재료의 기계적 거동
(Mechanical Behavior of Materials)

Elasticity of crystalline solids

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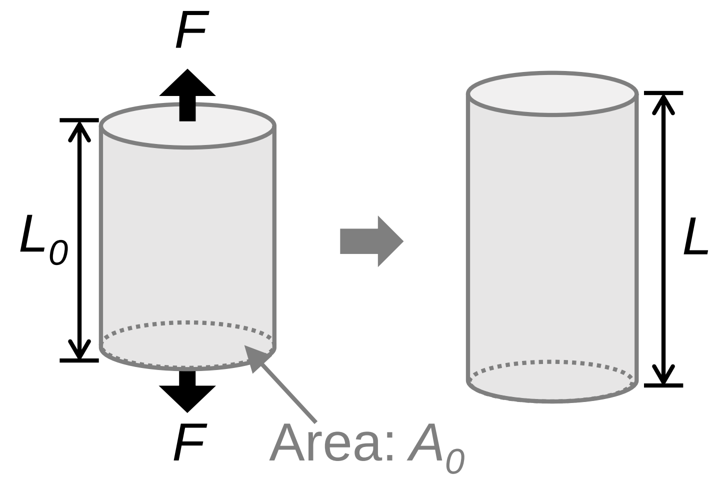
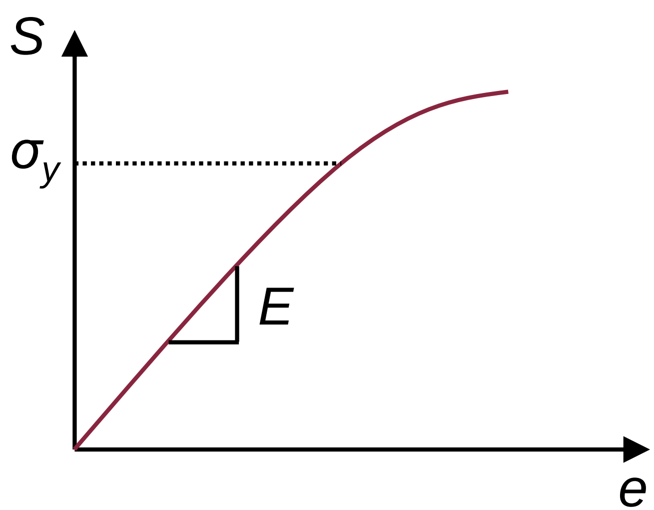
Objectives of the chapter





- When a small amount of load is applied to a material, elastic deformation occurs.
- For most metals the **load** (*F*) and **elongation** (L-L_0) are **proportional** to each other in the elastic range.
- In other words, the **stress** and **strain** relationship is **linear**.

Engineering stress: $S = \dfrac{F}{A_0}$

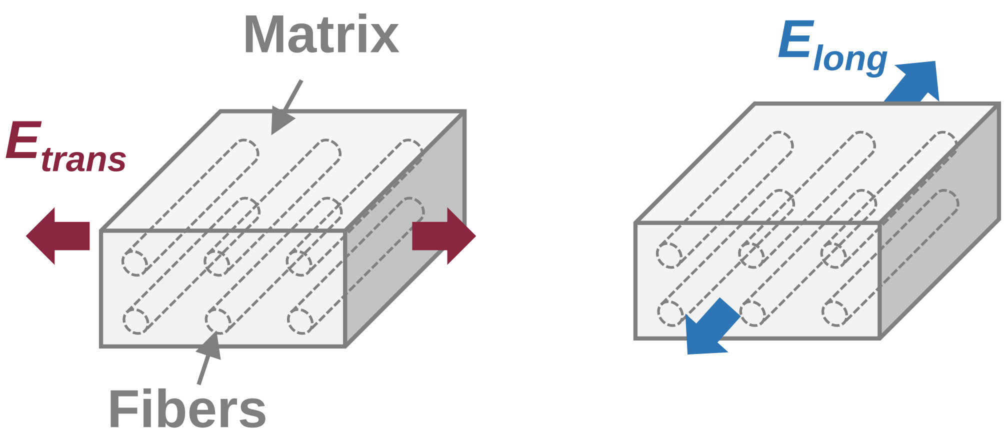
Engineering strain: $e = \dfrac{L - L_0}{L_0}$

Objectives of the chapter

- This linear relationship between the stress and strain is known as **Hooke's law**. For instance, in uniaxial tension:

$\sigma = E\varepsilon$ *: Hooke's law in uniaxial tension*

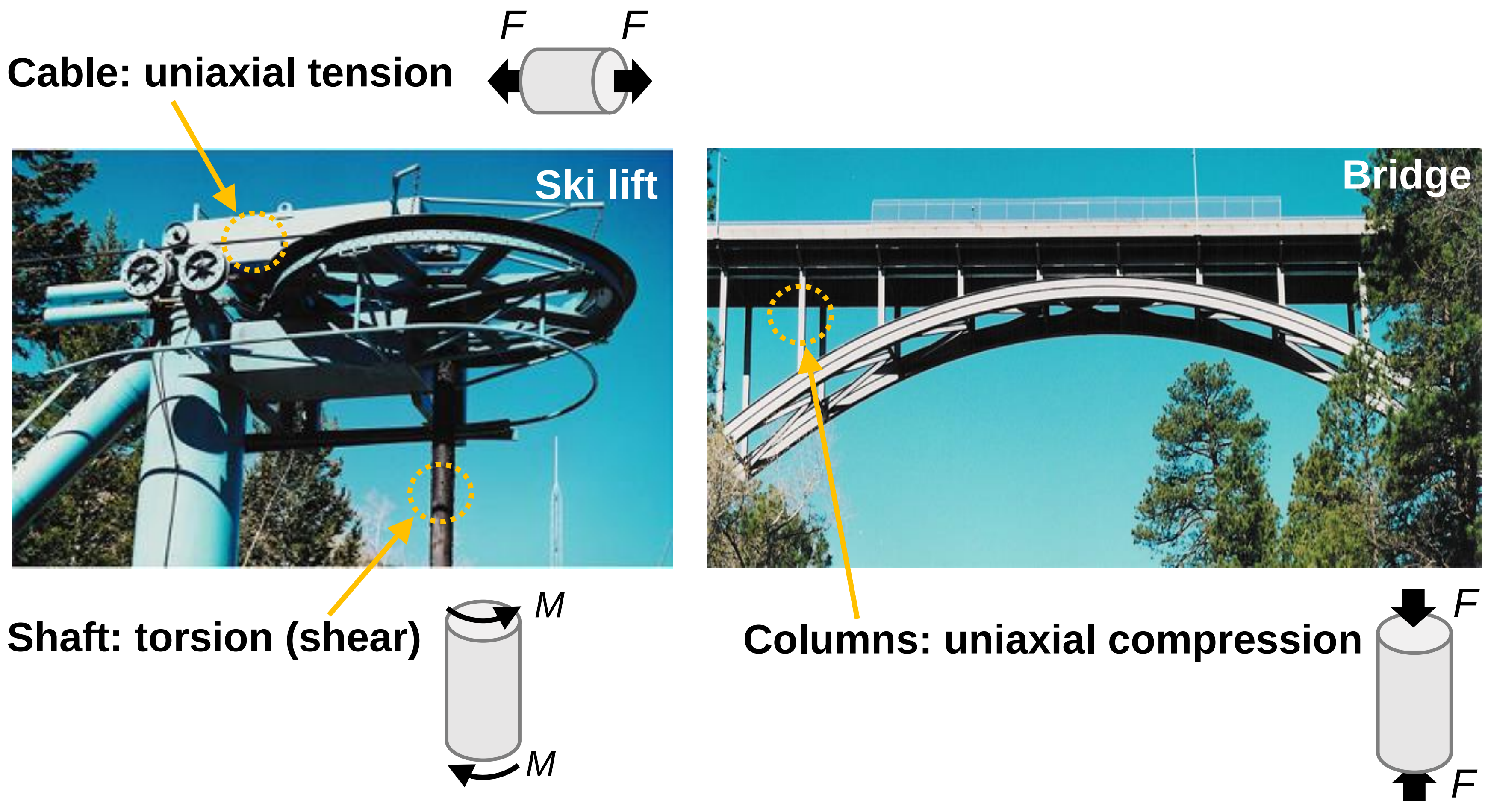
- This simple representation is not sufficient in reality for two reasons. First, the material property can be different depending on the loading direction (**material anisotropy**).



$E_{trans} \neq E_{long}$

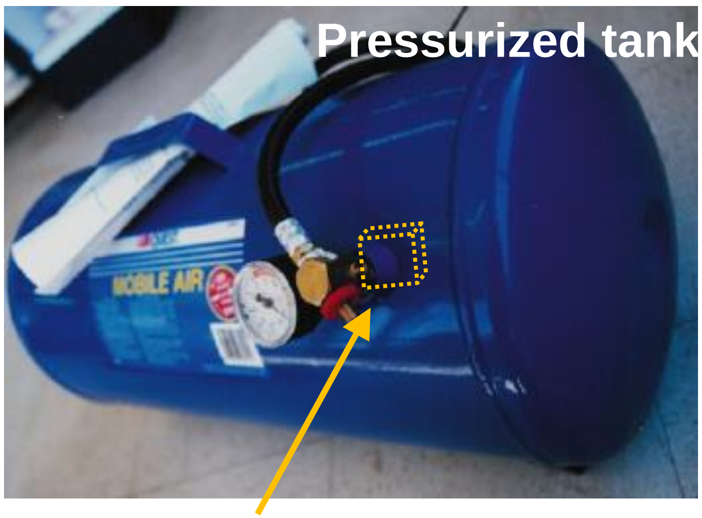
Objectives of the chapter

- Second, the **stress state** of a material may not be simply uniaxial but **multi-axial**.

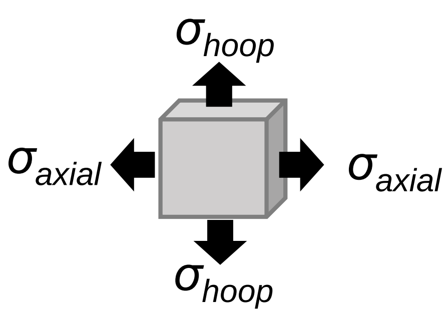


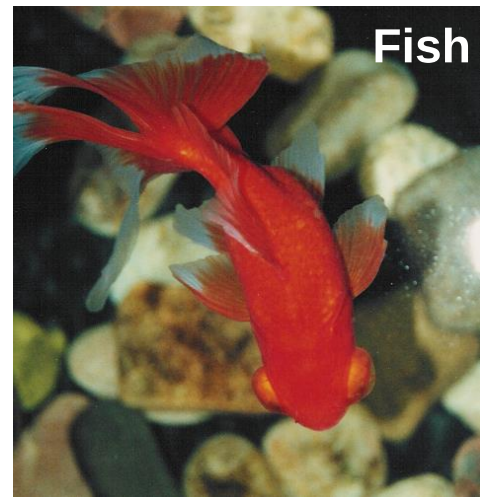
Objectives of the chapter

- Second, the **stress state** of a material may not be simply uniaxial but **multi-axial**.

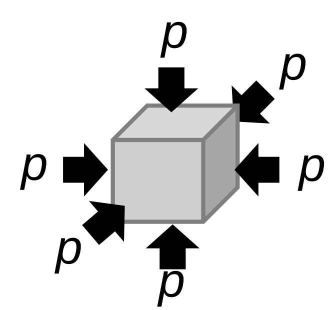


Tank wall: Biaxial tension





Hydrostatic compression



Objectives of the chapter

In this chapter, we are going to learn:

- How to construct **an anisotropic elasticity law** considering **three-dimensional** states of stress and strain

1-D

$$\sigma = E\varepsilon$$

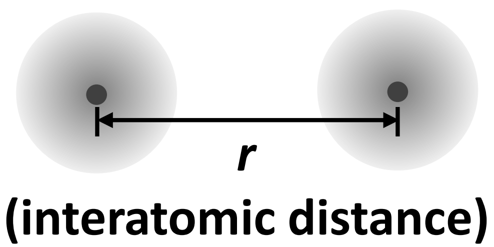
3-D

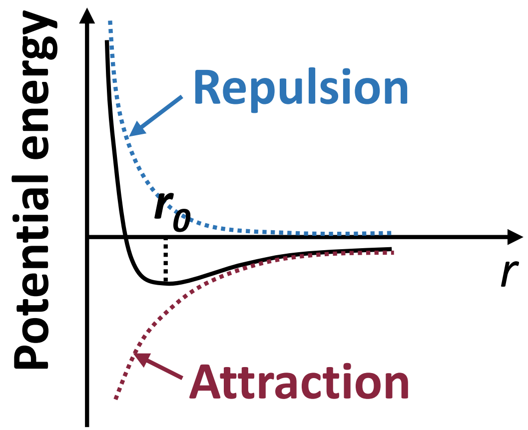
$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \overset{(?)}{\Longleftrightarrow} \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix}$$

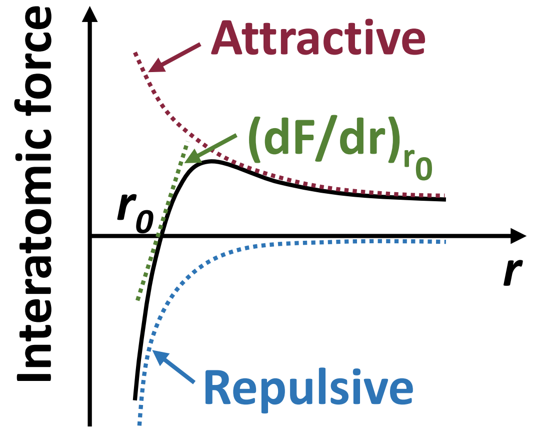
We will introduce 'stiffness' and 'compliance' tensors for this purpose

- How to **reduce** the number of elasticity constants for **single crystals having symmetry**

