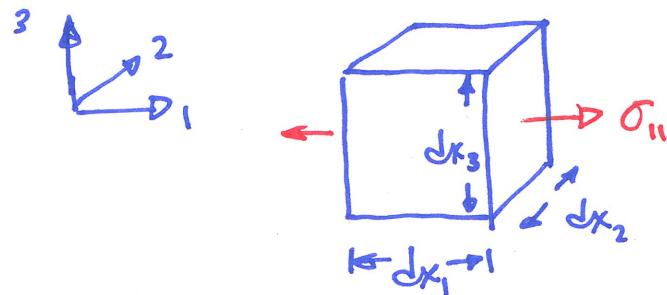


Atomistic basis for linear elasticity

Consider a cubic element:



dU = change in internal energy

dW = work done on material by σ_{11}

dq = heat absorbed by the material

$$dU = dW + dq$$

$$dW = \sigma_{11} dx_2 dx_3 dE_{11} dx_1$$

$$= \sigma_{11} dE_{11} V \text{ (assume } \sigma = \text{constant over volume } V)$$

$$dq = TdS \text{ (reversible process)}$$

T = temperature

dS = change in entropy

$$dU = V\sigma dE + TdS$$

- crystalline materials +
 - amorphous materials $T < T_g$
- $\left. \begin{array}{l} \frac{dS}{dE} \\ \text{small} \end{array} \right\}$

- rubber $\Rightarrow \frac{dS}{dE}$ significant

$$\sigma = \frac{1}{V} \frac{dU}{dE} - \frac{T}{V} \frac{dS}{dE}$$

Crystalline materials + amorphous materials ($T < T_g$)

Consider internal energy per atom or molecule, of atomic volume Ω

$$\sigma = \frac{1}{\Omega} \frac{du}{de}$$

u = internal potential energy

- have energy - separation curve $u(r)$

$$E = \frac{d\sigma}{de} = \frac{1}{\Omega} \frac{d^2u}{de^2}$$

- for a pair of atoms with central forces (act along line between center of atoms)

$$u(r) = -\frac{A}{r^m} + \frac{B}{r^n}$$

attractive term

(e.g. ionic crystals - electrostatic attraction)

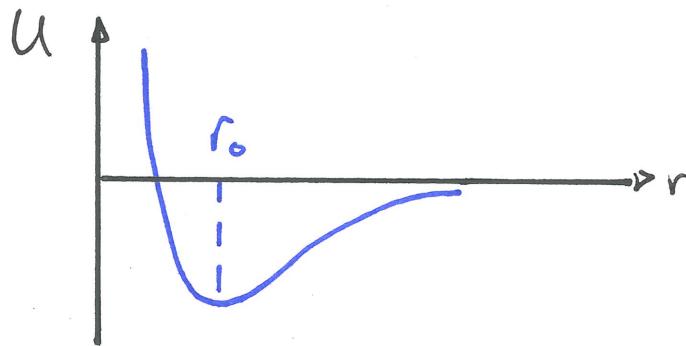
ionic crystals $m=1$

covalent; metals $m \sim 4-6$

repulsive term

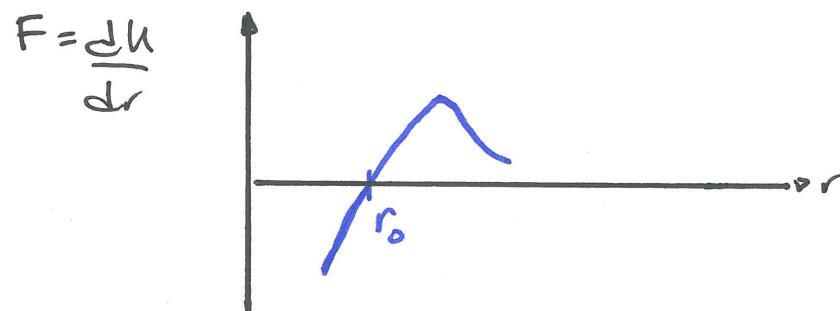
(atoms pressed close, electron shells overlap)

