Ch. 2. Mechanical Fundamentals

In order to understand mechanical properties of materials with respect to microstructures, we need to learn some terminologies and fundamental concepts.

Mechanical behaviors of materials are related to "What happens to a solid when forces are imposed on its boundaries".

In general, solid deforms i.e. changes volume and shape. Microstructure can change consequences:
- elastic
- amelastic
- plastic

1. elastic: deformation which is "instantaneous" and "recoverable"

surface traction $\rightarrow$ Traction $\rightarrow$ stresses $\rightarrow$ elastic strain

- e.g.: The spring
- The bouncing ball
- The bow
- The guitar string
2. *amelastic*: deformation which is recoverable but time-dependent

\[ \text{Traction} \rightarrow \text{stresses} \rightarrow \text{strain} = f(\text{time}) \]

3. *plastic*: deformation which is permanent (both "instantaneous" and time-dependent)

\[ \text{Traction} \rightarrow \text{stresses} \rightarrow \text{permanent strain} \]
4. Special kinds of mechanical response

creep - time dependent plastic flow under fixed stress

fracture - elastic or plastic or diffusion instability associated with internal defects such as cracks or cavities

fatigue - failure due to repeated loading
Basic definitions

Stress \((\sigma, \tau)\): intensity of load

simple loading: one component of stress

- Axial loading: normal stress

\[
\begin{align*}
\text{Tension} & \quad \sigma = \frac{P}{A} \\
\text{(Force} \ P \text{ is uniformly distributed over area} \ A \text{ for a long rod)} \\
\text{Compression} & \quad \sigma = \frac{P}{A}
\end{align*}
\]

In both cases, cohesive forces transmit applied forces.

- shear loading

\[
\begin{align*}
\text{Shear stress} & \quad \tau = \frac{P}{A}
\end{align*}
\]

unit of stress

\[
\begin{align*}
1 \ Pa & = 1 \ N/m^2 \\
1 \ psi & = 6.89 \times 10^4 \ dyne/cm^2 = 6.89 \times 10^3 \ N/m^2 \\
1 \ dyne/cm^2 & = 0.1 \ Pa
\end{align*}
\]
Why do we use 'stress', not 'force'? 

Even for the same material, twice the load is required to produce the same elongation if the cross-sectional area is doubled.

If we normalize the applied force by the area, 

\[ \sigma = \frac{P}{A} = \frac{2P}{2A} \cdot \frac{m}{m^2} = \frac{\Delta}{A} \rightarrow \text{The effect of area is removed.} \]

This is more important when we compare two different materials. We need to use the same geometry for comparison.

"Stress" gives you the force per unit area.

A. It is much easier to deform tungsten nanobar than a big aluminum bar. In this case, do you think that the big aluminum bar is stronger than a tungsten nanoparticle?
Simple loading is not enough to describe the full 3-dimensional stress state (at the point).

What is the state of stress at this point?

Let's consider an infinitesimal element of volume described by an orthogonal coordinate system (here Cartesian).

\[ \Delta f_{ij} \]
\[ i, j = x, y, z \]
\[ i = \text{direction of force} \]
\[ j = \text{plane normal} \]

Forces shown are positive forces on the positive faces of the element.
The stresses are defined as:

$$\sigma_{xx} = \lim_{\Delta A \to 0} \left( \frac{\Delta f_{xx}}{\Delta A} \right) \quad \text{where} \quad \Delta A = \Delta Y \Delta Z$$

(positive notation)

Tensorial

$$\sigma_{ij} \quad i, j = x, y, z \quad \text{or} \quad 1, 2, 3$$

Matrix

$$\begin{pmatrix}
\sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\
\sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\
\sigma_{zx} & \sigma_{zy} & \sigma_{zz}
\end{pmatrix}$$

Note:

Normal stress (i = j): $$\sigma_{ij} = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz})$$

Shear stress (i ≠ j): $$\sigma_{ij} = (\sigma_{xy}, \sigma_{yx}, \sigma_{xz}, \sigma_{zx}, \sigma_{yz}, \sigma_{zy})$$
Conditions for static equilibrium.

In order for a body (or infinitesimal element in the body) to remain still, summation of force and moment acting on the body has to be zero.

