HOMEWORK

Calculate Young's modulus for Al and Cu in the <111>, <100>, and <110> directions.

Module #5

Origins of elasticity
Elastic constants in isotropic materials
Elastic constants in anisotropic materials

READING LIST

DIETER: Ch. 2, Pages 47-60

Pages 21-36 in Hosford ; Ch. 2 in Roesler ;
Ch. 8 in Nye ; Ch. 3 in McClintock and Argon
Ch. 7 in Sines ; Ch. 6 in Wagoner and Chenot
Ch. 11 in Sadd

Elasticity

- Important because most engineering design is done in the elastic region. (Remember, plastic deformation generally constitutes failure.)

- Macroscopically, most polycrystalline materials are elastically isotropic.

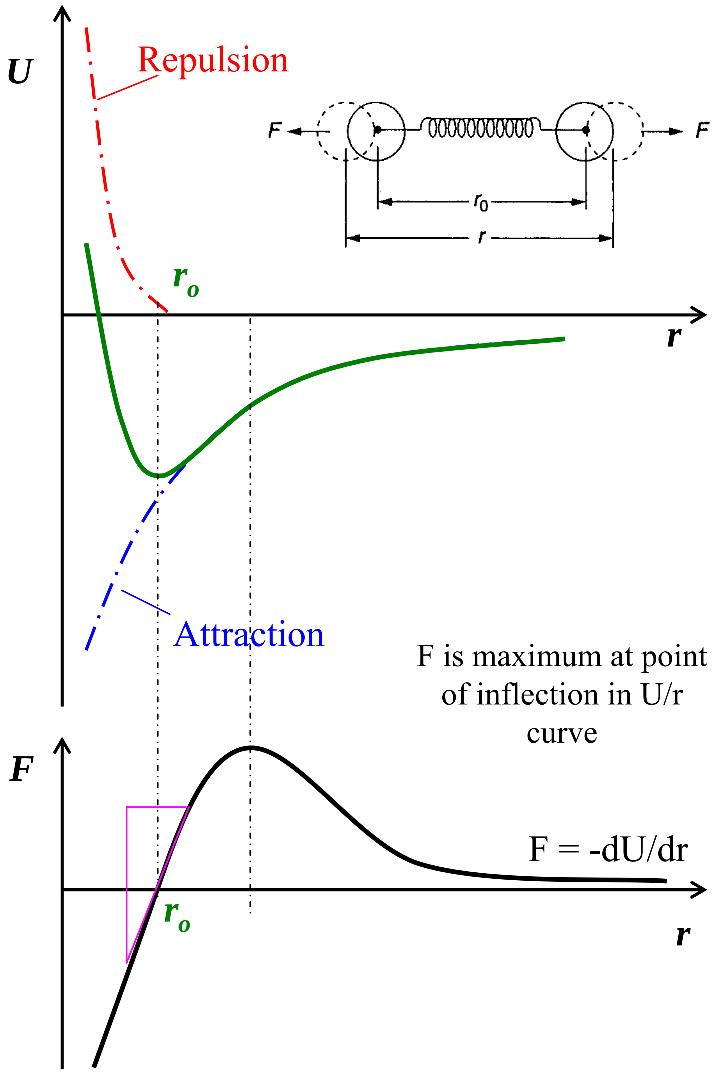
- Microscopically, elastic behavior is inherently anisotropic for individual grains.

- Polycrystalline materials can be anisotropic if they exhibit strong crystallographic textures.

Elasticity – cont’d

- Derived from atomic bonding forces originating from long range attractive forces which draw atoms together until short range repulsive forces become large enough to balance them out.

- As such, elastic properties are an aggregate effect of individual deformations of interatomic bonds.



F is maximum at point of inflection in U/r curve

Bulk Elastic Behavior

- Applied force is transmitted by the network of bonds constituting the material.
- Thus, elastic behavior depends quantitatively on the magnitude of the interatomic forces.
- Elastic properties do not depend on microstructure of the material.

Forces Between Atoms

- Bonds form when atoms either share (e.g., covalent and metallic bonds) or transfer (e.g., ionic bonds) electrons between atoms.

- This occurs to achieve a minimum in potential energy for the system corresponding to a stable electron configuration.

- This has been modeled for ionic systems as follows:

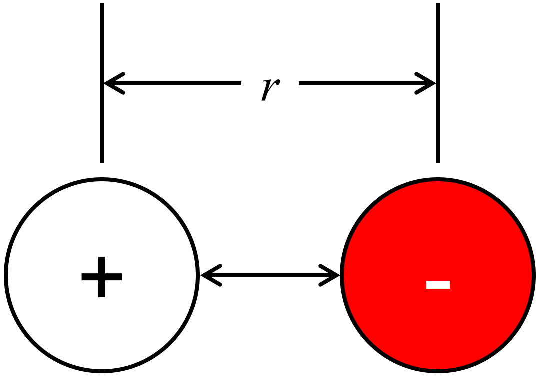
Ionic Bond

- Electron transfer from one atom to another occurs due to electrostatic interaction between oppositely charged ions (e.g., Na^+ and Cl^- in NaCl).

- Force of attraction between ions is $F_{attract}$

- Work is done to draw ions together. It is given by:

$$U_{attract} = \int_{\infty}^{r} F_{attract}\, dr = \frac{-q^2}{4\pi\varepsilon_o r} = \frac{-A}{r^m}$$



$$F_{attract} = \frac{q^2}{4\pi\varepsilon_o r^2}$$

---

q = charge of ion

ε_o = permittivity of free space

r = ionic separation distance

- Each atom maintains an electron cloud surrounding it. The outer surfaces of each atom are both negatively charged.

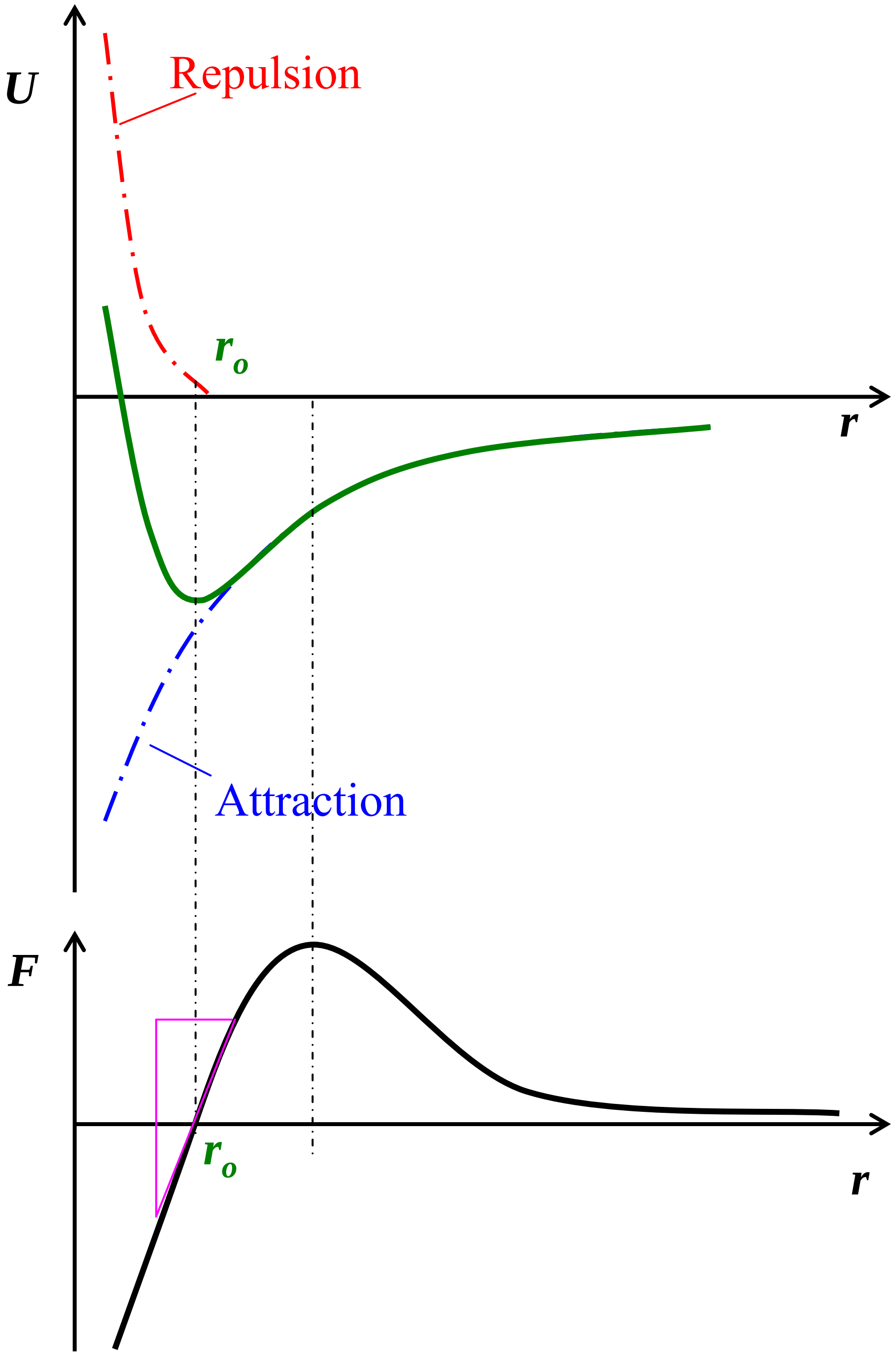
- Thus, at close distances, the electron clouds overlap and repel. The repulsive force can be written as:

$$U_{repel} = \frac{B}{r^n}$$

- The total energy of the system is thus the sum of the attractive and repulsive components. It can be expressed in general as:

$$U_{total} = U_{attract} + U_{repel} = \frac{-A}{r^m} + \frac{B}{r^n}$$

- This is the well known Lennard-Jones potential. You might recall this from your chemistry or physics courses.



- The minimum energy point corresponds to the equilibrium separation (i.e., the equilibrium bond length, r_o).

- The force between atoms is simply the derivative (i.e., the slope) of the energy versus distance plot.

$$F = \frac{-dU_{total}}{dr}$$

- The bond stiffness is the derivative of the force versus distance plot.

$$S = \frac{dF}{dr} = \frac{d^2U_{total}}{dr^2}$$

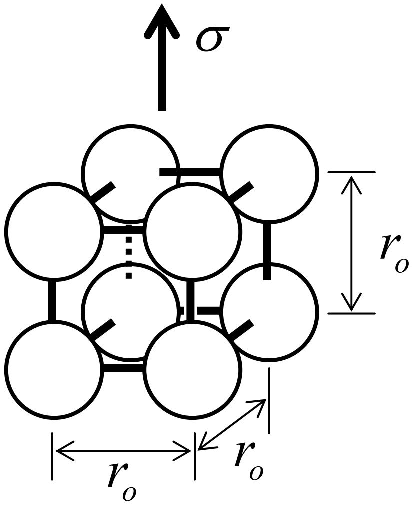
- At the equilibrium bond length, r_o, the variation of F with r is essentially linear, which means that the stiffness is essentially constant at small distances from r_o.

$$S_o = \left.\frac{dF}{dr}\right|_{r_o}$$

- Using this expression, the force to "stretch" n bonds in a solid is:

$$F = n\int_{r_o}^{r} S_o dr = nS_o\left(r - r_o\right)$$

where n is the number of bonds.



- The applied stress is:

$$\sigma = \frac{F}{A} = \frac{nS_o\left(r - r_o\right)}{nr_o^2}$$

- The strain can be expressed as:

$$\varepsilon = \frac{r - r_o}{r_o}$$

- Thus, stress becomes:

$$\sigma = \frac{F}{A} = \frac{nS_o\left(r - r_o\right)}{nr_o^2} = \frac{S_o}{r_o}\frac{\left(r - r_o\right)}{r_o} = \frac{S_o}{r_o}\varepsilon$$

- From Hooke's law:

$$\sigma = E\varepsilon$$

- Thus,

$$E = \frac{S_o}{r_o} = \frac{1}{r_o}\left.\frac{d^2U}{dr^2}\right|_{r=r_o}$$

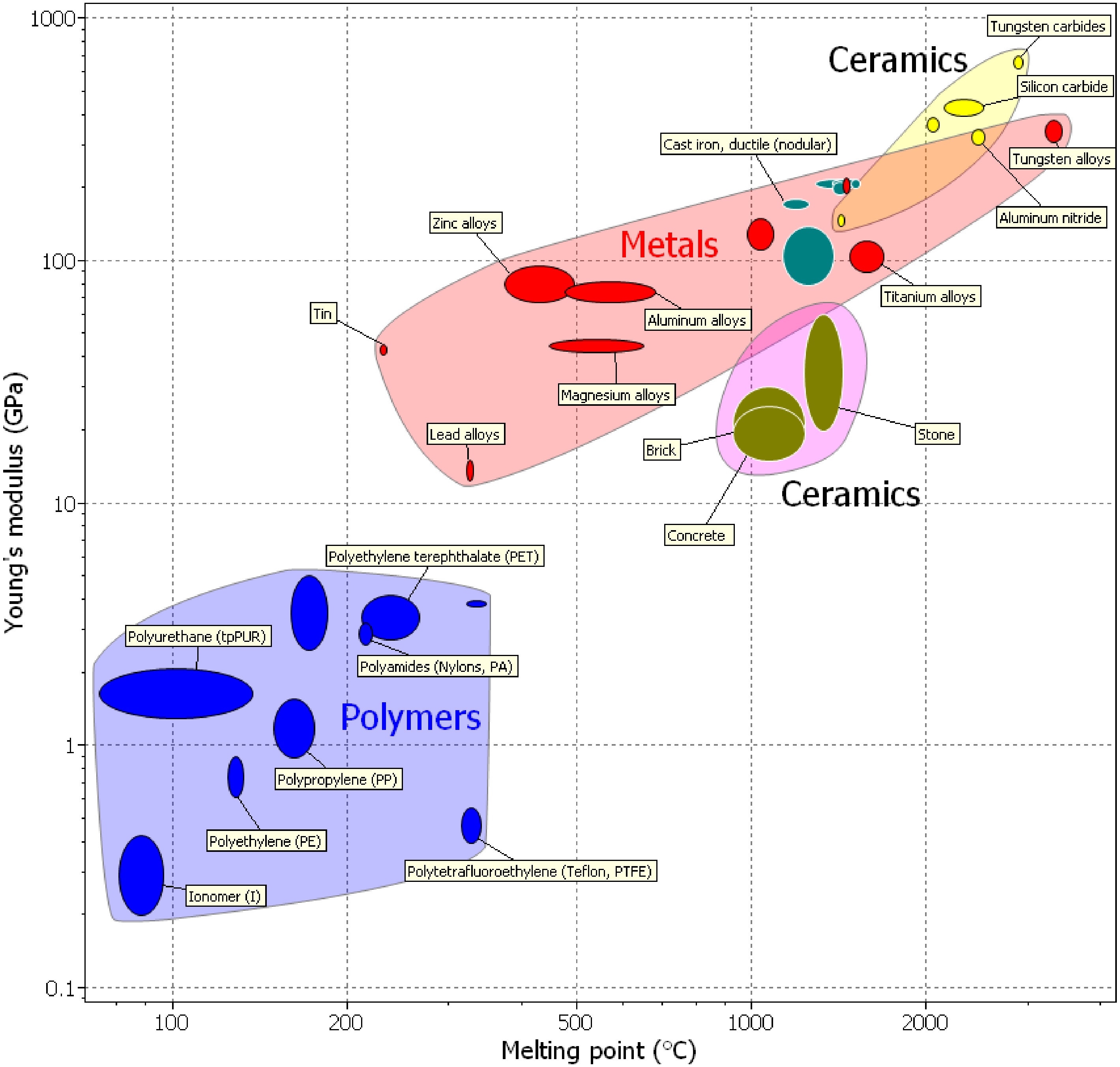
The derived expression shows that the modulus is dependent upon bonding.

