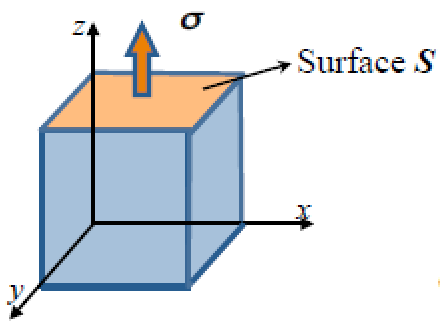
THE STRESS TENSOR



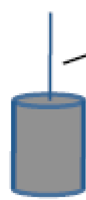
Normal tensile load, force ***F***

$$\boxed{\frac{F}{S} = \sigma}$$ **Stress**

dimension of it: $\frac{N}{m^2} = Pascal \cong \frac{100\ g_{(weight)}}{1\ m^2}$ (not a lot..)

More useful unit:

$$MPa = 10^6\ Pa = \frac{100\ g}{mm^2}$$



wire, 1 mm section

100 g

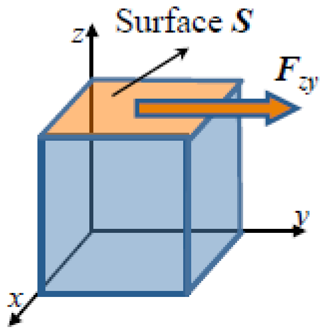
$$GPa = 1000\ MPa = \frac{100\ Kg}{mm^2}$$

Compare this for example with the Young's modulus $\boldsymbol{E = 211\ GPa}$ for **Fe**

(note of course, that fracture onsets much before a 211GPa tensile stress can be applied)

THE STRESS TENSOR

Orientation of stress



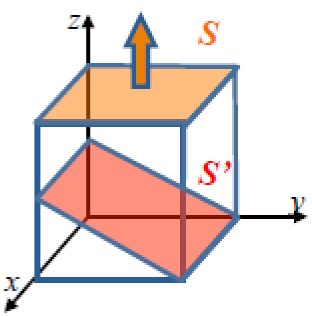
$$\frac{F_{zy}}{S} = \sigma_{zy}$$

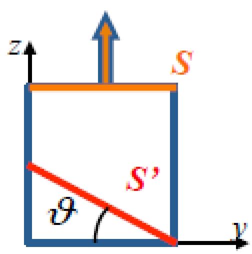
(z: on face **z**; y: in the **y** direction)

We get a 9-component **tensor** (matrix)

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

Example: traction

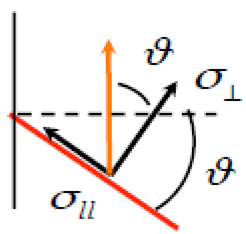




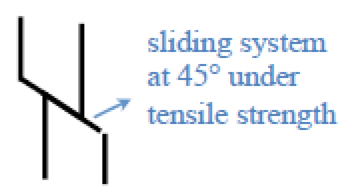
$$\sigma_0 = \frac{F}{S}; \quad S'\cos\vartheta = S \;\Rightarrow\; \sigma = \frac{F}{S'} = \frac{F}{S}\cos\vartheta = \sigma_0\cos\vartheta$$

The shear (or "parallel") component is

$$\sigma_{//} = \sigma_0 \cos\vartheta \sin\vartheta = \frac{1}{2}\sigma_0 \sin(2\vartheta)$$



This ($\sigma_{//}$) is the only relevant component for the deformation, so the maximum is at $\vartheta = 45°$



THE STRESS TENSOR

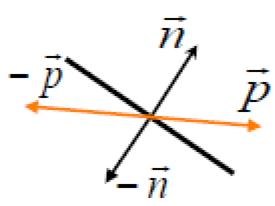
Q: How do we compute the stress on <u>any</u> surface? By a *left* product

A: $\vec{p} = \vec{n} \cdot \underline{\underline{\sigma}}$ $\quad \vec{p} =$ stress resolved on the surface identified by $\vec{n} = \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$

$$\left(n_x, n_y, n_z\right) \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} = \begin{pmatrix} n_x\sigma_{xx} + n_y\sigma_{yx} + n_z\sigma_{zx} \\ \dots \\ \dots \end{pmatrix}$$

Comment: if you "invert" the surface $(\vec{n} \rightarrow -\vec{n})$, $\rightarrow \vec{p} \rightarrow -\vec{p}$.

→the stress vector is "opposite" on "the other side" of the plane.

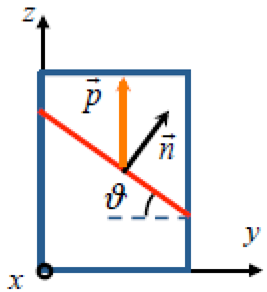


In practice, we always think of **two forces** (per unit surface) acting in opposite directions on the two sides of the chosen plane.

The total force is ∅ (uniform stress yields no acceleration), but "***tension***" (or "**compression**", "**shear**", etc.) is there.

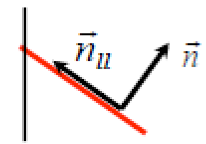
THE STRESS TENSOR

<u>Exercise</u>: we reconsider the previous example

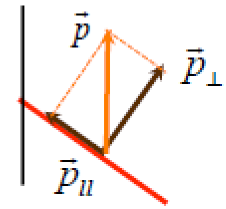


$$\vec{p} = \vec{n} \cdot \underline{\underline{\sigma}} \qquad \vec{n} = \begin{pmatrix} 0 & \sin\vartheta & \cos\vartheta \end{pmatrix} \qquad \vec{n}_\perp = \begin{pmatrix} 0 & -\cos\vartheta & \sin\vartheta \end{pmatrix}$$

$$\vec{p} = \begin{pmatrix} 0 & \sin\vartheta & \cos\vartheta \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sigma_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \sigma_0 \cos\vartheta \end{pmatrix}$$



$\vec{p}$ is directed in the '*z*' direction, and is $\propto \cos\vartheta$.



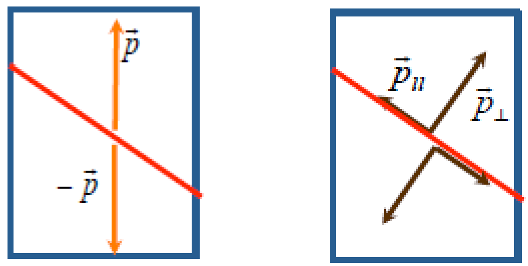
$$\vec{p}_\perp = (\vec{p} \cdot \vec{n}) \cdot \vec{n} = \begin{pmatrix} 0 & 0 & \sigma_0 \cos\vartheta \end{pmatrix} \begin{pmatrix} 0 \\ \sin\vartheta \\ \cos\vartheta \end{pmatrix} \cdot \begin{pmatrix} 0 \\ \sin\vartheta \\ \cos\vartheta \end{pmatrix} = \sigma_0 \cos^2\vartheta \cdot \begin{pmatrix} 0 \\ \sin\vartheta \\ \cos\vartheta \end{pmatrix}$$

$$\vec{p}_{II} = \vec{p} - \vec{p}_\perp = \begin{pmatrix} 0 \\ 0 \\ \sigma_0 \cos\vartheta \end{pmatrix} - \sigma_0 \cos^2\vartheta \cdot \begin{pmatrix} 0 \\ \sin\vartheta \\ \cos\vartheta \end{pmatrix} = \sigma_0 \cos\vartheta \left[\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} - \begin{pmatrix} 0 \\ \sin\vartheta\cos\vartheta \\ \cos^2\vartheta \end{pmatrix} \right] =$$

$$= \sigma_0 \cos\vartheta \begin{pmatrix} 0 \\ -\sin\vartheta\cos\vartheta \\ \sin^2\vartheta \end{pmatrix} = \sigma_0 \sin\vartheta\cos\vartheta \begin{pmatrix} 0 \\ -\cos\vartheta \\ \sin\vartheta \end{pmatrix} = \sigma_0 \sin\vartheta\cos\vartheta \cdot \vec{n}_{II}$$

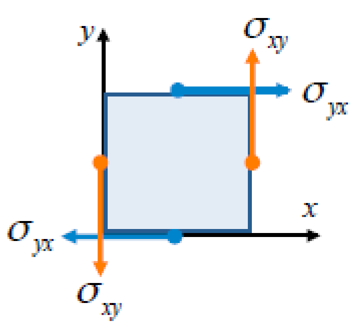
THE STRESS TENSOR

The situation in the previous exercise was:



Note that *both* the tensile and shear components are equal and opposite at the two sides

Symmetry of stress tensor, and vector representation



for couples to be ∅ (to avoid rotations), we **must** have

$$\sigma_{xy} = \sigma_{yx} \qquad \text{(true for all couples)}$$

$$\Rightarrow \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ & \sigma_{yy} & \sigma_{yz} \\ \text{symm.} & & \sigma_{zz} \end{pmatrix} \Rightarrow \begin{pmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ & \sigma_2 & \sigma_4 \\ & & \sigma_3 \end{pmatrix} \Rightarrow \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} \begin{matrix} \left.\right\} \text{Tensile} \\ \left.\right\} \text{Shear} \end{matrix}$$

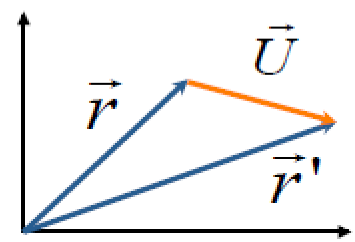
There are only 6 independent components of the stress tensor, **3⊥** and **3*//***.

