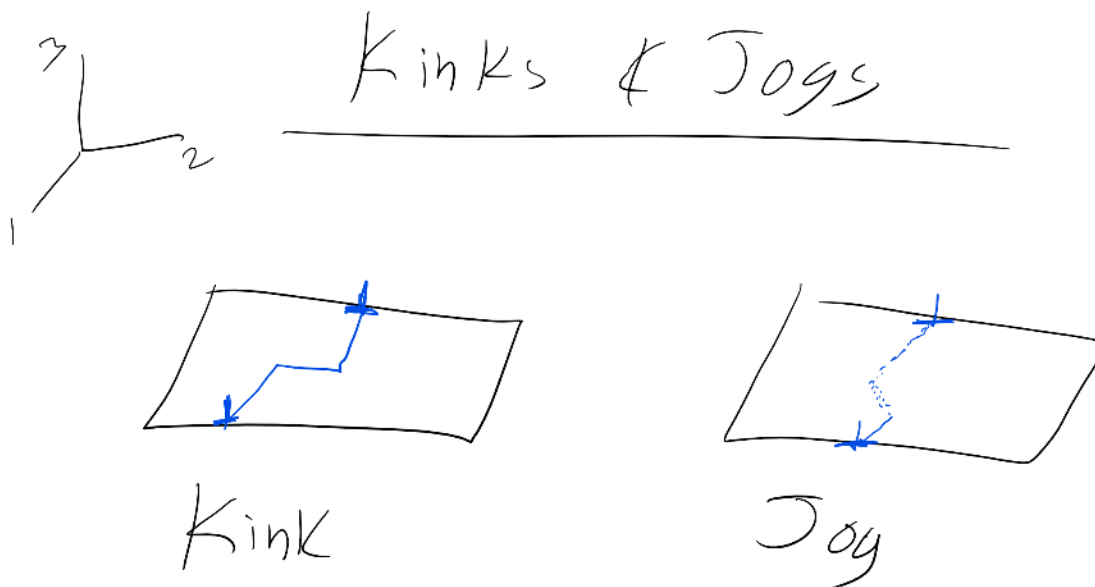


Figure Chapter9.15: Kinks vs. jogs.

For edge dislocations, jogs require mass transport (diffusion of atoms or vacancies) to move, while for screw dislocations, both steps are referred to as kinks. The motion of dislocations through kink propagation can be visualized as movement through a potential energy landscape — dislocations move through successive energy barriers, with each kink hopping from one potential minimum to the next.

Kink Motion

The formation and migration of kinks are thermally activated processes. The rate of kink motion depends on the applied stress τ , Burgers vector b , and temperature T . The forward and backward jump frequencies for kinks are:

$$\Gamma_+ \approx \nu \exp \left[-\frac{(\Delta G_k^m - \frac{\tau b^3}{2})}{kT} \right] \quad (\text{Chapter 9.65})$$

$$\Gamma_- \approx \nu \exp \left[-\frac{(\Delta G_k^m + \frac{\tau b^3}{2})}{kT} \right] \quad (\text{Chapter 9.66})$$

where ν is the attempt frequency, and ΔG_k^m is the migration free energy for kink motion. The net rate is:

$$\Gamma = \Gamma_+ - \Gamma_- \approx 2\nu \exp \left(-\frac{\Delta G_k^m}{kT} \right) \sinh \left(\frac{\tau b^3}{2kT} \right) \quad (\text{Chapter 9.67})$$

At low stresses, where $\sinh(x) \approx x$, this simplifies to:

$$\Gamma \approx \nu \exp \left(-\frac{\Delta G_k^m}{kT} \right) \frac{\tau b^3}{2kT} \quad (\text{Chapter 9.68})$$

The velocity of a single kink is then:

$$v_k = b\Gamma \quad (\text{Chapter 9.69})$$

If multiple kinks are distributed along the dislocation line, each separated by distance l , the average dislocation velocity becomes:

$$v = \frac{b^2 \nu}{l} \exp \left(-\frac{\Delta G_k^m}{kT} \right) \frac{\tau b^3}{2kT} = D_k \frac{\tau b^3}{2kT} \quad (\text{Chapter 9.70})$$

where D_k is the kink diffusivity, which follows Arrhenius behavior.