Modulus, and other elastic properties, are <u>structure</u> <u>insensitive</u>.

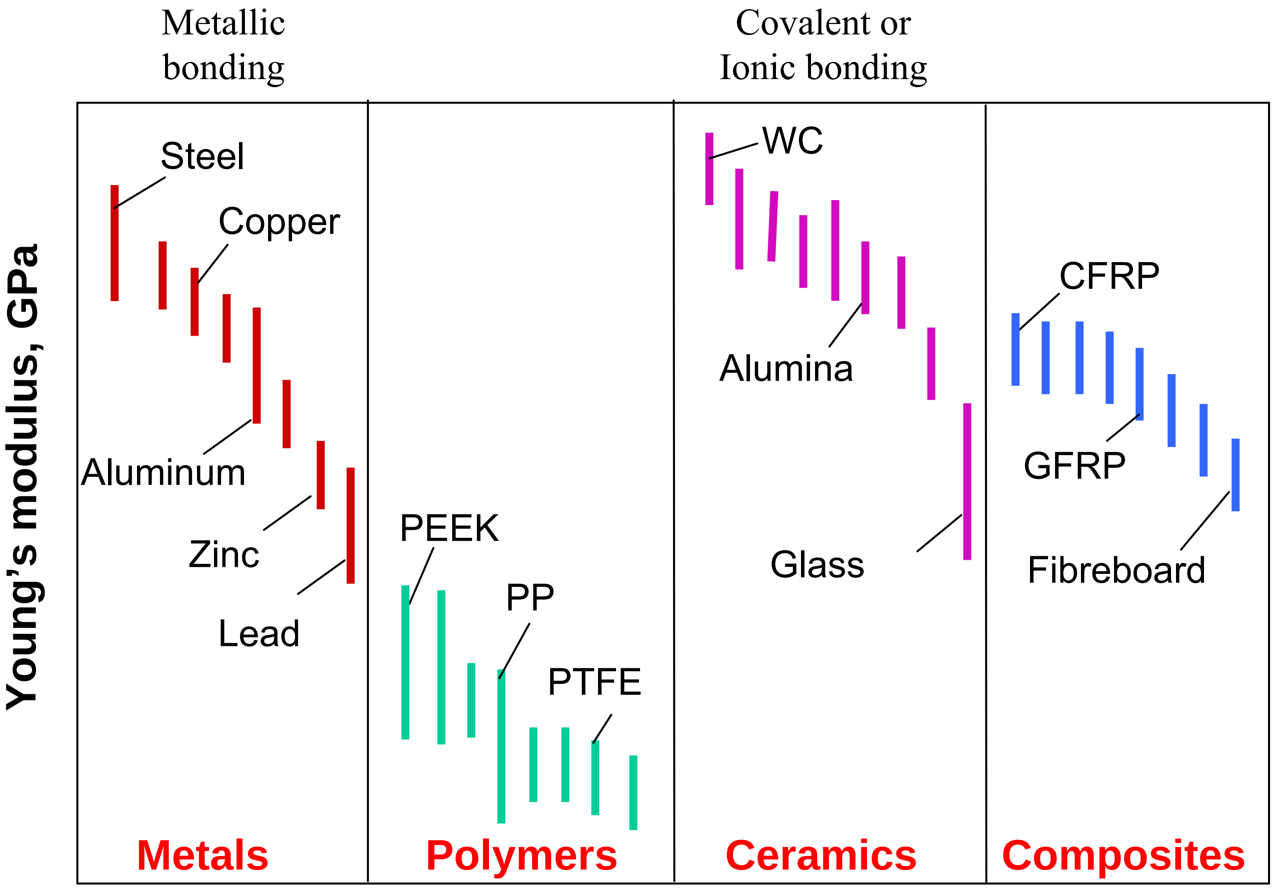
The directionality of elastic properties <u>does</u> depend upon atomic arrangement (crystallography) in single crystals. They tend to average out in polycrystals.

Bonding Type	Material, Substance	Bonding Energy		Melting Temperature °C
		kJ/mol	eV/Atom, Ion, Molecule	
Ionic	NaCl	640	3.3	801
	MgO	1000	5.2	2800
Covalent	Si	450	4.7	1410
	C (diamond)	713	7.4	>3550
Metallic	Hg	68	0.7	-39
	Al	324	3.4	660
	Fe	406	4.2	1538
	W	849	8.8	3410
van der Waals	Ar	7.7	0.08	-189
	Cl_2	31	0.32	-101
Hydrogen	NH_3	35	0.36	-78
	H_2O	51	0.52	0

[From W.D. Callister, Jr, Materials Science and Engineering: An Introduction, 7th Ed., (Wiley, New York, 2007) p.28]



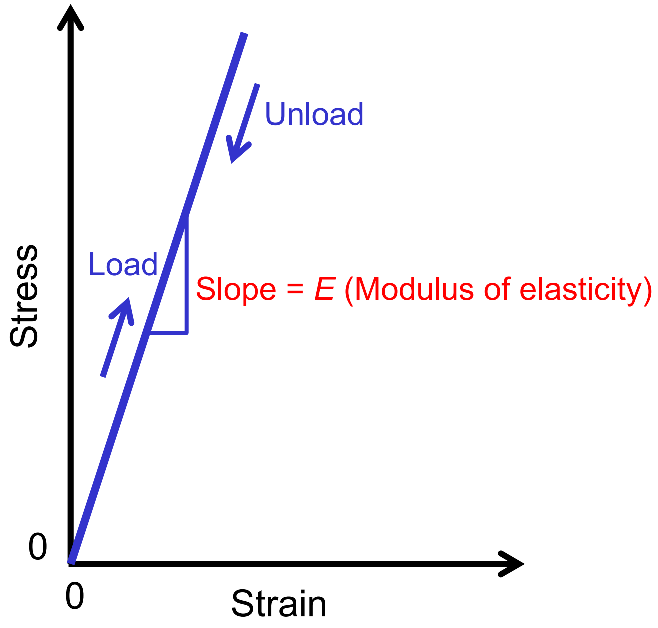
Ceramics
Tungsten carbides
Silicon carbide
Tungsten alloys
Aluminum nitride
Cast iron, ductile (nodular)
Zinc alloys
Metals
Titanium alloys
Aluminum alloys
Tin
Magnesium alloys
Lead alloys
Stone
Brick
Ceramics
Concrete
Polyethylene terephthalate (PET)
Polyurethane (tpPUR)
Polyamides (Nylons, PA)
Polymers
Polypropylene (PP)
Polyethylene (PE)
Polytetrafluoroethylene (Teflon, PTFE)
Ionomer (I)
Young's modulus (GPa)
1000
100
10
1
0.1
Melting point (°C)
100
200
500
1000
2000



Courtesy of Granta Design

A bar chart illustrating Young's moduli for some common examples of the primary classes of materials (i.e., metals, ceramics, polymers and composites). Ceramics tend to exhibit the highest elastic moduli and polymers the lowest. The elastic moduli of composites are between those of their constituents.

stress is related to strain for an isotropic solid



Stress-strain plot for a linearly elastic material

- Hooke's Law
  - Isotropic Solids (properties are the same in all directions)

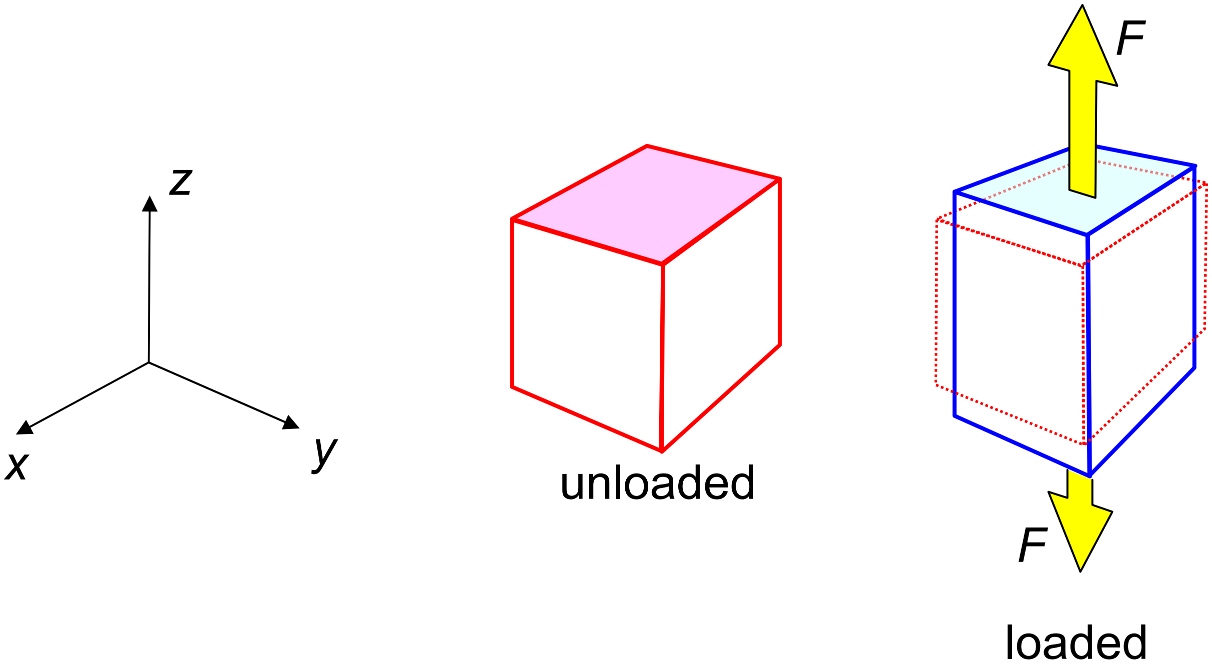
$$\sigma = \varepsilon E \text{ or } \varepsilon = \frac{1}{E}\sigma$$

  - Anisotropic solids (properties are directional)

Need different definition

  - Let's consider both cases

First consider the Poisson effect



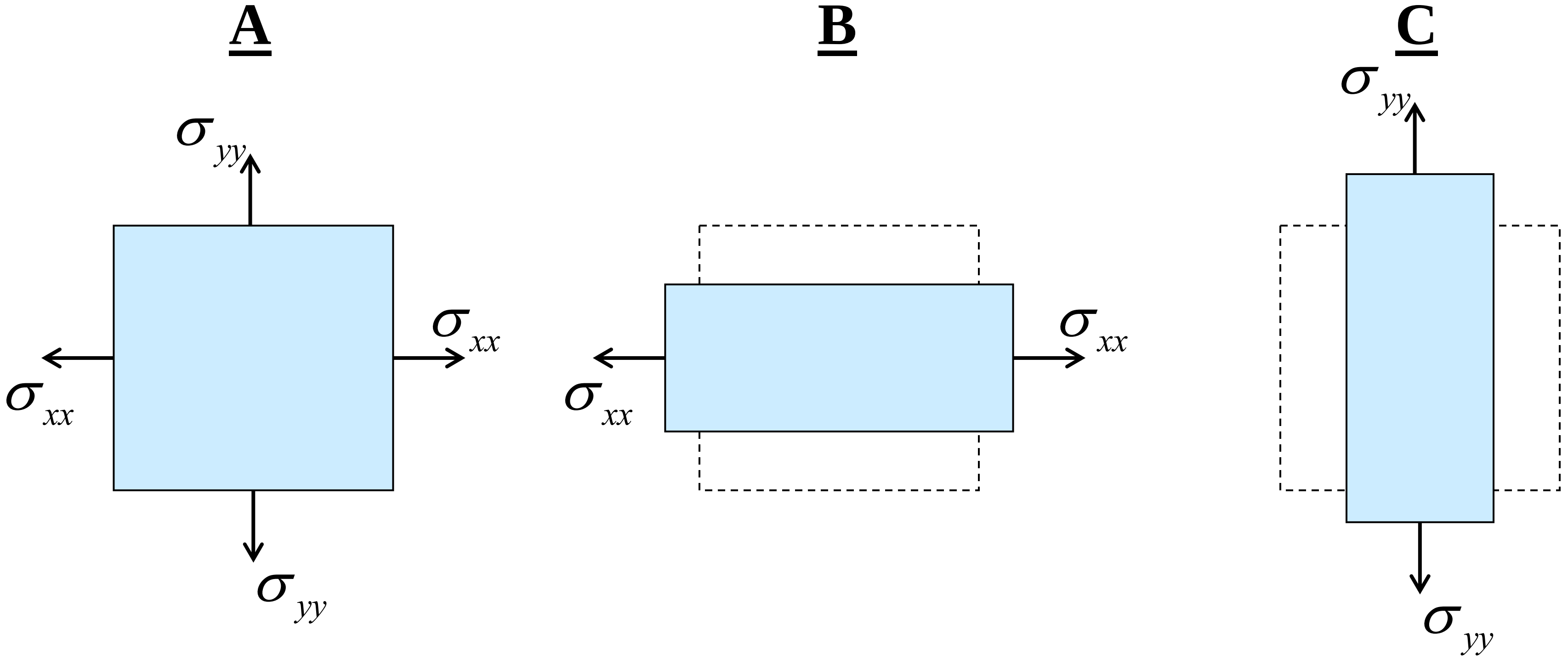
$$\nu(z,x) = -\frac{\varepsilon_x}{\varepsilon_z} \text{ and } \nu(z,y) = -\frac{\varepsilon_y}{\varepsilon_z}$$

A tensile stress along the *z* axis causes the material to stretch along the *z* axis and to contract along the *x* and *y* axes.

$$\text{Poisson's Ratio, } \nu = -\frac{\text{lateral strain}}{\text{longitudinal strain}}$$

Room-Temperature Poisson's Ratio for Selected Solids

Material Class	Material	ν
Metallic solid (crystalline)	Ag	0.38
	Al	0.34
	Au	0.42
	Cu	0.34
	α-Fe	0.29
	Ir	0.26
	Ni	0.31
	W	0.29
Covalent solid (crystalline)	Ge	0.28
	Si	0.27
	Al_2O_3	0.23
	TiC	0.19
Covalent Ionic Solid	MgO	0.19
Covalent Glass	Silica glass	0.20
Network Polymer	Bakelite	0.20
	Ebonite (hard rubber)	0.39
Elastomer	Natural rubber	0.49
Chain Polymer	Polystyrene	0.33
	Polyethylene	0.40
Van der Waal's Solid	Argon (at 0 K)	0.25



The strains resulting from this stress state must be the sum of the strains associated with loading along each individual axis.

$$\mathrm{B}:\ \varepsilon_{xx}^{\mathrm{B}} = \frac{\sigma_{xx}}{E},\quad \varepsilon_{yy}^{\mathrm{B}} = -\nu\varepsilon_{xx}^{\mathrm{B}} = -\nu\frac{\sigma_{xx}}{E}$$

$$\mathrm{C}:\ \varepsilon_{yy}^{\mathrm{C}} = \frac{\sigma_{yy}}{E},\quad \varepsilon_{xx}^{\mathrm{C}} = -\nu\varepsilon_{yy}^{\mathrm{C}} = -\nu\frac{\sigma_{yy}}{E}$$

$$\mathrm{A} = \mathrm{B}+\mathrm{C}:\ \varepsilon_{xx} = \varepsilon_{xx}^{\mathrm{B}} + \varepsilon_{xx}^{\mathrm{C}} = \frac{\sigma_{xx}}{E} - \nu\frac{\sigma_{yy}}{E}$$

(There's a similar expression for ε_{yy})

RECALL: Elastic Stress-Strain Relations

Stress		**Strain in the x-direction**	**Strain in the y-direction**	**Strain in the z-direction**
σ_{xx}	$\longrightarrow$	$\varepsilon_{xx} = \frac{\sigma_{xx}}{E}$	$\varepsilon_{yy} = -\frac{\nu\sigma_{xx}}{E}$	$\varepsilon_{zz} = -\frac{\nu\sigma_{xx}}{E}$
σ_{yy}	$\longrightarrow$	$\varepsilon_{xx} = -\frac{\nu\sigma_{yy}}{E}$	$\varepsilon_{yy} = \frac{\sigma_{yy}}{E}$	$\varepsilon_{zz} = -\frac{\nu\sigma_{yy}}{E}$
σ_{zz}	$\longrightarrow$	$\varepsilon_{xx} = -\frac{\nu\sigma_{zz}}{E}$	$\varepsilon_{yy} = -\frac{\nu\sigma_{zz}}{E}$	$\varepsilon_{zz} = \frac{\sigma_{zz}}{E}$

$$\varepsilon_{xx} = \frac{1}{E}\left[\sigma_{xx} - \nu\left(\sigma_{yy} + \sigma_{zz}\right)\right]$$

$$\varepsilon_{yy} = \frac{1}{E}\left[\sigma_{yy} - \nu\left(\sigma_{zz} + \sigma_{xx}\right)\right]$$

$$\varepsilon_{zz} = \frac{1}{E}\left[\sigma_{zz} - \nu\left(\sigma_{xx} + \sigma_{yy}\right)\right]$$

$$\tau_{xy} = G\gamma_{xy};\ \tau_{yz} = G\gamma_{yz};\ \tau_{xz} = G\gamma_{xz}$$

Variation in elastic strain for an **isotropic** **solid** because of the Poisson effect

Other Elastic Stress-Strain Relations for Isotropic Solids

- Bulk Modulus (K), also known as the *volumetric elastic modulus*:

$$K = \frac{\text{hydrostatic pressure}}{\text{volume change produced}} = \frac{\sigma_m}{\Delta} = \frac{-p}{\Delta} = \frac{1}{B}$$

where:

$-p$ = hydrostatic pressure,

$$\sigma_m = \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3}$$

Δ = dilatation (i.e., volume change) $= \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$,

B = compressibility.