THE STRAIN TENSOR

We start by defining a displacement vector caused by an elastic deformation. Each vector $\vec{r}$ is transformed by the deformation into a new vector $\vec{r}\,'$:

$$\vec{r} \rightarrow \vec{r}\,' = \vec{r} + \vec{U}(\vec{r})$$

$\vec{U}(\vec{r})$ → displacement vector, depends on $\vec{r}$



We next require that $\vec{U}(\vec{r})$ be **linear**: $\vec{U}(2\vec{r}) = 2\vec{U}(\vec{r})$

This is the same as writing:

$\vec{U} = \underline{\underline{\varepsilon}} \cdot \vec{r}$ where $\underline{\underline{\varepsilon}}$ is the 3x3 matrix defining **the Strain** tensor

$$\underline{\underline{\varepsilon}} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix}$$

Strain Matrix

THE STRAIN TENSOR

Meaning of the ε_{ij} **coefficients** (they are adimensional!)

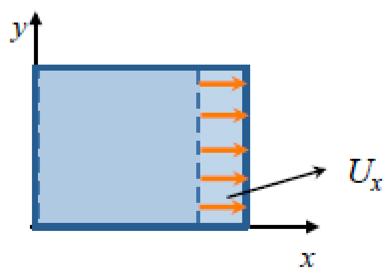
Let's have a look in 2D:

$$\begin{cases} U_x = \varepsilon_{xx} x + \varepsilon_{xy} y \\ U_y = \varepsilon_{yx} x + \varepsilon_{yy} y \end{cases} \Longleftrightarrow \vec{U} = \underline{\underline{\varepsilon}} \cdot \vec{r}$$

So we have, formally

$$\varepsilon_{xx} = \frac{\partial U_x}{\partial x}$$ Diagonal term

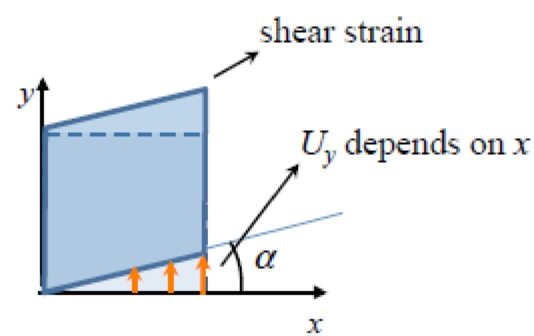
$$\varepsilon_{yx} = \frac{\partial U_y}{\partial x}$$ Off diagonal ("shear") term



$\frac{\partial U_x}{\partial x}$ ➡ Is the fractional elongation in the chosen direction

e.g. a deformation of 1 cm of a 1 m bar has:

$\frac{\partial U_x}{\partial x} = 0{,}01$ (everywhere, and it will add up to 2cm for a 2m bar)



The angle α is $\frac{\partial U_y}{\partial x}$ for small angles.

THE STRAIN TENSOR

We also have $\vec{r}\,' = (\underline{\underline{1}} + \underline{\underline{\varepsilon}})\ \vec{r}$ which we can write:

$$\vec{r}\,' = (\underline{\underline{1}} + \underline{\underline{\varepsilon}}_S + \underline{\underline{\varepsilon}}_A)\ \vec{r} \cong (\underline{\underline{1}} + \underline{\underline{\varepsilon}}_S)(\underline{\underline{1}} + \underline{\underline{\varepsilon}}_A)\ \vec{r}$$

$\cong$ for small strain values, such as ε = 0,01

$$\begin{cases} \underline{\underline{\varepsilon}}_S^{\ ij} = \dfrac{\varepsilon^{ij} + \varepsilon^{ji}}{2} & \text{Symmetric Matrix} \\ \underline{\underline{\varepsilon}}_A^{\ ij} = \dfrac{\varepsilon^{ij} - \varepsilon^{ji}}{2} & \text{Anti-symmetric Matrix} \end{cases}$$

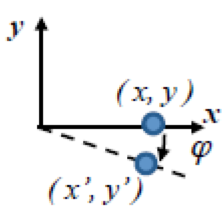
Q: But what is $(\underline{\underline{1}} + \underline{\underline{\varepsilon}}_A)$ **?** **A:** a *rotation*!

Example (in 2D):

$\begin{pmatrix} 1 & \phi \\ -\phi & 1 \end{pmatrix}$ with φ a small angle, can always be written, to 1st order, as $\begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix}$,

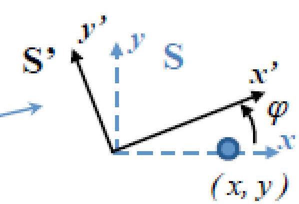
which is a rotation by φ in the *xy* plane. ⇒

$$x' = \cos\phi\ x + \sin\phi\ y$$
$$y' = -\sin\phi\ x + \cos\phi\ y$$



Master objects rotate clockwise,

or can be thought as a reference plane rotated anticlockwise.



THE STRAIN TENSOR

Now: rotations are irrelevant to elasticity (they're not, really, a "deformation").

So we will ignore $(\underline{\underline{1}} + \underline{\underline{\varepsilon}}_A)$ and use $\vec{r}\,' = (\underline{\underline{1}} + \underline{\underline{\varepsilon}}_S)\ \vec{r}$ as our only relevant deformation

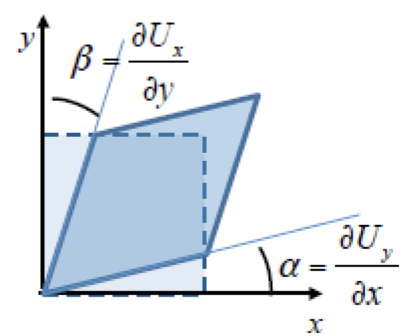
$$\underline{\underline{\varepsilon}} = \begin{pmatrix} \frac{\partial U_x}{\partial x} & \cdots & \cdots \\ \cdots & \frac{\partial U_y}{\partial y} & \varepsilon_{yz} \\ \cdots & \cdots & \frac{\partial U_z}{\partial z} \end{pmatrix} \qquad \varepsilon_{yz} = \frac{1}{2}\left(\frac{\partial U_y}{\partial z} + \frac{\partial U_z}{\partial y}\right)$$

This would seem to work, but the definition of the vector $\underline{\varepsilon} = \vec{\varepsilon}$ (6-D) is:

$$\underline{\varepsilon} = \begin{pmatrix} \frac{\partial U_x}{\partial x} \\ \frac{\partial U_y}{\partial y} \\ \frac{\partial U_z}{\partial z} \\ \left(\frac{\partial U_y}{\partial z} + \frac{\partial U_z}{\partial y}\right) \\ \left(\frac{\partial U_x}{\partial z} + \frac{\partial U_z}{\partial x}\right) \\ \left(\frac{\partial U_x}{\partial y} + \frac{\partial U_y}{\partial x}\right) \end{pmatrix}$$

$$\gamma = \beta + \alpha = \frac{\partial U_x}{\partial y} + \frac{\partial U_y}{\partial x}$$

There is no ½ !



.. Since we prefer to "read" from the vector the *total* angle of shear deformation

STRESS – STRAIN RELATIONS

Simple harmonic oscillator: $U = \frac{1}{2}kx^2$ $\quad \vec{F} = -\frac{\partial U}{\partial x} = -kx$

in some way $\underline{\sigma}$ is analogous to F

and $\underline{\varepsilon}$ is analogous to x

The correct expression is: $\boxed{\underline{\underline{\sigma}} = \underline{\underline{\underline{\underline{C}}}} \cdot \underline{\underline{\varepsilon}}}$ a full *tensor* relation

but in practice we use the vectors $\underline{\sigma}$, $\underline{\varepsilon}$: $\boxed{\underline{\sigma} = \underline{\underline{C}} \cdot \underline{\varepsilon}}$

where $\underline{\underline{C}}$ is a 6x6 matrix ⇒ "**Elastic Moduli**" or "**Stiffness Constants**"

Note: $[\,C_{ij}\,] = Pa$ ← They are pressures, dimensionally.