Background



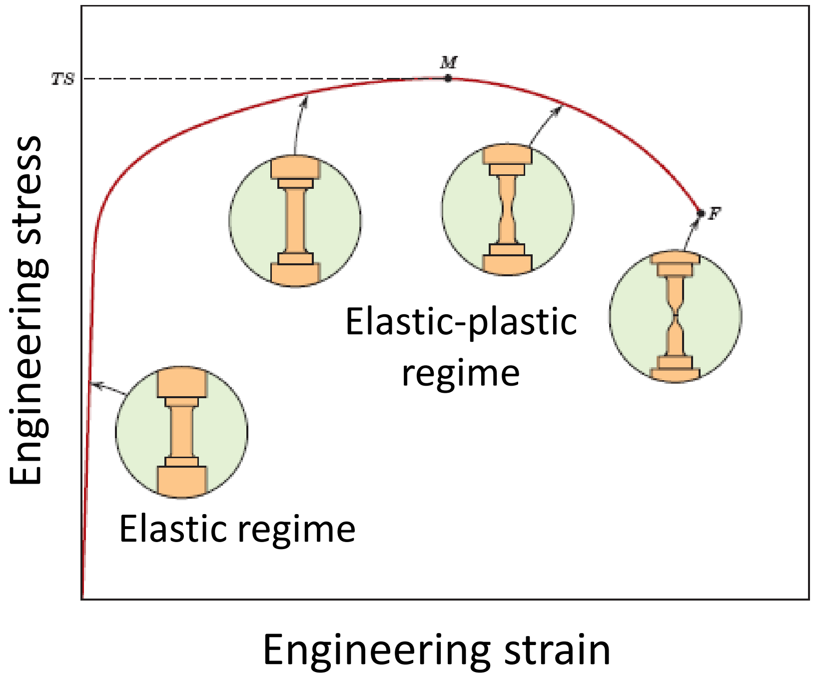




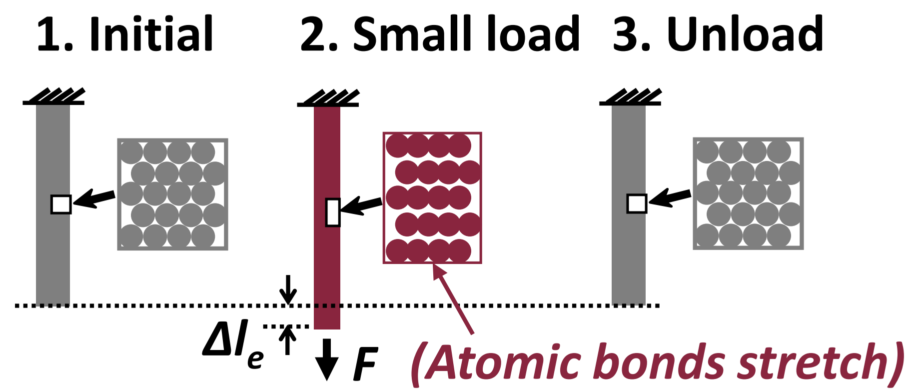
- Elastic deformation originates from the change of interatomic spacing under external loads.
- Therefore, the elastic modulus is proportional to the slope of the interatomic force-distance curve at the equilibrium spacing:

$$E \propto \left(\frac{dF}{dr}\right)_{r_0}$$

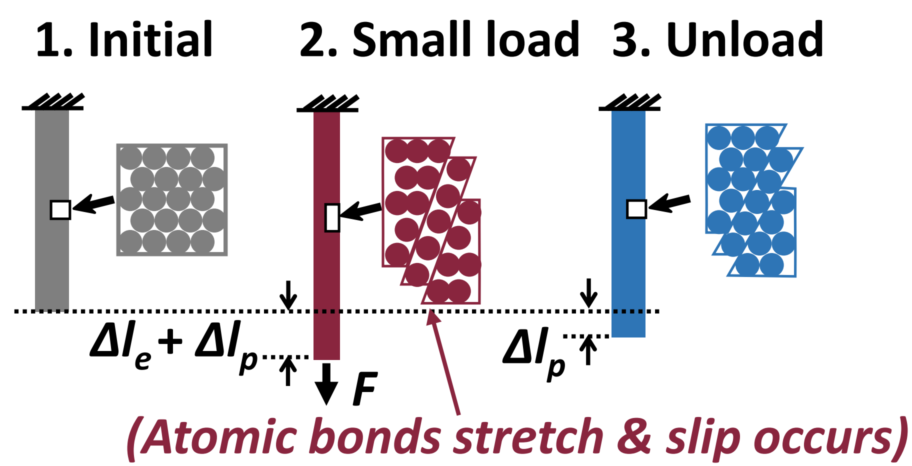
Background



Elastic deformation



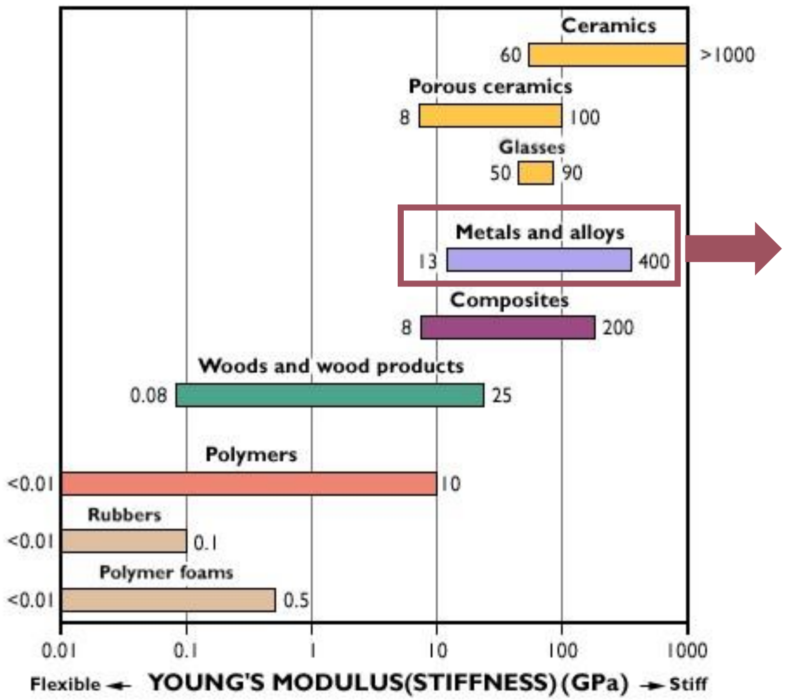
Elastic-plastic deformation



- Elastic deformation is reversible.
- **Plastic deformation is irreversible.**

Background

Elastic properties of engineering materials

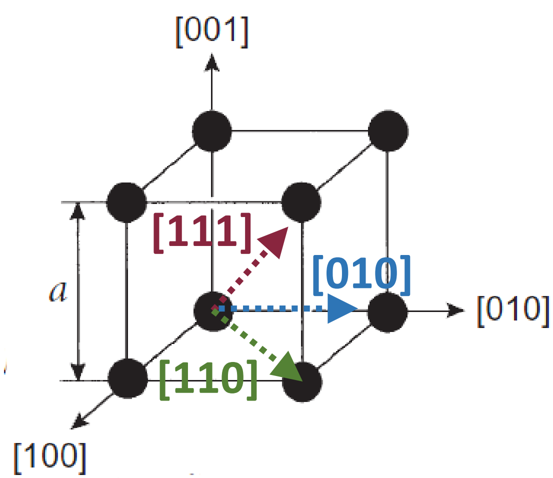


Metal alloy	Elastic modulus [GPa]	Shear modulus [GPa]	Poisson's ratio
Aluminum	69	25	0.33
Brass	97	37	0.34
Copper	110	46	0.34
Magnesium	45	17	0.29
Nickel	207	76	0.31
Steel	207	83	0.30
Titanium	107	45	0.34
Tungsten	407	160	0.28

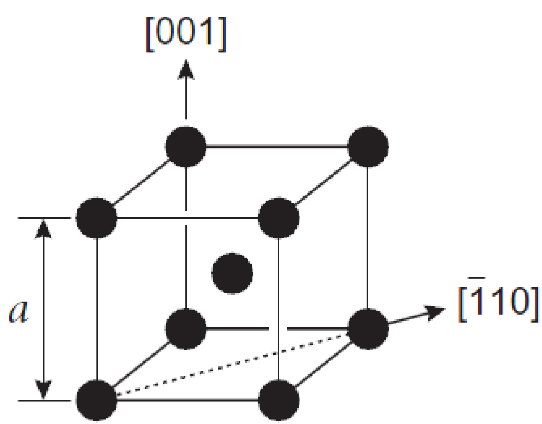
Background

- Consequently, the elastic behavior of a material is affected by the nature of **atomic bond** as well as **crystallographic structure**.
- For instance, in the simple cubic structure, the **elastic response** is different depending on the loading direction, i.e., **anisotropic**.

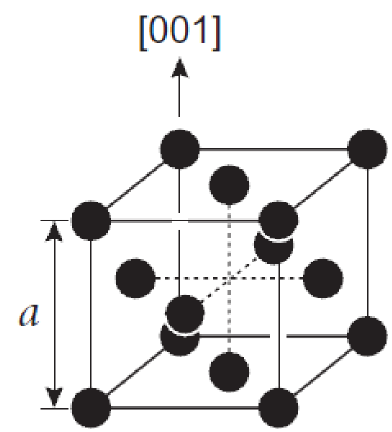
Simple cubic



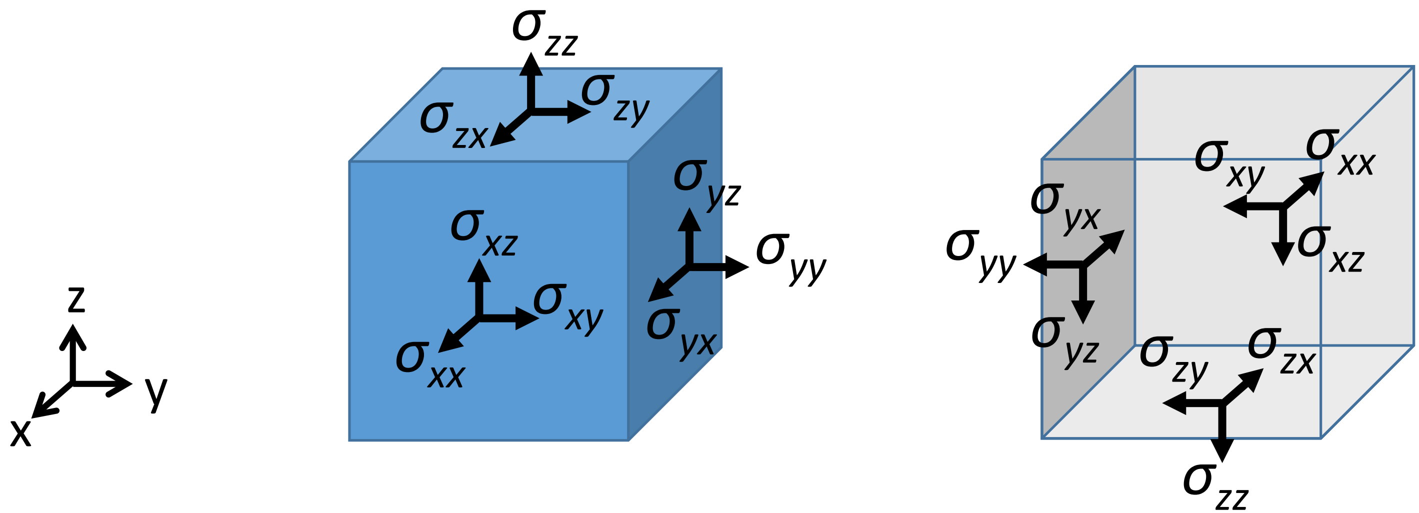
Body-centered cubic



Face-centered cubic



Stress and strain tensor



Using tensor notation: $\boldsymbol{\sigma_{ij}}$ **for** ***i=x,y,z*** **(surface normal) and**
j=x,y,z **(force direction)**

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

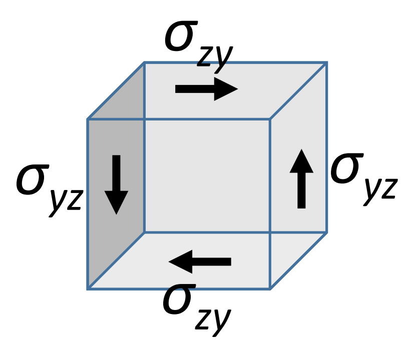
9 components

6 independent components

normal **shear**

$$\sigma_{ij} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix}$$

Sum of moments = 0 (equilibrium)



$\sigma_{yx} = \sigma_{xy}$

$\sigma_{zy} = \sigma_{yz}$

$\sigma_{zx} = \sigma_{xz}$

$(\sigma_{ij} = \sigma_{ji}$ for $i \neq j)$

Anisotropic elasticity

- We will keep the concept of **linear elasticity**, i.e., the stress-strain relationship is linear.
- Then, each stress component can be expressed as **a linear combination** of the strain components. For example,

$$
\begin{aligned}
\sigma_{xx} = {} & C_{xxxx}\varepsilon_{xx} + C_{xxxy}\varepsilon_{xy} + C_{xxxz}\varepsilon_{xz} \\
& + C_{xxyx}\varepsilon_{yx} + C_{xxyy}\varepsilon_{yy} + C_{xxyz}\varepsilon_{yz} \\
& + C_{xxzx}\varepsilon_{zx} + C_{xxzy}\varepsilon_{zy} + C_{xxzz}\varepsilon_{zz}
\end{aligned}
$$

Constants

$$
\begin{aligned}
\sigma_{xx} = {} & C_{xxxx}\varepsilon_{xx} + C_{xxxy}\varepsilon_{xy} + C_{xxxz}\varepsilon_{xz} \\
& + C_{xxyx}\varepsilon_{yx} + C_{xxyy}\varepsilon_{yy} + C_{xxyz}\varepsilon_{yz} \\
& + \boxed{C_{xxzx}}\varepsilon_{zx} + C_{xxzy}\varepsilon_{zy} + C_{xxzz}\varepsilon_{zz}
\end{aligned}
$$

Contribution of the strain component ε_{zx} to the stress component σ_{xx}

Using tensor notation:

$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$ for $i, j, k, l = x, y, z$

C_{ijkl} : **Stiffness tensor**

(The ratio of the stress component σ_{ij} to the strain component ε_{kl})

Anisotropic elasticity

- Alternatively, each strain component can be expressed as **linear combination** of the stress components.

$$\begin{aligned}\varepsilon_{xx} &= S_{xxxx}\sigma_{xx} + S_{xxxy}\sigma_{xy} + S_{xxxz}\sigma_{xz} \\ &+ S_{xxyx}\sigma_{yx} + S_{xxyy}\sigma_{yy} + S_{xxyz}\sigma_{yz} \\ &+ \boxed{S_{xxzx}}\sigma_{zx} + S_{xxzy}\sigma_{zy} + S_{xxzz}\sigma_{zz}\end{aligned}$$

Contribution of the stress component σ_{zx} to the stress component ε_{xx}

$\varepsilon_{ij} = S_{ijkl}\sigma_{kl}$ for $i, j, k, l = x, y, z$

S_{ijkl} : **Compliance tensor**

(The ratio of the strain component ε_{ij} to the strain component σ_{kl})

Remarks

- It is conventional to use the symbols 'C' for stiffness tensor and 'S' for compliance tensor.
- In general, $C_{xxxx} \neq 1/(S_{xxxx})$.