The equilibrium concentration of kinks per unit length is given by:

$$c_k = \frac{1}{l} = \frac{\exp \left(-\frac{\Delta G_k^f}{kT} \right)}{b} \quad (\text{Chapter 9.71})$$

where ΔG_k^f is the kink formation free energy. Combining these relationships gives a general mobility law for dislocations:

$$v = D_k \exp \left(-\frac{\Delta G_k^f}{kT} \right) \frac{\tau b^2}{kT} \quad (\text{Chapter 9.72})$$

At high stresses, dislocation velocity is governed by the nucleation and separation of kink pairs. The free energy for forming a kink pair is:

$$\Delta G_{kp}^f = 2\Delta G_k^f \left(1 - \frac{\tau}{\tau_{max}} \right)^2 \quad (\text{Chapter 9.73})$$

where τ_{max} is the threshold stress beyond which no thermal activation is required to move kinks.

Dislocation Climb

Dislocation climb, unlike glide, requires diffusion of vacancies or interstitials to or from the dislocation core. The emission and trapping rates of vacancies are given by:

$$\Gamma_{emit} = \nu \exp \left(-\frac{\Delta G_v^f}{kT} \right) \exp \left(-\frac{\Delta G_v^m - \frac{\sigma b^3}{2}}{kT} \right) \quad (\text{Chapter 9.74})$$

$$\Gamma_{trap} = \nu n_v \exp \left(-\frac{\Delta G_v^m + \frac{\sigma b^3}{2}}{kT} \right) \quad (\text{Chapter 9.75})$$

where σ is the applied stress and n_v is the equilibrium vacancy concentration. The net rate, assuming steady-state conditions and low stress, becomes:

$$\Gamma = \Gamma_{emit} - \Gamma_{trap} \approx \nu n_v \exp\left(-\frac{\Delta G_v^m}{kT}\right) \frac{\sigma b^3}{kT} \quad (\text{Chapter 9.76})$$

Since climb velocity is proportional to the jump rate:

$$v_j = b\Gamma \quad (\text{Chapter 9.77})$$

and if there is a concentration c_j of jogs along the dislocation line, the overall dislocation climb velocity is:

$$v = b^2 n_v c_j \nu \exp\left(-\frac{\Delta G_v^m}{kT}\right) \frac{\sigma b^3}{kT} = D_s \frac{c_j \sigma b^3}{kT} \quad (\text{Chapter 9.78})$$

where $D_s = D_v n_v$ is the self-diffusivity.

Orowan's Equation for Dislocation Motion

The relationship between dislocation motion and plastic strain rate was established by Orowan, who related the strain rate to the dislocation density and velocity.