Other Elastic Stress-Strain Relations for Isotropic Solids

- Now we can relate the elastic constants.

$$\varepsilon_{xx} = \frac{1}{E}\left[\sigma_{xx} - \nu\left(\sigma_{yy} + \sigma_{zz}\right)\right]$$

$$\varepsilon_{yy} = \frac{1}{E}\left[\sigma_{yy} - \nu\left(\sigma_{zz} + \sigma_{xx}\right)\right]$$

$$\varepsilon_{zz} = \frac{1}{E}\left[\sigma_{zz} - \nu\left(\sigma_{xx} + \sigma_{yy}\right)\right]$$

Summation yields:

$$\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} = \frac{1-2\nu}{E}\left(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}\right) = \frac{1-2\nu}{E}3\sigma_m = \Delta$$

$$\therefore$$

$$K = \frac{\sigma_m}{\Delta} = \frac{E}{3\left(1-2\nu\right)}$$

Other Relations Between Isotropic Elastic Constants

In terms of **Elastic constants**	$E,\ \nu$	$E,\ G$	$K,\ \nu$	$E,\ G$	$\lambda,\ \mu$
E [elastic]	$= E$	$= E$	$= 3(1-2\nu)K$	$= \dfrac{9K}{1+3K/G}$	$= \dfrac{\mu(3+2\mu/\lambda)}{2(1+\mu/\lambda)}$
ν	$= \nu$	$= -1+\dfrac{E}{2G}$	$= \nu$	$= \dfrac{1-2G/3K}{2+2G/3K}$	$= \dfrac{1}{2(1+\mu/\lambda)}$
G [shear]	$= \dfrac{E}{2(1+\nu)}$	$= G$	$= \dfrac{3(1-2\nu)K}{2(1+\nu)}$	$= G$	$= \mu$
K [bulk]	$= \dfrac{E}{3(1-2\nu)}$	$= \dfrac{E}{9-3E/G}$	$= K$	$= K$	$= \lambda+\dfrac{2\mu}{3}$
λ	$= \dfrac{E\nu}{(1+\nu)(1-2\nu)}$	$= \dfrac{E(1-2G/E)}{3-E/G}$	$= \dfrac{3K\nu}{1+\nu}$	$= K-\dfrac{2G}{3}$	$= \lambda$
μ	$= \dfrac{E}{2(1+\nu)}$	$= G$	$= \dfrac{3(1-2\nu)K}{2(1+\nu)}$	$= G$	$= \mu$

$\lambda,\ \mu$ = Lame constants

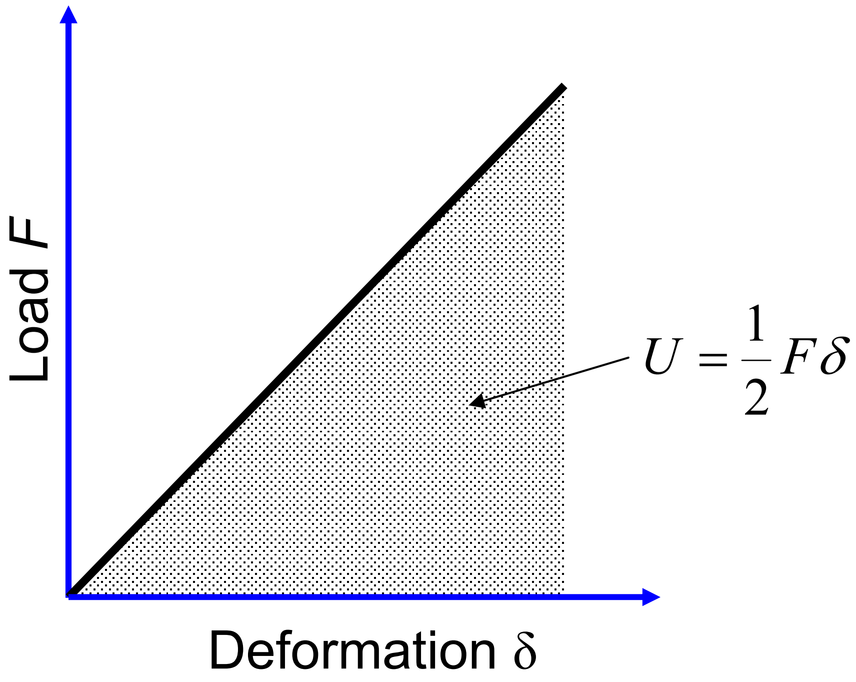
STRAIN ENERGY

Energy stored in a body due to deformation.

- Work to deform a body elastically is stored as elastic strain energy. It is recovered when the applied forces are released.

- Strain energy is proportional to the area under the load-deformation (stress-strain) curve.

- We will elaborate on this concept on the next few pages.



Strain Energy

- The first law of thermodynamics states:

  $$dU = \delta Q + \delta W = TdS - PdV$$

  where,

  dU = internal energy
  δQ = heat
  δW = mechanical work done

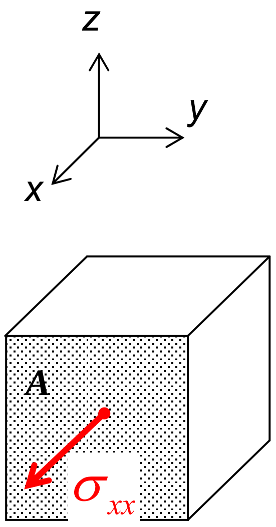
- <u>During</u> <u>elastic</u> <u>deformation</u>, the amount of heat generated is negligible.

- Thus the work done on the body is converted into internal energy and is fully recovered upon unloading.

ELASTIC STRAIN ENERGY – cont'd

- Consider an elemental cube that is subjected to only an elastic tensile stress along the *x*-axis. The elastic strain energy, *U*, is:

$$U = \frac{1}{2}(\text{load})(\text{deformation})$$



$$\sigma_{xx} = \frac{F}{A}$$

$$\varepsilon_{xx} = \frac{du}{dx}$$

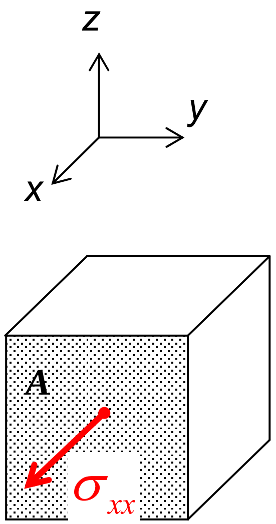
$$dU = \frac{1}{2}F\,du = \frac{1}{2}(\sigma_{xx}A)(\varepsilon_{xx}dx) = \frac{1}{2}(\sigma_{xx}\varepsilon_{xx})(A\,dx)$$

= total elastic energy absorbed by the material element.

Since *Adx* is the volume, the elastic strain energy per unit volume (i.e., the strain energy density) is:

$$U_o = \frac{dU}{A\,dx} = \frac{1}{2}(\sigma_{xx}\varepsilon_{xx}).$$

ELASTIC STRAIN ENERGY – cont'd



$$\sigma_{xx} = \frac{F}{A}$$

$$\varepsilon_{xx} = \frac{du}{dx}$$

From Hooke's law, $\varepsilon_{xx} = \dfrac{\sigma_{xx}}{E}$.

Therefore:

$$U_o = \frac{1}{2}\frac{\sigma_{xx}^2}{E} = \frac{1}{2}\varepsilon_{xx}^2 E \text{ [in tension]}$$

$$U_o = \frac{1}{2}\left(\tau_{xy}\gamma_{xy}\right) = \frac{1}{2}\frac{\tau_{xy}^2}{G} = \frac{1}{2}\gamma_{xy}^2 G \text{ [in pure shear]}$$

In three dimensions, the general expression for elastic strain energy is:

$$U_o = \frac{1}{2}\left(\sigma_{xx}\varepsilon_{xx} + \sigma_{yy}\varepsilon_{yy} + \sigma_{zz}\varepsilon_{zz} + \tau_{xy}\gamma_{xy} + \tau_{xz}\gamma_{xz} + \tau_{yz}\gamma_{yz}\right).$$

ELASTIC STRAIN ENERGY – cont’d

In tensor notation, these general expressions become:

$$U_o = \frac{1}{2}\sigma_{ij}\varepsilon_{ij} = \frac{1}{2}\frac{\sigma_{ij}^2}{E} = \frac{1}{2}\varepsilon_{ij}^2 E.$$

If we substite into these expressions, the variation in elastic strain for an isotropic solid, accounting for the Poisson effect, we get:

$$U_o = \frac{1}{2E}\left(\sigma_{xx}^2 + \sigma_{yy}^2 + \sigma_{zz}^2\right) - \frac{\nu}{E}\left(\sigma_{xx}\sigma_{yy} + \sigma_{yy}\sigma_{zz} + \sigma_{xx}\sigma_{zz}\right) + \frac{1}{2G}\left(\tau_{xy}^2 + \tau_{xz}^2 + \tau_{yz}^2\right)$$

[for a 3D isotropic solid]

Expressed in terms of strains and elastic constants:

$$U_o = \frac{1}{2}\lambda\Delta^2 + G\left(\varepsilon_{xx}^2 + \varepsilon_{yy}^2 + \varepsilon_{zz}^2\right) + \frac{1}{2}G\left(\gamma_{xy}^2 + \gamma_{xz}^2 + \gamma_{yz}^2\right)$$

ELASTIC STRAIN ENERGY – cont'd

$$U_o = \frac{1}{2}\left(\sigma_{xx}\varepsilon_{xx} + \sigma_{yy}\varepsilon_{yy} + \sigma_{zz}\varepsilon_{zz} + \tau_{xy}\gamma_{xy} + \tau_{xz}\gamma_{xz} + \tau_{yz}\gamma_{yz}\right)$$

The derivative of U_o with respect to any strain component yields the corresponding stress component, or:

$$\frac{\partial U_o}{\partial \varepsilon_{ij}} = \lambda\Delta + 2G\varepsilon_{ij} = \sigma_{ij}$$

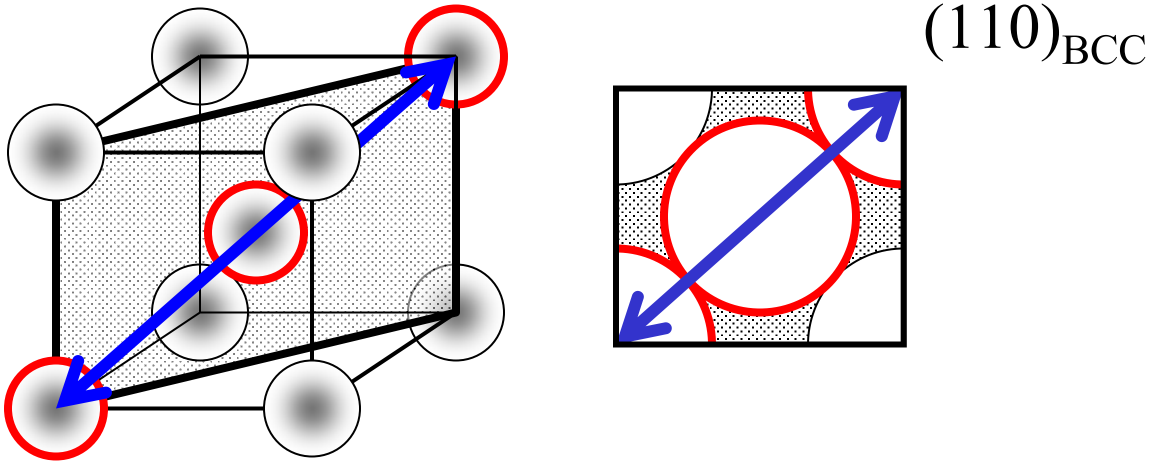
Similarly, the derivative of U_o with respect to any stress component yields the corresponding strain or:

$$\frac{\partial U_o}{\partial \sigma_{ij}} = \varepsilon_{ij}$$

You can use these terms to calculate stresses and strains in elasticty. Techniques for doing this include Castigliano's theorem, the theorem of least work, and the principal of virtual work.

Anisotropy and Single Crystals

- Forces between atoms are directional.



- They act along the “lines” connecting the atoms together.

Relations between stress and strain for anisotropic crystals

- Since force varies with direction, elastic constants will also vary.

- In general, we need to relate every stress component to every strain component.