$n \sim 9-12$

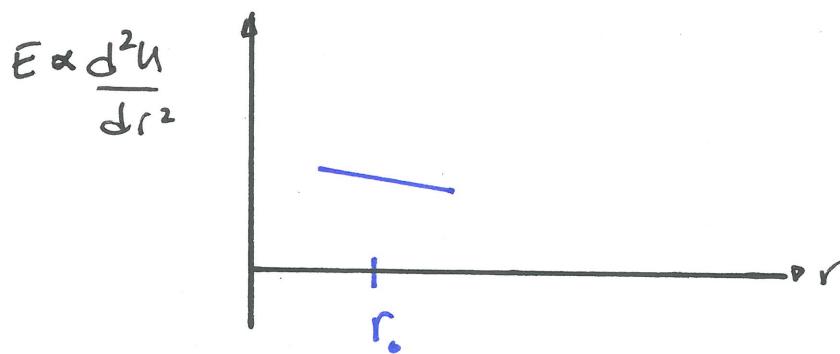


r_0 = equilibrium spacing

$$\epsilon = \frac{r - r_0}{r_0} = \frac{r}{r_0} - 1$$



F vs. r linear for small displacements about r_0
 \Rightarrow Hooke's Law



E decreases as r increases

- as heat material, it expands, $r_0 \uparrow$
- as heat, E decreases

$$E = \frac{d\sigma}{d\varepsilon} \Big|_{\varepsilon=0}$$

$$d\sigma = \frac{dF}{r^2}$$

$$\frac{d\sigma}{dr} = \frac{1}{r_0^2} \frac{dF}{dr}$$

$$\frac{dE}{dr} = \frac{1}{r_0}$$

$$E = \frac{d\sigma}{dr} \cdot \frac{dr}{d\varepsilon} \Big|_{\varepsilon=0} = \frac{1}{r_0} \frac{dF}{dr} \Big|_{r=r_0} = \frac{1}{r_0} \frac{d^2U}{dr^2} \Big|_{r=r_0}$$

- can find $\frac{d^2U}{dr^2} \Big|_{r=r_0}$ from energy - separation curve

- taking second derivative, can show:

$$E = \frac{A m (n-m)}{r_0^{m+3}}$$

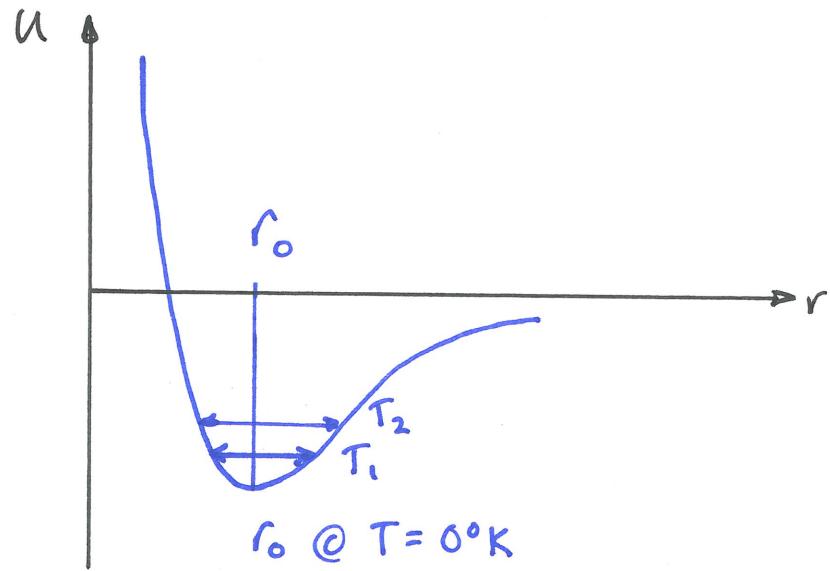
derivation m:

Meyers, M + Chawla, K (2009)

Mechanical Behaviors of Materials

Cambridge University Press.