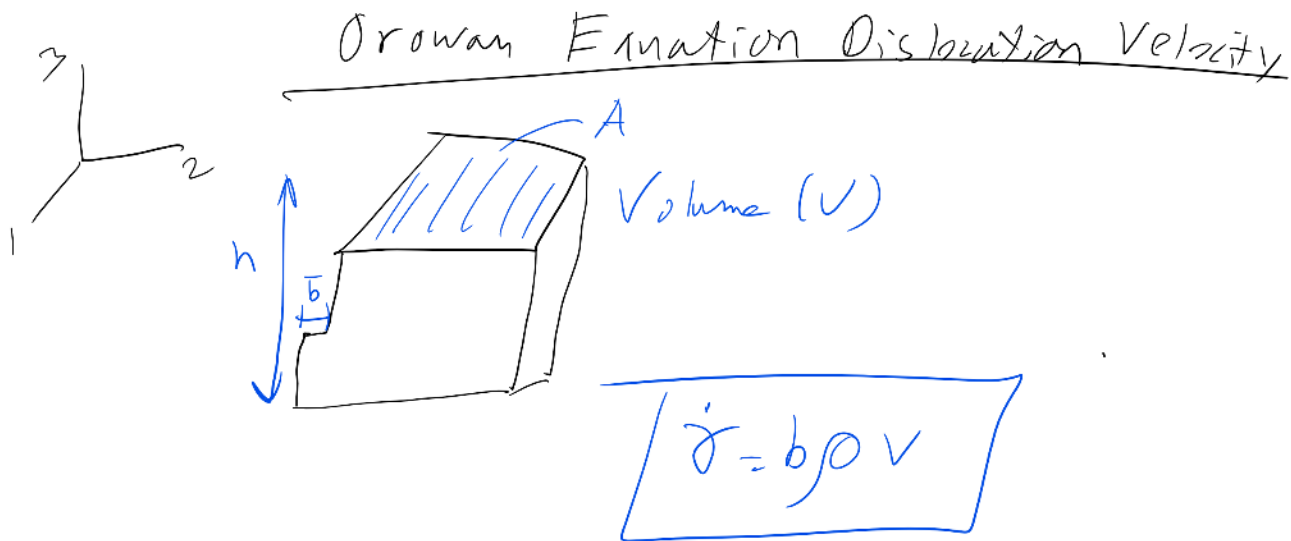


Figure Chapter9.16: Orowan's equation for dislocation motion.

The shear strain from the passage of one dislocation is:

$$\gamma = \frac{b}{h} = \frac{bA}{V} \quad (\text{Chapter 9.79})$$

For incremental dislocation motion dx :

$$d\gamma = b \frac{dA}{V} = \frac{b dx}{V} \quad (\text{Chapter 9.80})$$

For n dislocations:

$$d\gamma = \frac{n b dx}{V} \quad (\text{Chapter 9.81})$$

Since dislocation density $\rho = \frac{n}{V}$, we can express this as:

$$d\gamma = b \rho dx \quad (\text{Chapter 9.82})$$

and differentiating with respect to time gives:

$$\dot{\gamma} = b\rho v \quad (\text{Chapter 9.83})$$

This is the Orowan equation, a fundamental relationship linking the macroscopic plastic strain rate $\dot{\gamma}$ to microscopic dislocation properties. It tells us that plastic deformation rate increases with dislocation density, Burgers vector magnitude, and dislocation velocity.

Dislocation Reactions, Sources, and Sessile Dislocations

We have covered the forces on dislocations, their stress fields, and mobility. Now, we turn to interactions between dislocations that can either increase or decrease the yield strength of a material. These interactions are collectively referred to as dislocation reactions.

When two dislocations meet, they can react with one another, and these reactions can occur spontaneously if the total energy of the system decreases. The Burgers vector of the resulting dislocation is the vector sum of the Burgers vectors of the reactants.

According to Frank's Rule, the energy per unit length of a dislocation is proportional to the square of its Burgers vector. Therefore, a dislocation reaction is energetically favorable (spontaneous) if:

$$b_{product}^2 < b_1^2 + b_2^2 \quad (\text{Chapter 9.84})$$

A simple example of this is the annihilation of two dislocations with equal and opposite Burgers vectors, producing a perfect crystal with $b_{product} = 0$.

Generating New Dislocations

There are several mechanisms by which new dislocations can form in a material:

1. Generation from Dislocation Sources
2. Heterogeneous Nucleation
3. Homogeneous Nucleation

Generation of New Dislocations from Dislocation Sources

One of the most important and efficient ways to generate new dislocations is through the Frank–Read (FR) source. Imagine a dislocation segment pinned at both ends. When a shear stress is applied, the dislocation bows out in the direction of the applied force. The opposing force is the line tension due to the dislocation's curvature.

