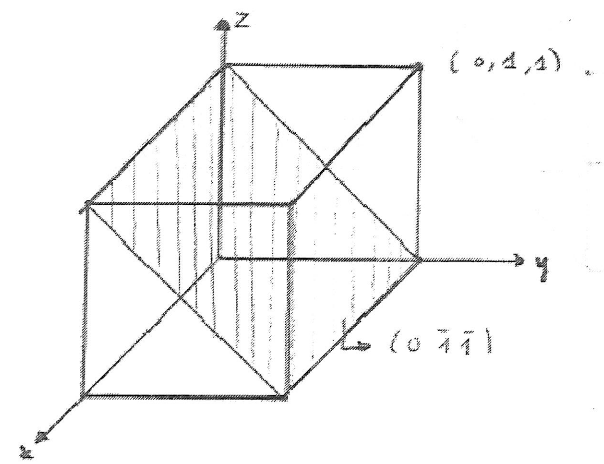
1.38. Sketch the following planes within the unit cell. Draw one cell for each solution. Show new origin and ALL necessary calculations.

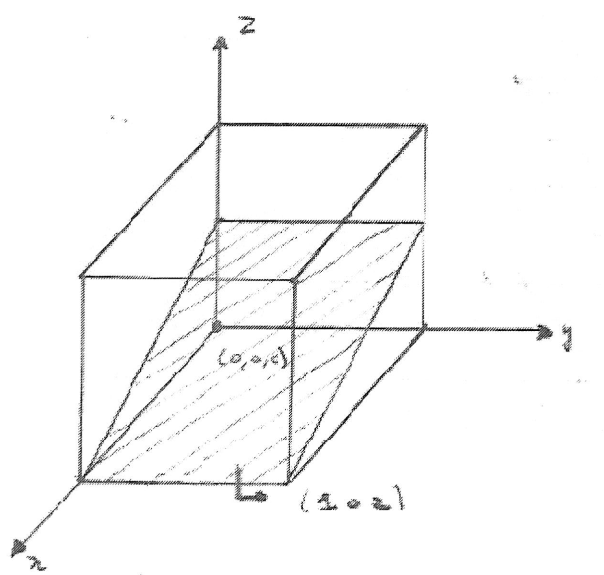
(a) $(0\bar{1}\bar{1})$,

$\Rightarrow$ intersections $\left(\infty, \frac{1}{-1}, \frac{1}{-1}\right)$, origin $(0, 1, 1)$



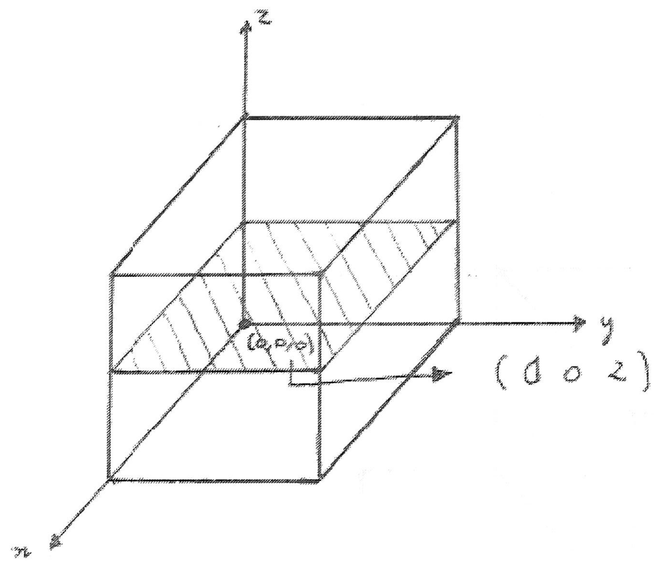
(b) (102),

$\Rightarrow$ intersections : $\left(\frac{1}{1}, \infty, \frac{1}{2}\right)$ origin $(0,0,0)$