Coefficient of thermal expansion



- at $T = 0^\circ\text{K}$, equilibrium spacing, r_0
- as T increases, atoms oscillate & move up potential well (since they have thermal energy)
- potential is asymmetric
- mean interatomic spacing shifts to right
- thermal expansion coefficient, α
- α related to shape of energy-separation curve

Thermal strain

- as heat materials, they expand
- α = coefficient of thermal expansion [$^\circ\text{K}^{-1}$]
- ΔT = change in temperature

$$\epsilon_T = \alpha \Delta T$$

- for isotropic material, uniform expansion in all directions

$$\epsilon_x = \epsilon_y = \epsilon_z = \alpha \Delta T$$

no shear strain from thermal expansion:

$$\gamma_{xz} = \gamma_{yz} = \gamma_{xy} = 0$$

Typical values of α

polymers: $50 - 500 \times 10^{-6} \text{ } ^\circ\text{K}^{-1}$ eg. PS $100 \times 10^{-6} \text{ } ^\circ\text{K}^{-1}$

metals: $5 - 50 \times 10^{-6} \text{ } ^\circ\text{K}^{-1}$ eg. Cu $16 \times 10^{-6} \text{ } ^\circ\text{K}^{-1}$

ceramics: $1 - 10 \times 10^{-6} \text{ } ^\circ\text{K}^{-1}$ eg. SiC $4.3 \times 10^{-2} \text{ } ^\circ\text{K}^{-1}$

glasses: $1 - 2 \times 10^{-6} \text{ } ^\circ\text{K}^{-1}$

Concrete: $14.5 \times 10^{-6} \text{ } ^\circ\text{K}^{-1}$

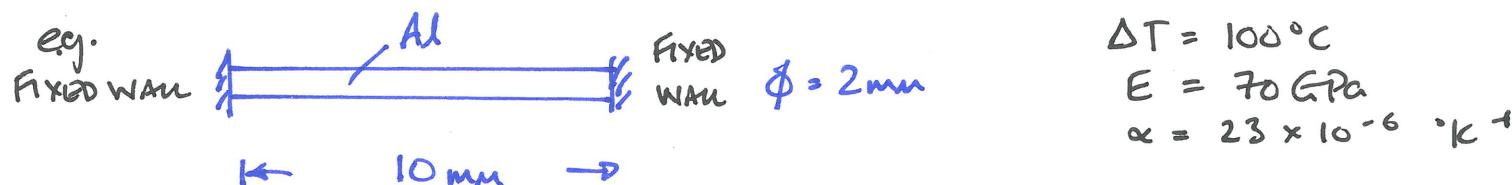
steel : $13 \times 10^{-6} \text{ } ^\circ\text{K}^{-1}$

Small difference means low stresses from ΔT
in reinforced concrete

bimetal bar: difference in α gives bending of the bar.

Thermal strain + stresses

- thermal strain can lead to stresses, if material is constrained



- If rod was free (not fixed at walls), it would have a thermal strain of:

$$\epsilon_T = \alpha \Delta T = 23 \times 10^{-6} (\text{ } ^\circ\text{K}^{-1}) \times (100 \text{ } ^\circ\text{K}) = 0.0023$$

- rigid walls don't move - push back on bar

$$\sigma = E \epsilon_T = (70 \text{ GPa}) (0.0023) = 161 \text{ MPa} \text{ in rod}$$

(note $\sigma_y = 276 \text{ MPa}$ for Al 6061 alloy)

- =
- in materials processing - heating materials with more than one component, then cooling, can induce residual stresses associated with different α of different materials
 - layered materials - thin films on substrates - different α in different layers generates thermal stresses under ΔT
-