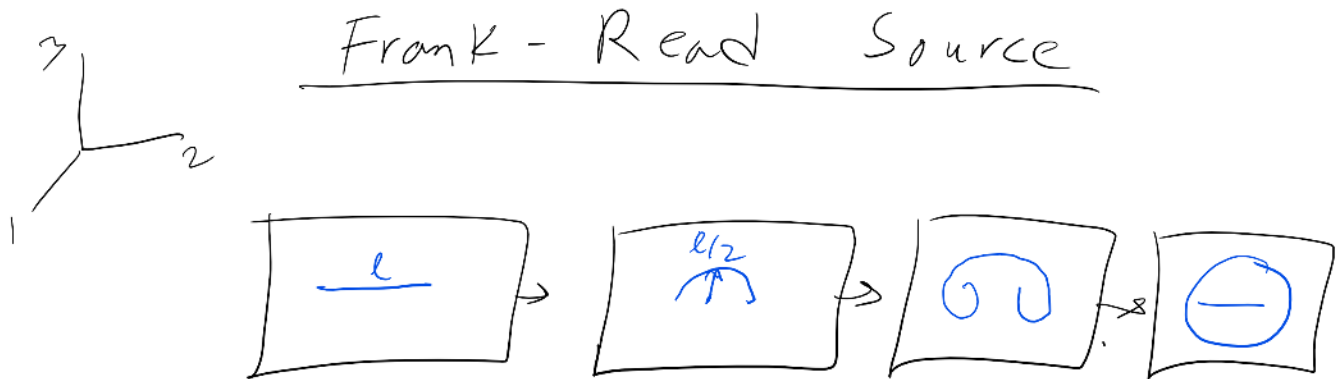


Figure Chapter9.17: Frank-Read source.

The curvature κ of the bowed-out dislocation is:

$$\kappa = \frac{1}{r} \quad (\text{Chapter 9.85})$$

Initially, when the dislocation is straight, the curvature is zero because $r \rightarrow \infty$. As the dislocation bows out, the curvature increases, reaching a maximum when $r = \frac{l}{2}$. The critical resolved shear stress required to reach this condition is found by equating the applied force per unit length ($\tau_c b$) to the maximum line tension ($\frac{Gb^2}{4\pi R}$):

$$\tau_c b = \frac{Gb^2}{2\pi l} \quad (\text{Chapter 9.86})$$

$$\tau_c = \frac{Gb}{2\pi l} \quad (\text{Chapter 9.87})$$

Beyond this point, further bowing reduces the curvature, and the dislocation eventually loops back on itself. The two opposing segments of the dislocation annihilate where they meet, leaving behind a closed dislocation loop and reestablishing the original pinned segment — now ready to repeat the process. This mechanism can produce a large number of dislocation loops from a single source under constant applied stress.

There also exists a single-ended version of this source, where the dislocation is pinned at only one end and spirals outward, known as a spiral Frank-Read source. Another related mechanism is the Bardeen-Herring (BH) source, which operates through dislocation climb rather than glide.