- Thus we must define two new elastic constants:

  - $C \equiv$ stiffness
  - $S \equiv$ compliance

- We also re-write Hooke's law as:

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

Stiffness is a 4th rank tensor

$3^4 = 81$ terms

$$\sigma_{ij} = \sum_{k=1}^{3}\sum_{l=1}^{3} C_{ijkl}\varepsilon_{kl}$$

$$\downarrow$$

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$$

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \\ \sigma_{zy} \\ \sigma_{xz} \\ \sigma_{yx} \end{pmatrix} = \begin{pmatrix}
C_{xxxx} & C_{xxyy} & C_{xxzz} & C_{xxyz} & C_{xxzx} & C_{xxxy} & C_{xxzy} & C_{xxxz} & C_{xxyx} \\
C_{yyxx} & C_{yyyy} & C_{yyzz} & C_{yyyz} & C_{yyxz} & C_{yyxy} & C_{yyzy} & C_{yyxz} & C_{yyyx} \\
C_{zzxx} & C_{zzyy} & C_{zzzz} & C_{zzyz} & C_{zzxz} & C_{zzxy} & C_{zzzy} & C_{zzxz} & C_{zzyx} \\
C_{yzxx} & C_{yzyy} & C_{yzzz} & C_{yzyz} & C_{yzxz} & C_{yzxy} & C_{yzzy} & C_{yzxz} & C_{yzyx} \\
C_{zxxx} & C_{zxyy} & C_{zxzz} & C_{zxyz} & C_{zxxz} & C_{zxxy} & C_{zxzy} & C_{zxxz} & C_{zxyx} \\
C_{xyxx} & C_{xyyy} & C_{xyzz} & C_{xyyz} & C_{xyxz} & C_{xyxy} & C_{xyzy} & C_{xyxz} & C_{xyyx} \\
C_{zyxx} & C_{zyyy} & C_{zyzz} & C_{zyyz} & C_{zyxz} & C_{zyxy} & C_{zyzy} & C_{zyxz} & C_{zyyx} \\
C_{xzxx} & C_{xzyy} & C_{xzzz} & C_{xzyz} & C_{xzxz} & C_{xzxy} & C_{xzzy} & C_{xzxz} & C_{xzyx} \\
C_{yxxx} & C_{yxyy} & C_{yxzz} & C_{yxyz} & C_{yxxz} & C_{yxxy} & C_{yxzy} & C_{yxxz} & C_{yxyx}
\end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \\ \varepsilon_{zy} \\ \varepsilon_{xz} \\ \varepsilon_{yx} \end{pmatrix}$$

Stress tensor

Elastic Stiffness

Strain tensor

EQUILIBRIUM CONSIDERATIONS

$$\sigma_{ij} = \sigma_{ji} \qquad \varepsilon_{kl} = \varepsilon_{lk}$$

$$C_{ijkl} = C_{jikl} \qquad C_{ijkl} = C_{jikl}$$

$$C_{ijkl} = C_{jikl} \qquad C_{ijkl} = C_{ijlk}$$

Allow us to reduce the number of constants from 81 to 36

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix} = \begin{pmatrix} C_{xxxx} & C_{xxyy} & C_{xxzz} & C_{xxyz} & C_{xxxz} & C_{xxxy} \\ C_{yyxx} & C_{yyyy} & C_{yyzz} & C_{yyyz} & C_{yyxz} & C_{yyxy} \\ C_{zzxx} & C_{zzyy} & C_{zzzz} & C_{zzyz} & C_{zzxz} & C_{zzxy} \\ C_{yzxx} & C_{yzyy} & C_{yzzz} & C_{yzyz} & C_{yzxz} & C_{yzxy} \\ C_{xzxx} & C_{xzyy} & C_{xzzz} & C_{xzyz} & C_{xzxz} & C_{xzxy} \\ C_{xyxx} & C_{xyyy} & C_{xyzz} & C_{xyyz} & C_{xyxz} & C_{xyxy} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{pmatrix}$$

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix} = \begin{pmatrix} C_{xxxx} & C_{xxyy} & C_{xxzz} & C_{xxyz} & C_{xxxz} & C_{xxxy} \\ C_{yyxx} & C_{yyyy} & C_{yyzz} & C_{yyyz} & C_{yyxz} & C_{yyxy} \\ C_{zzxx} & C_{zzyy} & C_{zzzz} & C_{zzyz} & C_{zzxz} & C_{zzxy} \\ C_{yzxx} & C_{yzyy} & C_{yzzz} & C_{yzyz} & C_{yzxz} & C_{yzxy} \\ C_{xzxx} & C_{xzyy} & C_{xzzz} & C_{xzyz} & C_{xzxz} & C_{xzxy} \\ C_{xyxx} & C_{xyyy} & C_{xyzz} & C_{xyyz} & C_{xyxz} & C_{xyxy} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{pmatrix}$$

$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \longrightarrow$ C_{ijkl} is the STIFNESS matrix

$$\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{pmatrix} = \begin{pmatrix} S_{xxxx} & S_{xxyy} & S_{xxzz} & S_{xxyz} & S_{xxxz} & S_{xxxy} \\ S_{yyxx} & S_{yyyy} & S_{yyzz} & S_{yyyz} & S_{yyxz} & S_{yyxy} \\ S_{zzxx} & S_{zzyy} & S_{zzzz} & S_{zzyz} & S_{zzxz} & S_{zzxy} \\ S_{yzxx} & S_{yzyy} & S_{yzzz} & S_{yzyz} & S_{yzxz} & S_{yzxy} \\ S_{xzxx} & S_{xzyy} & S_{xzzz} & S_{xzyz} & S_{xzxz} & S_{xzxy} \\ S_{xyxx} & S_{xyyy} & S_{xyzz} & S_{xyyz} & S_{xyxz} & S_{xyxy} \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix}$$

$\varepsilon_{ij} = S_{ijkl}\sigma_{kl} \longrightarrow$ S_{ijkl} is the COMPLIANCE matrix

Matrix/Contracted Notation

- We often replace the indices with matrix (contracted) notation for simplicity [Voigt, Lehrbuch der Kristallphysik (Teubner VErlag, Berlin, 1910)].

$$xx \rightarrow 11 \rightarrow 1 \quad yy \rightarrow 22 \rightarrow 2 \quad zz \rightarrow 33 \rightarrow 3$$

$$yz \rightarrow 23 \rightarrow 4 \quad xz \rightarrow 13 \rightarrow 5 \quad xy \rightarrow 12 \rightarrow 6$$

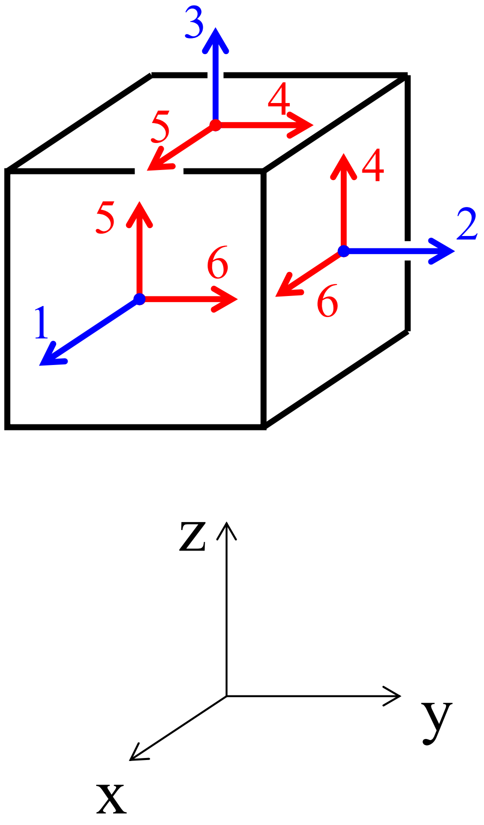
$$\begin{pmatrix} 11 & & 12 & \leftarrow & 13 \\ & \searrow & & & \uparrow \\ & & 22 & & 23 \\ & & & \searrow & \uparrow \\ & & & & 33 \end{pmatrix} \equiv \begin{pmatrix} 1 & & 6 & \leftarrow & 5 \\ & \searrow & & & \uparrow \\ & & 2 & & 4 \\ & & & \searrow & \uparrow \\ & & & & 3 \end{pmatrix}$$

- Thus, Hooke's law is often re-written in matrix form as:

$$\sigma_p = C_{\underset{\substack{\uparrow \\ \text{row}}}{p}\underset{\substack{\uparrow \\ \text{column}}}{q}}\varepsilon_q \quad \text{or} \quad \varepsilon_p = S_{pq}\sigma_q$$

Additional note about contracted notation

- Numbers 1-3 are associated with normal stresses and strains.
- Numbers 4-6 are associated with shear stresses and strains.
- On the next slide I attempt to show you which stresses and strains are related to each elastic constant.



TENSOR

$$\begin{array}{cc} & \begin{array}{cc} \sigma,\varepsilon & \sigma,\gamma \end{array} \\ C_{ijkl} = & \left(\begin{array}{ccc|ccc} C_{xxxx} & C_{xxyy} & C_{xxzz} & C_{xxyz} & C_{xxxz} & C_{xxxy} \\ C_{yyxx} & C_{yyyy} & C_{yyzz} & C_{yyyz} & C_{yyxz} & C_{yyxy} \\ C_{zzxx} & C_{zzyy} & C_{zzzz} & C_{zzyz} & C_{zzxz} & C_{zzxy} \\ \hline C_{yzxx} & C_{yzyy} & C_{yzzz} & C_{yzyz} & C_{yzxz} & C_{yzxy} \\ C_{xzxx} & C_{xzyy} & C_{xzzz} & C_{xzyz} & C_{xzxz} & C_{xzxy} \\ C_{xyxx} & C_{xyyy} & C_{xyzz} & C_{xyyz} & C_{xyxz} & C_{xyxy} \end{array}\right) \\ & \begin{array}{cc} \tau,\varepsilon & \tau,\gamma \end{array} \end{array}$$

CONTRACTED

$$\begin{array}{cc} & \begin{array}{cc} \sigma,\varepsilon & \sigma,\gamma \end{array} \\ C_{ijkl} = & \left(\begin{array}{ccc|ccc} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ \hline C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{array}\right) \\ & \begin{array}{cc} \tau,\varepsilon & \tau,\gamma \end{array} \end{array}$$

Contracted vs. Tensor Notation

- Contracted notation is simple and convenient for conducting matrix inversions.

►However, for coordinate transformations or invariant determination, it is more useful to use the stiffness and compliances in tensor notation.

Note the change from tensor notation to matrix notation. See Chapter 8 in Nye for details.

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

$\sigma_p = C_{pq}\varepsilon_q \longrightarrow$ C_{pq} is the STIFNESS matrix

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

$\varepsilon_p = S_{pq}\sigma_q \longrightarrow$ S_{pq} is the COMPLIANCE matrix

Stiffness and compliance matrices are also symmetric about the main diagonal

$$\begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{pmatrix} \rightarrow \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ \cdot & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ \cdot & \cdot & C_{33} & C_{34} & C_{35} & C_{36} \\ \cdot & \cdot & \cdot & C_{44} & C_{45} & C_{46} \\ \cdot & \cdot & \cdot & \cdot & C_{55} & C_{56} \\ \cdot & \cdot & \cdot & \cdot & \cdot & C_{66} \end{pmatrix}$$

$$\begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{21} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{31} & S_{32} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{41} & S_{42} & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & S_{53} & S_{54} & S_{55} & S_{56} \\ S_{61} & S_{62} & S_{63} & S_{64} & S_{65} & S_{66} \end{pmatrix} \rightarrow \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ \cdot & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ \cdot & \cdot & S_{33} & S_{34} & S_{35} & S_{36} \\ \cdot & \cdot & \cdot & S_{44} & S_{45} & S_{46} \\ \cdot & \cdot & \cdot & \cdot & S_{55} & S_{56} \\ \cdot & \cdot & \cdot & \cdot & \cdot & S_{66} \end{pmatrix}$$

Required number of components reduces to 21

The number can be further reduced by considering crystal symmetry

Neumann's Principle

- "The symmetry of any physical property of a crystal must include the symmetry elements of the point group of the crystal."
- Point groups are the group of macroscopic symmetry elements possessed by the structure of a crystal.*
- Crystals exhibit specific point symmetries.
- Crystal "properties" will include the point group but can exhibit more symmetry than the point group.

* Review pages 20-25 and 279-288 in Nye for a more complete treatment.

Possible Macroscopic Symmetry Elements

- Center of symmetry
- Mirror plane

► 1-, 2-, 3-, 4- or 6-fold rotation axes

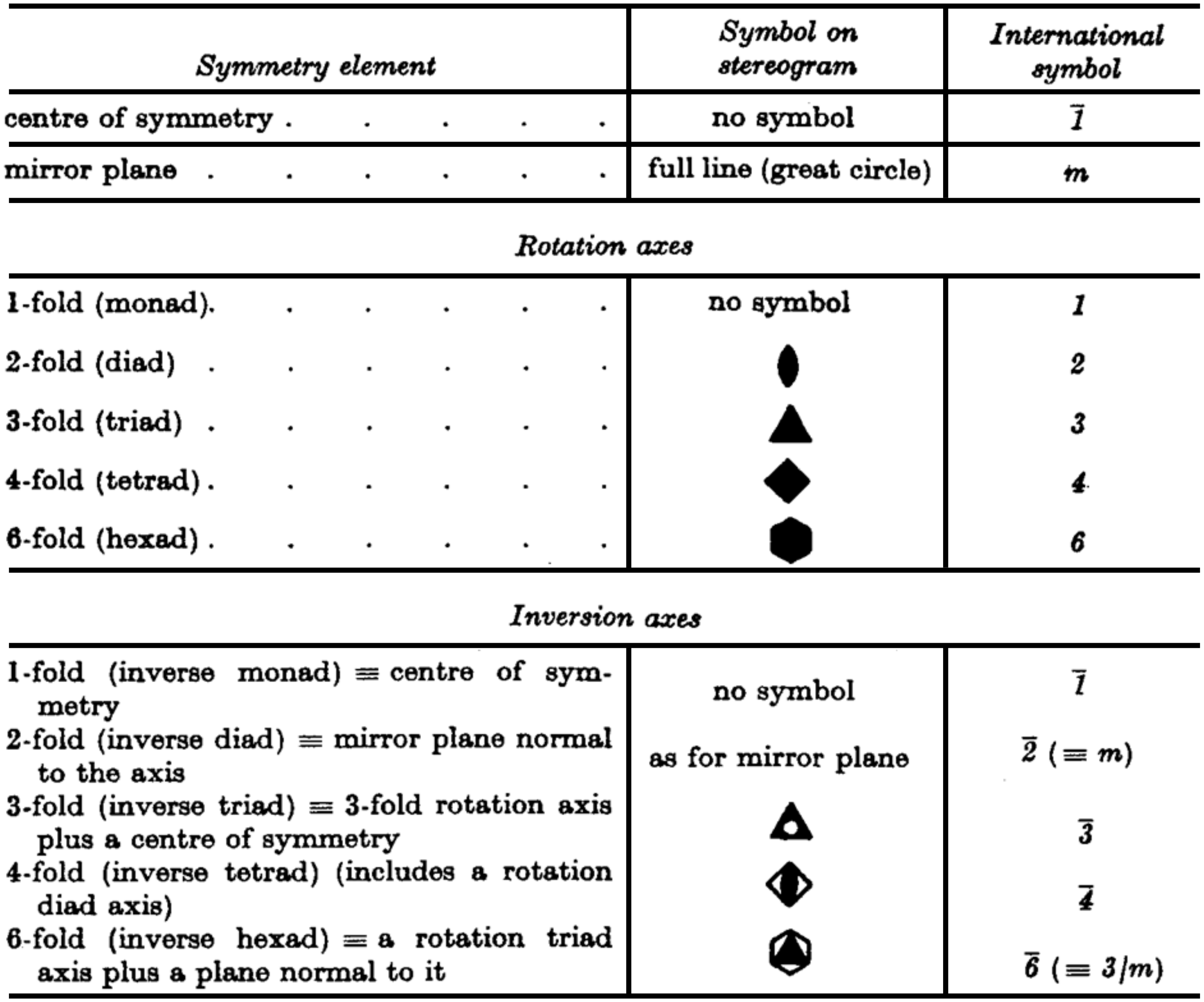
- 1-, 2-, 3-, 4- or 6-fold inversion axes

Crystal systems

- The 32 crystal classes (i.e., point groups) are conventionally grouped into seven crystal systems.

- The requirements for membership in a given crystal system is that the symmetry of the class should possess a certain minimum characteristic.

Symbolism for the symmetry elements of the 32 point groups

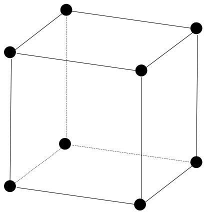


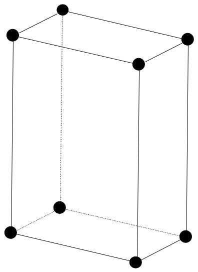
Symmetry element	*Symbol on stereogram*	*International symbol*
centre of symmetry	no symbol	$\bar{1}$
mirror plane	full line (great circle)	m
Rotation axes		
1-fold (monad).	no symbol	1
2-fold (diad)	⬮	2
3-fold (triad)	▲	3
4-fold (tetrad)	◆	4
6-fold (hexad)	⬢	6
Inversion axes		
1-fold (inverse monad) ≡ centre of symmetry	no symbol	$\bar{1}$
2-fold (inverse diad) ≡ mirror plane normal to the axis	as for mirror plane	$\bar{2}\ (\equiv m)$
3-fold (inverse triad) ≡ 3-fold rotation axis plus a centre of symmetry	◬	$\bar{3}$
4-fold (inverse tetrad) (includes a rotation diad axis)	◈	$\bar{4}$
6-fold (inverse hexad) ≡ a rotation triad axis plus a plane normal to it	⬡	$\bar{6}\ (\equiv 3/m)$

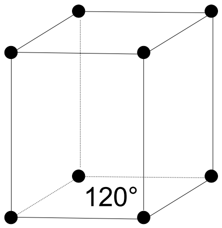
[Table from J.F. Nye, Physical Properties of Crystals, (Oxford University Press, Oxford, 1985) p. 280]

- We can describe shapes and arrangements of points within shapes in terms of the symmetry exhibited by them.