Moduli of rubbers

- polymers at temperatures above T_g are rubbers
- at $T < T_g$, structure is of random carbon chains, covalently bonded along the chain; may have covalent + van der Waals bonds between chains
- at T_g van der Waals bonds melt; usually covalent cross-links are infrequent
(if no covalent cross-links, polymer becomes a liquid at T_g)
- segments of the polymer chain between x-links are free to move

- if load rubber in tension/compression/shear, the chains slide over one another & the structure becomes more ordered

e.g. tension



(tangled wool analogy)

- structure straightens out + becomes more aligned, less random
- entropy decreases
- move chains relative to one another, but don't stretch C-C bonds along chain

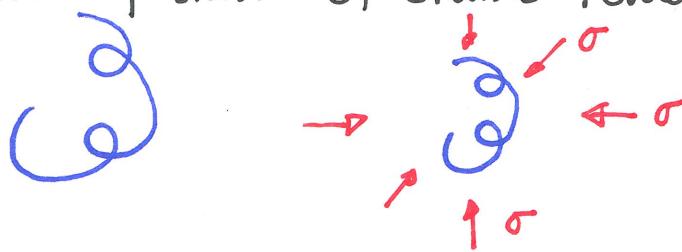
- last time: $E = \frac{1}{2} \frac{d^2 U}{d \epsilon^2} - \frac{T}{2} \frac{d^2 S}{d \epsilon^2}$

↓ ↓
 bond stretching term change in entropy term

- change in entropy term \gg bond stretching term.

$$E = -\frac{T}{2} \frac{d^2 S}{d \epsilon^2}$$

- in contrast, if rubber loaded hydrostatically ($\sigma_x = \sigma_y = \sigma_z = \sigma$)
the entire structure contracts uniformly without changing its configuration
- relative position of chains remains unchanged



- little change in entropy
- Instead, strain C-C bonds along chain

- bulk modulus $K = \sigma / \Delta V / V_0$, volumetric strain $\Delta V / V_0 = \Delta$
- for bulk modulus, bond stretching term \gg change in entropy term

$$K = \frac{1}{2} \frac{d^2 U}{d \Delta^2} \quad \Rightarrow K \gg E$$

- Note also, for isotropic materials (rubbers are isotropic)

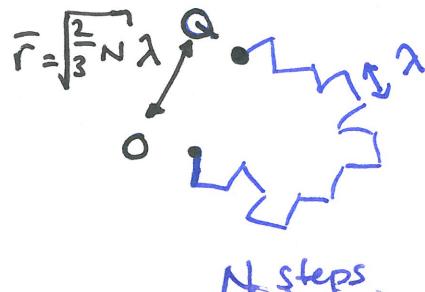
$$\nu = \frac{1}{2} - \frac{1}{6} \frac{E}{K} \quad \text{since } K \gg E \quad \nu \rightarrow \frac{1}{2} \quad (\text{but always } < \frac{1}{2})$$

Rubbers: Calculation of Young's moduli

$$E = -\frac{1}{2} \frac{d^2 S}{d \epsilon^2}$$

- need to calculate change in entropy with strain
- consider structure of rubbers: random chains

- portion of 1 chain between cross-links at O and Q



- each step one c-c bond, of length λ
- N C-C bonds between cross-links
- Chain builds up randomly
- F = most likely distance $O \rightarrow Q = \sqrt{\frac{2}{3} N} \lambda$

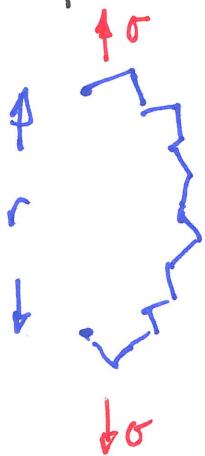
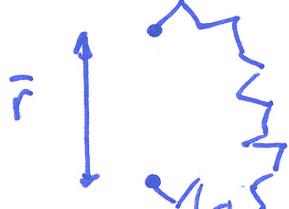
- Model structure as a random walk process
- entropy $S = k \ln \Omega'$
 - k = Boltzmann's constant
 - Ω' = no. of configurations
- random walk theory states that if one end of the chain is at the origin, O, the probability that the other end of the chain, Q, is a distance r from the origin is:

$$P = A \exp(-r^2/\bar{r}^2)$$

- $P \propto \Omega' \Rightarrow$ the more configurations, the higher the probability that the end Q is at r

$$\begin{aligned}\therefore S &= k \ln P \\ &= k \ln A - k \left(\frac{r}{\bar{r}}\right)^2 \\ &= C - k \left(\frac{r}{\bar{r}}\right)^2\end{aligned}$$