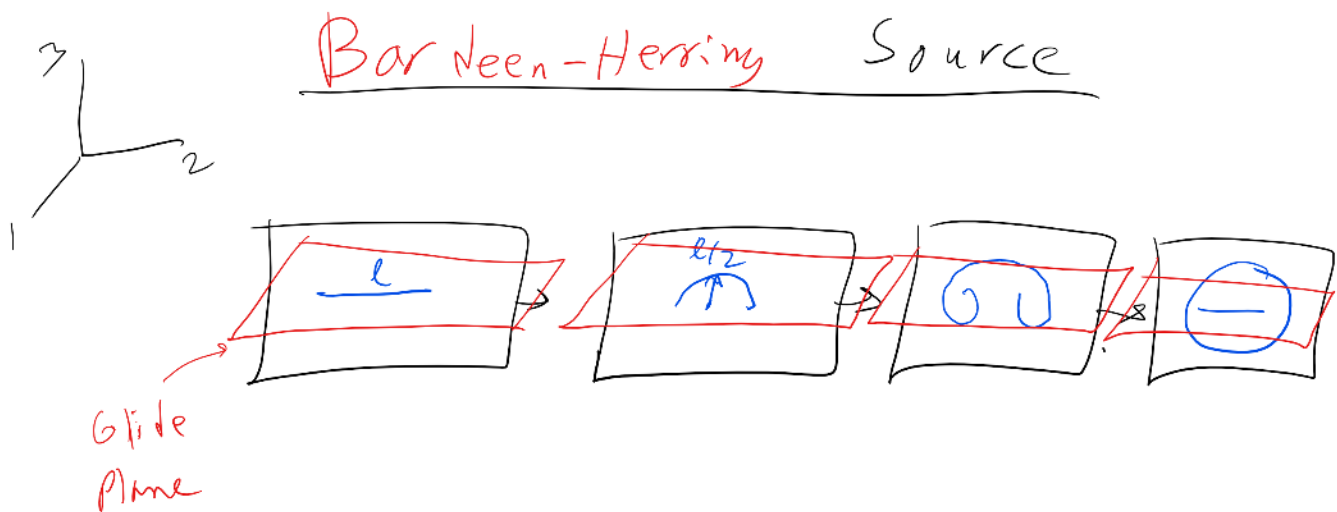


Figure Chapter9.18: Bardeen-Herring source.

Heterogeneous Dislocation Nucleation

Dislocations can also nucleate heterogeneously at existing defects such as grain boundaries, free surfaces, or other dislocations. This type of nucleation requires less stress than homogeneous nucleation because the presence of a defect reduces the energy barrier for dislocation formation. However, since the nucleus is on the atomic scale, linear elasticity theory cannot describe it accurately, and atomistic modeling is typically required.

Homogeneous Dislocation Nucleation

Homogeneous nucleation refers to dislocation formation within a perfect crystal, without the aid of preexisting defects. It requires extremely high stresses, close to the theoretical shear strength of the material ($\approx G/10$). Homogeneous nucleation typically involves the formation of dislocation loops, as dislocations cannot start or end inside a perfect lattice. This mechanism is rare and generally only occurs under very high applied stresses, such as during shock loading or intense deformation.

Formation of Sessile Dislocations

Certain dislocation reactions produce dislocations that are sessile — meaning they cannot move by glide. Sessile dislocations play a key role in strain hardening because they act as obstacles to dislocation motion, increasing the yield strength.

A well-known example occurs in FCC metals through the Lomer-Cottrell reaction. Two glissile dislocations on intersecting $\{111\}$ planes react to form a sessile dislocation along the line of intersection of the two planes.

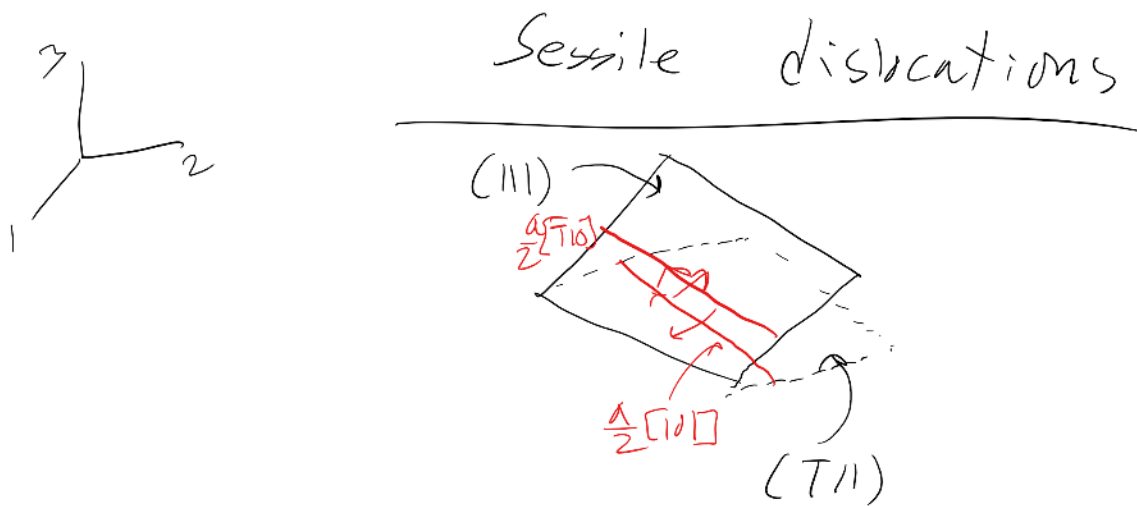


Figure Chapter9.19: Sessile dislocations.

An example reaction is:



The magnitudes of the Burgers vectors are $b_{\text{reactants}}^2 = a^2$ and $b_{\text{product}}^2 = \frac{a^2}{2}$, so the reaction is energetically favorable. The resulting dislocation lies on the (100) plane and has the slip system (100)[$\overline{0}11$], which is not a normal glide plane, making the dislocation sessile.