Anisotropic elasticity

- We need **nine equations** to express the entire set of stress (or strain) components.

$$\begin{aligned}\sigma_{xx} &= C_{xxxx}\varepsilon_{xx} + C_{xxxy}\varepsilon_{xy} + C_{xxxz}\varepsilon_{xz} \\ &+ C_{xxyx}\varepsilon_{yx} + C_{xxyy}\varepsilon_{yy} + C_{xxyz}\varepsilon_{yz} \\ &+ C_{xxzx}\varepsilon_{zx} + C_{xxzy}\varepsilon_{zy} + C_{xxzz}\varepsilon_{zz}\end{aligned}$$

Note: This matrix notation is equivalent to the tensor notation of

$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$ for $i, j, k, l = x, y, z$

$$\begin{bmatrix}\sigma_{xx}\\ \sigma_{xy}\\ \sigma_{xz}\\ \sigma_{yx}\\ \sigma_{yy}\\ \sigma_{yz}\\ \sigma_{zx}\\ \sigma_{zy}\\ \sigma_{zz}\end{bmatrix} = \begin{bmatrix} C_{xxxx} & C_{xxxy} & C_{xxxz} & C_{xxyx} & C_{xxyy} & C_{xxyz} & C_{xxzx} & C_{xxzy} & C_{xxzz} \\ C_{xyxx} & C_{xyxy} & C_{xyxz} & C_{xyyx} & C_{xyyy} & C_{xyyz} & C_{xyzx} & C_{xyzy} & C_{xyzz} \\ C_{xzxx} & C_{xzxy} & C_{xzxz} & C_{xzyx} & C_{xzyy} & C_{xzyz} & C_{xzzx} & C_{xzzy} & C_{xzzz} \\ C_{yxxx} & C_{yxxy} & C_{yxxz} & & & & & & \\ C_{yyxx} & C_{yyxy} & C_{yyxz} & & & & & & \\ C_{yzxx} & C_{yzxy} & C_{yzxz} & & & \ddots & & & \vdots \\ C_{zxxx} & C_{zxxy} & C_{zxxz} & & & & & & \\ C_{zyxx} & C_{zyxy} & C_{zyxz} & & & & & & \\ C_{zzxx} & C_{zzxy} & C_{zzxz} & & & \cdots & & & C_{zzzz} \end{bmatrix} \begin{bmatrix}\varepsilon_{xx}\\ \varepsilon_{xy}\\ \varepsilon_{xz}\\ \varepsilon_{yx}\\ \varepsilon_{yy}\\ \varepsilon_{yz}\\ \varepsilon_{zx}\\ \varepsilon_{zy}\\ \varepsilon_{zz}\end{bmatrix}$$

Stiffness (and also compliance) tensor contains 9 x 9 = 81 components!

Anisotropic elasticity

- The **81 components** of stiffness or compliance tensors are **not completely independent**.
- This implies that **it is possible to reduce the number of constants** and to simplify the expression.

Step-1) First, we can reduce the number of constants by taking only the six independent components of stress and strain.

Vector (or Voigt) notation for stress and strain:

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \Rightarrow \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{yz} \\ \sigma_{zx} \end{bmatrix} \Rightarrow \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} \begin{matrix} \left.\vphantom{\begin{matrix} a \\ a \\ a \end{matrix}}\right\} \text{normal} \\ \left.\vphantom{\begin{matrix} a \\ a \\ a \end{matrix}}\right\} \text{shear} \end{matrix}$$

$$\begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} \Rightarrow \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ 2\varepsilon_{xy} \\ 2\varepsilon_{yz} \\ 2\varepsilon_{zx} \end{bmatrix} = \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \gamma_{xy} \\ \gamma_{yz} \\ \gamma_{zx} \end{bmatrix} \Rightarrow \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

Anisotropic elasticity

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

Remarks

$[\sigma] = [C][\varepsilon] = [C][S][\sigma]$

$[C][S] = [I]$

$[C] = [S]^{-1}$ and $[S] = [C]^{-1}$

(But $C_{11} \neq S_{11}$ in general)

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{21} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{31} & S_{32} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{41} & S_{42} & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & S_{53} & S_{54} & S_{55} & S_{56} \\ S_{61} & S_{62} & S_{63} & S_{64} & S_{65} & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}$$

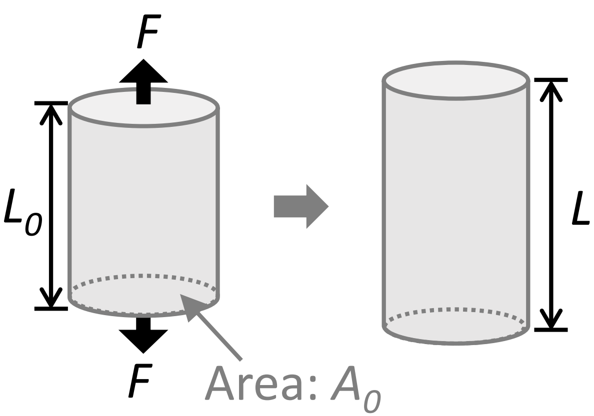
Then, we need only **6 x 6 = 36 constants** to express six stress components in terms of six strain components.

Anisotropic elasticity

Step-2) Next, consider the symmetry of stiffness and compliance tensors. This comes from the path-independent nature of linear elasticity.

Elastic strain energy

When an external load is applied, the work done to the material is stored as a form of elastic strain energy.



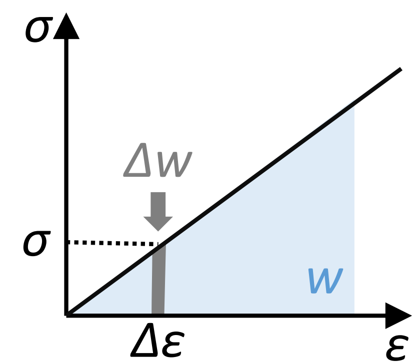
$$\Delta W = F\Delta L$$

1-D case:

$$\Delta w = \frac{\Delta W}{V_0} = \frac{F\Delta L}{A_0 L_0} = \sigma \Delta \varepsilon$$

$$w = \frac{1}{2}\sigma\varepsilon = \frac{1}{2}E\varepsilon^2$$

: Elastic strain energy per unit volume



Anisotropic elasticity

3-D case:

$$\Delta w = \sigma_1 \Delta\varepsilon_1 + \sigma_2 \Delta\varepsilon_2 + \sigma_3 \Delta\varepsilon_3 + \sigma_4 \Delta\varepsilon_4 + \sigma_5 \Delta\varepsilon_5 + \sigma_6 \Delta\varepsilon_6 \Rightarrow$$

For very small $\Delta\varepsilon_i$

$$\frac{\Delta w}{\Delta\varepsilon_i} \approx \frac{\partial w}{\partial\varepsilon_i} = \sigma_i$$

for i=1, …, 6.

$$w = \frac{1}{2}(\sigma_1\varepsilon_1 + \sigma_2\varepsilon_2 + \cdots \sigma_6\varepsilon_6)$$

Recall that $\sigma_1 = C_{11}\varepsilon_1 + C_{12}\varepsilon_2 + \cdots + C_{16}\varepsilon_6$

and $\sigma_2 = C_{21}\varepsilon_1 + C_{22}\varepsilon_2 + \cdots + C_{26}\varepsilon_6$

$$C_{12} = \frac{\partial\sigma_1}{\partial\varepsilon_2} = \frac{\partial}{\partial\varepsilon_2}\left(\frac{\partial w}{\partial\varepsilon_1}\right)$$

$$C_{21} = \frac{\partial\sigma_2}{\partial\varepsilon_1} = \frac{\partial}{\partial\varepsilon_1}\left(\frac{\partial w}{\partial\varepsilon_2}\right)$$

Since $\dfrac{\partial^2 w}{\partial\varepsilon_2\partial\varepsilon_1} = \dfrac{\partial^2 w}{\partial\varepsilon_1\partial\varepsilon_2}$ (this equality comes from the path-independent nature of linear elasticity)

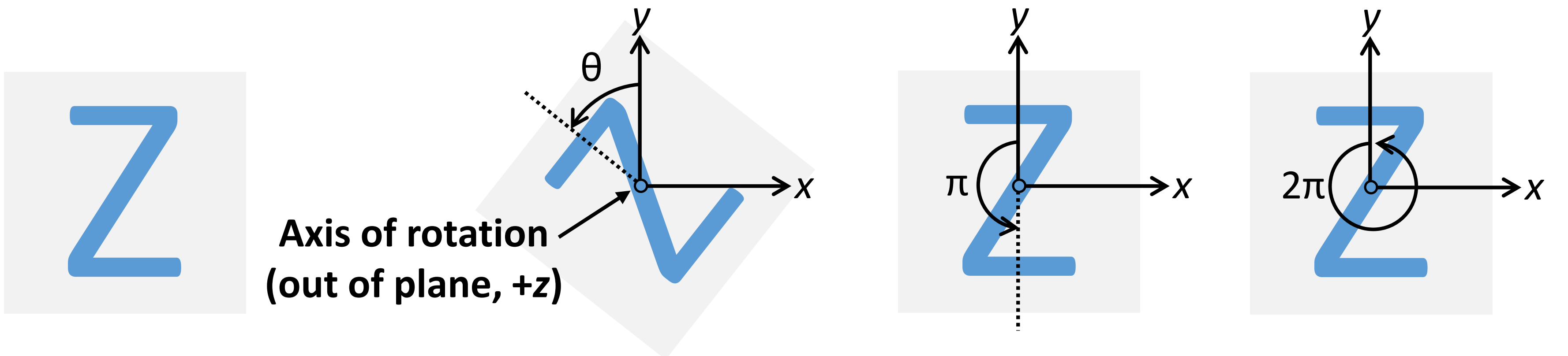
$C_{12} = C_{21}$ or, in general, $C_{ij} = C_{ji}$ for i, j = 1, …, 6.

Anisotropic elasticity

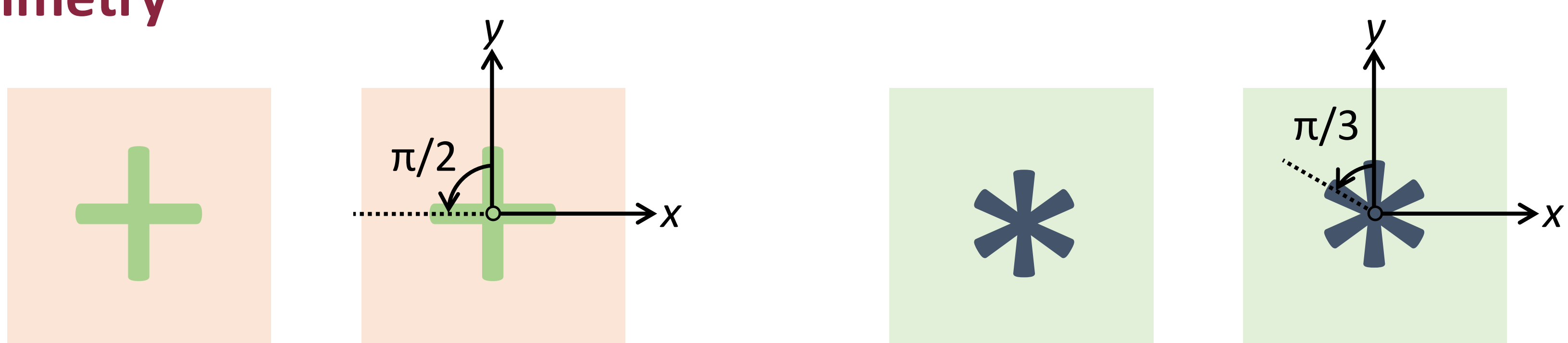
$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

This reduces the number of elasticity constants to **6+5+…+1 = 21** for **fully anisotropic materials.**

Rotational symmetry



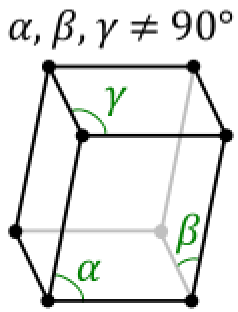
When we rotate the image by 0 < θ ≤ 2π, we can find **two rotated images** that are identical to the original image: **two-fold rotational symmetry**



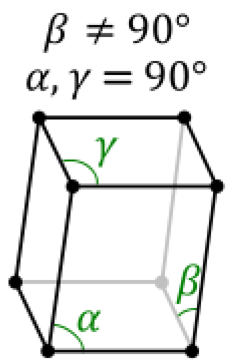
If we can find the identical image when it is rotated by a multiple of **2π/n**, this image is said to have **n-fold symmetry**.