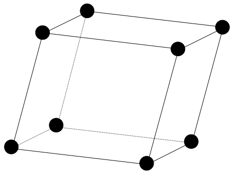
- In crystal systems, the symmetry of a class of crystals should possess a certain characteristic symmetry (i.e., certain minimum symmetry elements).

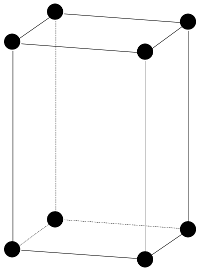

Cubic

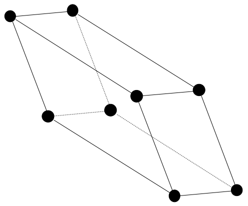

Orthorhombic

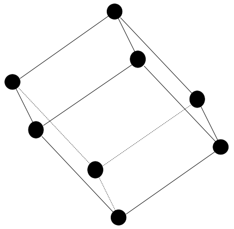


Hexagonal


Monoclinic


Tetragonal


Triclinic


Rhombohedral

We describe crystal symmetry relative to specific crystallographic axes and symmetry elements operating on those axes

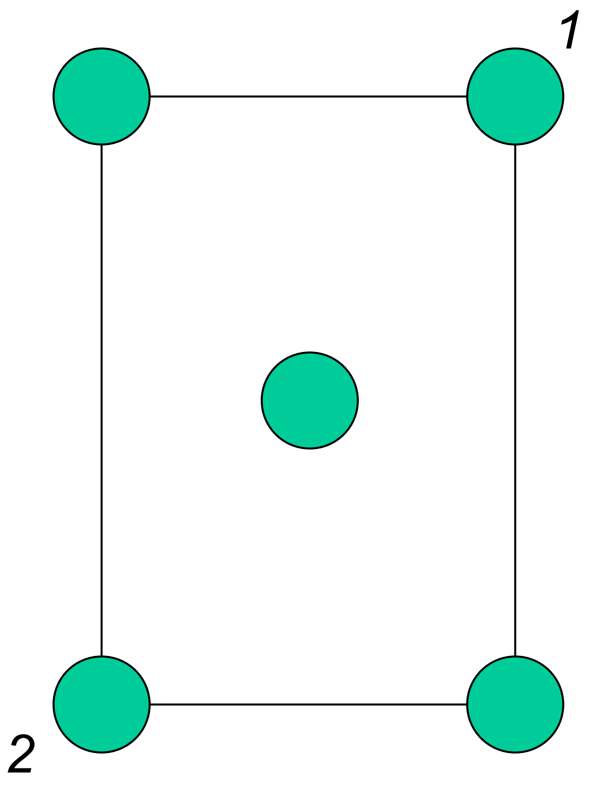
The order of Hermann-Mauguin symbols in point groups

Crystal System	Primary	Secondary	Tertiary
Triclinic	–	–	–
Monoclinic	$[010]$, unique axis b $[001]$, unique axis c	–	–
Orthorhombic	$[100]$	$[010]$	$[001]$
Tetragonal	$[001]$	$[100], [010]$	$[1\bar{1}0], [110]$
Trigonal, Rhombohedral Axes	$[111]$	$[1\bar{1}0], [01\bar{1}], [\bar{1}01]$	
Trigonal, Hexagonal Axes	$[001]$	$[100], [010], [\bar{1}\bar{1}0]$	
Hexagonal	$[001]$	$[100], [010], [\bar{1}\bar{1}0]$	$[1\bar{1}0], [120, [\bar{2}\bar{1}0]$
Cubic	$[100], [010], [001]$	$[111], [1\bar{1}\bar{1}], [\bar{1}1\bar{1}], [\bar{1}\bar{1}1]$	$[1\bar{1}0], [110], [01\bar{1}],$ $[011], [\bar{1}01], [101]$

Table adapted from R. Tilley, *Crystals and Crystal Structures*, John Wiley & Sons, Hoboken, NJ, 2006, p. 73.

The concept of crystal symmetry is illustrated on the next six viewgraphs.

You should review this and related literature on your own time.



- Rotation about the center point.
- 180° rotation moves point “1” to “2” but produces same pattern.
- Second 180° rotation moves original point (labeled with a “1”) back to its starting point.
- 2-fold rotation.

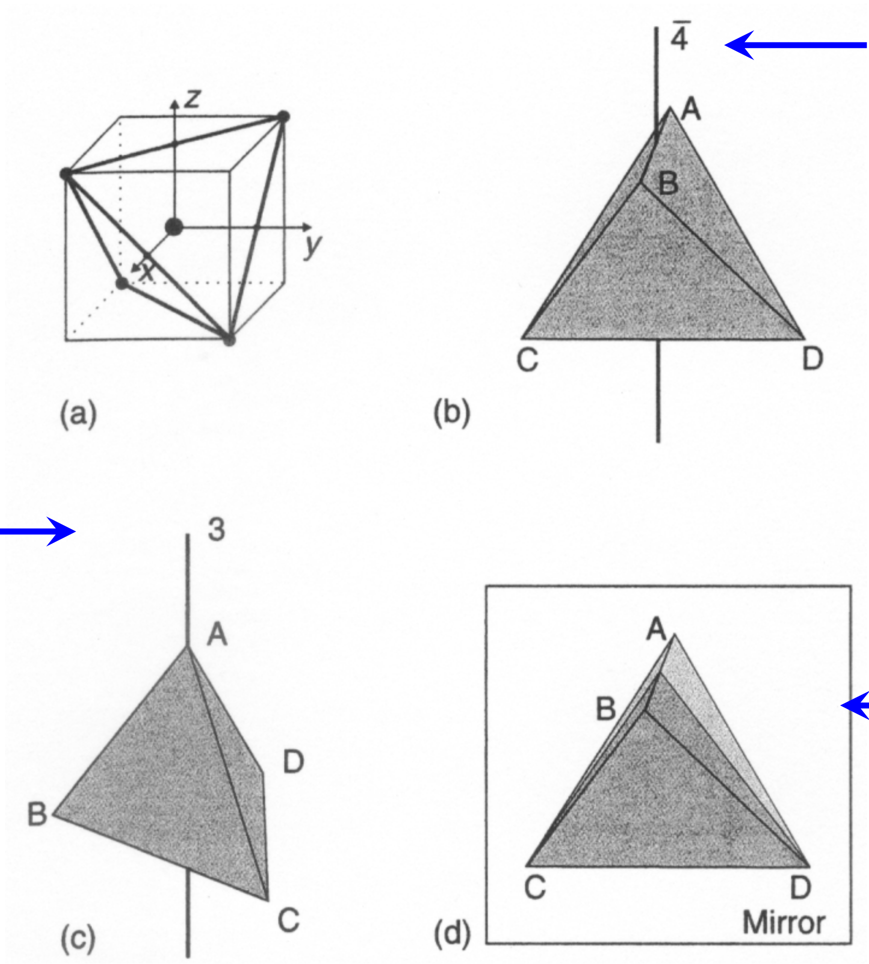
$\bar{4}3m$

Tetrahedron inscribed in a cube

4-fold inversion axes parallel to x,y,z (aka, <100>)

3-fold rotation axes parallel to cube diagonals (aka, <111>)

Mirror plane parallel to face diagonals (aka, <110>)



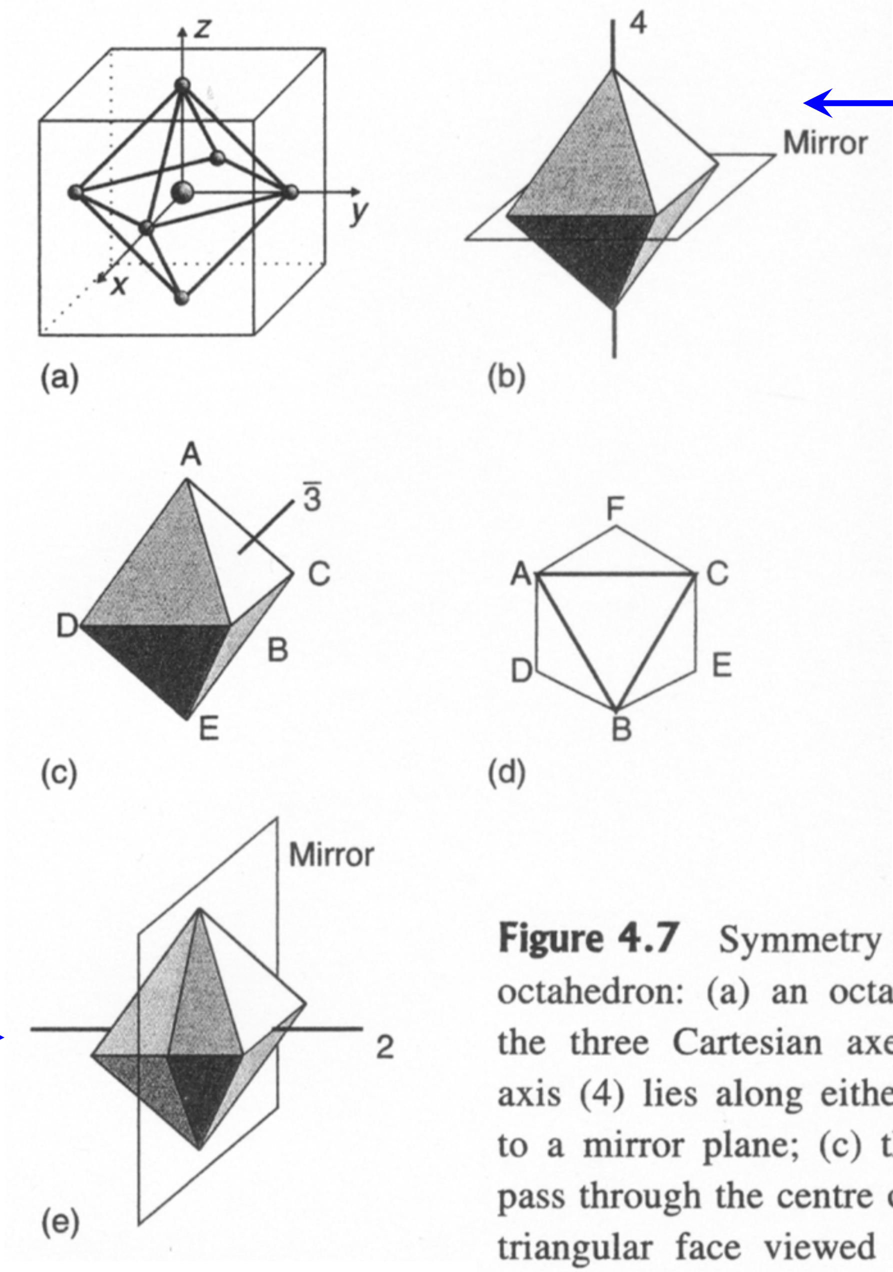
B*

Symmetry elements in a regular tetrahedron. (a) tetrahedron inscribed in a cube showing three Cartesian axes; (b) 4-fold inversion axes along *x* [100], *y* [010] and *z* [001]; (c) 3-fold rotation axes passing through vertex and center of opposite triangular face (i.e., [111]); (d) mirror planes parallel to [110]. Adapted from Fig. 4.6 in R. Tilley, *Crystals and Crystal Structures*, John Wiley & Sons, Hoboken, NJ, 2006.

$4\bar{3}m$

Octahedron
inscribed in a cube

4-fold rotation axes
parallel to x,y,z
(aka, <100>) with
perpendicular
mirror plane.



3-fold inversion
axes parallel to
cube diagonals
(aka, <111>)

2-fold rotation axes
parallel to face
diagonals
(aka, <111>) with
perpendicular
mirror plane.

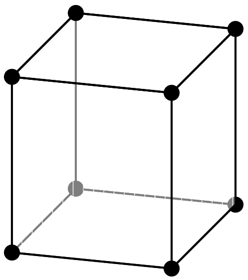
R. Tilley, *Crystals and Crystal Structures*,
John Wiley & Sons,
Hoboken, NJ, 2006.

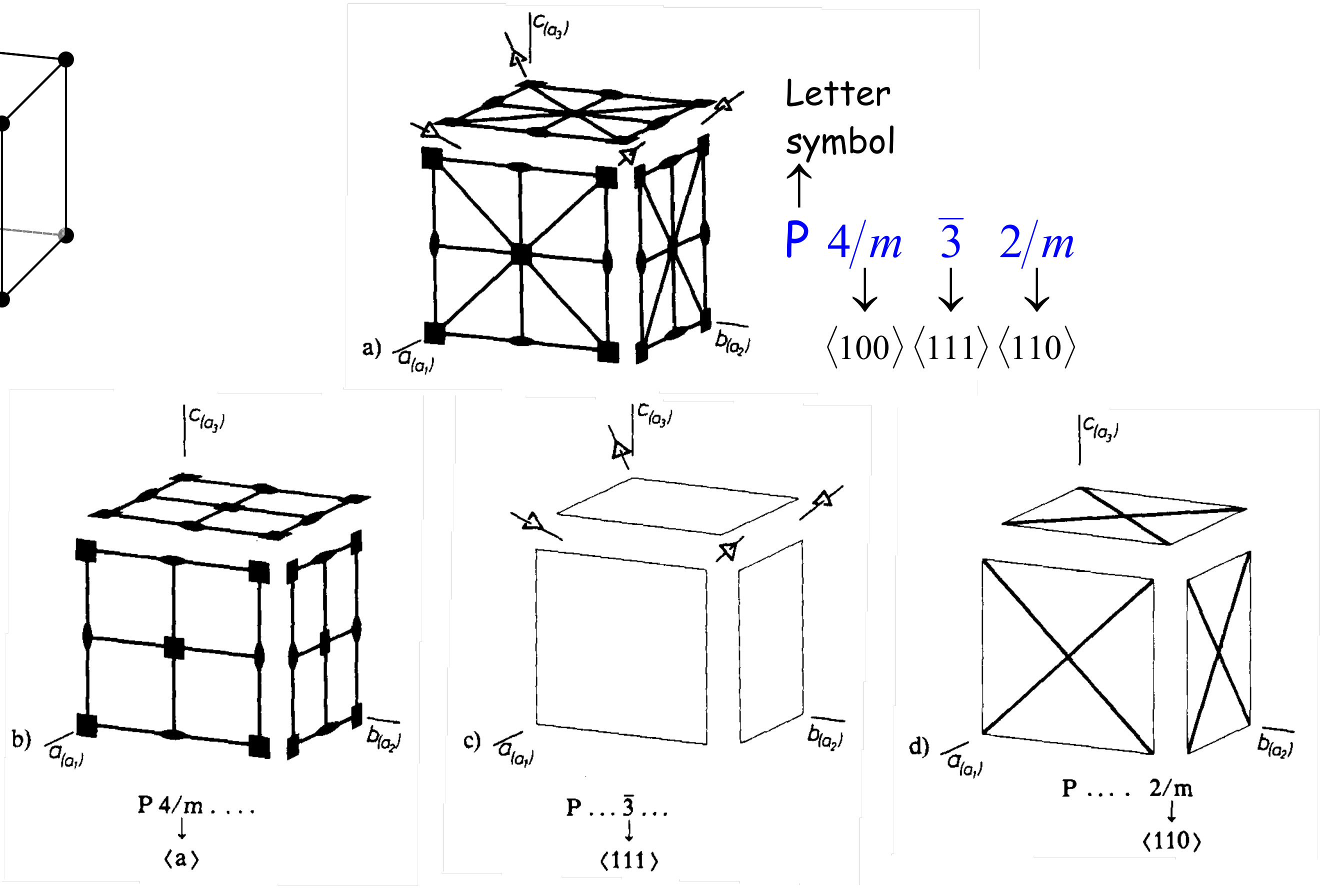
Figure 4.7 Symmetry elements present in a regular octahedron: (a) an octahedron in a cube, showing the three Cartesian axes; (b) each tetrad rotation axis (4) lies along either x-, y- or z and is normal to a mirror plane; (c) three-fold inversion axes ($\bar{3}$) pass through the centre of each triangular face; (d) a triangular face viewed from above; (d) diad axes through the centre of each edge lie normal to mirror planes

B*

We describe lattice shapes and arrangements of lattice points in the same way.