Because sessile dislocations require energy input to dissociate and move, they act as pinning points, preventing the motion of other dislocations. Even short sessile segments can effectively block gliding dislocations, leading to increased hardening. In low stacking fault energy (SFE) FCC metals, dislocations may dissociate into partials (Shockley partials), leading to similar blocking effects.

Types of Plastic Behavior and Yield Criteria

We have now built a foundation for understanding plasticity from the atomistic perspective, so we can step back and take a more macroscopic view of how materials yield. There are several types of plastic behavior that materials can exhibit.

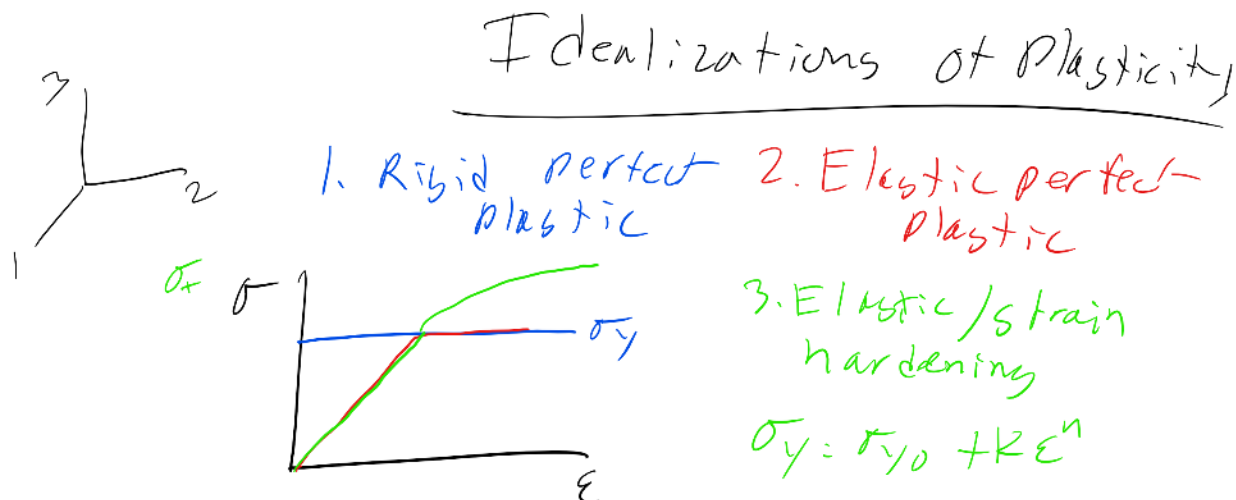


Figure Chapter9.20: Idealizations of plasticity.

Rigid/Perfectly Plastic Behavior

In a rigid or perfectly plastic material, the material behaves as if it were completely rigid (infinite Young's modulus) up to the yield point. Once yielding occurs, the material deforms plastically at a constant stress. There is no strain hardening or softening.

Elastic/Perfectly Plastic Behavior

A more realistic model assumes that the material exhibits elastic behavior up to the yield point, after which plastic deformation occurs at a constant yield stress.

Elastic/Strain Hardening Behavior

Many ductile materials exhibit strain hardening, where the stress required to continue plastic deformation increases with strain. After yielding, the true stress-strain relationship can be expressed as:

$$\sigma = \sigma_y + k\epsilon^n \quad (\text{Chapter 9.89})$$

where n is the strain-hardening exponent, typically ranging from 0.1 to 0.5 for metals.

Elastic/Strain Softening Behavior

Some materials, such as certain polymers and metallic glasses, exhibit strain softening after yielding — the stress decreases with continued strain.

These idealized material behaviors allow us to model and predict how materials respond once they enter the plastic regime. Next, we turn to the criteria that define when yielding begins.