Crystal systems

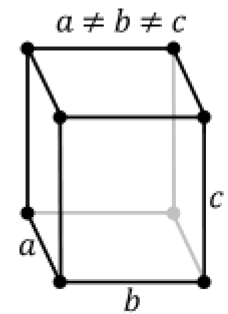
Triclinic



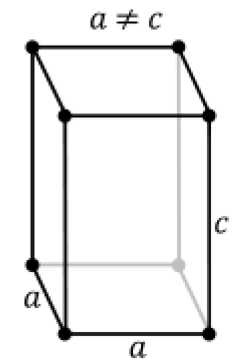
Monoclinic



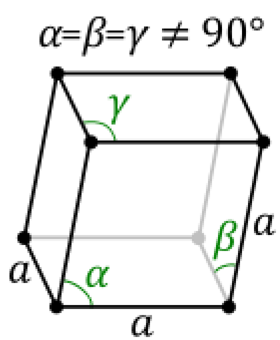
Orthorhombic



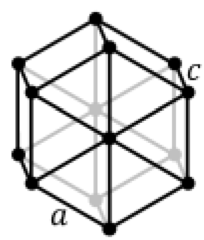
Tetragonal



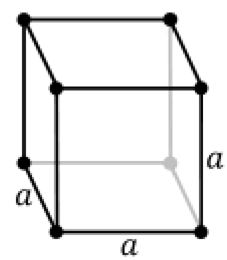
Rhombohedral



Hexagonal

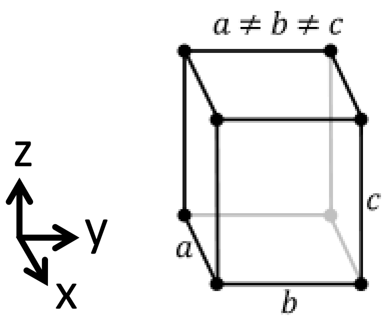


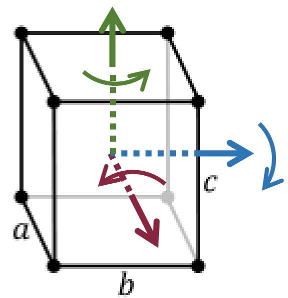
Cubic



Crystal systems

Example: Orthorhombic crystal

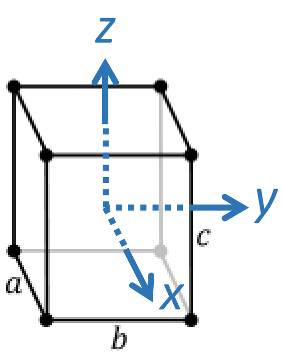




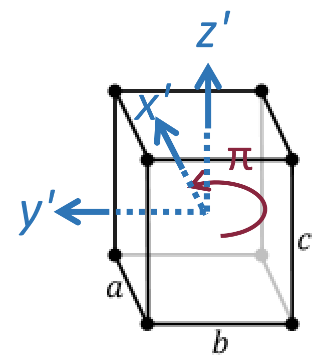
- Four-fold symmetry with respect to x-, y- and z-axis.
- Orthorhombic crystal has 3 four-fold axes of rotational symmetry.

Crystal system	Lattice parameter relationships	Defining symmetry
Triclinic	$a \neq b \neq c$, $\alpha \neq \beta \neq \gamma \neq 90°$	-
Monoclinic	$a \neq b \neq c$, $\alpha = \gamma = 90° \neq \beta$	1 two-fold axis
Orthorhombic	$a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$	3 two-fold axes
Tetragonal	$a = b \neq c$, $\alpha = \beta = \gamma = 90°$	1 four-fold axis
Rhombohedral	$a = b = c$, $\alpha = \beta = \gamma \neq 90°$	1 three-fold axis
Hexagonal	$a = b \neq c$, $\alpha = \beta = 90°$, $\gamma = 120°$	1 six-fold axis
Cubic	$a = b = c$, $\alpha = \beta = \gamma = 90°$	4 three-fold axes

Elasticity constants of orthorhombic crystal



Rotate the crystal (or equivalently, rotate the coordinate axes) by π with respect to the z-axis



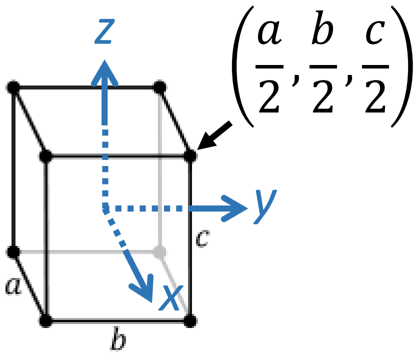
- For orthorhombic (= orthotropic) crystals this rotation must not affect the crystal structure. material property.
- This implies that the **stiffness tensor** must be **identical** for these two crystals.

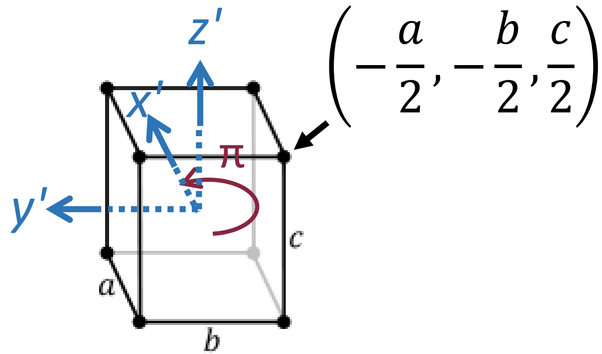
$$[\sigma] = [C][\varepsilon] \qquad \boxed{[C] = [C']} \qquad [\sigma'] = [C'][\varepsilon']$$

Stress-strain relationship written in the original coordinate system (x, y, z)

Stress-strain relationship written in the rotated coordinate system (x', y', z')

Elasticity constants of orthorhombic crystal





Rotation by π with respect to the z-axis

$$x' = -x$$
$$y' = -y$$
$$z' = z$$

$x' = -x$ and $x' = -x$

$$\begin{bmatrix} \sigma'_{xx} \\ \sigma'_{yy} \\ \sigma'_{zz} \\ \sigma'_{xy} \\ \sigma'_{yz} \\ \sigma'_{zx} \end{bmatrix} = \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ -\sigma_{yz} \\ -\sigma_{zx} \end{bmatrix} \text{ or } \begin{bmatrix} \sigma'_{1} \\ \sigma'_{2} \\ \sigma'_{3} \\ \sigma'_{4} \\ \sigma'_{5} \\ \sigma'_{6} \end{bmatrix} = \begin{bmatrix} \sigma_{1} \\ \sigma_{2} \\ \sigma_{3} \\ \sigma_{4} \\ -\sigma_{5} \\ -\sigma_{6} \end{bmatrix}$$

$z' = z$ and $x' = -x$

$$\begin{bmatrix} \varepsilon'_{xx} \\ \varepsilon'_{yy} \\ \varepsilon'_{zz} \\ \gamma'_{xy} \\ \gamma'_{yz} \\ \gamma'_{zx} \end{bmatrix} = \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \gamma_{xy} \\ -\gamma_{yz} \\ -\gamma_{zx} \end{bmatrix} \text{ or } \begin{bmatrix} \varepsilon'_{1} \\ \varepsilon'_{2} \\ \varepsilon'_{3} \\ \varepsilon'_{4} \\ \varepsilon'_{5} \\ \varepsilon'_{6} \end{bmatrix} = \begin{bmatrix} \varepsilon_{1} \\ \varepsilon_{2} \\ \varepsilon_{3} \\ \varepsilon_{4} \\ -\varepsilon_{5} \\ -\varepsilon_{6} \end{bmatrix}$$

Elasticity constants of orthorhombic crystal

If we express $[\sigma] = [C][\varepsilon]$ with their components

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ \vdots & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & \cdots & & & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

If we express $[\sigma'] = [C'][\varepsilon'] = [C][\varepsilon']$ with their components

$$\begin{bmatrix} \sigma'_1 \\ \sigma'_2 \\ \sigma'_3 \\ \sigma'_4 \\ \sigma'_5 \\ \sigma'_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ \vdots & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & \cdots & & & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon'_1 \\ \varepsilon'_2 \\ \varepsilon'_3 \\ \varepsilon'_4 \\ \varepsilon'_5 \\ \varepsilon'_6 \end{bmatrix} \Leftarrow \boxed{\begin{bmatrix} \sigma'_1 \\ \sigma'_2 \\ \sigma'_3 \\ \sigma'_4 \\ \sigma'_5 \\ \sigma'_6 \end{bmatrix} = \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ -\sigma_5 \\ -\sigma_6 \end{bmatrix} \text{ and } \begin{bmatrix} \varepsilon'_1 \\ \varepsilon'_2 \\ \varepsilon'_3 \\ \varepsilon'_4 \\ \varepsilon'_5 \\ \varepsilon'_6 \end{bmatrix} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ -\varepsilon_5 \\ -\varepsilon_6 \end{bmatrix}}$$

Elasticity constants of orthorhombic crystal

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ -\sigma_5 \\ -\sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ \vdots & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & \cdots & & & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ -\varepsilon_5 \\ -\varepsilon_6 \end{bmatrix}$$

We can rewrite the above expression as

$$\underbrace{\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}}_{[\sigma]} = \underbrace{\begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & -C_{15} & -C_{16} \\ & C_{22} & C_{23} & C_{24} & -C_{25} & -C_{26} \\ \vdots & & C_{33} & C_{34} & -C_{35} & -C_{36} \\ & & & C_{44} & -C_{45} & -C_{46} \\ & & & & C_{55} & C_{56} \\ & & \cdots & & & C_{66} \end{bmatrix}}_{\textbf{This must be identical to } [C]} \underbrace{\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}}_{[\varepsilon]}$$

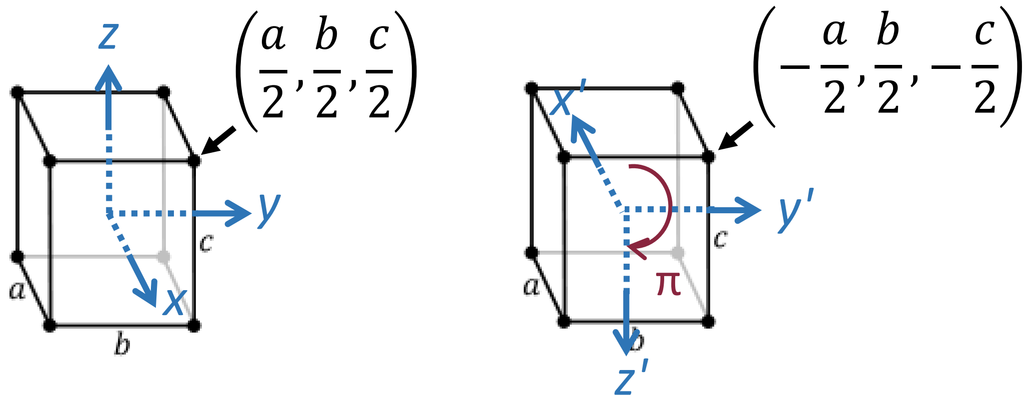
The symmetry condition can be satisfied only when we have:

$$C_{15} = -C_{15} = 0$$
$$C_{25} = -C_{25} = 0$$
$$C_{35} = -C_{35} = 0$$
$$C_{45} = -C_{45} = 0$$

$$C_{16} = -C_{16} = 0$$
$$C_{26} = -C_{26} = 0$$
$$C_{36} = -C_{36} = 0$$
$$C_{46} = -C_{46} = 0$$

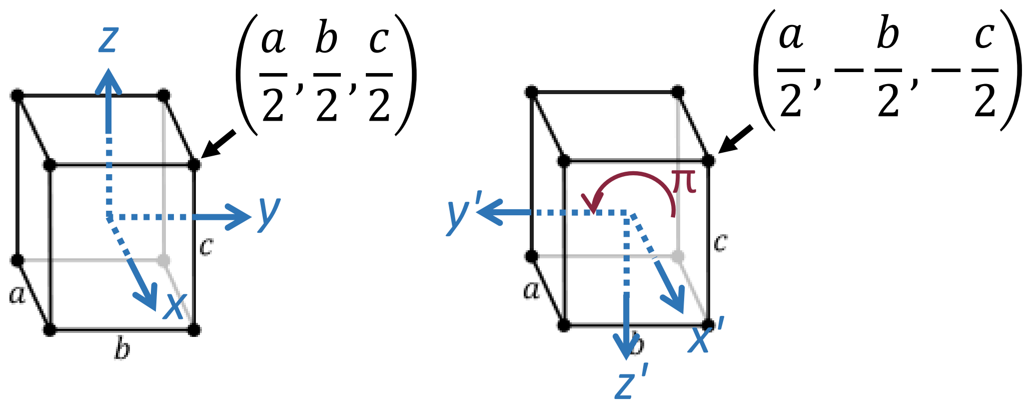
Elasticity constants of orthorhombic crystal

- We have two more two-fold axes of symmetry: *x*- and *y*-axes.



Rotation by π with respect to the y-axis

$$x' = -x$$
$$y' = y$$
$$z' = -z$$



Rotation by π with respect to the x-axis

$$x' = x$$
$$y' = -y$$
$$z' = -z$$

- If we repeat the same procedures for these two rotations...