Of course, we can invert this relation to give $\boxed{\underline{\varepsilon} = \underline{\underline{S}} \cdot \underline{\sigma}}$

where $\underline{\underline{S}} = \underline{\underline{C}}^{-1}$ The "**Elastic Compliance**" 6x6 Matrix

..we next look at noteworthy derived modules, within the cubic symmetry

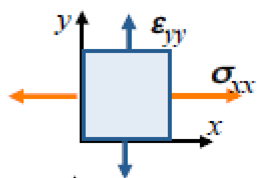
SYMMETRY OF $\underline{\underline{C}}$ IN A CUBIC CRYSTAL

We assume to have a cubic isotropic crystal:

from equations like $\sigma_1 = C_{11}\varepsilon_1 + C_{12}\varepsilon_2 + C_{13}\varepsilon_3 + C_{14}\varepsilon_4 + C_{15}\varepsilon_5 + C_{16}\varepsilon_6$

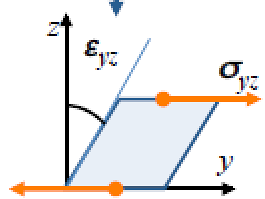
- $C_{11} = \dfrac{\partial \sigma_1}{\partial \varepsilon_1} = \dfrac{\partial \sigma_{xx}}{\partial \varepsilon_{xx}} = C_{22} = C_{33}$ since all axes are equivalent by symmetry
- also $\dfrac{\partial \sigma_1}{\partial \varepsilon_2} = C_{12} = \dfrac{\partial \sigma_{xx}}{\partial \varepsilon_{yy}}$

  $\therefore\ C_{12} = C_{13} = C_{23}$



is how much the stress on the x face along x direction depends on the yy strain.

- also $C_{44} = \dfrac{\partial \sigma_4}{\partial \varepsilon_4} = \dfrac{\partial \sigma_{yz}}{\partial \varepsilon_{yz}}$



and is the same for all axes couples:

$$C_{44} = C_{55} = C_{66}$$

$$\Rightarrow \underline{\underline{C}} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

Note: all other elements are 0 by symmetry!

For instance $C_{14} = \dfrac{\partial \sigma_1}{\partial \varepsilon_4} = \dfrac{\partial \sigma_{xx}}{\partial U_{yz}}$

Since opposite-sign shear strains in the yz plane must give opposite stress due to this linear relation, and same stress due to the mirror symmetry: the xx stress generated by yz shearing *must* be zero.

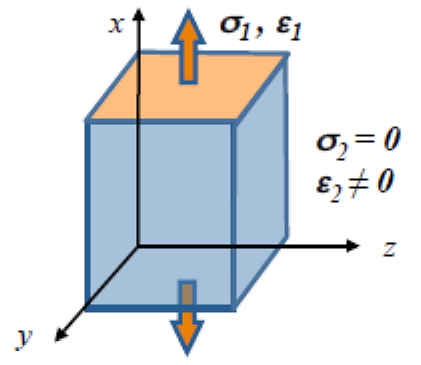
$$\frac{\partial \sigma_{xx}}{\partial -(U_{yz})} = -C_{14} = C_{14} = \text{(therefore) } \emptyset$$

ELASTIC MODULI

1) **Young's Module *E***

Normally written as $\sigma = E\varepsilon$, has the meaning:

the stress (tensile) vs. deformation (in the same direction).



$$\sigma_1 = C_{11}\varepsilon_1 + C_{12}\varepsilon_2 + C_{12}\varepsilon_3$$

$$\sigma_2 = C_{12}\varepsilon_1 + C_{11}\varepsilon_2 + C_{12}\varepsilon_3$$

Normally we have $\varepsilon_2 = \varepsilon_3 < 0$ if $\varepsilon_1, \sigma_1 > 0$.

By symmetry $\varepsilon_2 = \varepsilon_3$, and noting that $\sigma_2 = \sigma_3 = 0$,

actually we define: $\boxed{\nu = -\frac{\varepsilon_2}{\varepsilon_1}}$ **Poisson's Module** (This is not a pressure, just a number. So it's better to call it "**Poisson's Ratio**")

Limit of constant volume, defining a cube of edge "*a*", under uniaxial stress:

$$V = a^3 \qquad V' = (1+\varepsilon_1)a \cdot (1+\varepsilon_2)^2 a^2$$

$$V = V' \longrightarrow 1 = (1+\varepsilon_1)\cdot(1+2\varepsilon_2+\varepsilon_2{}^2) = 1+\varepsilon_1+2\varepsilon_2+O(\varepsilon^3)$$

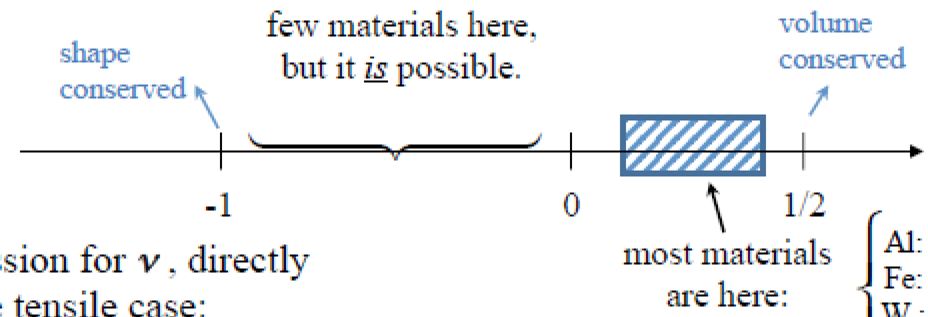
thus: $\nu = -\frac{\varepsilon_2}{\varepsilon_1} = \frac{1}{2}$ ← Poisson Ratio for constant volume

ELASTIC MODULI

Limit of constant shape

$$\varepsilon_2 = \varepsilon_1 \qquad \nu = -1$$

so, Poisson's Ratio ν :



Al: 0,345
Fe: 0,293
W : 0,280
a "stiffening" progression?

We can get another expression for ν, directly from the C_{ij}'s, for the pure tensile case:

$$\sigma_1 = C_{11}\varepsilon_1 + 2C_{12}\varepsilon_2$$

$$\sigma_2 = C_{12}\varepsilon_1 + (C_{11} + C_{12})\varepsilon_2 = 0 \Rightarrow \boxed{\nu = -\frac{\varepsilon_2}{\varepsilon_1} = \frac{C_{12}}{C_{11} + C_{12}}}$$

Poisson's Ratio

Let's go back to Young's Module. From the first equation:

$$\sigma_1 = (C_{11} - 2\nu C_{12})\varepsilon_1$$

$$\therefore \; E = C_{11} - 2\nu\, C_{12} = C_{11} - 2\frac{C_{12}}{C_{11} + C_{12}} \cdot C_{12} = \frac{C_{11}^2 + C_{11}C_{12} + 2C_{12}^2}{C_{11} + C_{12}}$$

$$\boxed{E = \frac{(C_{11} - C_{12})(C_{11} + 2C_{12})}{(C_{11} + C_{12})}}$$

Young's Module (as a function of the elastic moduli)

Al: 70,3
Fe: 211 GPa
W: 411

definitely stiffening up!

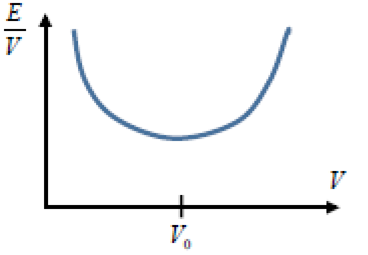
ELASTIC MODULI

2) Bulk Modulus *B*

Quite simply, the "spring" for volumic compression/expansion.

energy per unit volume under compression/expansion:
→ it's again a pressure!

$$\frac{E}{V} = \frac{1}{2}B\left(\frac{V - V_0}{V}\right)^2$$



➡ **B** is also a **pressure**.