Symmetry of the Cubic *P*-Lattice





Letter symbol
↑
P $4/m$ $\bar{3}$ $2/m$
↓ ↓ ↓
⟨100⟩ ⟨111⟩ ⟨110⟩

Primary **Secondary** **Tertiary**

Four 3-fold rotation axes parallel to cube diagonals (aka, <111>)

Fig. 6.24. a Space group P 4/m $\bar{3}$ 2/m . In the other diagrams, only the symmetry elements corresponding to the symmetry directions ⟨a⟩, ⟨111⟩, ⟨110⟩ are shown.
b P 4/m . . . ., **c** P . . . $\bar{3}$ . . ., **d** P 2/m
↓ ↓ ↓
⟨a⟩ ⟨111⟩ ⟨110⟩

Adapted from W. Borchardt-Ott, *Crystallography, 2nd Edition*, (Springer, Berlin, Germany, 1995) p. 99

- There are only 32 crystal classes derived from the 7 crystal systems (i.e., shapes).
- Each has a certain characteristic symmetry.
- They are presented on stereograms on this viewgraph and the two that follow.

B*

Table 21

Symmetry elements and conventions for the choice of axes in the 32 crystal classes

Symbols of centrosymmetrical classes are enclosed in boxes

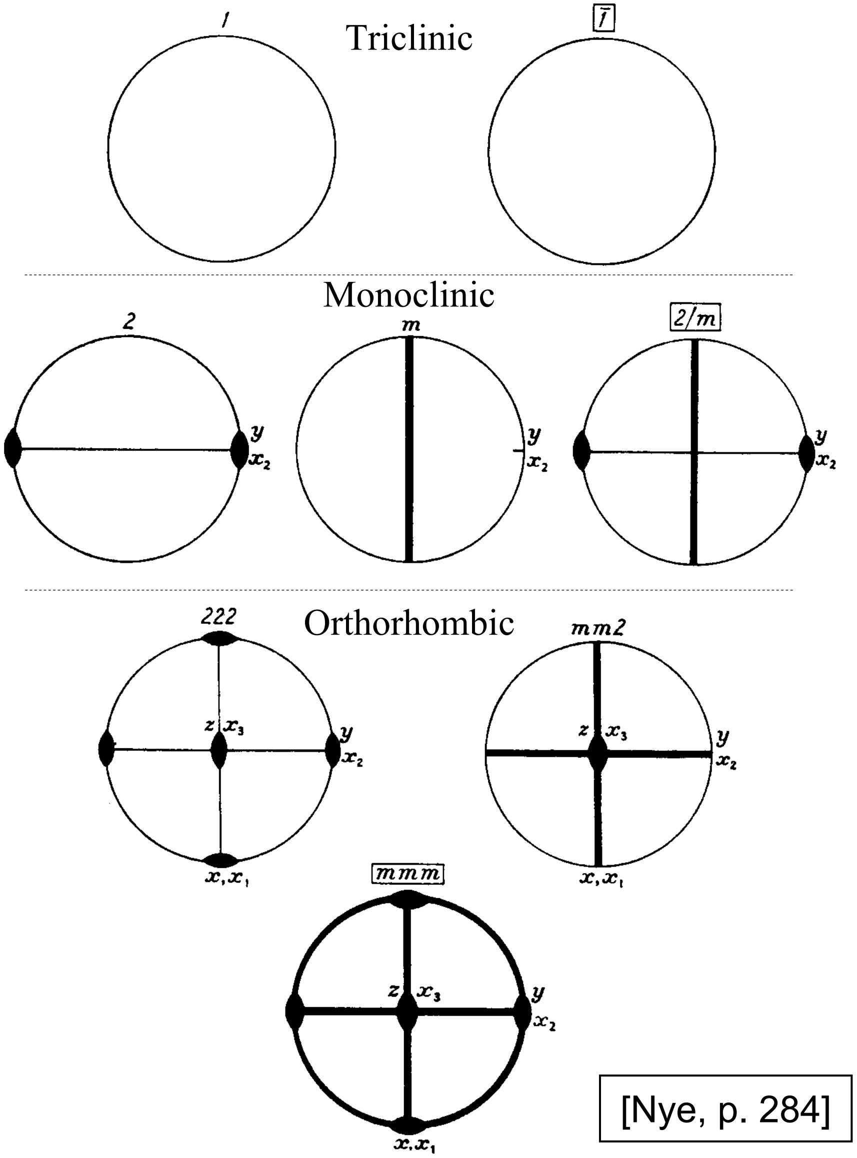


Table 21.3

[Nye, p. 284]

Tetragonal

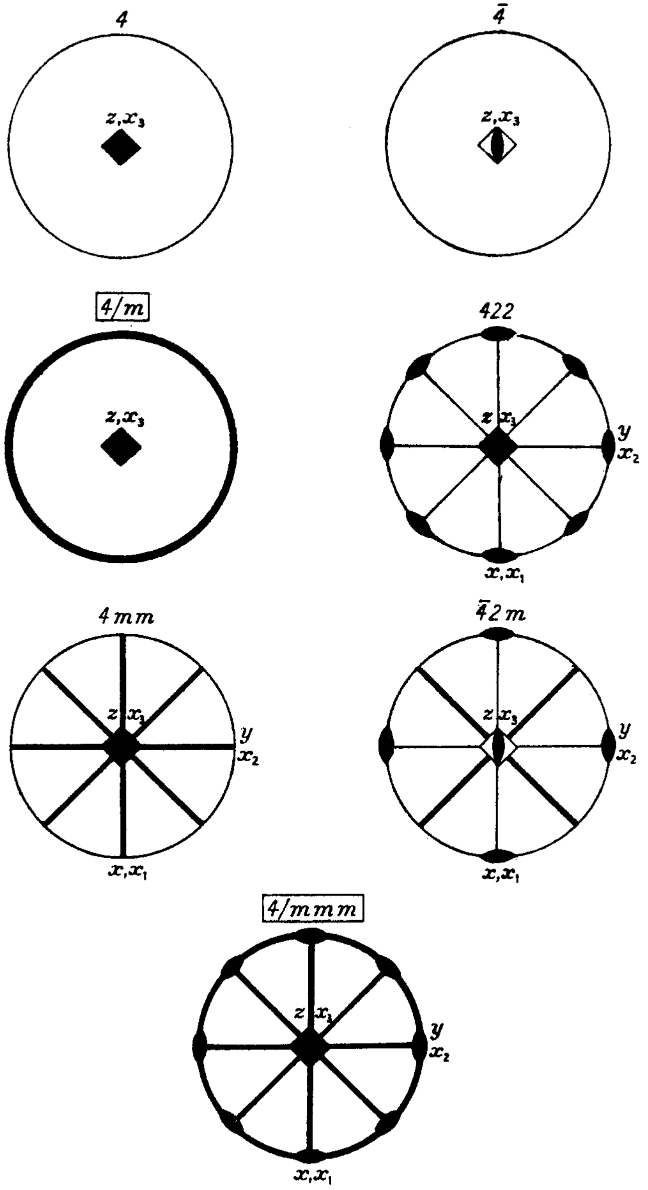


Table 21.2

Trigonal

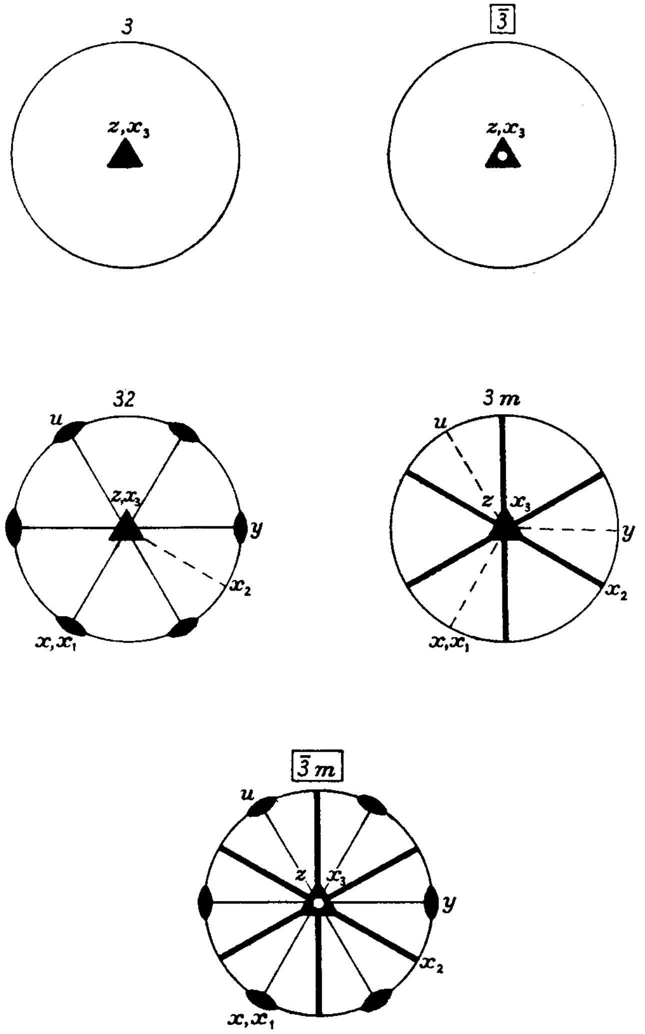


Table 21.3

[Nye, pp. 285-286]

B*

Hexagonal

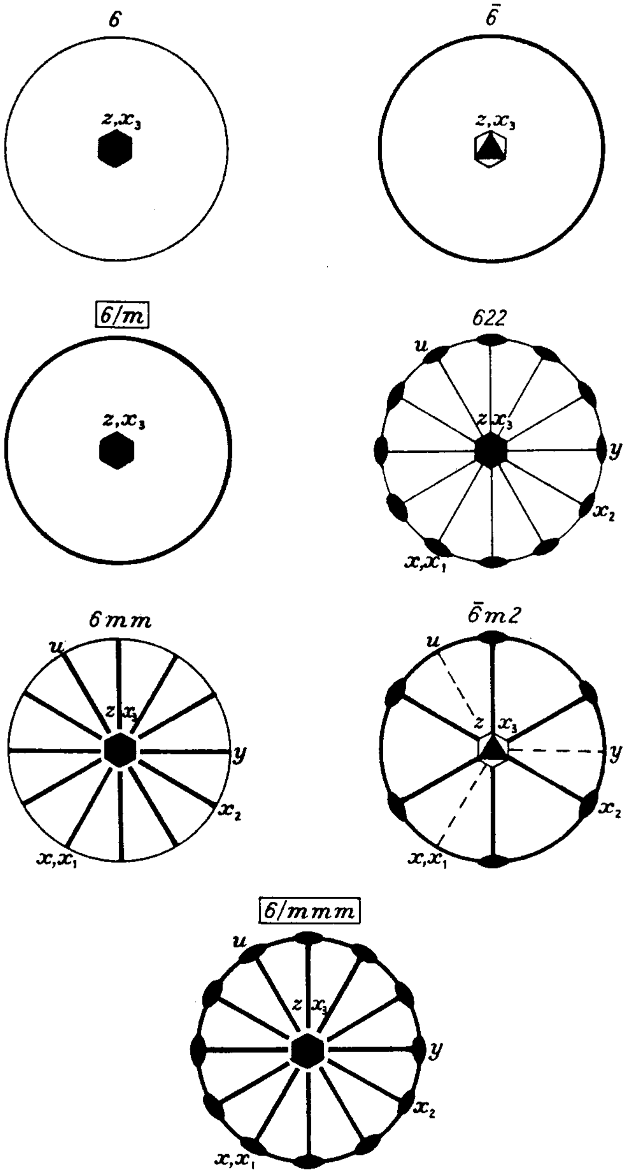


Table 21.4

Cubic

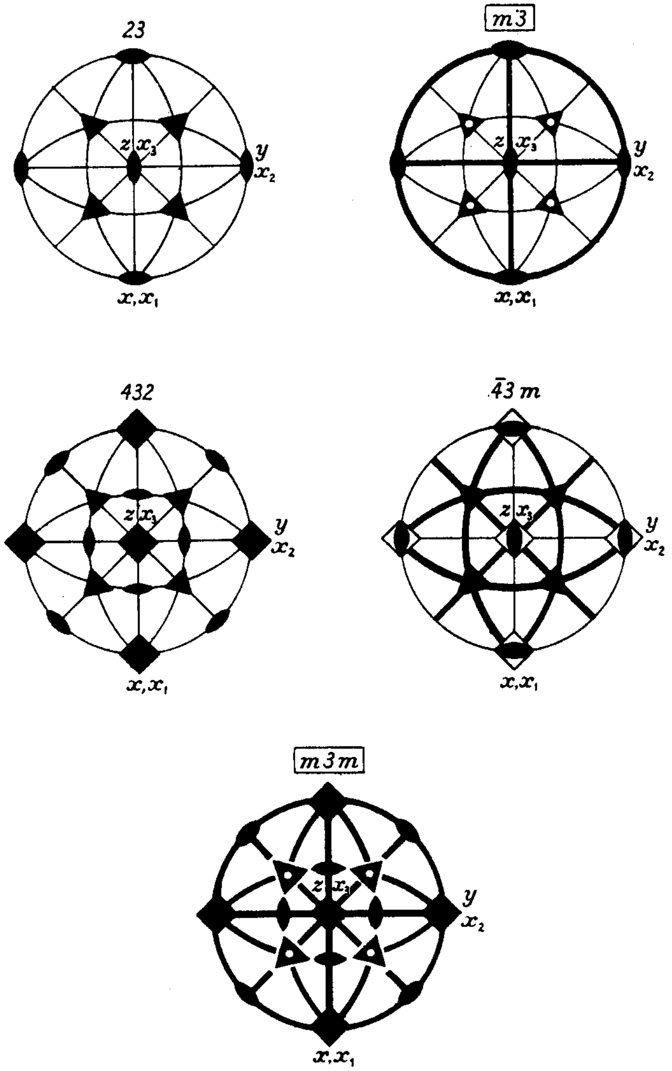
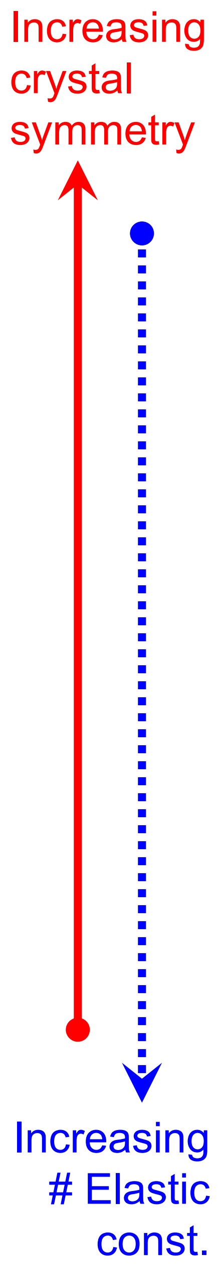


Table 21.5

[Nye, pp. 287-288]

Influence of Crystal Symmetry on Number of Elastic Constants

Crystal System	**Axial Relation-ships**	**Interaxial Angles**	**Minimum Symmetry Elements**	**Number of Elastic Constants**
Cubic	*a* = *b* = *c*	$\alpha = \beta = \gamma = 90°$	**Four 3-fold rotation** or rotoinversion axes parallel to body diagonals	3
Hexagonal	*a* = *b* ≠ *c*	$\alpha = \beta = 90°$; $\gamma = 120°$	**One 6-fold rotation** or rotoinversion axis parallel to *z*-axis	5
Tetragonal	*a* = *b* ≠ *c*	$\alpha = \beta = \gamma = 90°$	**One 4-fold rotation** or rotoinversion axis parallel to *z*-axis	6 or 7
Rhombohedral (Trigonal)	*a* = *b* = *c*	$\alpha = \beta = \gamma \neq 90°$	**One 3-fold rotation** or rotoinversion axis parallel to *z*-axis	5, 6 or 7
Orthorhombic	*a* ≠ *b* ≠ *c*	$\alpha = \beta = \gamma = 90°$	**Three 2-fold rotation** or rotoinversion axes parallel to *x*,*y*,*z*-axes	9
Monoclinic	*a* ≠ *b* ≠ *c*	$\alpha = \gamma = 90° \neq \beta$	**One 2-fold rotation** or rotoinversion axis parallel to *y*-axis	13
Triclinic	*a* ≠ *b* ≠ *c*	$\alpha \neq \beta \neq \gamma \neq 90°$	- None - **One 1-fold rotation** or rotoinversion axis	21


Increasing crystal symmetry

Increasing # Elastic const.