1) Moment equilibrium

Consider moments (with respect to G) acting on an elemental area $dA (= dx\,dy)$

\[
\tau_{xy} + \left( \frac{\partial \tau_{xy}}{\partial y} \right) \frac{dy}{2} = 0
\]

\[
\tau_{yx} + \left( \frac{\partial \tau_{yx}}{\partial x} \right) \frac{dx}{2} = 0
\]

\[
\tau_{yx} \cdot \left( \frac{\partial \tau_{xy}}{\partial y} \right) \frac{dy}{2} - \left( \tau_{xy} - \frac{\partial \tau_{xy}}{\partial x} \frac{dx}{2} \right) dy \cdot \frac{dx}{2} + \left( \tau_{yx} - \frac{\partial \tau_{yx}}{\partial y} \frac{dy}{2} \right) dx \cdot \frac{dy}{2} = 0
\]

\[
\sum_{G} M_{G} = 0
\]

\[
\left( \tau_{yx} + \frac{\partial \tau_{yx}}{\partial x} \frac{dx}{2} \right) dy \cdot \frac{dx}{2} + \left( \tau_{yx} - \frac{\partial \tau_{yx}}{\partial x} \frac{dx}{2} \right) dy \cdot \frac{dx}{2} - \left( \tau_{xy} - \frac{\partial \tau_{xy}}{\partial y} \frac{dy}{2} \right) dx \cdot \frac{dy}{2} = 0
\]

\[
\tau_{xy} = \tau_{yx}
\]

Likewise,

\[
\tau_{xz} = \tau_{zx} \quad (\text{from } y-z \text{ plane})
\]

\[
\tau_{xz} = \tau_{zx} \quad (\text{from } x-z \text{ plane})
\]
Results

The stress tensor is symmetric.
\[ \rightarrow 9 \text{ stress components are reduced into 6 components.} \]

\[
\sigma_{ij} = \begin{pmatrix}
\sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\
\sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\
\sigma_{zx} & \sigma_{zy} & \sigma_{zz}
\end{pmatrix} = \begin{pmatrix}
\sigma_1 & 0 & 0 \\
0 & \sigma_2 & 0 \\
0 & 0 & \sigma_3
\end{pmatrix}
\]

\( i \) force equilibrium

* spatial variation of stress component.

If stress varies from place to place we have to be concerned with how it can vary. The stress components may be varied arbitrarily - the conditions of equilibrium must be satisfied. These conditions are used to determine how stresses are distributed in solids.

Consider an element of volume where the stress components are not constant.

Force equilibrium (see the figure at the next page).

\[
\frac{\partial \sigma_{xx} \Delta x}{\partial x} \Delta y \Delta z + \frac{\partial \sigma_{xy} \Delta y}{\partial y} \Delta x \Delta z + \frac{\partial \sigma_{xz} \Delta z}{\partial z} \Delta x \Delta y = 0 = \Sigma F_x
\]
Equilibrium equation is

\[ \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} = 0; \quad \frac{\partial \sigma_{ij}}{\partial x_j} = 0 \]

Note: Repeated \( j \) means sum over \( j = 1, 2, 3 \) or \( x, y, z \)

Similar relations for \( \sum F_y = \sum P_z = 0 \).

General result

\[ \frac{\partial \sigma_{ij}}{\partial x_j} = 0 \quad \text{for} \quad i = 1, 2, 3 \quad (x, y, z) \]

sum over \( j = 1, 2, 3 \quad (x, y, z) \).

These equations must be satisfied for any internal stress distributions.
The principal stress tensor is

\[
\sigma_p = \begin{pmatrix}
\sigma_1 & 0 & 0 \\
0 & \sigma_2 & 0 \\
0 & 0 & \sigma_3
\end{pmatrix}.
\]

Property of transformation: \(\sigma_{11} + \sigma_{22} + \sigma_{33} = \sigma_1 + \sigma_2 + \sigma_3\).

**Examples**

**Uniaxial Tension**

\[
\sigma_p = \begin{pmatrix}
\sigma_1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}.
\]

**Biaxial Tension**

\[
\sigma_p = \begin{pmatrix}
\sigma_1 & 0 & 0 \\
0 & \sigma_2 & 0 \\
0 & 0 & 0
\end{pmatrix}.
\]

**Hydrostatic Pressure**

\[
\sigma_p = \begin{pmatrix}
-p & 0 & 0 \\
0 & -p & 0 \\
0 & 0 & -p
\end{pmatrix}.
\]

**Triaxial Tension**

\[
\sigma_p = \begin{pmatrix}
\sigma_1 & 0 & 0 \\
0 & \sigma_2 & 0 \\
0 & 0 & \sigma_3
\end{pmatrix}.
\]

When any one of \(\sigma_1, \sigma_2, \sigma_3\) is zero we have a condition called *plane stress*.
Transformation of stress

Why do we need it? e.g. 2D stress field.

\[ \sigma_y = \frac{P}{A} \]
\[ \sigma_x = 0 \]
\[ \tau_{xy} = 0 \]

Q: \( \sigma_y' = ? \)
\( \sigma_x' = ? \)
\( \tau_{xy}' = ? \)
Why do we need 'transformation of stress'? 