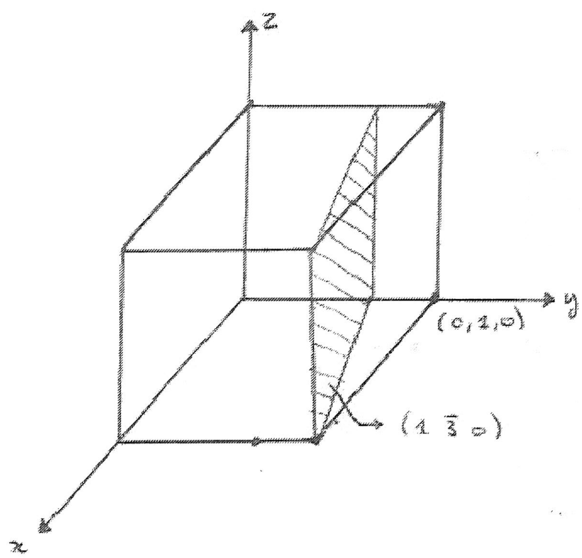
(c) (002),

$\Rightarrow$ intersections $(\infty, \infty, \frac{1}{2})$ origin $(0,0,0)$



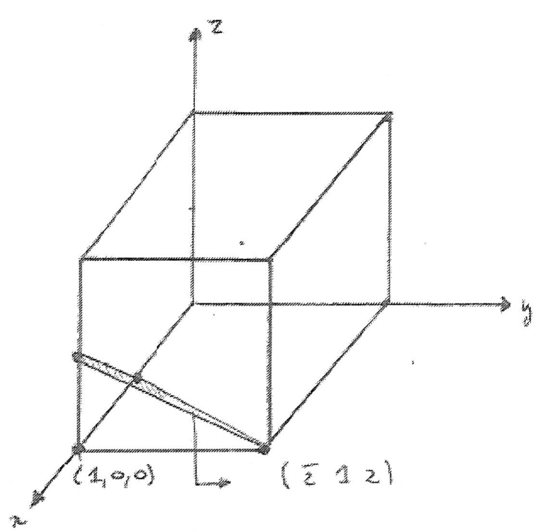
(d) $(1\bar{3}0)$,

⇒ intersections $(1, -\frac{1}{3}, \infty)$ origin $(0,1,0)$



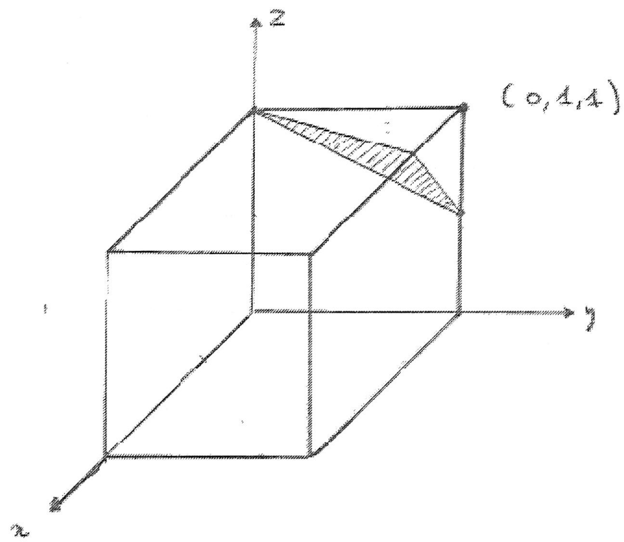
(e) $(\bar{2}12)$,

⇒ intersections $(-\frac{1}{2}, 1, \frac{1}{2})$ origen $(1,0,0)$



(f) $(3\overline{1}\overline{2})$

⇒ intersections $\left(\frac{1}{3}, -\frac{1}{1}, -\frac{1}{2}\right)$ origin $(0,1,1)$