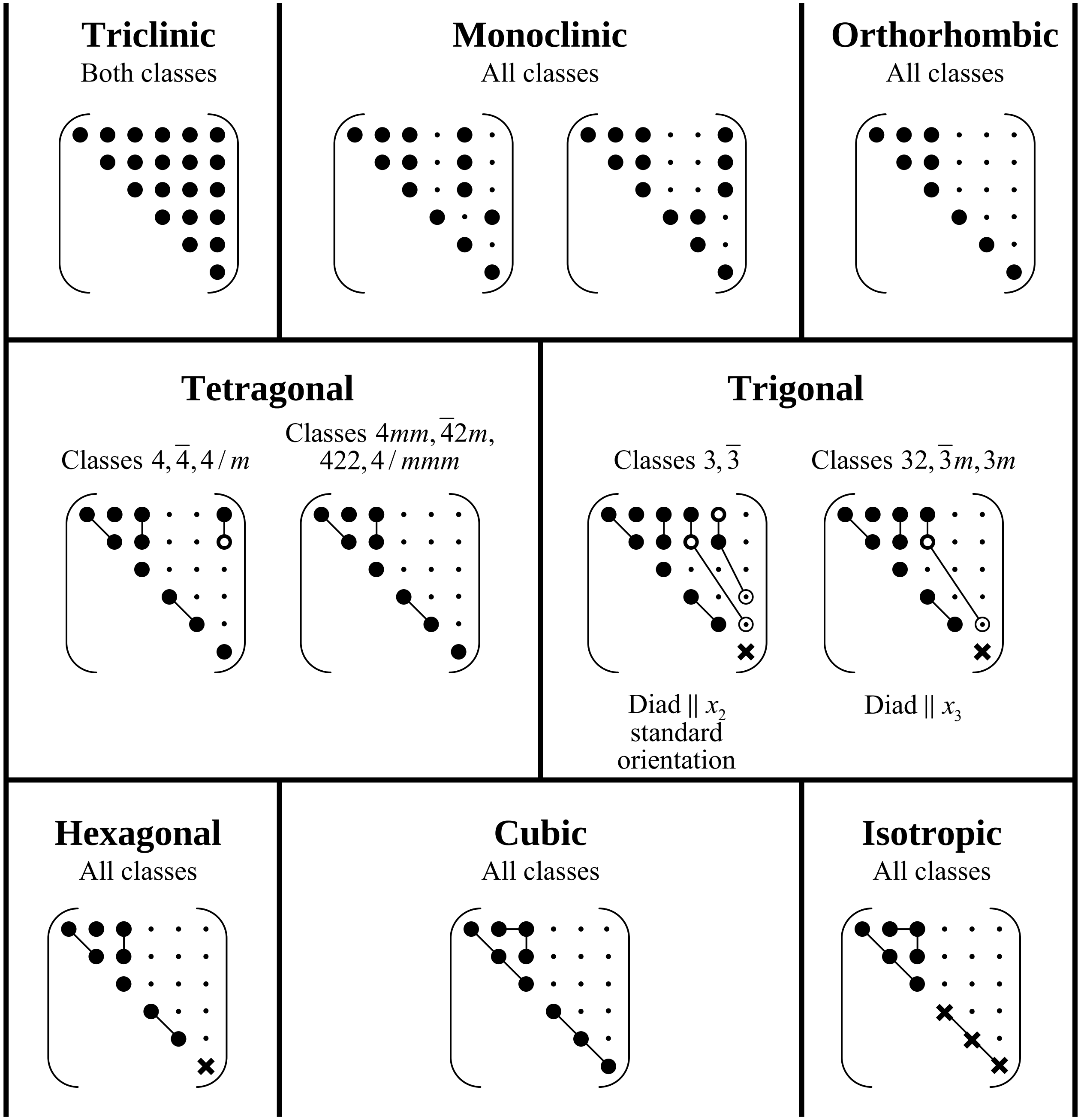
More Reading Regarding the Reduction of Elastic Constants with Increasing Symmetry

- A clear explanation of the reduction in the number of elastic constants due to crystal symmetry is provided in Chapter 6 of Wagoner and Chenot (pp. 196-207).

- Excellent explanations are also provided in Nye (i.e., Ch. 8 and Appendix B) and in Reid (Ch. 3).

- You are urged, but not required, to review some of this material.

Form of the elastic constant matrices for different symmetries.



· Zero component ($s = 0$, $c = 0$)

● Non-zero component ($s \neq 0$, $c \neq 0$)

●–● Equal components

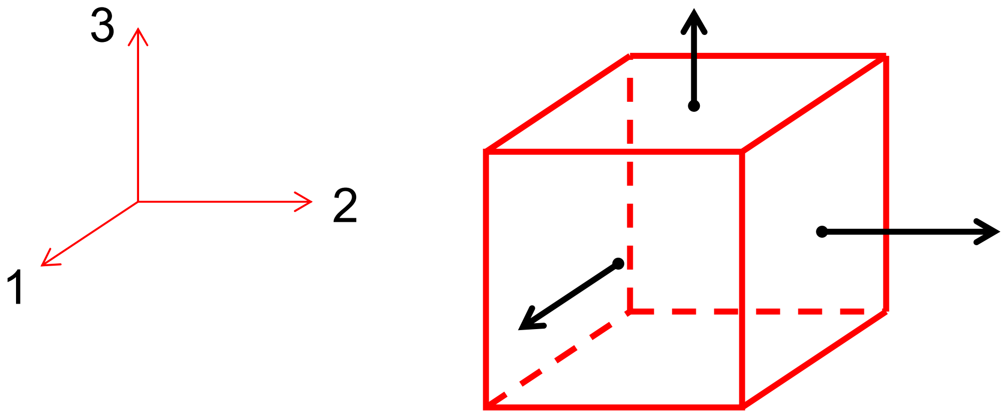
●–○ Numerically equal but opposite

●–⊙ ⊙ = 2● for s; ⊙ = ●/2 for c

✖ ✖=$2(s_{11}-s_{22})$ or $(c_{11}-c_{22})/2$

Figure adapted from J.F. Nye, Physical Properties of Crystals, Oxford University Press (1985), p. 140-141.

Cubic Symmetry and Elastic Constants

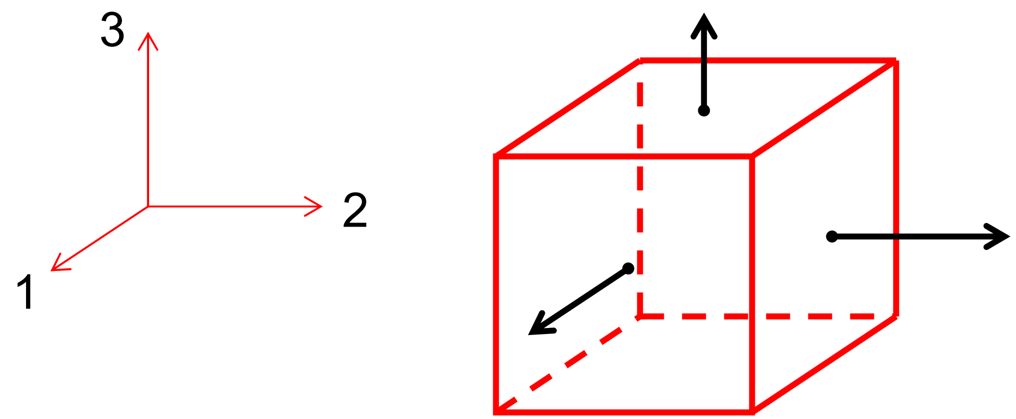


- Application of a stress along the [100] direction evokes a certain elastic response. Stresses applied along the [010] or [001] axes will evoke an equivalent elastic response. Thus:
  - $C_{11} = C_{22} = C_{33}$

- Similarly, applied shear stresses will evoke equivalent responses along the following axes:
  - $C_{44} = C_{55} = C_{66}$; $C_{12} = C_{13} = C_{23}$

- The number of independent elastic constants for a cubic material is 3.

Isotropy considerations



- Cubic materials are not necessarily isotropic.

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

$$A = \boxed{\begin{array}{c} \left(C_{11} - C_{12}\right)/2C_{44} \\ \text{or} \\ 2\left(S_{11} - S_{12}\right)/S_{44} \end{array}}$$

NOTE: Some books (Ex., Hertzberg) present an inverted version of this equation. However, the implications are still the same.

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

FOR CUBIC SOLIDS

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

$$C_{44} = \frac{C_{11} - C_{22}}{2}$$

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

$$S_{44} = 2\left(S_{11} - S_{22}\right)$$

We can assume that <u>most</u> polycrystalline solids are isotropic but not all.

Many parameters are used to describe the elastic properties of materials

$$E = \frac{1}{S_{11}} \qquad G = \frac{1}{S_{44}} = \frac{1}{2\left(S_{11} - S_{12}\right)} \qquad \nu = -\frac{S_{12}}{S_{11}}$$

These expressions are for isotropic solids. They are interrelated

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

See Ch. 8 in Nye, Ch. 13 in Newnham, or Ch. 10 in Gersten for a more thorough explanation.

Wikipedia also provides a nice discussion.

Elastic Moduli in Cubic Materials

We can use the different relations among elastic constants to ascertain elastic moduli in any crystallographic orientation

$$\frac{1}{E_{hkl}} = S_{11} - 2\left(S_{11} - S_{12} - \frac{1}{2}S_{44}\right)\left(\alpha^2\beta^2 + \beta^2\gamma^2 + \alpha^2\gamma^2\right)$$

Where α, β, and γ are the direction cosines between the $[hkl]$ crystal direction and the [100], [010], and [001] directions (*i.e.*, the x,y,z axes).

$\alpha = \cos(\angle[hkl][100])$; $\beta = \cos(\angle[hkl][010])$; $\gamma = \cos(\angle[hkl][010])$

TABLE 1.3 Stiffness and Compliance Constants for Selected Crystals[a]

	(10^{10} Pa)			(10^{-11} Pa^{-1})		
Material	c_{11}	c_{12}	c_{44}	s_{11}	s_{12}	s_{44}
Cubic						
Aluminum	10.82	6.13	2.85	1.57	−0.57	3.51
Copper	16.84	12.14	7.54	1.50	−0.63	1.33
Gold	18.60	15.70	4.20	2.33	−1.07	2.38
Iron	23.70	14.10	11.60	0.80	−0.28	0.86
Lithium fluoride	11.2	4.56	6.32	1.16	−0.34	1.58
Magnesium oxide	29.3	9.2	15.5	0.401	−0.096	0.648
Molybdenum[b]	46.0	17.6	11.0	0.28	−0.08	0.91
Nickel	24.65	14.73	12.47	0.73	−0.27	0.80
Sodium chloride[b]	4.87	1.26	1.27	2.29	−0.47	7.85
Spinel ($MgAl_2O_4$)	27.9	15.3	15.3	0.585	−0.208	0.654
Titanium carbide[b]	51.3	10.6	17.8	0.21	−0.036	0.561
Tungsten	50.1	19.8	15.14	0.26	−0.07	0.66
Zinc sulfide	10.79	7.22	4.12	2.0	−0.802	2.43

	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	s_{11}	s_{12}	s_{13}	s_{33}	s_{44}
Hexagonal										
Cadmium	12.10	4.81	4.42	5.13	1.85	1.23	−0.15	−0.93	3.55	5.40
Cobalt	30.70	16.50	10.30	35.81	7.53	0.47	−0.23	−0.07	0.32	1.32
Magnesium	5.97	2.62	2.17	6.17	1.64	2.20	−0.79	−0.50	1.97	6.10
Titanium	16.0	9.0	6.6	18.1	4.65	0.97	−0.47	−0.18	0.69	2.15
Zinc	16.10	3.42	5.01	6.10	3.83	0.84	0.05	−0.73	2.84	2.61

[a] Data adapted from H. B. Huntington, *Solid State Physics*, Vol. 7, Academic, New York, 1958, p. 213, and K. H. Hellwege, *Elastic, Piezoelectric and Related Constants of Crystals*, Springer-Verlag, Berlin, 1969, p. 3.

[b] Note that $E_{100} > E_{111}$.

R.W. Hertzberg, Deformation & Fracture Mechanics of Engineering Materials, 4th ed., (John Wiley & Sons, New York, 1996) p. 14.

Example Problem

- Compute the elastic modulus for tungsten in the <110> direction.

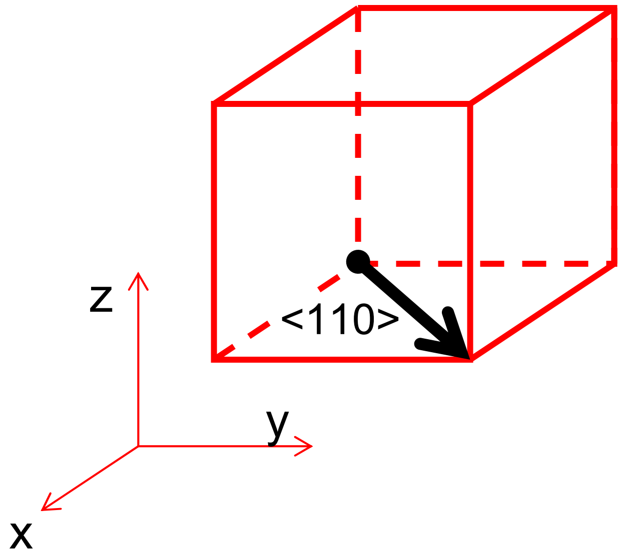
We need the direction cosines for the unit vectors in the cubic lattice.