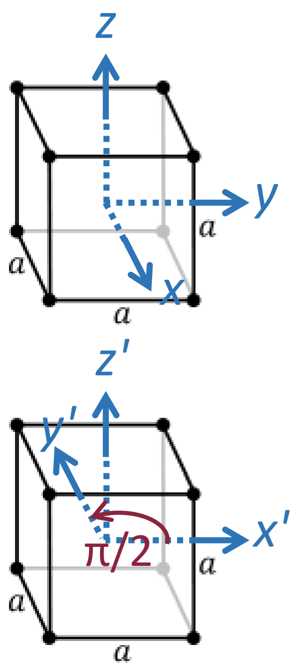
Elasticity constants of orthorhombic crystal

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ \vdots & & & C_{44} & 0 & 0 \\ & & & & C_{55} & 0 \\ & & & \cdots & & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ & S_{22} & S_{23} & 0 & 0 & 0 \\ & & S_{33} & 0 & 0 & 0 \\ \vdots & & & S_{44} & 0 & 0 \\ & & & & S_{55} & 0 \\ & & & \cdots & & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}$$

Orthorhombic (= orthotropic) materials have **9 independent elasticity constants**.

Elasticity constants of cubic crystal



- Cubic crystals automatically satisfy the symmetry condition of orthorhombic crystal.
- Therefore, we can utilize the stiffness matrix of orthorhombic crystal with 9 constants.
- We can further reduce the number of constants using the additional symmetry conditions of cubic crystals.

Rotation by π/2 with respect to the z-axis

$$x' = y$$
$$y' = -x$$
$$z' = z$$

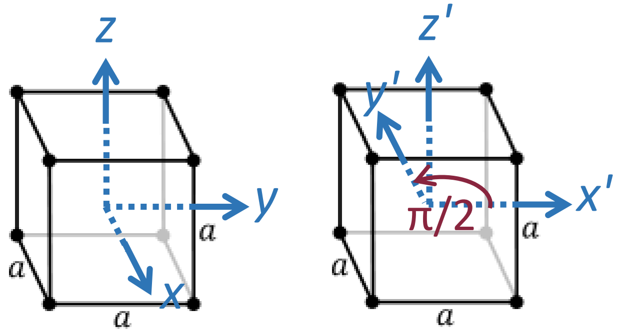
Rotation by π/2 with respect to the y-axis

$$x' = -z$$
$$y' = y$$
$$z' = x$$

Rotation by π/2 with respect to the x-axis

$$x' = x$$
$$y' = z$$
$$z' = -y$$

Elasticity constants of cubic crystal



Rotation by π/2 with respect to the z-axis

$$x' = y$$
$$y' = -x$$
$$z' = z$$

$x' = y$ and $x' = y$

$$\begin{bmatrix} \sigma'_{xx} \\ \sigma'_{yy} \\ \sigma'_{zz} \\ \sigma'_{xy} \\ \sigma'_{yz} \\ \sigma'_{zx} \end{bmatrix} = \begin{bmatrix} \sigma_{yy} \\ \sigma_{xx} \\ \sigma_{zz} \\ -\sigma_{xy} \\ -\sigma_{zx} \\ \sigma_{yz} \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} \sigma'_{1} \\ \sigma'_{2} \\ \sigma'_{3} \\ \sigma'_{4} \\ \sigma'_{5} \\ \sigma'_{6} \end{bmatrix} = \begin{bmatrix} \sigma_{2} \\ \sigma_{1} \\ \sigma_{3} \\ -\sigma_{4} \\ -\sigma_{6} \\ \sigma_{5} \end{bmatrix}$$

$z' = z$ and $x' = y$

Insert these to the equation

$$[\sigma'] = [C'][\varepsilon'] = [C][\varepsilon']$$

Elasticity constants of cubic crystal

$$\begin{bmatrix} \sigma_2 \\ \sigma_1 \\ \sigma_3 \\ -\sigma_4 \\ -\sigma_6 \\ \sigma_5 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ \vdots & & & C_{44} & 0 & 0 \\ & & & & C_{55} & 0 \\ & & \cdots & & & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_2 \\ \varepsilon_1 \\ \varepsilon_3 \\ -\varepsilon_4 \\ -\varepsilon_6 \\ \varepsilon_5 \end{bmatrix}$$

This symmetry condition requires

$$C_{11} = C_{22}$$
$$C_{13} = C_{23}$$
$$C_{55} = C_{66}$$

We can rewrite the above expression as

$$\underset{[\sigma]}{\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}} = \underbrace{\begin{bmatrix} C_{22} & C_{12} & C_{23} & 0 & 0 & 0 \\ & C_{11} & C_{13} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ \vdots & & & C_{44} & 0 & 0 \\ & & & & C_{66} & 0 \\ & & \cdots & & & C_{55} \end{bmatrix}}_{\textbf{This must be identical to } [C]} \underset{[\varepsilon]}{\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}}$$

If we repeat the same procedure for the other two rotations we can also find

$$C_{11} = C_{22} = C_{33}$$
$$C_{12} = C_{23} = C_{13}$$
$$C_{44} = C_{55} = C_{66}$$

Elasticity constants of cubic crystal

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ & C_{11} & C_{22} & 0 & 0 & 0 \\ \vdots & & C_{11} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & \cdots & & C_{44} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ & S_{11} & S_{12} & 0 & 0 & 0 \\ \vdots & & S_{11} & 0 & 0 & 0 \\ & & & S_{44} & 0 & 0 \\ & & & & S_{44} & 0 \\ & & & \cdots & & S_{44} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}$$

Cubic crystals have **only 3 independent elasticity constants**.

Elasticity constants of other crystals

Monoclinic

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & C_{15} & 0 \\ \vdots & C_{22} & C_{23} & 0 & C_{25} & 0 \\ & & C_{33} & 0 & C_{35} & 0 \\ & & & C_{44} & 0 & C_{46} \\ & & & & C_{55} & 0 \\ \text{13 constants} & & & & \cdots & C_{66} \end{bmatrix}$$

Rhombohedral

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & 0 & 0 \\ \vdots & C_{11} & C_{13} & -C_{14} & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & C_{14} \\ \text{6 constants} & & & & \cdots & (C_{11}-C_{12})/2 \end{bmatrix}$$

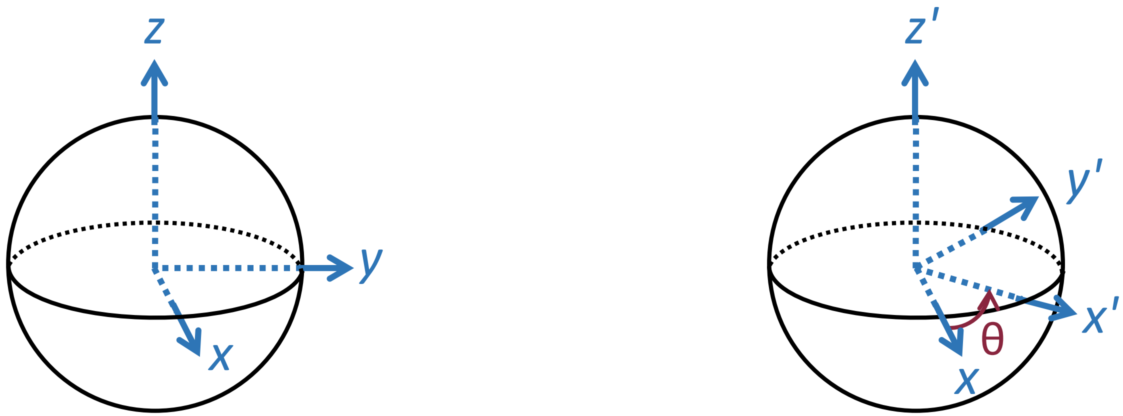
Tetragonal

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ \vdots & C_{11} & C_{13} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ \text{6 constants} & & & & \cdots & C_{66} \end{bmatrix}$$

Hexagonal

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ \vdots & C_{11} & C_{13} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ \text{5 constants} & & & & \cdots & (C_{11}-C_{12})/2 \end{bmatrix}$$

Elasticity constants of isotropic material



- **Isotropic** materials exhibit **the same property along any direction**.
- Therefore, the stiffness tensor is preserved for any rotation.
- Considering that isotropic material automatically satisfy the cubic and hexagonal symmetries, we can utilize the previous results to obtain the isotropic stiffness tensor:

Elasticity constants of isotropic material

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ & C_{11} & C_{22} & 0 & 0 & 0 \\ \vdots & & C_{11} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & \cdots & & & C_{44} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} \quad \text{where} \quad C_{44} = \frac{\mathrm{C}_{11} - \mathrm{C}_{22}}{2}$$

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ & S_{11} & S_{12} & 0 & 0 & 0 \\ \vdots & & S_{11} & 0 & 0 & 0 \\ & & & S_{44} & 0 & 0 \\ & & & & S_{44} & 0 \\ & & \cdots & & & S_{44} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} \quad \text{where} \quad S_{44} = 2(\mathrm{S}_{11} - \mathrm{S}_{22})$$

Isotropic materials have **only 2 independent elasticity constants**.

Elasticity constants of isotropic material

It is conventional to designate C_{12} and C_{44} as λ and μ, which are called **Lamé constants**.

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} \lambda+2\mu & \lambda & \lambda & 0 & 0 & 0 \\ & \lambda+2\mu & \lambda & 0 & 0 & 0 \\ \vdots & & \lambda+2\mu & 0 & 0 & 0 \\ & & & \mu & 0 & 0 \\ & & & & \mu & 0 \\ & & \cdots & & & \mu \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

Recall the elasticity constants we learned in the previous lectures:

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ & 1-\nu & \nu & 0 & 0 & 0 \\ \vdots & & 1-\nu & 0 & 0 & 0 \\ & & & (1-2\nu) & 0 & 0 \\ & & & & (1-2\nu) & 0 \\ & & \cdots & & & (1-2\nu) \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

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

$$K = \frac{E}{3(1-2\nu)}$$

(Generalized Hooke's law for isotropic material)

Elasticity constants of isotropic material

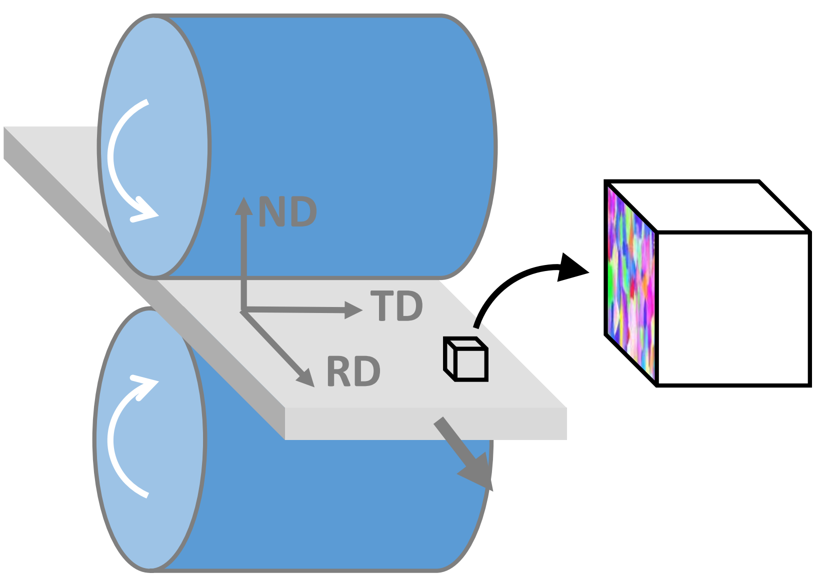
- Because there are **only two independent constants** in **isotropic elasticity**, E, ν, G, K, λ, and μ are not completely independent.
- If any two of these constants are given, the other constants can be determined.

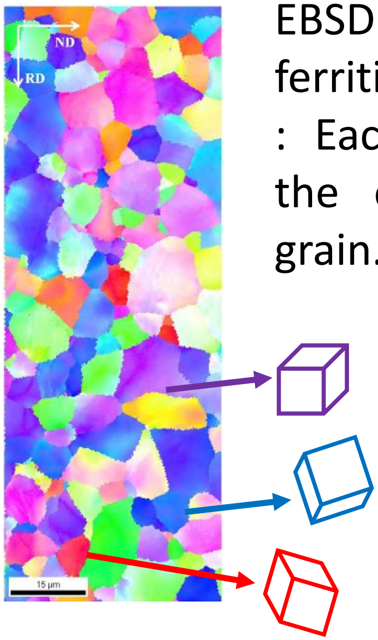
$(G = 2\mu)$

Known Elastic Constants	E	ν	μ	κ	λ
Shear modulus μ, Bulk modulus κ	$\frac{9\kappa\mu}{3\kappa+\mu}$	$\frac{3\kappa-2\mu}{6\kappa+2\mu}$	μ	κ	$\frac{3\kappa-2\mu}{3}$
Young's modulus E, Poisson's ratio ν	E	ν	$\frac{E}{2(1+\nu)}$	$\frac{E}{3(1-2\nu)}$	$\frac{E\nu}{(1+\nu)(1-2\nu)}$
Young's modulus E, Shear modulus μ	E	$\frac{E-2\mu}{2\mu}$	μ	$\frac{E\mu}{3(3\mu-E)}$	$\frac{\mu(E-2\mu)}{3\mu-E}$
Young's modulus E, Bulk modulus κ	E	$\frac{3\kappa-E}{6\kappa}$	$\frac{3\kappa E}{9\kappa-E}$	κ	$\frac{3\kappa(3\kappa-E)}{9\kappa-E}$
Shear modulus μ, Lame's constant λ	$\frac{\mu(3\lambda+2\mu)}{\lambda+\mu}$	$\frac{\lambda}{2(\lambda+\mu)}$	μ	$\frac{3\lambda+2\mu}{3}$	λ

Elastic property of polycrystal

- Most of crystalline materials are polycrystal.
- The elastic property that we typically observe with these materials is therefore the averaged value over a large number of crystals.





EBSD image of a thin ferritic stainless steel
: Each color represents the orientation of the grain.