- If strain the chain, so that the end moves to r



$$\epsilon = \frac{r - \bar{r}}{\bar{r}} = \frac{r}{\bar{r}} - 1$$

$$\frac{d\epsilon}{dr} = \frac{1}{\bar{r}}$$

$$\frac{dS}{dr} = -\frac{2kr}{\bar{r}^2}$$

$$E = -\frac{T}{2} \frac{d^2S}{d\epsilon^2} = \frac{2kT}{N\lambda^3} \leftarrow \text{volume of 1 chain}$$

- If n_v = no chains per unit volume = $1/N\lambda^3$

$$\frac{d^2S}{dr^2} = -\frac{2k}{\bar{r}^2}$$

$$E = 2n_v kT \quad \text{exact calculation: } E = 3n_v kT$$

$$\frac{1}{r^2} \frac{d^2S}{d\epsilon^2} = -\frac{2k}{\bar{r}^2}$$

$$\therefore \frac{d^2S}{d\epsilon^2} = -2k$$

- approximations:

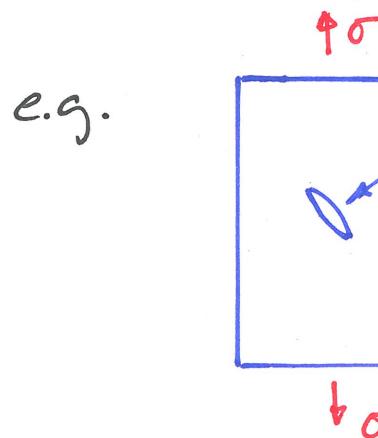
- single chain, not network
- 3D calculation of strain not accounted for.

Notes:

- ① E increases with no. chains/volume, n_v
i.e. with degree of cross-linking
- ② E increases with temperature, T
 - tendency of chain to go back to random configuration increases as thermal energy of rubber increases
- ③ nonlinear elastic behavior can be analyzed by considering large def^{in.}.
find slope of σ - ϵ curve increases with strain; as straighten C-C chains, stiffness increases

Stress transformations

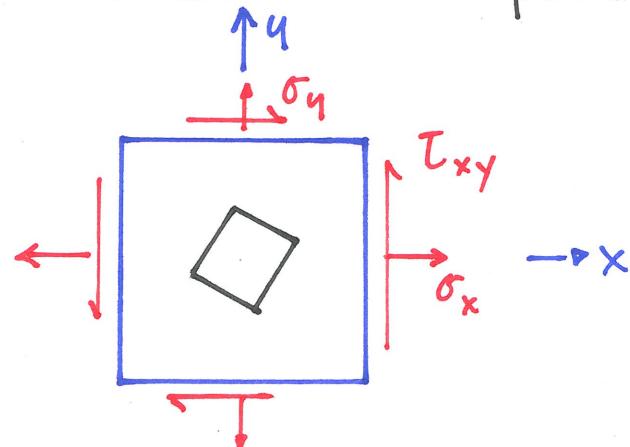
- sometimes want to find stress state at orientation different from applied stress



Crack:
normal, shear
stresses on crack
face = ?