E.g. 1) Dislocation dynamics
- the motion of dislocations
  - in-plane motion: glide
  - out-of-plane motion: climb

\[ \sigma \rightarrow \text{glide} \]
\[ \tau \rightarrow \text{(shear stress)} \]
\[ \tau \rightarrow \text{climb} \]
\[ \rightarrow \text{slip plane} \]

E.g. 2) Fracture analysis
- random distribution of microcrack
- Brittle fracture is sensitive to the maximum tensile stress.

[Diagram of crack propagation and microcrack]
< purpose of stress transformation >

Want to obtain $\sigma'_x$, $\sigma'_y$, $\tau'_{xy}$ (stress components in new coordinate) as a function of $\sigma_x$, $\sigma_y$, $\tau_{xy}$ (stress components in the old coordinate), which is known or measured.

Let's consider 2-D stress field, $\sigma_x$, $\sigma_y$, $\tau_{xy}$.

![Diagram showing stress components and angle $\theta$.]

Let $\Delta A =$ Area of side AB, then

$A_{OA} = \Delta A \cos \theta$, $A_{OB} = \Delta A \sin \theta$

Apply the force equilibrium condition on a new coordinate:

$$\sum F_{x'} = 0$$

$$\sigma'_x \Delta A - \sigma_x (\Delta A \cos \theta) \cos \theta - \tau_{xy} (\Delta A \cos \theta) \sin \theta - \sigma_y (\Delta A \sin \theta) \sin \theta - \tau_{xy} (\Delta A \sin \theta) \cos \theta = 0$$

$$\sum F_{y'} = 0$$

$$\tau_{xy} \Delta A + \sigma_x (\Delta A \cos \theta) \sin \theta - \tau_{xy} (\Delta A \sin \theta) \cos \theta - \sigma_y (\Delta A \sin \theta) \cos \theta + \tau_{xy} (\Delta A \sin \theta) \sin \theta = 0$$
Simplifying and rearranging eqs 1 and 2 yield

1) \[ \sigma_x' = \sigma_x \cos^2 \theta + \sigma_y \sin^2 \theta + 2 \tau_{xy} \sin \theta \cos \theta \]
\[ \tau_{xy}' = \tau_{xy} (\cos^2 \theta - \sin^2 \theta) + (\sigma_y - \sigma_x) \sin \theta \cos \Theta \]

To get \( \sigma_y' \), substitute \( \theta + \frac{\pi}{2} \) for \( \theta \) in the equation for \( \sigma_x' \):

2) \[ \sigma_y' = \sigma_x \sin^2 \theta + \sigma_y \cos^2 \theta - 2 \tau_{xy} \sin \theta \cos \theta \]

\( \sin \theta \rightarrow \cos \theta \)
\( \cos \theta \rightarrow -\sin \theta \)

3) The matrix form of eq 3

\[
\begin{pmatrix}
\sigma_x' \\
\sigma_y' \\
\tau_{xy}'
\end{pmatrix} =
\begin{pmatrix}
c^2 & s^2 & 2cs \\
s^2 & c^2 & -2cs \\
-2cs & cs & c^2 - s^2
\end{pmatrix}
\begin{pmatrix}
\sigma_x \\
\sigma_y \\
\tau_{xy}
\end{pmatrix}
\]

\( c = \cos \theta \)
\( s = \sin \theta \)
iii) To aid in computation, it is convenient to express eq. (3) in terms of double angle (2Θ) using the trigonometric identities

\[ \cos^2 \Theta = \frac{1 + \cos 2\Theta}{2} \]
\[ \sin^2 \Theta = \frac{1 - \cos 2\Theta}{2} \]
\[ 2 \sin \Theta \cos \Theta = \sin 2\Theta \]

The equation for stress transformation (in terms of 2Θ) becomes

\[ \sigma_x' = \frac{1}{2} (\sigma_x + \sigma_y) + \frac{1}{2} (\sigma_x - \sigma_y) \cos 2\Theta + \tau_{xy} \sin 2\Theta \]
\[ \sigma_y' = \frac{1}{2} (\sigma_x + \sigma_y) - \frac{1}{2} (\sigma_x - \sigma_y) \cos 2\Theta - \tau_{xy} \sin 2\Theta \]
\[ \tau_{xy}' = -\frac{1}{2} (\sigma_x - \sigma_y) \sin 2\Theta + \tau_{xy} \cos 2\Theta \]

Note

\[ \sigma_x + \sigma_y = \sigma_x' + \sigma_y' = \text{const.} \]

implying that the sum of the normal stresses on two (three) mutually perpendicular planes is invariant, i.e. independent of \( \Theta \).
Graphical Method of Stress transformation
(Mohr's circle).