Summary

- At the beginning of this chapter we had **81** elasticity constants for **fully anisotropic material**.

$$
\begin{bmatrix} \sigma_{xx} \\ \sigma_{xy} \\ \sigma_{xz} \\ \sigma_{yx} \\ \sigma_{yy} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{zy} \\ \sigma_{zz} \end{bmatrix} = \begin{bmatrix} C_{xxxx} & C_{xxxy} & C_{xxxz} & C_{xxyx} & C_{xxyy} & C_{xxyz} & C_{xxzx} & C_{xxzy} & C_{xxzz} \\ C_{xyxx} & C_{xyxy} & C_{xyxz} & C_{xyyx} & C_{xyyy} & C_{xyyz} & C_{xyzx} & C_{xyzy} & C_{xyzz} \\ C_{xzxx} & C_{xzxy} & C_{xzxz} & C_{xzyx} & C_{xzyy} & C_{xzyz} & C_{xzzx} & C_{xzzy} & C_{xzzz} \\ C_{yxxx} & C_{yxxy} & C_{yxxz} & & & & & & \\ C_{yyxx} & C_{yyxy} & C_{yyxz} & & & & & & \\ C_{yzxx} & C_{yzxy} & C_{yzxz} & & & \ddots & & & \vdots \\ C_{zxxx} & C_{zxxy} & C_{zxxz} & & & & & & \\ C_{zyxx} & C_{zyxy} & C_{zyxz} & & & & & & \\ C_{zzxx} & C_{zzxy} & C_{zzxz} & & & \cdots & & & C_{zzzz} \end{bmatrix} \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{xy} \\ \varepsilon_{xz} \\ \varepsilon_{yx} \\ \varepsilon_{yy} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{zy} \\ \varepsilon_{zz} \end{bmatrix}
$$

Summary

- But we found that there are only **21 independent constants** out of 81, owing to (1) the symmetry of stress and strain tensors and (2) path-independent nature of elastic strain energy.

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ \vdots & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & & \cdots & & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

Summary

- We could further reduce the number of independent constants for single crystals using their symmetry (**Higher symmetry → less number of constants**)
- Finally we found that there are **only two** independent constants for **isotropic materials**.

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} \lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\ & \lambda + 2\mu & \lambda & 0 & 0 & 0 \\ & & \lambda + 2\mu & 0 & 0 & 0 \\ & & & \mu & 0 & 0 \\ & & & & \mu & 0 \\ & & & & & \mu \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

Exercises (1)

Problem Uniaxial tension tests were performed for some metal alloys. From these experiments the Young's modulus and Poisson's ratio of the materials could be obtained, as given in the table below. If we assume these materials are isotropic, what will be the shear and bulk moduli of these materials?

Table Elastic constants of some metal alloys

	E [GPa]	ν [-]	G [GPa]	K [GPa]
Al	70.5	0.34		
Be	309.0	0.05		
α-Fe	208.2	0.29		
Mg	44.3	0.29		
Cu	122.5	0.34		

Exercises (2)

Problem Show that the stiffness or compliance tensor of tetragonal crystal has six independent constants as below:

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{11} & C_{13} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & C_{66} \end{bmatrix} \qquad \begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ & S_{11} & C_{13} & 0 & 0 & 0 \\ & & S_{33} & 0 & 0 & 0 \\ & & & S_{44} & 0 & 0 \\ & & & & S_{44} & 0 \\ & & & & & S_{66} \end{bmatrix}$$

Approach

(1) Note that the tetragonal symmetry satisfies the orthotropic symmetry.

(2) Then, consider the additional symmetry conditions of tetragonal crystal.

Exercises (3)

Problem α-Fe has a cubic crystal structure. Three elasticity constants for Fe can be found in the table below. When uniaxial tension is applied to a single crystal of α-Fe along [100] direction, what will be the elastic modulus?

Approach
(1) Choose which of the expressions will be useful: $[\sigma] = [C][\varepsilon]$ or $[\varepsilon] = [S][\sigma]$
(2) Calculate the stress and strain along the tensile direction (the *x*-direction in this example).
(3) The elastic modulus is then the ratio $\sigma_{\mathrm{xx}}/\varepsilon_{\mathrm{xx}}$.

Table Elastic constants of some cubic crystals

	C_{11} [GPa]	C_{12} [GPa]	C_{44} [GPa]	S_{11} [TPa^{-1}]	S_{12} [TPa^{-1}]	S_{44} [TPa^{-1}]
Cr	339.8	58.6	99.0	3.10	-0.46	10.10
α-Fe	231.4	134.7	116.4	7.56	-2.78	8.59
K	3.7	3.14	1.88	1223.9	56.19	53.19

Exercises (4)

Problem Consider a single crystal of α-Fe again. When uniaxial tension is applied along [110] direction, what will be the elastic modulus?

Approach
(1) Express the applied stress as a stress tensor in the crystallographic coordinate system (*Hint: use the transformation of stress tensor that we learned in the previous chapter*).
(2) Calculate the resultant strain using the stress-strain relationship for cubic crystal.
(3) Calculate strain along the loading direction [110].
(3) The elastic modulus is then the ratio $\sigma_{[110]}/\varepsilon_{[110]}$.

Appendix
- Slides from Prof. Han

Elasticity

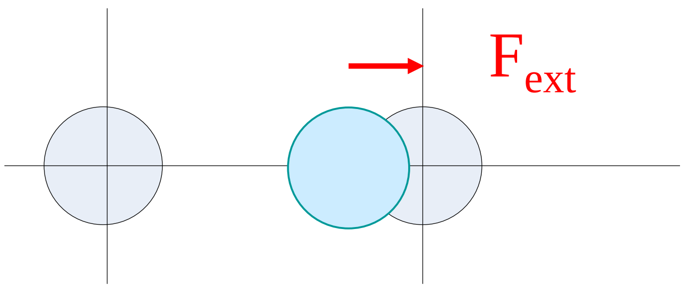
- Elasticity are extremely important because engineering design is done in the elastic region.

- Material fracture is related to elastic properties because the elastic energy release is one of driving force for fracture.

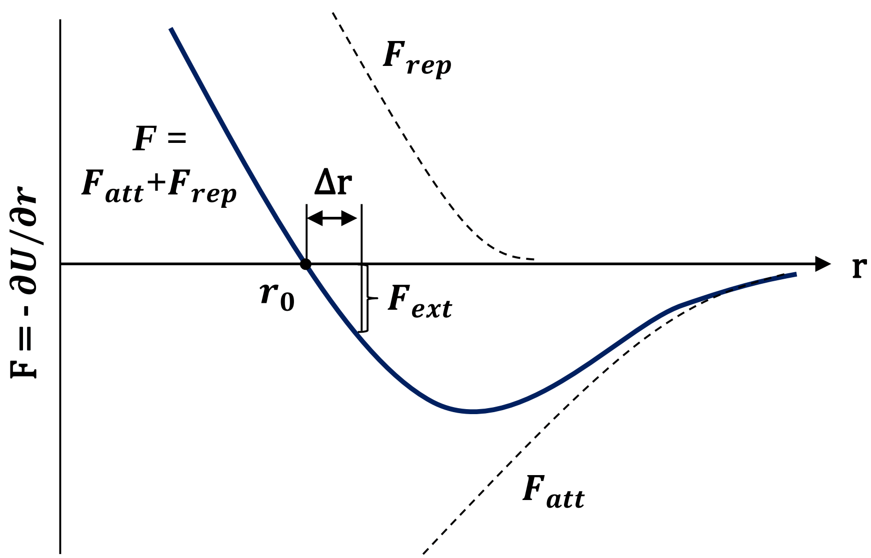
- Elastic behavior is inherently anisotropic for individual grains. However, most polycrystalline materials are elastically isotropic. Polycrystalline materials can be anisotropic if they are textured.

Basis for linear elasticity

- **Consider two atoms**

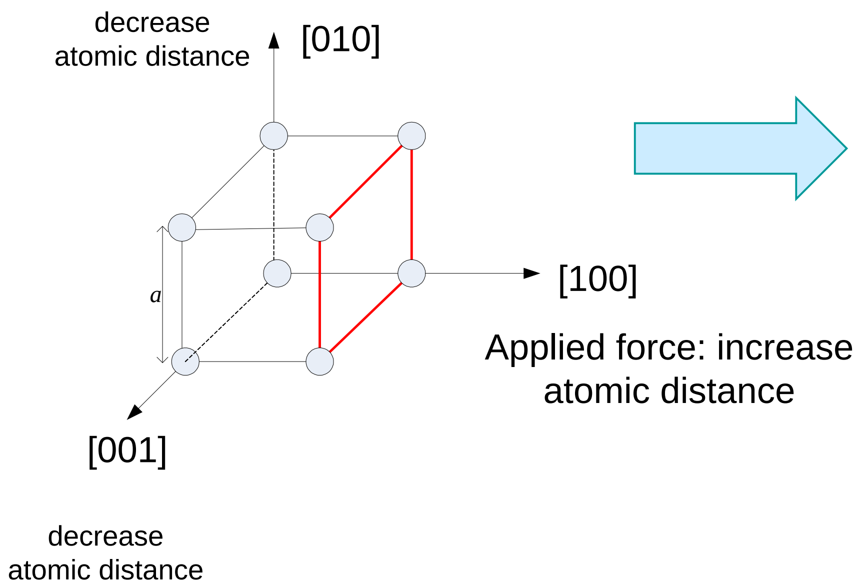


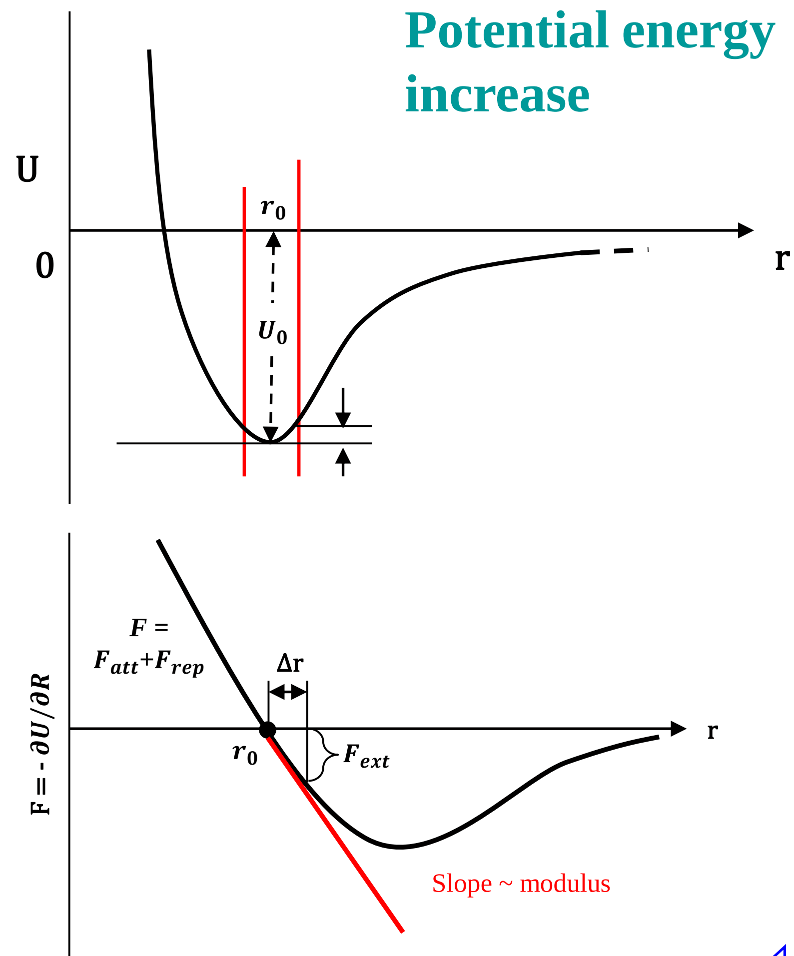
F_{ext} is a force that should be applied to separate the atom from r_o position ; external force



Basis for linear elasticity
(Young's modulus)

- **Consider cubic crystal material**

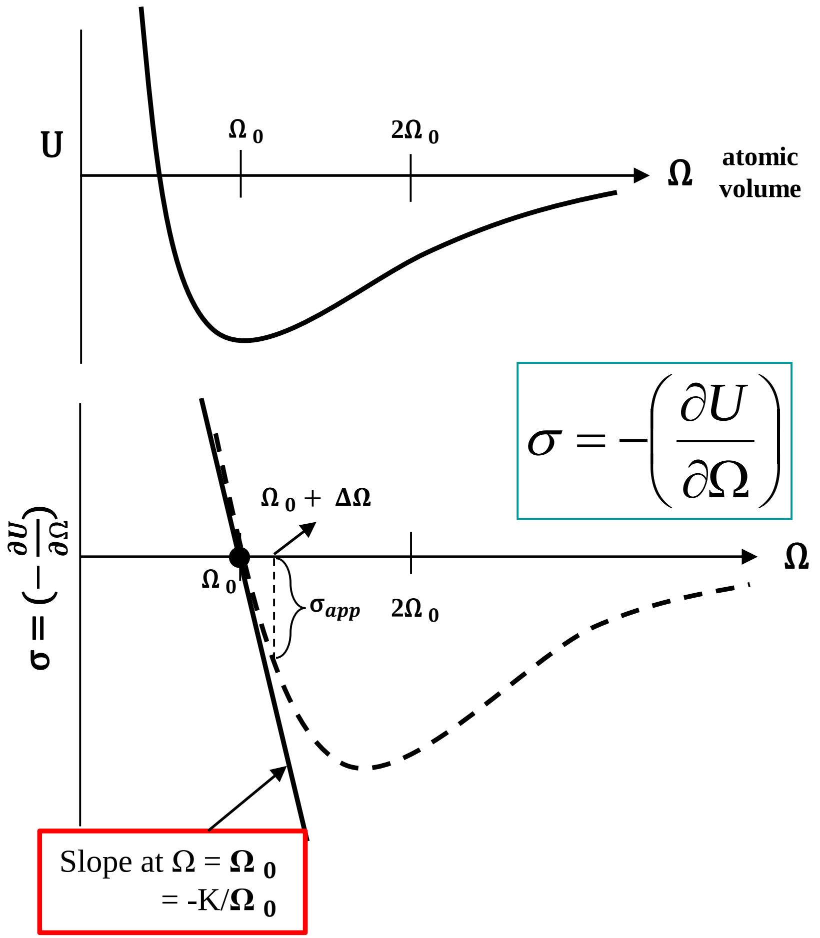




- **Slope : modulus**

Basis for linear elasticity
(Bulk modulus)