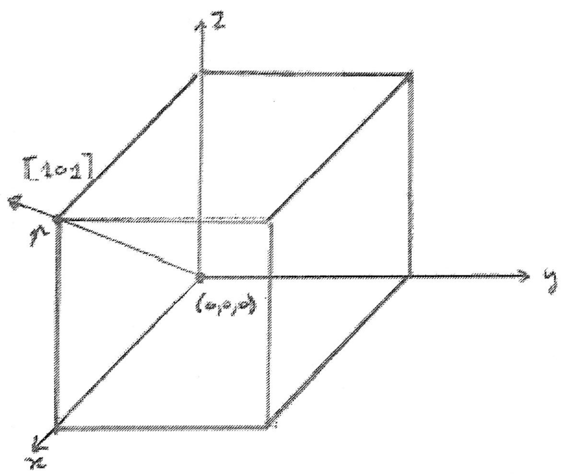
1.39. Sketch the following directions within the unit cell. Draw one cell for each solution. Show new origin and ALL necessary calculations.

a) $[1\,0\,1] \Rightarrow \bar{v} = \bar{i} + \bar{k}$

origin $(0,0,0)$ point $p(x,y,z)$

$$\Rightarrow \bar{v} = (x-0)\bar{i} + (y-0)\bar{j} + (z-0)\bar{k} = \bar{i} + \bar{k}$$

$$\Rightarrow \begin{cases} x = 1 \\ y = 0 \\ z = 1 \end{cases}$$

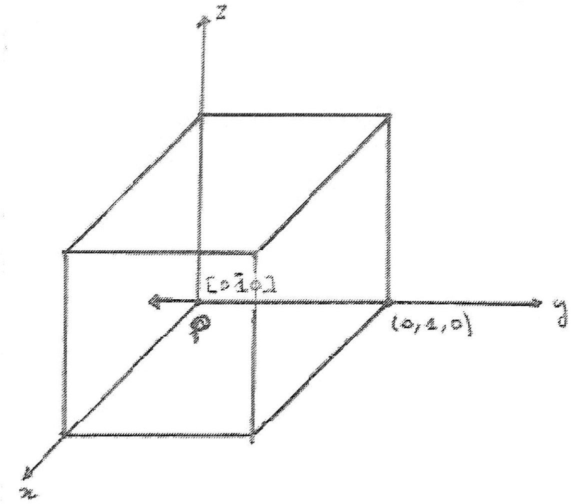


b) $[0\,\bar{1}\,0] \Rightarrow \bar{v} = -\bar{j}$

origin $(0,1,0)$ point $p(x,y,z)$

$$\Rightarrow \bar{v} = (x-0)\bar{i} + (y-1)\bar{j} + (z-0)\bar{k} = -\bar{j}$$

$$\Rightarrow \begin{cases} x = 0 \\ y = 0 \\ z = 0 \end{cases}$$



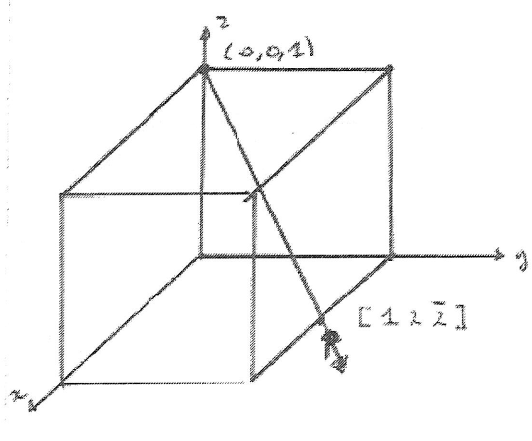
a) $[1\ 2\ \bar{2}]$

$$2\bar{v} = \bar{i} + 2\bar{j} - 2\bar{k}$$
$$\bar{v} = \frac{1}{2}\bar{i} + \bar{j} - \bar{k}$$

origin $(0,0,1)$ point $p(x,y,z)$

$$\Rightarrow \bar{v} = (x-0)\bar{i} + (y-0)\bar{j} + (z-1)\bar{k} = \frac{1}{2}\bar{i} + \bar{j} - \bar{k}$$