For isotropic compression: $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = \varepsilon$; $\sigma_1 = \sigma_2 = \sigma_3 = \sigma$

$$\Rightarrow \begin{cases} \sigma_1 = (C_{11} + 2C_{12})\varepsilon_1 \\ \sigma_2 = (C_{11} + 2C_{12})\varepsilon_2 \\ \ldots\ldots \end{cases}$$

they are equal!

$$V \rightarrow V' = (1 + \varepsilon)^3 V_0 \rightarrow \Delta V = 3\varepsilon V_0 \rightarrow \left(\frac{\Delta V}{V}\right)^2 = 9\varepsilon^2$$

So the energy density is $\frac{E}{V} = \frac{9}{2}B\varepsilon^2$

ELASTIC MODULI

To relate this to the C_{ij}'s we need a general expression for the Elastic energy density:

Harmonic oscillator

$$U = \frac{1}{2}kx^2$$

$$\begin{pmatrix} \sigma = kx \\ \varepsilon = x \end{pmatrix}$$

⇒

Stress/strain

$$u = \frac{1}{2}\underline{\sigma} \cdot \underline{\varepsilon}$$

Most natural guess for the elastic energy density (it's correct, but we will have to prove it later)

For the Bulk Modulus we get:

$$u = \frac{1}{2}\sigma_1\varepsilon_1 + \sigma_2\varepsilon_2 + \sigma_3\varepsilon_3$$

∴ given the above...

$$= \frac{3}{2}(C_{11} + 2C_{12})\varepsilon^2$$

so:

$$\frac{9}{2}B\varepsilon^2 = \frac{3}{2}(C_{11} + 2C_{12})\varepsilon^2$$

⇒

$$\boxed{B = \frac{(C_{11} + 2C_{12})}{3}}$$

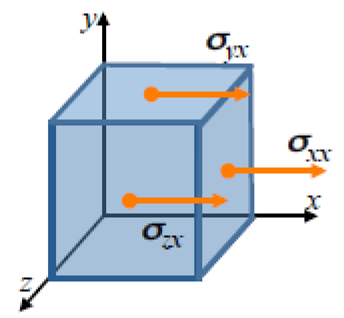
Bulk Modulus

(as a function of the elastic moduli C_{ij})

ELASTIC MODULI

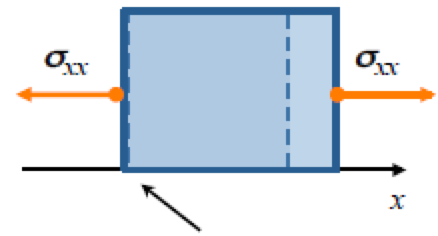
Let's now check the energy density expression: $u = \frac{1}{2}\underline{\sigma} \cdot \underline{\varepsilon}$

$\Delta L = \int \vec{F} \cdot \vec{U} dxdydz$ total work made by the forces which deform the cube (= by the applied stress)



For instance, the work associated with σ_{xx} becomes

$\sigma_{xx}\Delta y\Delta z \cdot$ (average length increase along x)



we can fix this point, so this quantity becomes $\frac{\partial U_x}{\partial x} \cdot \frac{\Delta x}{2}$

adding the other two contributions we have:

$$\Delta L = \sigma_{xx}\Delta y\Delta z \frac{1}{2}\frac{\partial U_x}{\partial x}\Delta x + \sigma_{yx}\Delta x\Delta z \frac{1}{2}\frac{\partial U_x}{\partial y}\Delta y + \sigma_{zx}\Delta x\Delta y \frac{1}{2}\frac{\partial U_x}{\partial z}\Delta z$$

$$\therefore \quad \frac{\Delta L}{\Delta V} = \frac{1}{2}\sigma_1\varepsilon_1 + \frac{1}{2}\sigma_4\frac{\partial U_x}{\partial y} + \frac{1}{2}\sigma_5\frac{\partial U_x}{\partial z}$$

adding similar expressions for the work associated with displacements along y and z we get:

$$\frac{\Delta L}{\Delta V} = \frac{1}{2}(\sigma_1\varepsilon_1 + \sigma_2\varepsilon_2 + \sigma_3\varepsilon_3) + \frac{1}{2}\sigma_4\left(\frac{\partial U_x}{\partial y} + \frac{\partial U_y}{\partial x}\right) + \ldots \quad = \frac{1}{2}\vec{\sigma} \cdot \vec{\varepsilon} \qquad \text{QED}$$

ELASTIC MODULI

<u>Exercise</u>: Elastic density in a cubic crystal

$$E = \frac{1}{2}\underline{\sigma}\cdot\underline{\varepsilon} = \frac{1}{2}\left(\sigma_1\varepsilon_1 + \sigma_2\varepsilon_2 + \sigma_3\varepsilon_3 + \sigma_4\varepsilon_4 + \sigma_5\varepsilon_5 + \sigma_6\varepsilon_6\right)$$

$$= \frac{1}{2}C_{ij}\sigma_i\varepsilon_j = \frac{1}{2}\begin{bmatrix} C_{11}\varepsilon_1{}^2 + C_{12}\varepsilon_1\varepsilon_2 + C_{12}\varepsilon_1\varepsilon_3 + \\ + C_{12}\varepsilon_1\varepsilon_2 + C_{11}\varepsilon_2{}^2 + C_{12}\varepsilon_2\varepsilon_3 + \\ + C_{12}\varepsilon_1\varepsilon_3 + C_{12}\varepsilon_2\varepsilon_3 + C_{11}\varepsilon_3{}^2 + \\ + C_{44}\left(\varepsilon_4{}^2 + \varepsilon_5{}^2 + \varepsilon_6{}^2\right) \end{bmatrix}$$

$$= \frac{1}{2}\left[C_{11}\left(\varepsilon_1{}^2 + \varepsilon_2{}^2 + \varepsilon_3{}^2\right) + 2C_{12}\left(\varepsilon_1\varepsilon_2 + \varepsilon_1\varepsilon_3 + \varepsilon_2\varepsilon_3\right) + C_{44}\left(\varepsilon_4{}^2 + \varepsilon_5{}^2 + \varepsilon_6{}^2\right)\right]$$

(a simple enough formula…)

For the Bulk Modulus: $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = \varepsilon$, $\varepsilon_4 = \varepsilon_5 = \varepsilon_6 = 0$ $\Rightarrow$ $E = \frac{3}{2}(C_{11} + 2C_{12})\varepsilon^2$

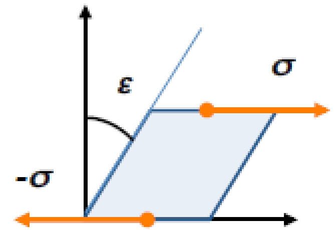
as already seen from a direct calculation

ELASTIC MODULI

3) Shear Modulus G

Quite simply, the stiffness under shear deformation.

$$\sigma = G\varepsilon \qquad \text{so:} \qquad G = C_{44}$$



Summary

$$\begin{cases} \nu = \dfrac{C_{12}}{C_{11}+C_{12}} \\ E = \dfrac{(C_{11}-C_{12})(C_{11}+2C_{12})}{(C_{11}+C_{12})} \\ B = \dfrac{(C_{11}+2C_{12})}{3} \\ G = C_{44} \end{cases}$$

We have 4 moduli from just 3 elastic constants, so they are not independent e.g., :

$$E = 3\cdot\frac{(C_{11}+2C_{12})}{3}\cdot\frac{(C_{11}+C_{12}-2C_{12})}{(C_{11}+C_{12})}$$

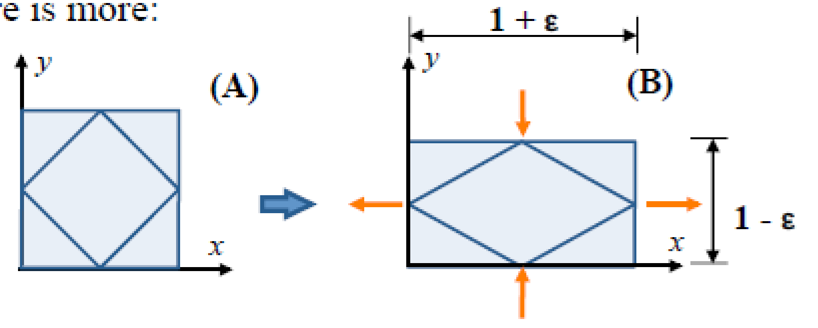
$$= 3\cdot\frac{(C_{11}+2C_{12})}{3}\cdot\left(1-2\frac{C_{12}}{(C_{11}+C_{12})}\right)$$

$$\Rightarrow \boxed{E = 3B(1-2\nu)}$$

ISOTROPIC SOLIDS

For isotropic solids there is more:

We deform this:



$\varepsilon_2 = -\varepsilon_1 = -\varepsilon$ *given* deformations along two dimensions

$\sigma_1 = (C_{11} - C_{12})\varepsilon_1$

$\sigma_2 = C_{12}\varepsilon_1 + C_{11}\varepsilon_2 = (C_{12} - C_{11})\varepsilon_1 = -\sigma_1$ the two stresses are also opposite

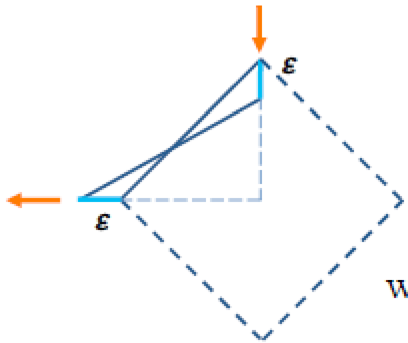
Clearly, the central square gets sheared (in isotropic solids the 45° rotation is irrelevant)

The energy density is $u = \frac{1}{2}C_{44}\varepsilon_{shear}^2$ while it is also $u = (C_{11} - C_{12})\varepsilon^2$

total shear angle

All we need is to calculate the shear angle in plot B in terms of the strain ε

ISOTROPIC SOLIDS



the angle goes from 45° to (45° - ϑ), i.e. goes *down* by a **small angle ϑ**.