Yielding Criteria

To predict yielding under complex, multiaxial loading states, several yield criteria have been developed. Before introducing them, we make the following assumptions:

1. Plastic flow occurs at constant volume.
2. Modest hydrostatic pressure does not cause yielding ($p < E/100$).

3. The material is perfectly plastic.
4. The material is isotropic.

Under these assumptions, we can apply the Rankine, Tresca, and von Mises yield criteria.

Rankine Criterion

The Rankine or maximum normal stress criterion states that a material yields when the maximum principal stress σ_1 reaches the yield stress observed in uniaxial tension:

$$\sigma_1 \geq \sigma_y \quad (\text{Chapter 9.90})$$

This criterion does not account for shear stresses and therefore cannot accurately describe yielding in most ductile materials.

Tresca Criterion

The Tresca or maximum shear stress criterion assumes that yielding occurs when the maximum shear stress reaches the critical value measured under uniaxial loading. The maximum shear stress is given by:

$$\tau_{max} = \frac{\sigma_1 - \sigma_3}{2} \quad (\text{Chapter 9.91})$$

and yielding occurs when:

$$\sigma_1 - \sigma_3 \geq \sigma_y \quad (\text{Chapter 9.92})$$

This model improves upon Rankine's by incorporating shear stresses, but experimental evidence during World War I and II showed it to be a poor predictor for certain metals, such as those used in submarine hulls.

Von Mises Criterion

The von Mises or maximum shear deformation energy criterion states that yielding occurs when the distortion energy reaches the same value as at the onset of yielding in a uniaxial tension test. The effective stress is defined as:

$$\sigma_{eff} = \sqrt{\frac{1}{2}[(\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + 6(\sigma_{23}^2 + \sigma_{31}^2 + \sigma_{12}^2)]} \quad (\text{Chapter 9.93})$$

Yielding occurs when:

$$\sigma_{eff} \geq \sigma_y \quad (\text{Chapter 9.94})$$

In terms of the principal stresses:

$$\sigma_{eff} = \sqrt{\frac{1}{2}[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2]} \geq \sigma_y \quad (\text{Chapter 9.95})$$

When these yield surfaces are plotted in principal stress space, the von Mises yield locus forms a cylinder, while the Tresca criterion forms a hexagon. The von Mises surface provides a smoother, more accurate description of yielding in ductile materials and is widely used in modern engineering design.

Polymer Yielding: Shear Banding and Crazing

Shear Banding

Shear bands are localized zones of intense plastic deformation and chain alignment, typically thousands of nanometers wide. They nucleate at stresses near $G/10$ and continue to grow as stress increases. Shear bands form at approximately 45° to the applied tensile axis (the planes of maximum shear stress) and are highly temperature-dependent.

Interestingly, the yield stress in compression is generally higher than in tension. This asymmetry is especially pronounced in polymers, where tensile loading tends to open free volume and promote chain alignment, making yielding easier.

Crazing

Crazes are another form of localized plastic deformation, distinct from cracks. They consist of microvoids and fibrils that span the deformed region. Crazes form perpendicular to the applied tensile axis, with fibrils aligned parallel to the loading direction. They do not form under compressive stress.

Shear banding and crazing can be thought of as polymer-specific manifestations of yielding. In modeling, the von Mises criterion can be modified to account for shear banding, and the Tresca criterion can be applied to describe crazing.

Strengthening Mechanisms

We have previously seen how dislocation motion controls plastic deformation, and we now know that yield stress depends on the ease with which dislocations move. One of the most powerful aspects of materials science is that we can intentionally modify a material's structure to change how dislocations move — and thereby tune the yield strength. This ability to tailor mechanical properties based on structure–processing relationships is a central theme of the materials tetrahedron.

The general principle is simple: the yield stress increases when it becomes harder for dislocations to move or propagate. Obstacles to dislocation motion raise the stress required for yielding. There are four primary strengthening mechanisms:

1. Work Hardening
2. Solute Strengthening
3. Grain Size Strengthening
4. Precipitate/Particle Strengthening

Work Hardening (Lattice Resistance)

Dislocation density is a measure of the total length of dislocations per unit volume or, equivalently, the number of dislocations per area of a slip plane. It is given by:

$$\rho = \frac{N}{A} \quad (\text{Chapter 9.96})$$

where N is the number of dislocations in area A . A heavily cold-worked material typically has a dislocation density on the order of 10^{14} m^{-2} , while a well-annealed material may have only 10^7 m^{-2} .