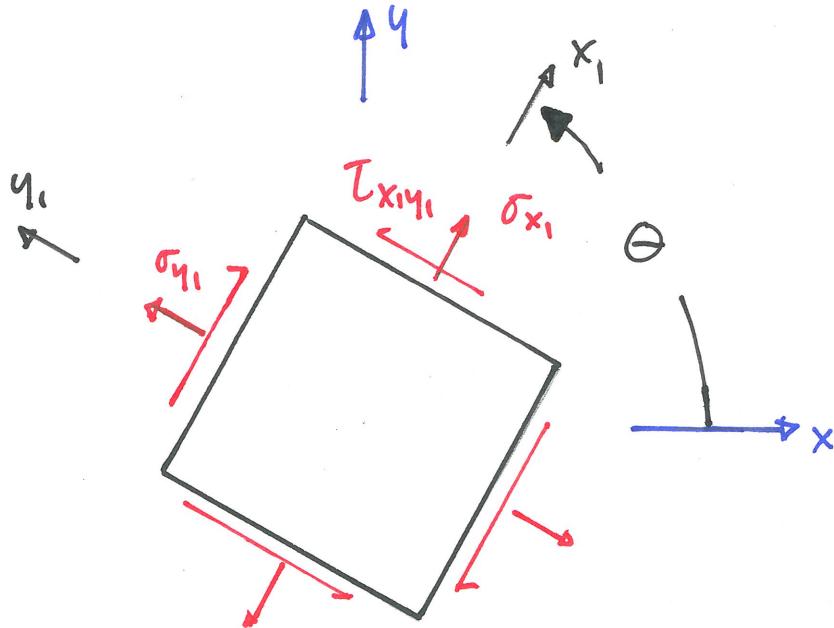
- stresses vary with orientation
at the crack

- in general, consider element in plane stress
- all stresses in one plane; usually take to be x-y plane $\sigma_z = 0$ $\sigma_{xz} = 0$ $\sigma_{yz} = 0$



what is equivalent stress state
on rotated element?

(shear stress often τ_{xy})



② positive counter clockwise (ccw)

define x_1, y_1 axes rotated by θ ccw
with respect to xy axes.

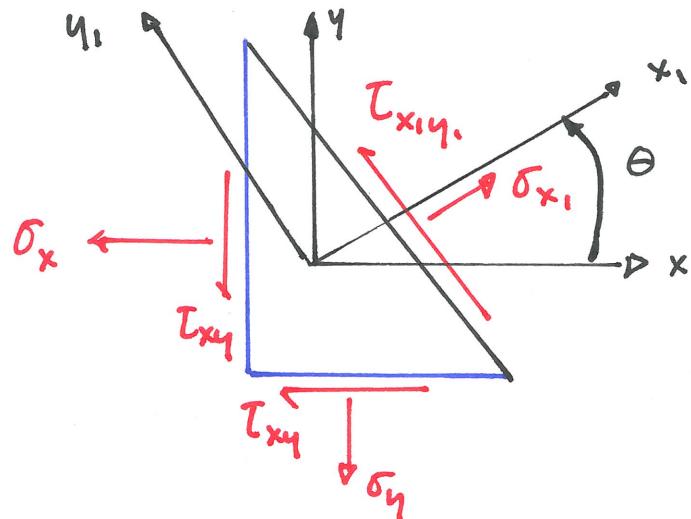
$$\sigma_{x_1} = f_1(\sigma_x, \sigma_y, \tau_{xy}, \theta)$$

$$\sigma_{y_1} = f_2(\sigma_x, \sigma_y, \tau_{xy}, \theta)$$

$$\tau_{x_1 y_1} = f_3(\sigma_x, \sigma_y, \tau_{xy}, \theta)$$

- ① want to find these relationships
- ② want to find maximum normal stress] "principal stresses"
- ③ " " " minimum " "] "principal stresses"
- ④ " " " maximum shear stress