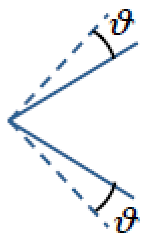
$$\tan\left(\frac{\pi}{4}-\vartheta\right)\cong\left(\frac{1-\varepsilon}{1+\varepsilon}\right)\cong\boxed{1-2\varepsilon}$$

where ε is the strain $|\varepsilon_1|=|\varepsilon_2|$ above.

while also:

$$\tan\left(\frac{\pi}{4}-\vartheta\right)\cong\tan\left(\frac{\pi}{4}\right)+\left.\frac{\partial\tan}{\partial\vartheta}\right|_{\vartheta=\pi/4}\cdot(-\vartheta)$$

$$=1+\left[1+\tan^2\left(\frac{\pi}{4}\right)\right]\cdot(-\vartheta)=\boxed{1-2\vartheta}$$



$$\Rightarrow\ 1-2\vartheta=1-2\varepsilon\ \Rightarrow\ \vartheta=\varepsilon$$

The total shear angle is, thus $\varepsilon_{shear}=2\vartheta=2\varepsilon$

Finally, equating we get $(C_{11}-C_{12})\varepsilon^2=\frac{1}{2}C_{44}4\varepsilon^2$ ⇒

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

True in **isotropic** solids

Sometimes an **anisotropy ratio** is defined to check the deviations from this rule in single crystals.

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

Anisotropy Ratio

Confronting the different anisotropy ratios in table 10.3:

- Al: 1,22
- Fe: 2,41
- W: 1,02

CALCULATION OF ELASTIC MODULI

We go back to our noteworthy modules:

$$E = \frac{(C_{11} - C_{12})(C_{11} + 2C_{12})}{(C_{11} + C_{12})} = 2G \cdot (1 + \nu)$$

we already knew that $E = 3B(1 - 2\nu)$

ISOTROPIC SOLIDS
=
there are only two independent constants: C_{11}, C_{12}

Example 1: (Table 10.2 - Aluminum)

$$B = \frac{E}{3(1 - 2\nu)} = \frac{70{,}3}{3(1 - 2 \cdot 0{,}345)} = 75{,}59\ GPa \qquad (\text{meas.}: 76{,}0)$$

$$G = \frac{E}{2(1 + \nu)} = \frac{70{,}3}{2(1 + 0{,}345)} = 26{,}133\ GPa \qquad (\text{meas.}: 26{,}1)$$

In practice, by accurate tensile load σ, ε_1, ε_2 are known. This gives ν and E $\longrightarrow$ B,G $\longrightarrow$ all C's.

Example 2: (Crystal Table 10.3 - Aluminum)

$C_{11} = 107$

$C_{12} = 61$

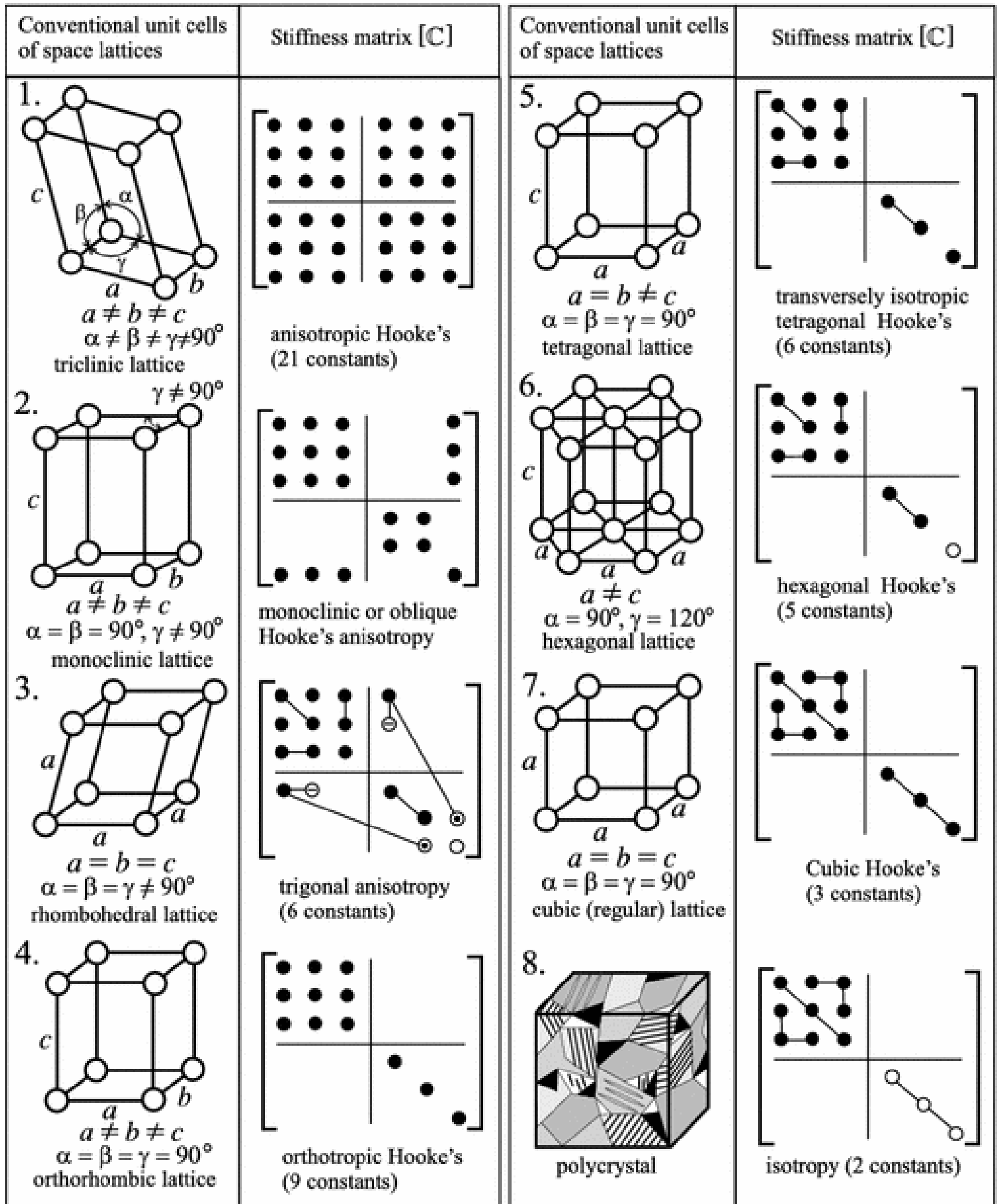
$\Rightarrow$

$$\nu = \frac{C_{12}}{C_{11} + C_{12}} = \frac{61}{168} = 0.363 \qquad (\text{meas.}: 0.345)$$

$$E = \frac{(C_{11} - C_{12})(C_{11} + 2C_{12})}{(C_{11} + C_{12})} = \frac{(107 - 61)(107 + 122)}{168} = 62{,}7\ GPa \qquad (\text{meas.}: 70{,}3)$$

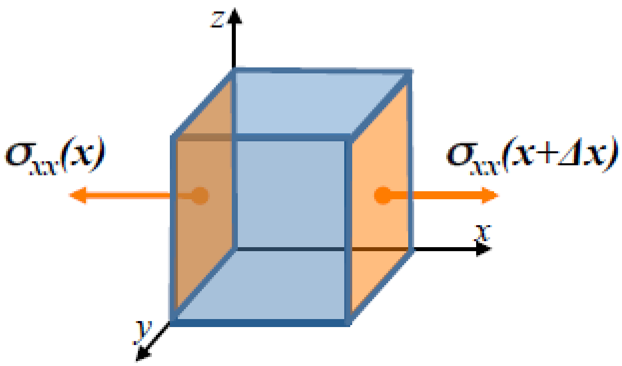
$$B = \frac{C_{11} + 2C_{12}}{3} = \frac{107 + 122}{3} = 76{,}3\ GPa \qquad (\text{meas.}: 76{,}0)$$