$$\Rightarrow \begin{cases} x = \frac{1}{2} \\ y = 1 \\ z = 0 \end{cases}$$



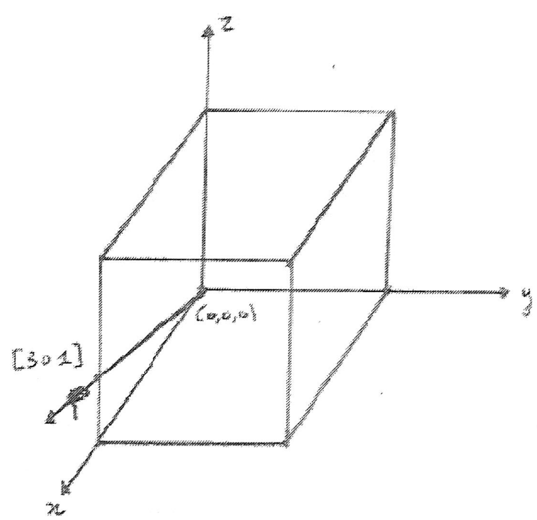
b) [3 0 1]

$$3\bar{v} = 3\bar{i} + \bar{k}$$
$$\bar{v} = \bar{i} + \frac{1}{3}\bar{k}$$

origin $(0,0,0)$ point $p(x,y,z)$

$$\Rightarrow \bar{v} = (x-0)\bar{i} + (y-0)\bar{j} + (z-0)\bar{k} = \bar{i} + \frac{1}{3}\bar{k}$$

$$\Rightarrow \begin{cases} x = 1 \\ y = 0 \\ z = \frac{1}{3} \end{cases}$$



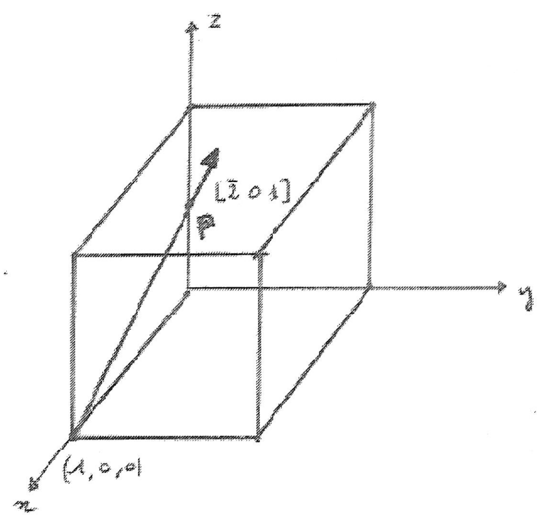
c) [$\bar{2}$ 0 1]

$$2\bar{v} = -2\bar{i} + \bar{k}$$
$$\bar{v} = -\bar{i} + \frac{1}{2}\bar{k}$$

origin $(1,0,0)$ point $p(x,y,z)$

$\Rightarrow \bar{v} = (x-1)\,\bar{i} + (y-0)\,\bar{j} + (z-0)\,\bar{k} = -\bar{i} + \frac{1}{2}\bar{k}$

$$\Rightarrow \begin{cases} x = 0 \\ y = 0 \\ z = \frac{1}{2} \end{cases}$$



d) [2 $\bar{1}$ 3]