- Consider static equilibrium of a wedge:



$$\text{AREA OF LEFT FACE} = A_0$$

$$\text{AREA OF BOTTOM FACE} = A_0 \tan \theta$$

$$\text{AREA OF INCLINED FACE} = \frac{A_0}{\cos \theta}$$

$$\sum F_x = 0$$

$$\sum F_y = 0$$

Algebra, Trig identities see Geret Goodno p 592-93

$$\sigma_{x_1} = \frac{\sigma_x + \sigma_y}{2} + \left(\frac{\sigma_x - \sigma_y}{2} \right) \cos 2\theta + \tau_{xy} \sin 2\theta$$

$$\tau_{x_1y_1} = - \left(\frac{\sigma_x - \sigma_y}{2} \right) \sin 2\theta + \tau_{xy} \cos 2\theta$$

σ_{y_1} obtained from eq'n for σ_{x_1} with $\theta = \Theta + 90^\circ$

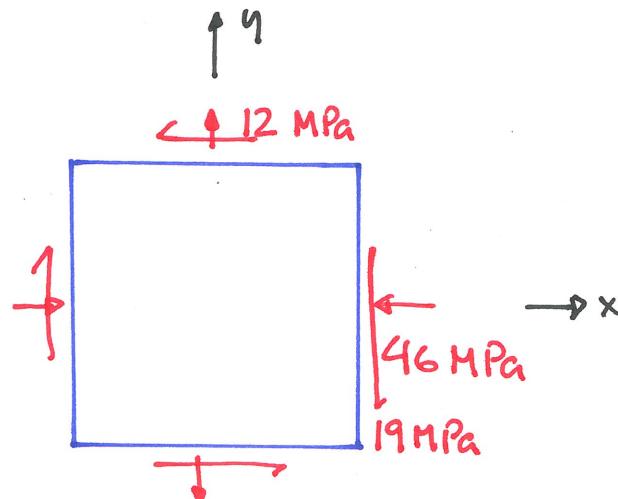
$$\sigma_{y_1} = \left(\frac{\sigma_x + \sigma_y}{2} \right) - \left(\frac{\sigma_x - \sigma_y}{2} \right) \cos 2\theta - \tau_{xy} \sin 2\theta$$

Note also: $\sigma_{x_1} + \sigma_{y_1} = \sigma_x + \sigma_y$

- sum of normal stresses acting on two \perp faces of an element in plane stress is constant, independent of θ

Example:

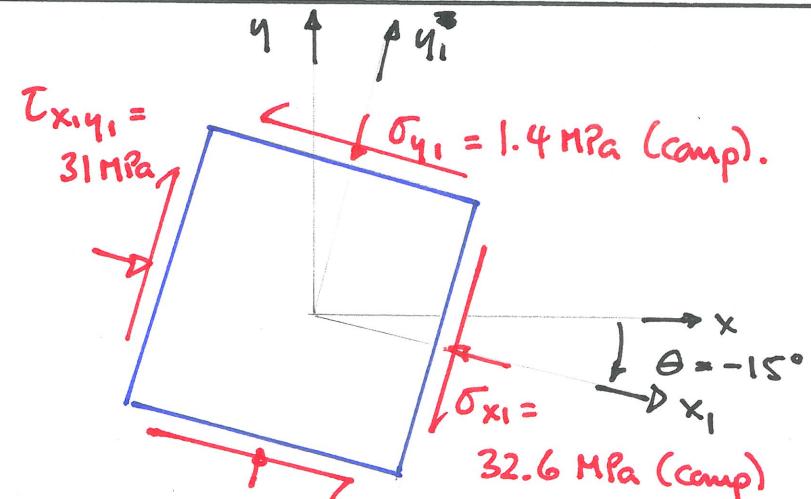
- element sees stress state shown below
- calculate stress state on element rotated 15° cw
- sketch stresses on rotated element.



$$\sigma_x = -46 \text{ MPa}$$

$$\sigma_y = 12 \text{ MPa}$$

$$\tau_{xy} = -19 \text{ MPa}$$



$$\sigma_{x_1} = -32.6 \text{ MPa}$$

$$\sigma_{y_1} = -1.4 \text{ MPa}$$

$$\tau_{x_1 y_1} = -31.0 \text{ MPa}$$