- **Relate elastic modulus to volume change**



$$F = -\left(\frac{\partial U}{\partial \Omega}\right) \times \text{area}$$

$$\sigma = -\left(\frac{\partial U}{\partial \Omega}\right)$$

- **Bulk modulus**

$$K = -\Omega_0 \left(\frac{\partial \sigma}{\partial \Omega}\right)_{\Omega_0} = \Omega_0 \left(\frac{\partial^2 U}{\partial \Omega^2}\right)_{\Omega_0}$$

Basis for linear elasticity
(Bulk modulus)

- Alkali metal
- Covalent bonded
- Diamond cubic

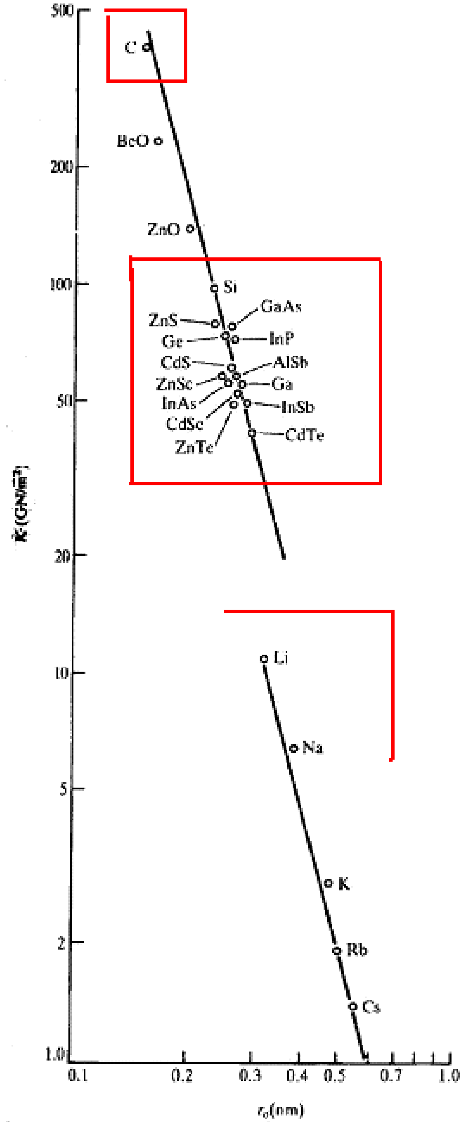


Figure 2.7
Bulk moduli of the alkali metals and tetrahedral covalently bonded crystals as a function of their interatomic spacing. The slope of −4 observed on these logarithmic coordinates shows $K \sim (r_0)^{-4}$. The generally higher moduli of the covalent solids is indicative of their inherently stronger bonding. *(Data obtained from J. J. Gilman, Micromechanics of Flow in Solids, McGraw-Hill, New York, 1969, Chap. 2, pp. 29–41.)*

Basis for linear elasticity
(Temperature effect)

- **Bulk (Young's) moduli relates to**
  - **Curvature of bonding energy**
- **Bonding energy correlates with the melting temperature**

$$U_0 \propto kT_m \qquad k = 1.38\times10^{-3}\, J/atom\, K$$

$$E \propto \frac{kT_m}{\Omega}$$

- **Temperature (heat) increases atomic vibration**
  - **Thermal energy added**
  - **Potential increased**
  - **Curvature of bonding energy decreases**

Range of Elastic Moduli

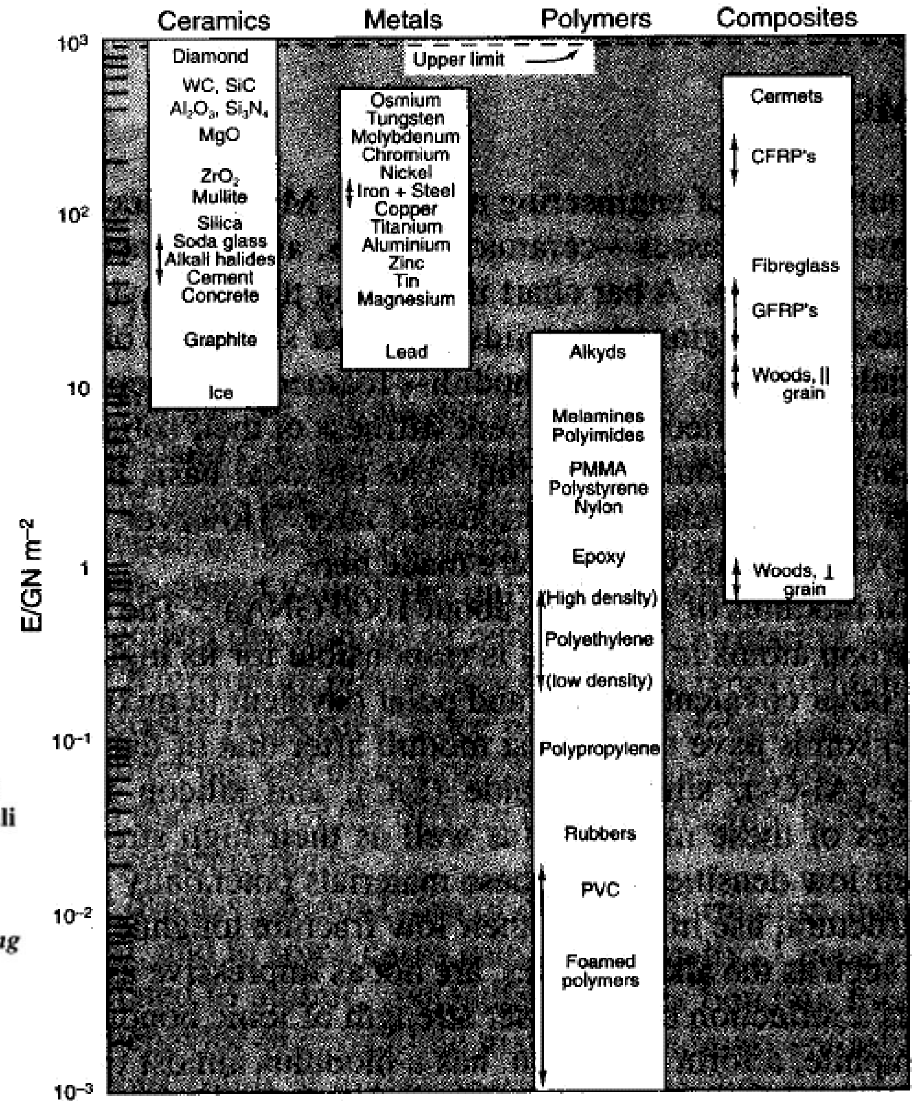


Figure 2.1

A bar chart illustrating elastic moduli values of the primary material classes (ceramics, metals, and polymers) and of composites (a hybrid of materials from the different primary classes). Although there is considerable variation in elastic moduli within a given material class, ceramics as a whole have the highest elastic moduli and polymers the lowest. Moduli of composites are intermediate to those of their constituents. It is noteworthy that elastic moduli of engineering solids span about six orders of magnitude. (*From Michael F. Ashby and David R. H. Jones, Engineering Materials I—An Introduction to their Properties and Applications, Pergamon Press, Oxford, 1980.*)

Basis for linear elasticity
(anisotropy)

- The forces between atoms, molecules, or ions in crystals depends on the distances between them. Thus, they also vary with crystallographic direction so it should not be surprising that crystalline moduli are anisotropic.

Hooke's Law in One Dimension

Robert Hooke [1635-1702] first drew attention to the linear relation between the impressed force and the resulting displacement, and in recognition of this we have *Hooke's Law*. By definition, this holds for all linear elastic solids, and for the example of the wire it simply states that the applied uniaxial stress σ is linearly related to the longitudinal strain ε. In one dimension, this relation can be written either as

$$\sigma = C\,\varepsilon \qquad \text{or} \qquad \varepsilon = S\,\sigma$$

where C is known as the *stiffness* and S as the *compliance*. In one dimension, the stiffness is also referred to as *Young's modulus or elastic modulus*.

Hooke's Law in Three Dimensions

The alternative forms of *Hooke's law* are best written in the repeated suffix notation

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \quad \text{and} \quad \varepsilon_{ij} = S_{ijkl}\sigma_{kl}$$

Each of these statements of *Hooke's law* stands for 9 equations each having nine terms on the right-hand side, altogether making 81 components of the stiffness or compliance.

$$\varepsilon_{ij} = S_{ijkl}\sigma_{kl} \;=\; \varepsilon_{ji} = S_{jikl}\sigma_{kl}$$

The number of independent components of compliance is reduced to 36.

An exactly parallel argument can be used to conclude that the stiffness, C_{ijkl} **, also has just 36 components.**

Hooke's Law in Three Dimensions

Changing Reference Axes.

The *compliance* or *stiffness* constants defined by these equations are themselves tensors and consequently they obey the transformation law for a *fourth-rank tensor*

$$S'_{ijkl} = a_{im} a_{jn} a_{ko} a_{lp} S_{mnop} \qquad \textit{and} \qquad C'_{ijkl} = a_{im} a_{jn} a_{ko} a_{lp} C_{mnop}$$

Contracted or Matrix Notation.

The compliance (or stiffness) is a fourth rank tensor and so its components have four subscripts. A more economical notation has been devised for the components of compliance (or stiffness) having only two subscripts; this is called *the contracted or matrix notation.* Each pair of subscripts of the tensor components is replaced by a single subscript according to the following table;

Tensor	11	22	33	23 or 32	13 or 31	12 or 21
Contracted	1	2	3	4	5	6

Hooke's Law in Three Dimensions

$$\begin{bmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{bmatrix} \qquad \begin{bmatrix} \varepsilon_{12} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix} = \begin{bmatrix} \varepsilon_1 & \varepsilon_6/2 & \varepsilon_5/2 \\ \varepsilon_6/2 & \varepsilon_2 & \varepsilon_4/2 \\ \varepsilon_5/2 & \varepsilon_4/2 & \varepsilon_3 \end{bmatrix}$$

$$\sigma_{ij} = C_{ijkl}\, \varepsilon_{kl} \quad \Rightarrow \quad \sigma_i = C_{ij}\, \varepsilon_j$$

$$\varepsilon_{ij} = S_{ijkl}\, \sigma_{kl} \quad \Rightarrow \quad \varepsilon_i = S_{ij}\, \sigma_j$$

pS_{ijkl} (in the tensor notation) is equal to S_{mn} (in the matrix notation) where m and n correspond to ij and kl, respectively

$$pS_{ijkl} = S_{mn}$$

where p **= 1 when both m and n are 1, 2 or 3 (**$S_{1111} = S_{11}$, $S_{1122} = S_{12}$ **……)**
p **= 2 when either m or n are 1, 2 or 3 (2**$S_{1123} = S_{14}$, **2**$S_{1113} = S_{15}$ **……)**
p **= 4 when both m and n are 4, 5 or 6 (4**$S_{1223} = S_{64}$, **4**$S_{1212} = S_{66}$ **……)**

Hooke's Law in Three Dimensions

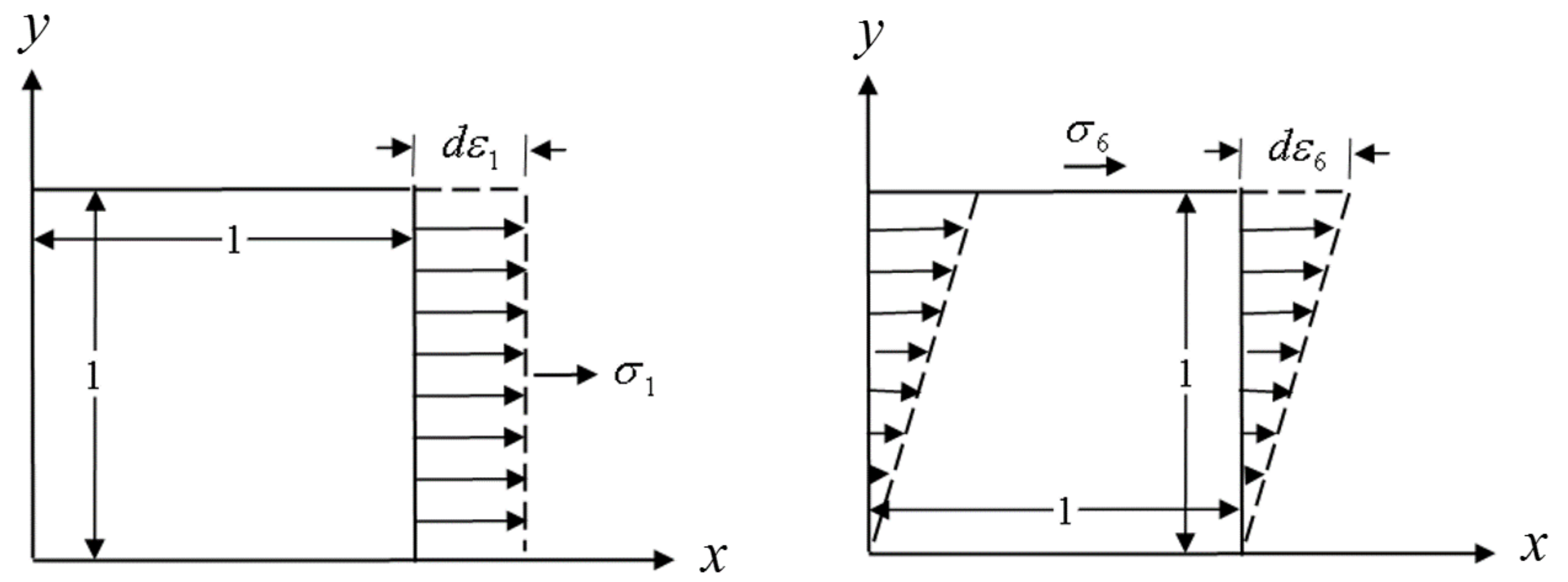
$$\begin{bmatrix}\sigma_1\\\sigma_2\\\sigma_3\\\sigma_4\\\sigma_5\\\sigma_6\end{bmatrix}=\begin{bmatrix}C_{11}&C_{12}&C_{13}&C_{14}&C_{15}&C_{16}\\C_{21}&C_{22}&C_{23}&C_{24}&C_{25}&C_{26}\\C_{31}&C_{32}&C_{33}&C_{34}&C_{35}&C_{36}\\C_{41}&C_{42}&C_{43}&C_{44}&C_{45}&C_{46}\\C_{51}&C_{52}&C_{53}&C_{54}&C_{55}&C_{56}\\C_{61}&C_{62}&C_{63}&C_{64}&C_{65}&C_{66}\end{bmatrix}\begin{bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\\\varepsilon_4\\\varepsilon_5\\\varepsilon_6\end{bmatrix}$$