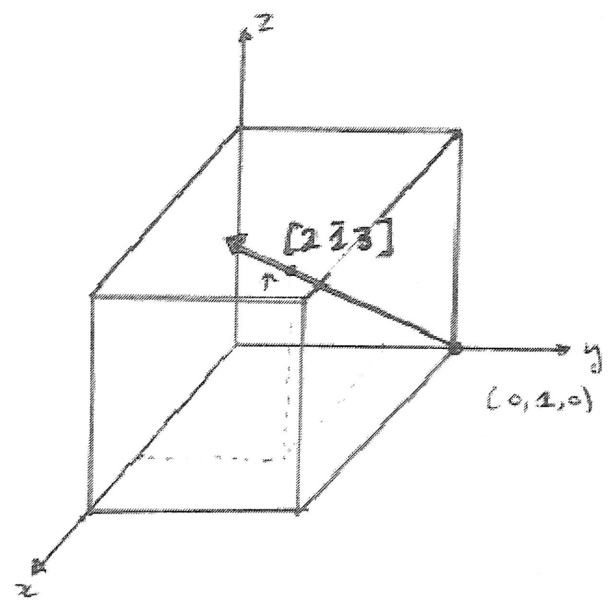
$3\bar{v} = 2\bar{i} - \bar{j} + 3\bar{k}$

$\bar{v} = \frac{2}{3}\bar{i} - \frac{1}{3}\bar{j} + \bar{k}$

origin (0, 1, 0) point ↑ (x, y, z)

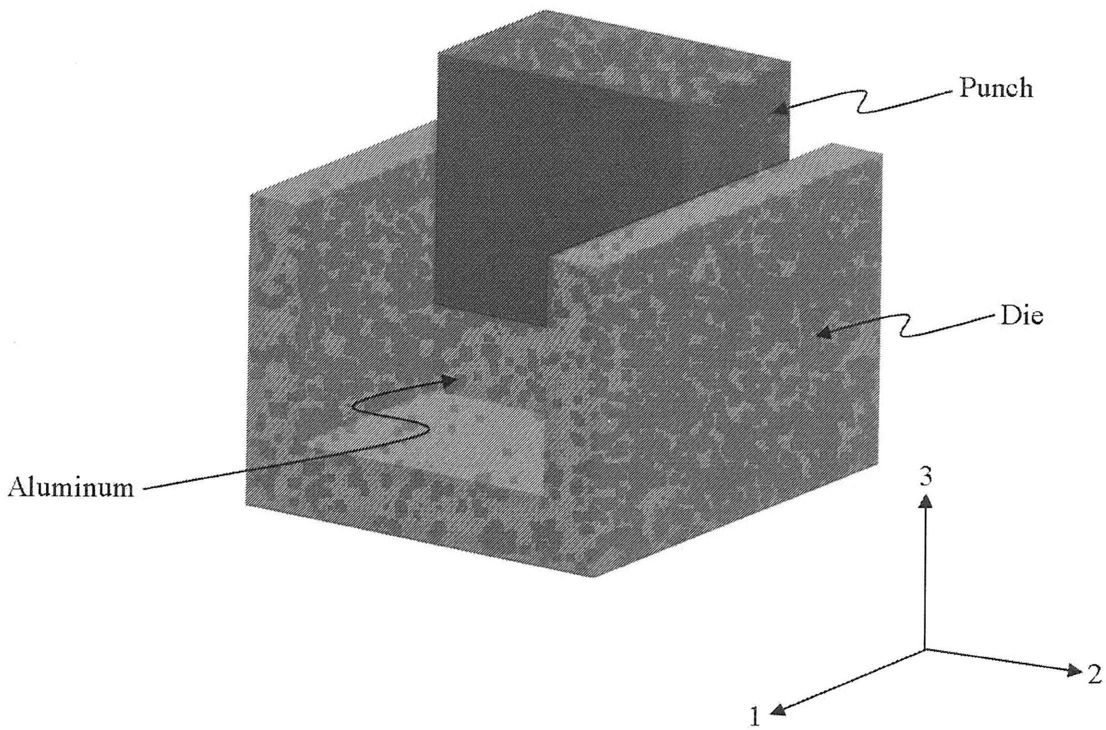
$\Rightarrow \bar{v} = (x-0)\,\bar{i} + (y-1)\,\bar{j} + (z-0)\,\bar{k} = \frac{2}{3}\bar{i} - \frac{1}{3}\bar{j} + \bar{k}$

$$\Rightarrow \begin{cases} x = \frac{2}{3} \\ y = \frac{2}{3} \\ z = 1 \end{cases}$$


z
[2 $\bar{1}$ 3]
r
y
(0,1,0)
x

2.2 An aluminum polycrystalline specimen is being elastically compressed in plane strain. If the true strain along the compression direction is -2×10^{-4}, what are the other two longitudinal strains?