Symmetry of Stiffneess Matrixes for the Crystalline Systems



ELASTIC WAVES

A very simple theory of elastic waves:



The little cube will now **move**, as it is not in equilibrium: the stress values $\boldsymbol{\sigma}_{xx}$ at the two ends of the cube do *not* cancel out

We next construct the $F = M \cdot a$ equation

$$F = \left[\sigma_{xx}(x+\Delta x) - \sigma_{xx}(x)\right] \cdot \Delta y \Delta z$$ → net force along x

$$Ma = \frac{\partial \sigma_{xx}}{\partial x} \Delta x \Delta y \Delta z$$

(we suppose there is just a compressive wave, no shear, no ε_2) ⇨ $\sigma_1 = C_{11} \cdot \varepsilon_1$

$$M \frac{\partial^2 U_x}{\partial t^2} = \frac{\partial}{\partial x}(C_{11}\varepsilon_{xx}) \cdot Volume \Longrightarrow \rho \frac{\partial^2 U_x}{\partial t^2} = C_{11} \frac{\partial}{\partial x} \frac{\partial U_x}{\partial x}$$

⇨ $$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{\left(\frac{C_{11}}{\rho}\right)} \frac{\partial^2}{\partial t^2} \right) U_x(x,t) = 0$$

The wave equation for a simple compressive (longitudinal) wave

ELASTIC WAVES

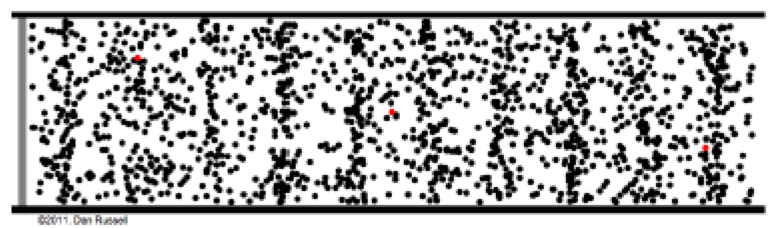
Note: if we allow for a complete treatment, the full equation is

$$\rho \frac{\partial^2 U_x}{\partial t^2} = C_{11} \frac{\partial^2 U_x}{\partial x^2} + C_{44}\left(\frac{\partial^2 U_x}{\partial y^2} + \frac{\partial^2 U_x}{\partial z^2} \right) + \left(C_{12} + C_{44}\right)\left(\frac{\partial^2 U_y}{\partial x \partial y} + \frac{\partial^2 U_z}{\partial x \partial z} \right) + $$

similar terms for the y and z components

For example in pure shear mode, for a purely transversal y-polarised wave propagating along the x axis, the equation is:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{\left(\frac{C_{44}}{\rho}\right)} \frac{\partial^2}{\partial t^2} \right) U_y(y,t) = 0$$

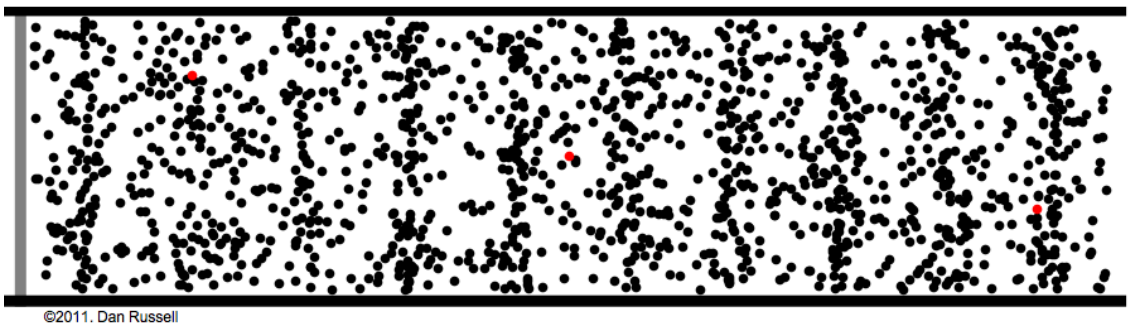


An estimate for the *speed of sound*:

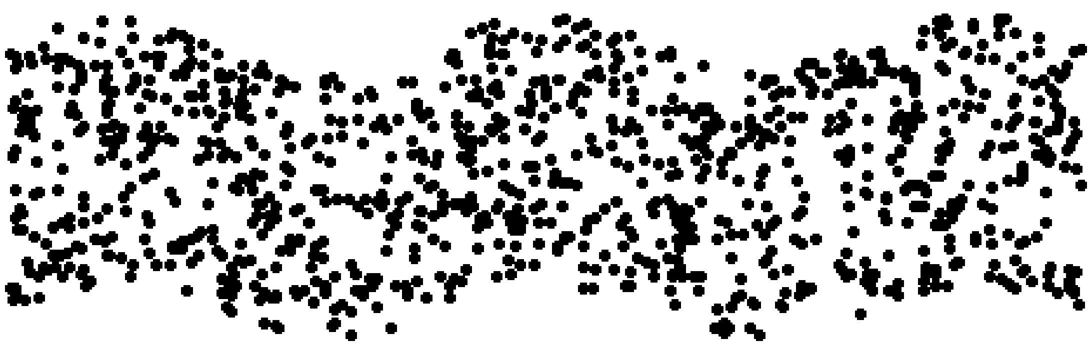
$$c = \sqrt{\frac{C_{11}}{\rho}} \cong \sqrt{\frac{200\ GPa}{10\ tons/m^3}} = \sqrt{\frac{200\times 10^9}{10^4}} \cong 4\times 10^3\ m/\sec$$