<hkl> = <110>

$\alpha = 1/\sqrt{2}$

$\beta = 1/\sqrt{2}$

$\gamma = 0$



Example Problem – cont'd

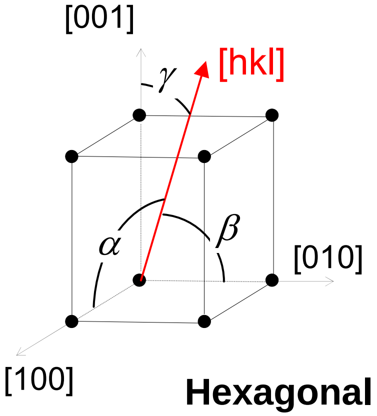
$$\frac{1}{E_{hkl}} = S_{11} - 2\left(S_{11} - S_{12} - \frac{1}{2}S_{44}\right)\left(\alpha^2\beta^2 + \beta^2\gamma^2 + \alpha^2\gamma^2\right)$$

$$\frac{1}{E_{110}} = 0.26 - 2\left(0.26 - (-0.07) - \frac{1}{2}(0.66)\right)\left(\frac{1}{4} + 0 + 0\right)$$

$$= 0.26 - (0)(1/4)$$

$$E_{110} = \underline{\underline{384.6\ \text{GPa}}}$$

Elastic Moduli in Hexagonal Crystals

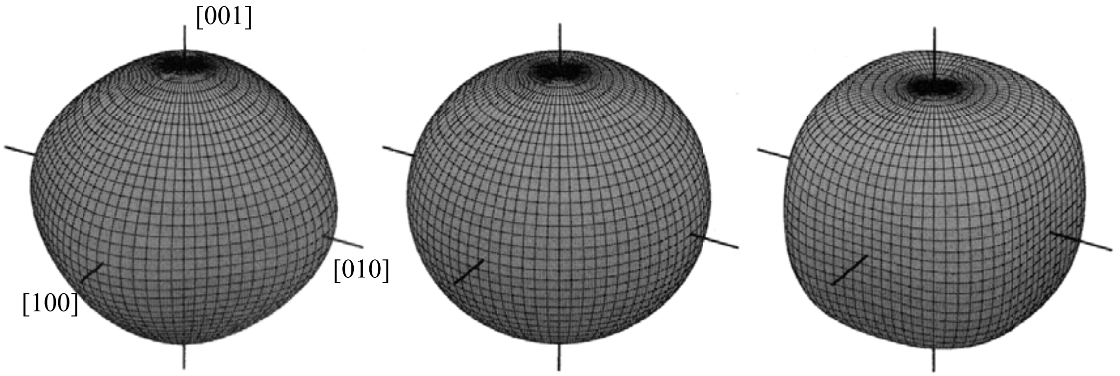


$$\frac{1}{E_{hkl}} = S_{11}(1-\gamma^2)^2 + S_{33}\gamma^4 + \gamma^2\left(1-\gamma^2\right)\left(2S_{13}+S_{44}\right)$$

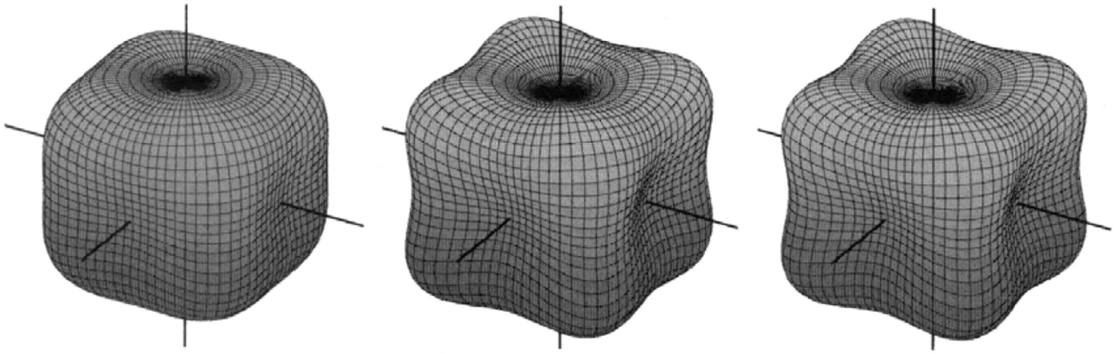
- $\alpha = \cos(\angle[hkl][100])$; $\beta = \cos(\angle[hkl][010])$; $\gamma = \cos(\angle[hkl][010])$ for the hexagonal unit cell.

- In hexagonal crystals, E_{hkl} depends only on the direction cosine γ which lies perpendicular to the basal plane.

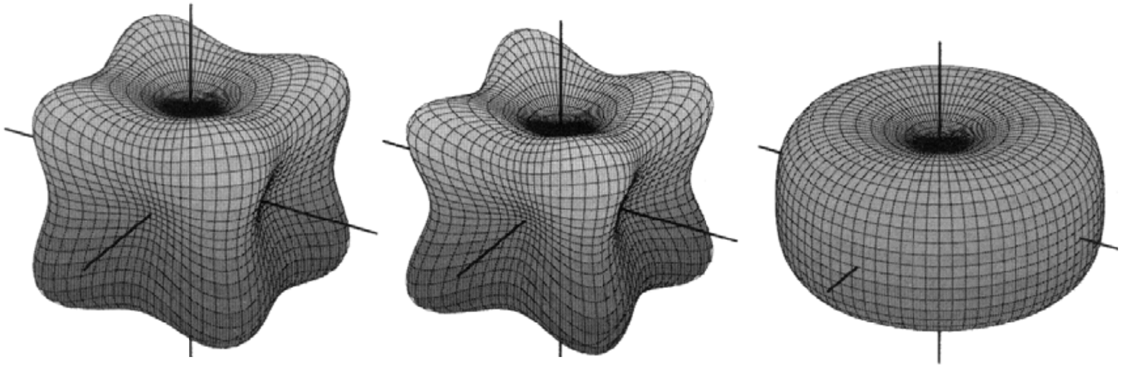
- As a result the modulus of elasticity in hexagonal crystals is isotropic everywhere in the basal plane.



(a) Titanium carbide $A = 0.88$ (b) Tungsten, $A = 1.00$ (c) Aluminum, $A = 1.23$



(d) Silicon, $A = 1.57$ (b) Gold, $A = 1.89$ (f) α Iron, $A = 2.13$



(g) Nickel, $A = 2.50$ (h) Copper, $A = 3.22$ (i) Zinc $E_{(0001)} / E_{(10\underline{1}0)} = 2.13$

Fig. 2.10 from Roesler et al. Orientation dependence of Young's modulus for some materials. In each spatial direction, the distance of the surface from the origin is a measure of Young's modulus. For example, Copper is elastically soft along <100> type directions and is elastically stiff along <111> type directions.

We can describe anisotropy in terms of the Zener ratio:

$$\boxed{A = \frac{2\left(S_{11} - S_{12}\right)}{S_{44}} = \frac{2C_{44}}{\left(C_{11} - C_{12}\right)}}$$

When $A = 1$, the material is isotropic. As A deviates, the material becomes more anisotropic.

Elastic properties of polycrystals

- In single crystals elastic constants are determined by bonding between atoms. As such, most single crystals are mechanically anisotropic.

- In polycrystals, the anisotropic behavior of each grain “averages out” because: (a) grain orientations tend to be random; and (b) the deformation of one grain is dependent on the deformation of its neighbor.

- Exceptions occur when the material is textured (i.e., the grains exhibit a preferred orientation).

- Page 34 in Hosford lists some possibilities.

Temperature dependence of elastic moduli

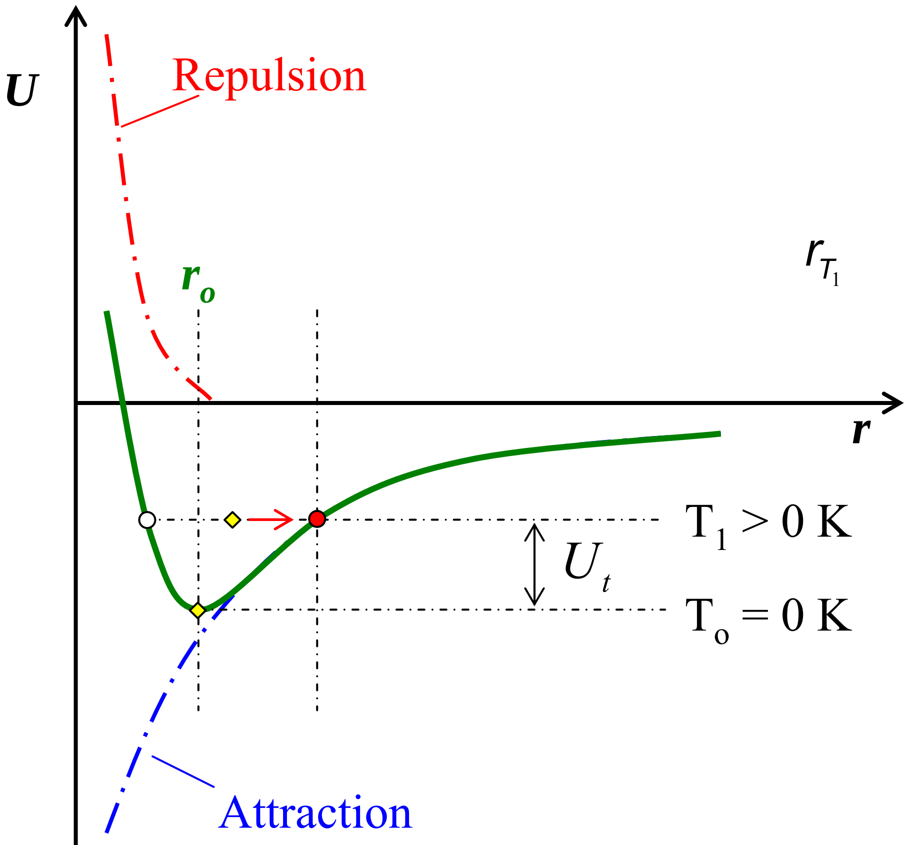
- Young's modulus does vary with temperature.
- For metals and ceramics there are some general rules of thumb for temperatures lower than half of the melting temperature.

$$\text{Metals: } E(T) = E(0\ \text{K}) \cdot \left(1 - 0.5\frac{T}{T_{mp}}\right)$$

$$\text{Ceramics: } E(T) = E(0\ \text{K}) \cdot \left(1 - 0.3\frac{T}{T_{mp}}\right)$$

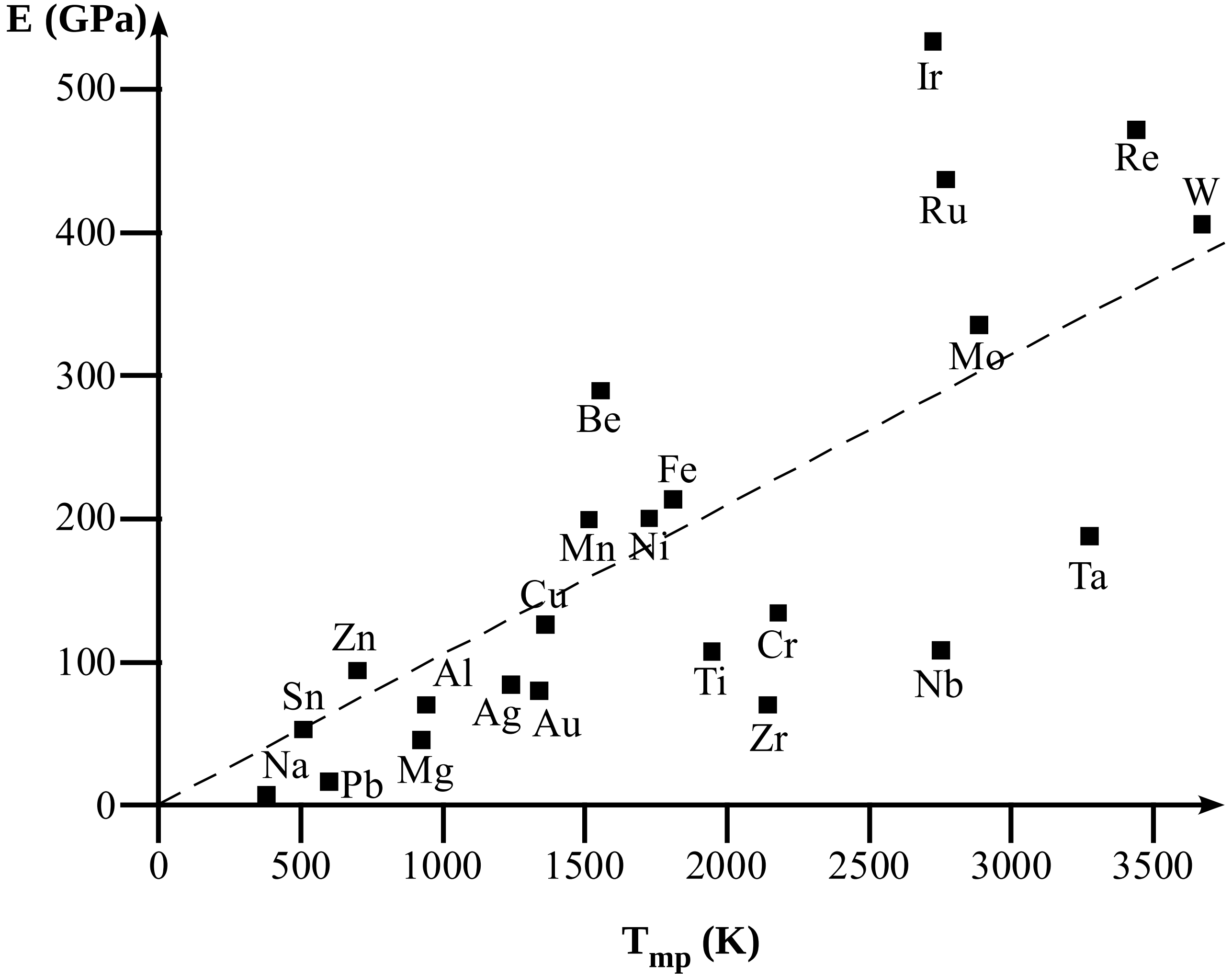
- Different rules apply for polymers.

Origin of *T* dependence



- Raising *T* increases the energy of the atoms by an amount U_t causing them to oscillate about their equilibrium positions.
- The repulsive interaction is short range in comparison to the attractive interaction.
- The mean distance between atoms thus grows when temperature is increased due to oscillation.
- Thermal expansion increases and *E* decreases with increasing *T*.

Young's modulus also tends to scale with T_{mp} for similar reasons.

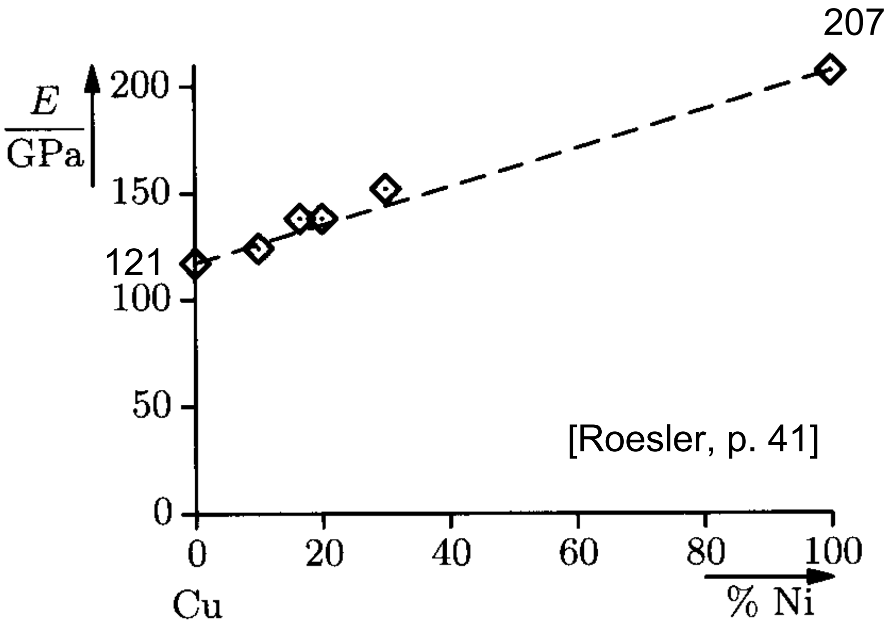


Influence of alloying

- Alloying generally has little influence on the stiffness of materials. This is because the solubility of alloying elements is generally very small (<10%).

- As noted by Roesler et al., the elastic modulus for Al alloys varies by roughly 10% while their strengths can be significantly altered by alloying.

- The Cu-Ni system is an exception to the rule. Ni is 100% soluble in Ni.



[Roesler, p. 41]