The average distance between dislocations can be approximated as:

$$\rho = \frac{1}{l^2} \quad (\text{Chapter 9.97})$$

where l is the spacing between dislocations. The increase in yield stress due to dislocation interactions can then be written as:

$$\Delta\sigma_y = \alpha G b \sqrt{\rho} \quad (\text{Chapter 9.98})$$

where G is the shear modulus, b is the Burgers vector, and α is a material constant (typically near 1).

Plastic deformation increases dislocation density as new dislocations are generated. As these dislocations interact and tangle, they impede each other's motion, making further deformation more difficult — this is work hardening. Rolling, drawing, or hammering metals are practical examples of inducing work hardening.

Alternatively, annealing a material (heating to elevated temperature) allows dislocations to climb and annihilate at free surfaces, reducing dislocation density and restoring ductility. During annealing, the grain size increases roughly as $d \sim t^{1/2}$, where t is time.

When solute atoms are added to a host metal, they can distort the local lattice because of differences in atomic size or modulus. These localized stress fields interact with dislocations and impede their motion.

The increase in yield strength due to solute atoms can be expressed as:

$$\Delta\sigma_y = G b \sqrt{c_{sol}} \epsilon_{sol}^{3/2} \quad (\text{Chapter 9.99})$$

where c_{sol} is the solute concentration and ϵ_{sol} is the lattice strain caused by size mismatch between solute and solvent atoms. The modulus mismatch between solute and solvent atoms can also contribute to strengthening.

The strengthening effect increases with solute concentration up to the solubility limit. This mechanism explains why solid-solution alloys (e.g., brass, bronze, stainless steel) are stronger than their pure metal components.

Grain Size Strengthening

Another effective way to increase strength is by reducing grain size. Grain boundaries act as barriers to dislocation motion, since dislocations cannot easily transmit across boundaries with different crystallographic orientations.

The Hall–Petch relationship describes this effect:

$$\Delta\sigma_y = \frac{\kappa}{d_g} \quad (\text{Chapter 9.100})$$

where κ is a material constant and d_g is the grain diameter. Smaller grains provide more grain boundaries, leading to higher yield strength.

However, this strengthening effect does not continue indefinitely. When the grain size becomes very small (below about 10 nm), dislocations cannot form or pile up inside the grain, and other deformation mechanisms such as grain boundary sliding dominate. As a result, the yield strength eventually decreases — a phenomenon known as the inverse Hall–Petch effect.

Precipitate/Particle Strengthening

In precipitation-hardened or particle-strengthened materials, dislocations encounter second-phase particles that serve as obstacles to motion. Depending on particle size and spacing, dislocations can either cut through the particles or bow around them.

If the dislocation cuts through particles, the strengthening effect is given by:

$$\Delta\sigma_y = \frac{\gamma_{p-m}\pi r_p}{bl} = \kappa^3 \sqrt{r_p f_p} \quad (\text{Chapter 9.101})$$

where:

- γ_{p-m} is the interfacial energy between the particle and the matrix,
- r_p is the particle radius,
- l is the average spacing between particles,
- f_p is the particle volume fraction, and
- κ is a constant related to particle geometry.

When dislocations bypass particles through bowing (the Orowan mechanism), the strengthening effect is:

$$\Delta\sigma_y = \frac{Gb}{l - 2r_p} \quad (\text{Chapter 9.102})$$

where G is the shear modulus, b is the Burgers vector, l is the particle spacing, and r_p is the particle radius.

For small particles, cutting is energetically more favorable because the interfacial energy penalty is low. For large particles, bowing becomes more favorable because cutting would require the creation of a large new interfacial area. Increasing the volume fraction of particles reduces the critical radius for transition between cutting and bowing, since more interfaces are created during cutting.

These four strengthening mechanisms — work hardening, solute strengthening, grain size strengthening, and precipitate strengthening — are often combined in engineering materials to achieve the desired balance of strength, ductility, and toughness.

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