↖ typical numbers for a metal

Bulk Acoustic Waves – BAW

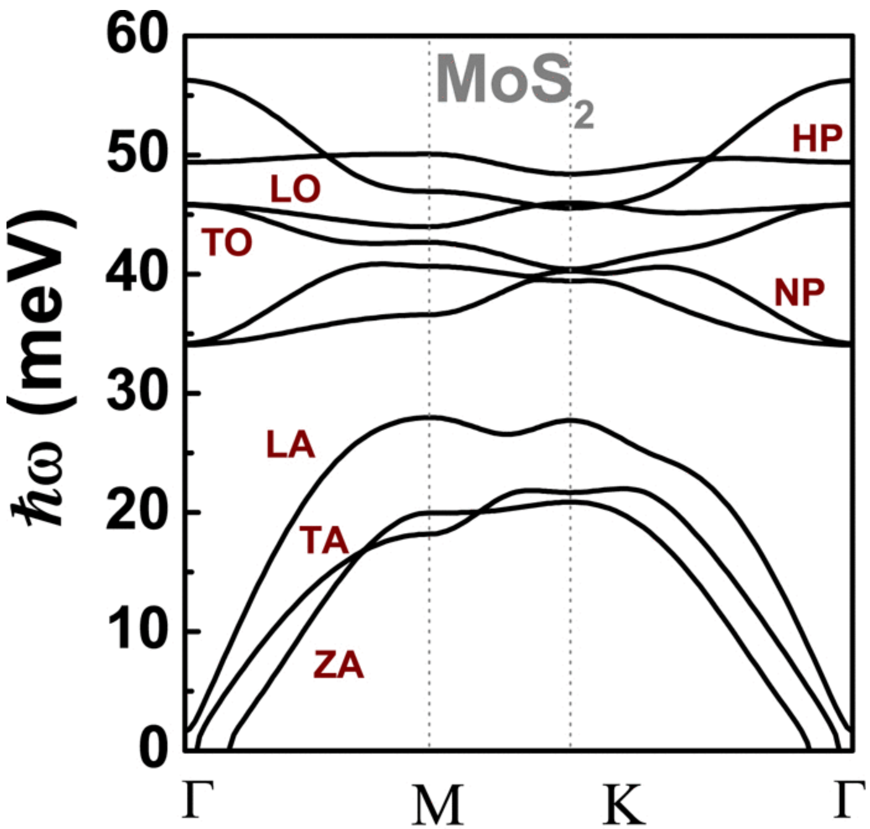


Longitudinal



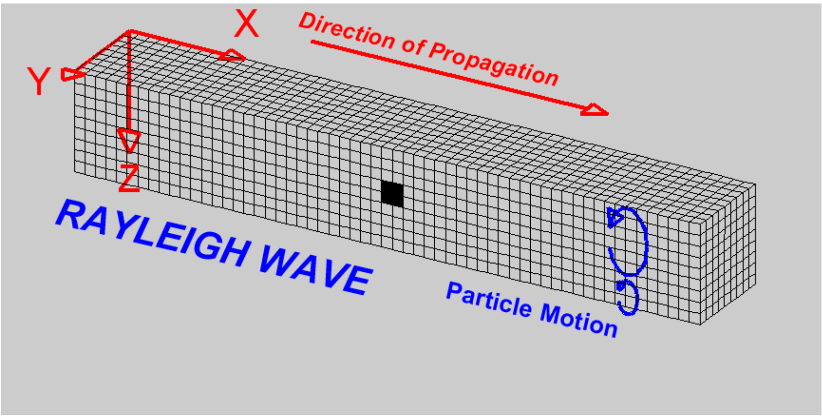
Transversal

Transversal and Longitudinal Phonons

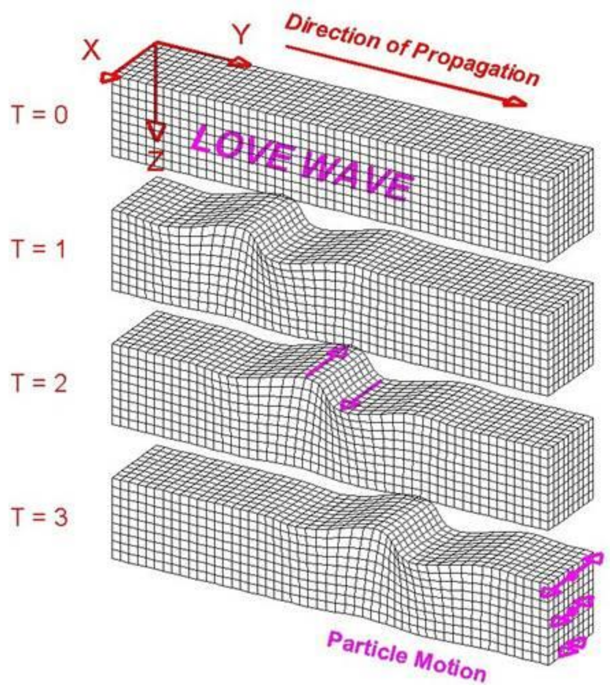


Surface Acoustic Waves – SAW

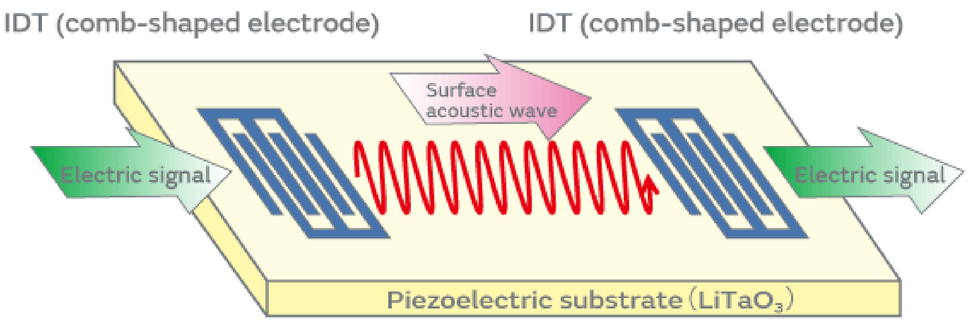
Rayleigh Waves



Love Waves

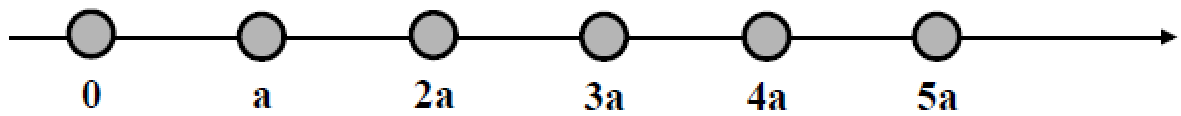


Application: SAW signal filters



1D PHONONS

We now want to investigate vibrations in solids, using a 1D model:



Atomic position are at $x_j = j \cdot a$ and we will define a displacement U_j :

$x_j \rightarrow x_j' = x_j + U_j$ as we did when defining the displacement vector field

Q: What is the elastic energy in this "solid"?

$$\mathrm{E} = \frac{1}{2}\sum_n \left(\frac{1}{2}K\left(U_n - U_{n-1}\right)^2 + \frac{1}{2}K\left(U_n - U_{n+1}\right)^2 \right)$$

where the force on a particular atom $\bar{j}$ is $-\frac{\partial \mathrm{E}}{\partial U_{\bar{j}}} = -K\left(U_{\bar{j}} - U_{\bar{j}-1}\right) - K\left(U_{\bar{j}} - U_{\bar{j}+1}\right)$

We now guess an the solution in wave form: $U_j \quad \forall j$

$$U_j = U_0 e^{i(kx_j - \omega t)}$$

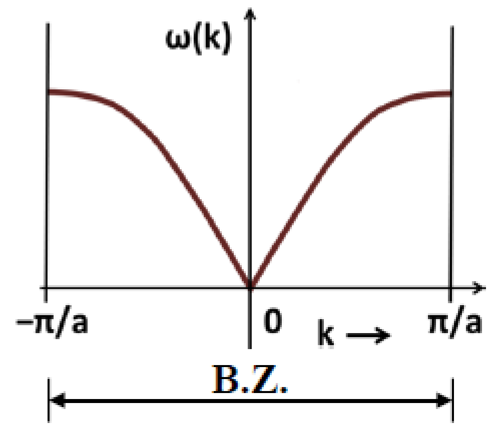
where $k \in B.Z.$ of the crystal, since $k \rightarrow k' = k + G$ must give the same results

1D PHONONS

$F = m \cdot a$ then becomes

$$+M\omega^2 U_0 = +K\left(2U_j - U_{j+1} - U_{j-1}\right)$$
$$= KU_0\left[2 - 2\frac{\left(e^{ika} + e^{-ika}\right)}{2}\right]$$
$$= 2KU_0\left[1 - \cos(ka)\right] = 4KU_0 sin^2\left(\frac{ka}{2}\right)$$

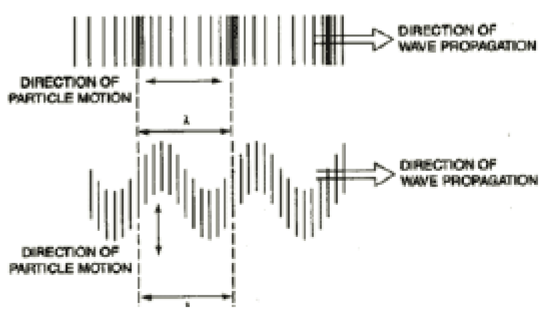
$$\therefore\ \omega^2 = \left(\frac{4K}{M}\right)\cdot sin^2\left(\frac{ka}{2}\right) \Rightarrow \boxed{\omega(k) = 2\sqrt{\frac{K}{M}}\cdot\left|sin\left(\frac{ka}{2}\right)\right|}$$



This gives the *ω(k) dispersion relation* for these particular "sound" waves.
Note that we have just postulated the energy function, but we have NOT specified if these are compressive waves i.e.,

longitudinally polarized:

or **transverse waves**:



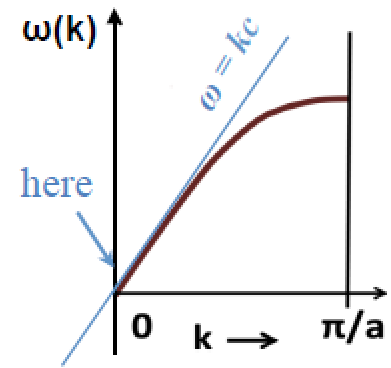
here *Uj* is orthogonal to $\vec{k} \,//\, \hat{x}$

1D PHONONS

Coming back to the formula $\omega(k) = 2\sqrt{\frac{K}{M}} \cdot \left| sin\left(\frac{ka}{2}\right)\right|$, there are two limits:

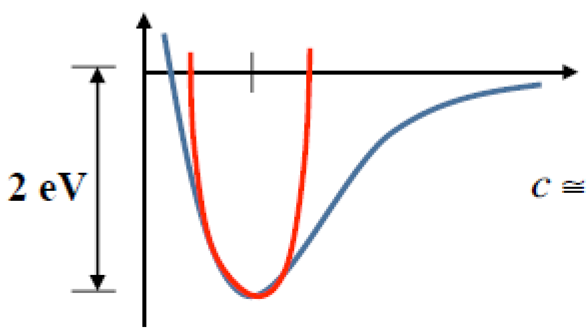
Elastic (or "acoustic") limit: $k \to 0 \quad \lambda \to \infty (k = 2\pi/\lambda)$

$$\omega(k) \approx 2\sqrt{\frac{K}{M}} \cdot \frac{ka}{2} = \sqrt{\frac{K}{M}}a \cdot k \longrightarrow \sqrt{\frac{K}{M}}a = c \text{ (speed of sound)}$$