The figure below shows the conditions of the test.



Strains

$\varepsilon_{22} = 0$ (rigid die wall provides the constraint)

$$\varepsilon_{33} = -2\ x\ 10^{-4}\ (given)$$

$$\varepsilon_{11} = ?$$

Stresses

$\sigma_{11} = 0$ because the material is free to flow in direction 1

$$\sigma_{22}, \sigma_{33} \neq 0$$

Hooke's Law

$$\varepsilon_{11} = \frac{1}{E}\left[0 - \nu\left(\sigma_{22} + \sigma_{33}\right)\right]$$

$$\varepsilon_{22} = 0 = \frac{1}{E}\left[\sigma_{22} - \nu\sigma_{33}\right]$$

$$\varepsilon_{33} = -2\,x\,10^{-4} = \frac{1}{E}\left[\sigma_{33} - \nu\sigma_{12}\right]$$

$$\varepsilon_{22} = \frac{1}{E}\left[\sigma_{22} - \nu\sigma_{33}\right] = 0$$

$$\therefore \sigma_{22} = \nu\sigma_{33}$$

$$\varepsilon_{33} = \frac{1}{E}\left[\sigma_{33} - \nu\left(\sigma_{11} + \sigma_{22}\right)\right]$$

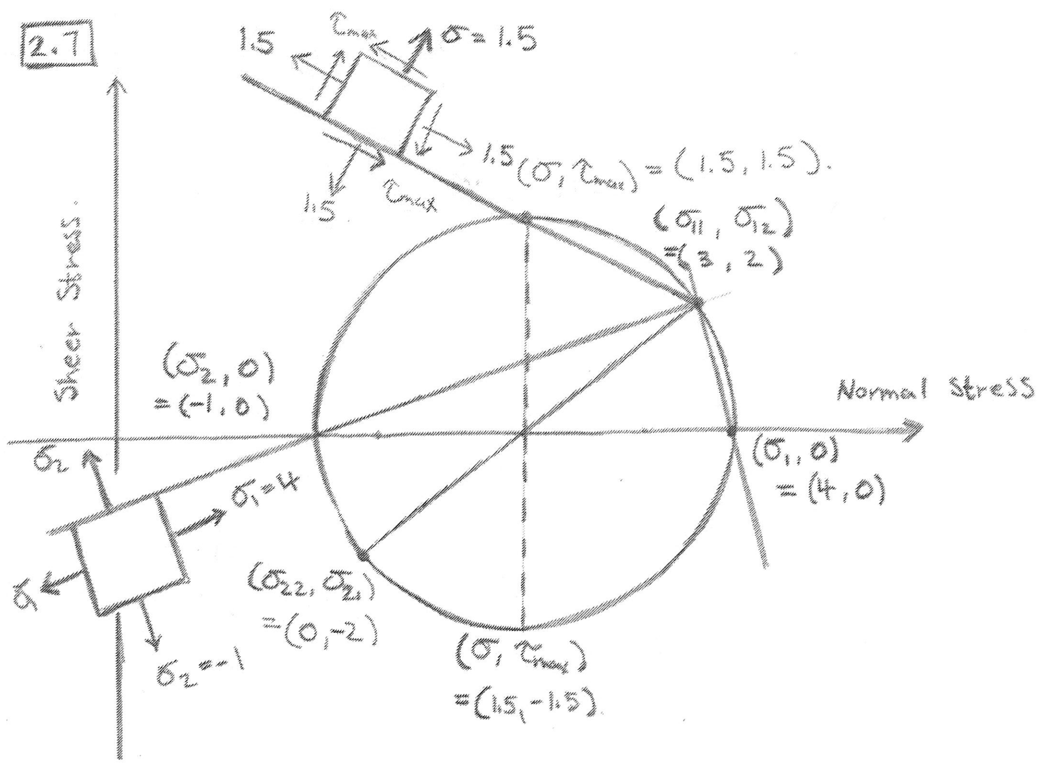
$$= \frac{1}{E}\left[\sigma_{33} - \nu\sigma_{22}\right] = \frac{\sigma_{33}}{E}\left[1 - \nu^2\right]$$