Rewriting the transformation rule

\[ \sigma'_x = \frac{1}{2} (\sigma_x + \sigma_y) + \frac{1}{2} (\sigma_x - \sigma_y) \cos 2\theta + \tau_{xy} \sin 2\theta \]
\[ \tau'_{xy} = -\frac{1}{2} (\sigma_x - \sigma_y) \sin 2\theta + \tau_{xy} \cos 2\theta \]

For convenience, let \( \sigma'_x = \sigma \) and \( \tau'_{xy} = \tau \) and rewrite eq. 1

\[ \sigma = \frac{\sigma_x + \sigma_y}{2} \]
\[ \tau = -\frac{\sigma_x - \sigma_y}{2} \sin 2\theta + \tau_{xy} \cos 2\theta \]

Square eq. 2 on each side and expand

\[ \left( \sigma - \frac{\sigma_x + \sigma_y}{2} \right)^2 = \left( \frac{\sigma_x - \sigma_y}{2} \right)^2 \cos^2 2\theta + \tau_{xy}^2 \sin^2 2\theta + (\sigma_x - \sigma_y) \tau_{xy} \cos 2\theta \sin 2\theta \]
\[ \tau^2 = \left( \frac{\sigma_x - \sigma_y}{2} \right)^2 \sin^2 2\theta + \tau_{xy}^2 \cos^2 2\theta - (\sigma_x - \sigma_y) \tau_{xy} \cos 2\theta \sin 2\theta \]

Add the above equations together

\[ \left( \sigma - \frac{\sigma_x + \sigma_y}{2} \right)^2 + \tau^2 = \left( \frac{\sigma_x - \sigma_y}{2} \right)^2 + \tau_{xy}^2 \]  

Note: \((x-a)^2 + y^2 = r^2\) is the equation of a circle with a radius of \(r\), centered at \((x, y) = (a, 0)\) in the x-y coordinate.
Thus, Eq. 3) is the equation representing a circle with a radius of $\sqrt{\frac{(\sigma_x-\sigma_y)^2}{2} + \tau_{xy}^2}$, centered at $\sigma = \frac{\sigma_x + \sigma_y}{2}$ in the \(\sigma-\tau\) coordinate.

**Sign convention:** the positive shear stress is the negative value in the Mohr's Circle (with \(\sigma_x\) only)

\[
(\sigma_x, -\tau_{xy}) \quad \text{x axis} \\
(\sigma_y, \tau_{xy}) \quad \text{y axis}
\]
properties of Mohr's circle.

1. mean stress: \( \sigma_m = \frac{\sigma_x + \sigma_y}{2} = \text{center of circle} \).
2. principal stress (\( \tau_{xy} = 0 \)): \( \sigma_1 > \sigma_2 \).
3. maximum shear stress: \( \tau_{\max} = \frac{\sigma_1 - \sigma_2}{2} \).

\( \vec{m} \) in 3 D.

1. mean stress: \( \sigma_m = \frac{\sigma_x + \sigma_y + \sigma_z}{3} \).
2. principal stress: \( \sigma_1 > \sigma_2 > \sigma_3 \).
3. maximum shear stress: \( \tau_{\max} = \frac{\sigma_1 - \sigma_3}{2} \).
3D transformation of stress

tensor transformation,

$$\sigma_{ij}' = \sum_{i=1}^{3} \sum_{j=1}^{3} \sigma_{ij} l_{ii} l_{jj}$$

where \( l_{ii} = \cos \theta_{ii} \) → directional cosine

angle between \( x_i' \) and \( x_i \) axis.

\[
\begin{align*}
\sigma_{11}' &= \sum_{i=1}^{3} \sigma_{ij} l_{i1} l_{j1} \\
\sigma_{22}' &= \sum_{i=1}^{3} \sigma_{ij} l_{i2} l_{j2} \\
\sigma_{33}' &= \sum_{i=1}^{3} \sigma_{ij} l_{i3} l_{j3}
\end{align*}
\]
How to construct the 3D Mohr’s circle.

First, we need to perform the 3D stress transformation to obtain three principal stresses, \( \sigma_1, \sigma_2 \), and \( \sigma_3 \).

In the principal stress axes, the stress state becomes

\[
\sigma_{i'j'} = \begin{pmatrix}
\sigma_{xx'} & 0 & 0 \\
0 & \sigma_{yy'} & 0 \\
0 & 0 & \sigma_{zz'}
\end{pmatrix} \quad \text{(No shear stresses.)}
\]

Suppose that the body is under the 3D stress state, \( \sigma_{ij} \), in the original coordinate system.