Thus, the speed of sound can be obtained from the "springs", the distances, and the masses of the atoms

To estimate c in a solid, we start from a chemical bond, supposing 2 eV are gained along the approximating parabola in ~ 1Å



$$\frac{1}{2}K(1\,\mathring{A})^2 = 2\ eV \to K = 4\ eV/\mathring{A}^2 \text{ ; in silicon } \begin{cases} a:\ 2.34\ \mathring{A} \\ M:\ 28 \end{cases}$$

$$c \cong \sqrt{\frac{4 \cdot 1{,}6 \times 10^{-19}}{10^{-20} \cdot 28 \times 10^{-27}}} \cdot 2 \times 10^{-10} = \sqrt{\frac{16 \cdot 1{,}6}{28} 10^{8}} \cong \sqrt{10^{8}} = 10^{4}$$

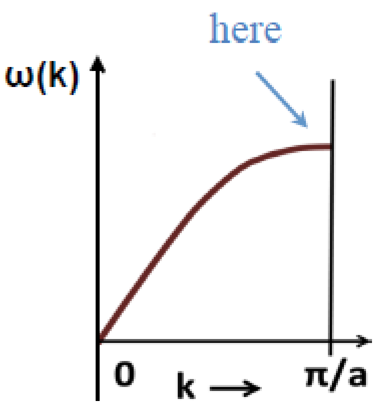
..expect anything between 1000 and 10000 m/sec

Silicon	8.400 m/sec
Diamond	12.000 m/sec
Aluminum	6.420 m/sec
Iron	5.130 m/sec

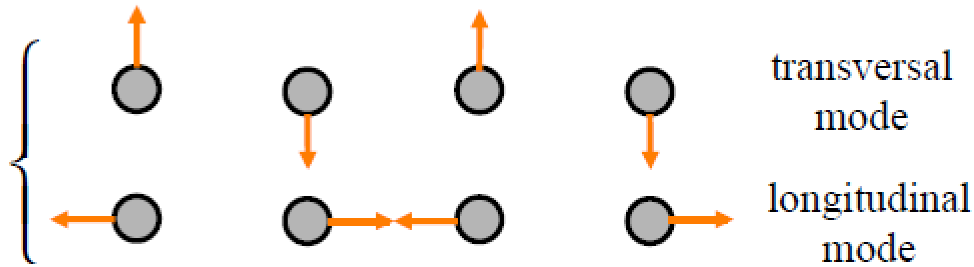
Silicon ⟶ $\lambda\nu = 8400$ m/sec for $\begin{cases} \nu = 8{,}4 \text{ kHz} \\ \lambda = 1 \text{ m} \end{cases}$

1D PHONONS

Optical limit: $k \to \pi/a$ (at the BZ boundary)



$$\omega = 2\sqrt{\frac{K}{M}} \cdot (1)$$



that is, nearest neighbour atoms are in anti-phase:

$$U_j = U_0 e^{i\left(\frac{\pi}{a}x_j\right)}$$ but $e^{i\pi} = -1$ ⇨ the phase gained for a "***a***" displacement is π

Typical frequencies = ? if we use the former estimate's numbers:

$$\omega = 2\sqrt{\frac{K}{M}} = 2\sqrt{\frac{4 \cdot 1{,}6 \times 10^{-19}}{10^{-20} \cdot 28 \times 10^{-27}}} \cong 2\sqrt{2 \cdot 10^{27}} \cong 10^{14} = 100THz$$

typical phononic frequency

⇨ $$\hbar\omega = 10^{-34} \cdot 10^{14} = 10^{-20}\,J$$

~0.1 eV ⟶ **infrared** light frequencies!!

SPEED OF SOUND, REPRISED

We now have ***c*** from two theories:

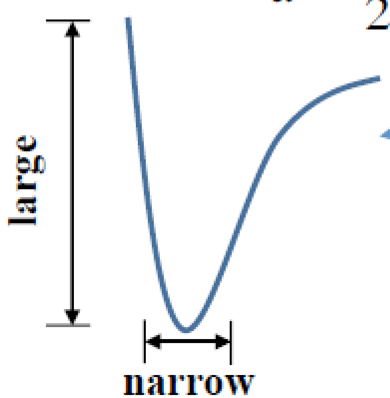
classical elastic theory: $\sqrt{\dfrac{C_{11}}{\rho}}$ atomistic theory: $\sqrt{\dfrac{K}{M}a^2}$

Clearly, the elastic constant derives from the stiffness of the chemical bond

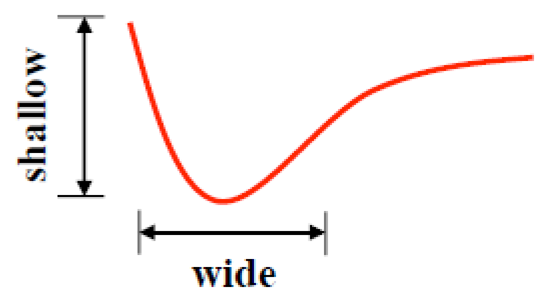
$$c = \sqrt{\left(\frac{K}{a}\right)\frac{a^3}{M}} = \sqrt{\frac{(K/a)}{\rho}} \quad \text{so} \quad C_{11} \approx \frac{K}{a}$$

In our estimate $K \cong 4 \; eV/\overset{\circ}{A}^2; \qquad a \cong 2\overset{\circ}{A}$

$$\text{so} \quad C_{11} \approx \frac{K}{a} = \frac{4eV}{2\overset{\circ}{A}^3} = \frac{2 \cdot 1{,}6 \times 10^{-19}}{10^{-30}} Pa = 3.2 \times 10^{11} Pa = 320 \; GPa$$



This will clearly correspond to a much higher speed of sound than this,



…and for a given bond strength lighter atoms → faster sound

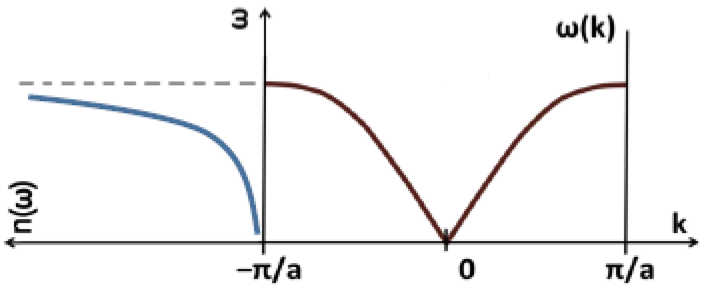
3D PHONONS

Q: What happens to phonons in the full 3D case? theref

A: $\forall \vec{k} \in \mathrm{BZ}$ there will be an acceptable **wave** = vibrational (phononic) mode

conceptually it's all as before, there will be a **phonon spectrum** $\omega(\vec{k}) \quad \vec{k} \in \mathrm{BZ}$

and a density of states ***n(ω)*** "counting" all the vibrational modes



n(ω) carries the information on how many "phonon modes" there are for any given interval of frequency (per unit volume of sample).

Note on density of states ***n(ω)***:
since $\vec{k} \in \mathrm{BZ}$, for a side ***L*** sample

$\left\{ \begin{array}{l} L = N \cdot a \text{ in a} \\ \text{1m 1D crystal} \\ N \sim 10^{10}\text{ ; a = 1Å} \end{array} \right.$

$\Rightarrow \quad k \cdot L = m \cdot 2\pi$; with $m = 0, \ \pm 1; \ \pm 2; \ \cdots$

We in fact have only N possible values of k: $\quad k_m = \frac{2\pi}{L} m \ ; \quad m = 0, \ \pm 1; \ \pm 2; \ \cdots \ \pm N/2$

so the "density" of states in the 1D BZ is $\quad \frac{dk}{dn} = \frac{2\pi}{L} \qquad \frac{dn}{d\omega} = \left(\frac{dn}{dk}\right)\left(\frac{dk}{d\omega}\right) = \frac{L}{2\pi} \frac{1}{(d\omega/dk)}$

1D density of states singular for zero group velocity…

3D case: $\left\{ \begin{array}{l} \text{in a sample of volume } L^3\text{, in a BZ} \\ (d^3k) \text{ there will be } \frac{L^3}{(2\pi)^3} d^3k \text{ waves.} \end{array} \right.$

$$dn = \frac{d^3k}{(2\pi)^3}$$

3D density of vibrational modes per unit volume of BZ and unit volume of specimen