$$\varepsilon_{11} = \frac{1}{E}\left[\sigma_{11} - \nu\left(\sigma_{22} + \sigma_{33}\right)\right] = -\frac{\nu}{E}\left(\sigma_{22} + \sigma_{33}\right)$$

$$= -\frac{\nu}{E}\left(\sigma_{33} + \nu\sigma_{33}\right) = \frac{-\nu\sigma_{33}(1+\nu)}{E}$$

$$= \frac{-\nu(1+\nu)}{E} \cdot \frac{E\varepsilon_{33}}{\left(1-\nu^2\right)} = -\left(\frac{\nu}{1-\nu}\right)\varepsilon_{33}$$

$$\varepsilon_{11} = -\left(\frac{0.345}{1-0.345}\right)\left(-2\times10^{-4}\right) = 1.05\times10^{-4}$$



$\sigma_{11} = 3$ $\qquad$ $A = (\sigma_{11}, \sigma_{12}) = (3,2)$

$\sigma_{12} = 2$ $\qquad$ $B = (\sigma_{22}, -\sigma_{12}) = (0,-2)$

$\sigma_{22} = 0$

Slope from A-B = $\dfrac{\Delta Y}{\Delta X} = \dfrac{2-(-2)}{3-(0)} = \dfrac{4}{3}$

$$Y = \frac{4}{3}x + B$$

For Pt. A: $\quad 2 = \dfrac{4}{3}(3) + b$

$$b = -2$$

$$Y = \frac{4}{3}x - 2$$

Find X intercept when Y = 0

$$0 = \frac{4}{3}x - 2$$

$$X = \frac{3}{2}$$

$$\text{Center} = \left(\frac{3}{2}, 0\right)$$

$$\text{Radius} = \sqrt{\left(3 - \frac{3}{2}\right)^2 + (2 - 0)^2} = 2.5$$

$$\tan 2\theta = \left(\frac{2 - 0}{3 - \frac{3}{2}}\right)$$

$$\sigma_1 = \frac{3}{2} + 2.5 = 4$$

$$\sigma_2 = \frac{3}{2} - 2.5 = -1$$

$$2\theta = \tan^{-1}\left(\frac{4}{3}\right) = 53$$

$$\text{Maximum Shear} = \tau = 1.5$$

2.5

$$\theta = 26.56^\circ$$

$\boxed{2.34}$ Consider a solid subjected to hydrostatic pressure, p, that results in a dilation or volumetric strain given by
$V/V = \varepsilon_p$.

The bulk modulus, K, is defined by the ratio p/ε_p. Using the generalized Hooke's law, show that

$K = E/3(1-2v)$,

where E is the Young's modulus and v is the Poisson's ratio.

Assume initial volume $V_i = 1$

$$V_f = (1+\varepsilon_{11})(1+\varepsilon_{22})(1+\varepsilon_{33})$$

$$V_f = 1+\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}$$

$$V_f - V_i = \Delta V = 1+\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33} - 1 = \varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}$$

Hydrostatic pressure implies $\varepsilon_{11} = \varepsilon_{22} = \varepsilon_{33}$

$$\Delta V = 3\varepsilon_{11}$$

$$K = \frac{p}{3\varepsilon_{11}}$$

Equation 2.11: $\varepsilon_{11} = \dfrac{1}{E}\left(\sigma_{11} - v(\sigma_{22}+\sigma_{33})\right)$