$$\begin{bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\\\varepsilon_4\\\varepsilon_5\\\varepsilon_6\end{bmatrix}=\begin{bmatrix}S_{11}&S_{12}&S_{13}&S_{14}&S_{15}&S_{16}\\S_{21}&S_{22}&S_{23}&S_{24}&S_{25}&S_{26}\\S_{31}&S_{32}&S_{33}&S_{34}&S_{35}&S_{36}\\S_{41}&S_{42}&S_{43}&S_{44}&S_{45}&S_{46}\\S_{51}&S_{52}&S_{53}&S_{54}&S_{55}&S_{56}\\S_{61}&S_{62}&S_{63}&S_{64}&S_{65}&S_{66}\end{bmatrix}\begin{bmatrix}\sigma_1\\\sigma_2\\\sigma_3\\\sigma_4\\\sigma_5\\\sigma_6\end{bmatrix}$$

$[\sigma]= [C][\varepsilon]$ **and** $[\varepsilon]= [S][\sigma]$

$[C] = [S]^{-1}$ **or** $[S] = [C]^{-1}$

Elastic Strain Energy



Normal strain $d\varepsilon_1$ due to normal stress σ_1 .

Shear strain $d\varepsilon_6$ due to shear stress σ_6 .

The works done by these stresses is $\sigma_1\, d\varepsilon_1$ and $\sigma_6\, d\varepsilon_6$.

$$\boxed{dw = C_{ij}\varepsilon_j d\varepsilon_i}$$

Elastic Strain Energy

If the straining is carried out isothermally and reversibly, the energy expended is equal to the change in free energy ($d\phi$) of the body.

$$d\phi = C_{ij}\,\varepsilon_j\,d\varepsilon_i \qquad \text{or} \qquad \frac{\partial\phi}{\partial\varepsilon_i} = C_{ij}\,\varepsilon_j$$

$$\frac{\partial}{\partial\varepsilon_j}\left(\frac{\partial\phi}{\partial\varepsilon_i}\right) = C_{ij}$$

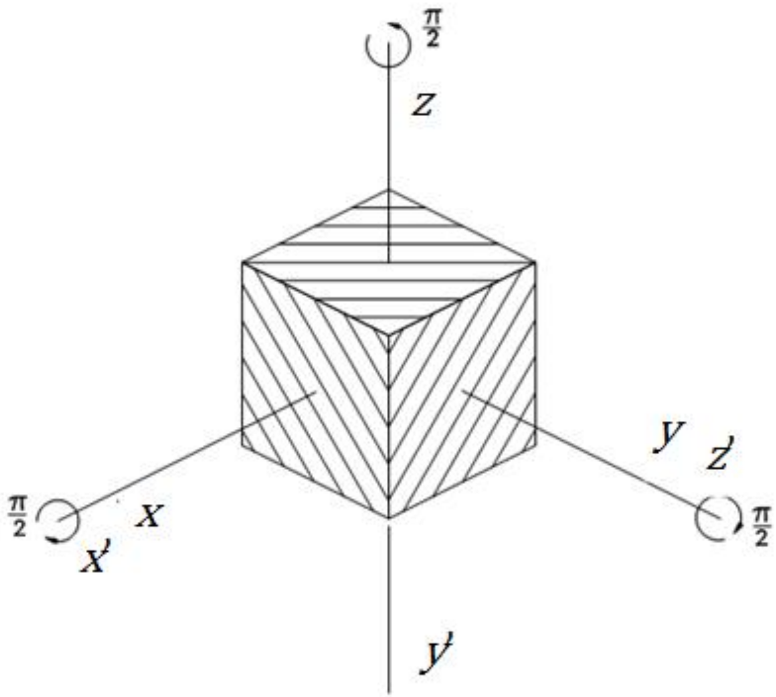
Since the free energy is a state property, this is a perfect differential and the order of differentiation is immaterial.

$$\boxed{C_{ij} = C_{ji}}$$

The matrix array of the components of stiffness is symmetrical. There can be no more than twenty-one independent components of stiffness.

$$\varphi = w = (1/2)\,C_{ij}\,\varepsilon_i\,\varepsilon_j = (1/2)\,\sigma_i\,\varepsilon_i = (1/2)\,S_{ij}\,\sigma_i\,\sigma_j$$

Effect of Materials Symmetry on Elastic Constants (*Cubic System*)



Three fourfold axes of rotation in cubic symmetry

If the crystal is rotated through $\pi/2$ about a fourfold axis,

	x	y	z
x'	1	0	0
y'	0	0	-1
z'	0	1	0

$$\Downarrow$$

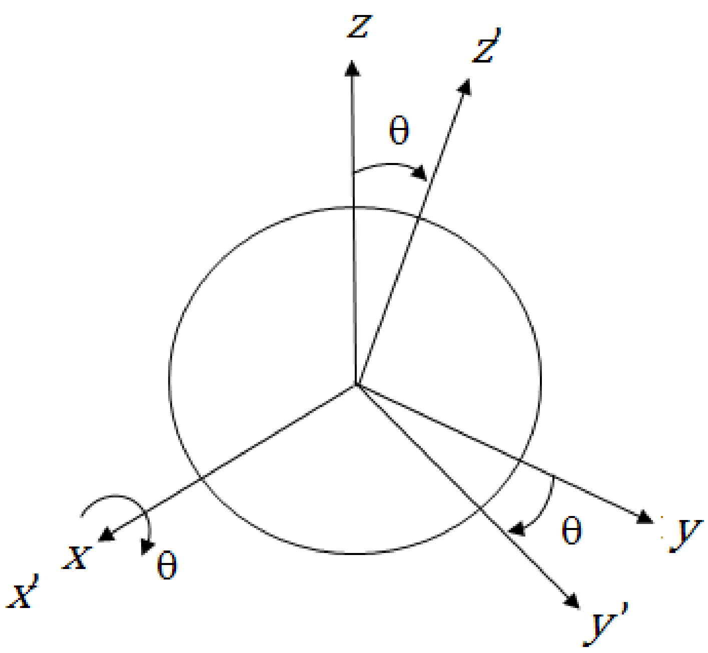
$$\begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$

There are only three independent components of stiffness and three of compliance.

Effect of Materials Symmetry on Elastic Constants (*Cubic System*)

Material class	Material	C_{11} (10^{10} N/m^2)	C_{12} (10^{10} N/m^2)	C_{44} (10^{10} N/m^2)	Anisotropy ratio $(C_{11} - C_{12})/2C_{44}$
Metals	Ag	12.4	9.3	4.6	0.34
	Al	10.8	6.1	2.9	0.81
	Au	18.6	15.7	4.2	0.35
	Cu	16.8	12.1	7.5	0.31
	α-Fe	23.7	14.1	11.6	0.41
	Mo	46.0	17.6	11.0	1.29
	Na	0.73	0.63	0.42	0.12
	Ni	24.7	14.7	12.5	0.40
	Pb	5.0	4.2	1.5	0.27
	W	50.1	19.8	15.1	1.00
Covalent solids	Si	16.6	6.4	8.0	0.64
	Diamond	107.6	12.5	57.6	0.83
	TiC	51.2	11.0	17.7	1.14
Ionic solids	LiF	11.2	4.6	6.3	0.52
	MgO	29.1	9.0	15.5	0.65
	NaCl	4.9	1.3	1.3	1.38

Effect of Materials Symmetry on Elastic Constants (*Isotropic System*)



A rotation of θ about x-axis in isotropic material

Obviously, this includes cubic symmetry as a special case. Accordingly, let us transform the stiffness tensor of cubic material for a rotation of θ about x-axis,

	x	y	z
x'	1	0	0
y'	0	$\cos\theta$	$-\sin\theta$
z'	0	$\sin\theta$	$\cos\theta$

$$\begin{bmatrix} (\lambda+2\mu) & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & (\lambda+2\mu) & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & (\lambda+2\mu) & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix}$$

We conclude that there are two independent components of stiffness.

Effect of Materials Symmetry on Elastic Constants (*Isotropic System*)

We can determine the compliances simply by taking the inverse of the matrix of stiffness components,

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

$$S_{11} = \frac{\mu+\lambda}{\mu(3\lambda+2\mu)}$$

$$S_{12} = \frac{-\lambda}{2\mu(3\lambda+2\mu)}$$

Suppose that an elastically isotropic sample is acted on solely *uniaxial stress* along x-axis,

$\varepsilon_1 = S_{11}\,\sigma_1$ or $\sigma_1/\varepsilon_1 = 1/S_{11}$ → ***Young's modulus,* E=1/S_{11}**

$\varepsilon_2 = \varepsilon_3 = S_{12}\,\sigma_1$ $-\varepsilon_2/\varepsilon_1 = -\varepsilon_3/\varepsilon_1 = -S_{12}/S_{11}$ → ***Poisson's ratio,* ν=-S_{12}/S_{11}**

Effect of Materials Symmetry on Elastic Constants (*Isotropic System*)

Suppose now that the sole applied stress is *a shear stress σ_4*,

$$\sigma_4 = \mu \varepsilon_4 \qquad \varepsilon_4 = 2(S_{11} - S_{12})\sigma_4 \quad \Rightarrow \quad \textit{Shear modulus, } G = \frac{E}{2(1+\nu)}$$

Let us consider the effect of *a hydrostatic stress σ_m*,

$$\Delta = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 = 3\,\sigma_m (S_{11} + 2S_{12}) \quad \Rightarrow \quad \textit{Bulk modulus, } B = \frac{E}{3(1-2\nu)}$$

$$\frac{B}{G} = \frac{2(1+\nu)}{3(1-2\nu)} \qquad \nu = \frac{3(B/G)-2}{6(B/G)+2}$$

One extreme of properties is reached when *B* >> *G*, whereupon ν → 1/2. At the other extreme we have *B/G* → 0, with ν approaching a value of -1, and so the possible value range of Poisson's ratio is -1 < ν < 1/2. Poisson's ratio of zero arises when *B/G* = 2/3.

Isotropy considerations

$$\begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ \cdot & C_{11} & C_{12} & 0 & 0 & 0 \\ \cdot & \cdot & C_{11} & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & C_{44} & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & C_{44} & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & C_{44} \end{pmatrix}$$

$$C_{44} = \frac{C_{11} - C_{12}}{2}$$

$$\begin{pmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ \cdot & S_{11} & S_{12} & 0 & 0 & 0 \\ \cdot & \cdot & S_{11} & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & S_{44} & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & S_{44} & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & S_{44} \end{pmatrix}$$

$$S_{44} = 2(S_{11} - S_{12})$$

For these systems, anisotropy is defined by the Zener ratio:

When the Zener ratio = 1, the material is isotropic.

$$(C_{11} - C_{12}) / 2C_{44}$$

$$or$$

$$S_{44} / 2(S_{11} - S_{12})$$

Elastic Moduli in Cubic Materials

We can use the different relations among elastic constants to ascertain elastic moduli along any orientation,

$$\frac{1}{E_{ijk}} = S_{11} - 2\left(S_{11} - S_{12} - \frac{1}{2}S_{44}\right)\left(l_{i1}{}^{2}l_{j2}{}^{2} + l_{j2}{}^{2}l_{k3}{}^{2} + l_{i1}{}^{2}l_{k3}{}^{2}\right)$$

where l_{i1}, l_{j2}, l_{k3} equal the direction cosines between the [ijk] direction and the [100], [010], and [001] directions.
(i.e., axes *x*, *y*, and *z*)

Elastic Moduli in Cubic Materials

Material class	Material*	$E_{polycrystal}$ (10^9 N/m^2)	$E_{<111>}$ (10^9 N/m^2)	$E_{<100>}$ (10^9 N/m^2)	$E_{<100>}/E_{<111>}$	Anisotropy ratio†
Metals	Al	70	76	64	0.84	0.81
	Au	78	117	43	0.37	0.35
	Cu	121	192	67	0.35	0.31
	α-Fe	209	276	129	0.47	0.41
	W	411	411	411	1.00	1.00
Covalent solids	Diamond	—	1200	1050	0.88	0.83
	TiC	—	429	476	1.11	1.14
Ionic solids	MgO	310	343	247	0.72	0.65
	NaCl	37	32	44	1.38	1.38

*For the materials listed $E_{<111>} = E_{max}$ and $E_{<100>} = E_{min}$ except for TiC and NaCl, for which the reverse applies.
†Note: $E_{<100>}/E_{<111>}$ should scale with the anisotropy ratio (Table 2.2).