The principal stress state can be found by performing tensor transformation of \( \sigma_{ij} \). Transformed stress state should satisfy \( \sigma_{xy'} = \sigma_{yz'} = \sigma_{zx'} = 0 \).

From the tensor transformation

\[
\sigma_{i'j'} = \sum_i \sum_j \sigma_{ij} l_i' l_j'
\]

Thus,

\[
\sigma_{xy'} = \sigma_{ij} l_i' l_{y'} = 0
\]

\[
= \begin{pmatrix}
\sigma_{xx} & \tau_{xy} & \tau_{xz} \\
\tau_{xy} & \sigma_{yy} & \tau_{yz} \\
\tau_{xz} & \tau_{yz} & \sigma_{zz}
\end{pmatrix}
\begin{pmatrix}
l_{x'} l_{y'} \\
l_{x'} l_{y'} \\
l_{x'} l_{y'}
\end{pmatrix}
\]

9 variables:

\( l_{x'}, l_{y'}, l_{x'z}, l_{yx}, l_{gy}, l_{yz}, l_{zx}, l_{zy}, l_{zx} \).
\[ \sigma_{y'z'} \Rightarrow \sigma_{ij} ly' i l z' j \rightarrow \text{the same 9 variables} \]
\[ \sigma_{z'x'} \Rightarrow \sigma_{ij} l z' i l x' j \rightarrow \text{the same 9 variables}. \]

Now, we have 9 variables and 3 equations.

From geometry, it is easy to get

(i)
\[ l x'^{2} + l x'^{2} y + l x'^{2} z = 1 \]
\[ l y'^{2} x + l y'^{2} y + l y'^{2} z = 1 \]
\[ l z'^{2} x + l z'^{2} y + l z'^{2} z = 1. \]

(ii)
\[ l x' l y' x + l x' l y' y + l x' l y' z = 0 \]
\[ l x' l z' x + l y' l z' y + l x' l z' z = 0 \]
\[ l y' l z' x + l y' l z' y + l y' l z' z = 0. \]

In fact, the direction vectors of the new axes in old coordinate system are
\[ \vec{v}_x' = [l x', l x' y, l x' z] \]
\[ \vec{v}_y' = [l y' x, l y' y, l y' z] \]
\[ \vec{v}_z' = [l z' x, l z' y, l z' z]. \]

These three vectors are mutually perpendicular to each other.

So,
\[ \vec{v}_x' \cdot \vec{v}_y' = \vec{v}_y' \cdot \vec{v}_z' = \vec{v}_z' \cdot \vec{v}_x' = 0. \]

(iii)
\[ l x'^{2} y + l y'^{2} y + l z'^{2} x = 1 \]
\[ l x'^{2} z + l y'^{2} z + l z'^{2} y = 1 \]
\[ l z'^{2} z + l y'^{2} z + l z'^{2} z = 1. \]
Now, we get 9 variables and 6 independent equations. These relations reduces 9 variables to 3 independent ones.

Therefore,

\[ l_x z', l_x y', l_z z', l_y z', l_y y', l_z y', l_z z' \]

Only three are independent.

Finally, we have three equations with three independent variables (directional cosines).

\[
\begin{align*}
\sigma_{x'y'} &= \sigma_{j} l_{x'} l_{y'} = 0, \\
\sigma_{y'z'} &= \sigma_{j} l_{y'} l_{z'} = 0, \\
\sigma_{x'z'} &= \sigma_{j} l_{z'} l_{x'} = 0.
\end{align*}
\]

By using the computer software such as MATLAB or Mathematica, we can easily solve the simultaneous equations. The, we can get all components of directional cosines. To transform \( \sigma_{ij} \) into \( \sigma'_{ij} \) in the principal axes.

\[ \Rightarrow \sigma_{1}, > \sigma_{2} > \sigma_{3}. \]
Once we know $\sigma_\text{III}, \sigma_\text{II}, \sigma_\text{I}$, we can draw the 3D Mohr's circle.

$\tau_{\text{max}} = \frac{\sigma_\text{I} - \sigma_\text{III}}{2}$. 
Use of the transformation law to calculate a resolved shear stress

Consider BCC single crystal subjected to tension in [010] direction.

Calculate resolved shear stress on $(\overline{1}2\overline{1})\langle\overline{1}1\overline{1}\rangle$ twinning system in terms of $\sigma_{22}$.

$$\sigma'_{12} = \frac{\sqrt{2}}{3} \sigma_{22}$$