Hydrostatic pressure implies $= \sigma_{11} = \sigma_{22} = \sigma_{33} = p$

$$\varepsilon_{11} = \frac{1}{E}(p - 2\nu p) = \frac{p}{E}(1 - 2\nu) \quad (1)$$

$$K = \frac{p}{\varepsilon_p} = \frac{p}{\frac{\Delta V}{V}} = \frac{p}{\Delta V} = \frac{p}{3\varepsilon_{11}}$$

Substitute in Equation (1) for ε_{11}

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

2.47 The potential energy of two atoms, a distance r apart, is

$$U = -\frac{A}{r^m} + \frac{B}{r^n}.$$

Given that the atoms form a stable molecule at a separation $r = r_0$, with a binding energy $U = U_0$, derive:

(a) the expressions for the constants A and B in terms of m, n, r_0, and U_0;

(b) the expressions for the stiffness S of the bond at arbitrary r and at r_0;

(c) the expression for the distance r^* of the maximum tensile force (needed to break the bond between atoms), and the expression for that force ($F*$).

(d) Given that m=2, n=10, and that the atoms form a stable molecule at a separation r_0 =0.3 nm, with a binding energy U_0=−4 eV, evaluate A, B, $r*$, $F*$, and the stiffness $S0$ of the bond at $r = r_0$.

$$U = \frac{-A}{r^m} + \frac{B}{r^n}$$

Atoms form a stable molecule at a separation $r = r_0$ with a binding energy $U = U_0$

a) $U = \dfrac{-A}{r^m} + \dfrac{B}{r^n}$ at equilibrium $r = r_0$, $\dfrac{dU}{dr} = 0$

$$\frac{dU}{dr} = \frac{mA}{r^{m+1}} - \frac{nB}{r^{n+1}} = 0 \qquad \text{Equation (1)}$$

Stable molecule $r = r_0$, $U = U_0$

$$U_0 = \frac{-A}{r_0^{\ m}} + \frac{B}{r^n} \qquad \text{Equation (2)}$$

There are two equations and two unknowns, so we can solve them

$$\frac{A}{r^{m+1}} = \frac{nB}{r^{n+1}} \qquad (1)$$

$$\frac{A}{r^m \cdot r} = \frac{nB}{r^n \cdot r} \Rightarrow A = r_0^{\ m-n} nB$$

$\Uparrow$

Plug into Equation (2)

$$U_0 = \frac{-r_0^{\ m-n} nB}{r_0^{\ m}} + \frac{B}{r_0^{\ n}}$$

$$U_0 = \frac{-nB}{r_0^{\ n}} + \frac{B}{r_0^{\ n}} \Rightarrow B = \frac{U_0 r_0^{\ n}}{1-n}$$

$$A = r_0^{\ m-n} n\left(\frac{U_0 r_0^{\ n}}{1-n}\right) = \frac{n r_0^{\ m} U_0}{1-n}$$

b)

Equation 2.52: $E = \dfrac{A(n-1)}{r_0^{\ 4}}$, $\qquad A = \dfrac{e^2}{4\pi\varepsilon_0}$

$e = 1.6 \times 10^{-19} eV$

$$\varepsilon_0 = 8.8 \times 10^{-12} \frac{c^2}{nm^2}$$

$$\boxed{E = \frac{e^2(n-1)}{4\pi\varepsilon_0 r_0^{\ 4}}}$$

c) $\dfrac{dU}{dr} = F$ At Maximum in F, $\dfrac{d^2U}{dr^2} = 0$

$$\frac{dU}{dr} = \frac{mA}{r^{m+1}} - \frac{nB}{r^{n+1}}$$

$$\frac{d^2U}{dr^2} = \frac{m(m+1)A}{r^{m+2}} - \frac{n(n+1)B}{r^{n+2}} = 0$$

$$\frac{m(m+1)A}{n(n+1)B} = \frac{r^{m+2}}{r^{n+2}} = r_*^{\ m-n}$$

$$\frac{m(m+1)nr_0^{\ m}U_0(1-n)}{n(n+1)(1-n)r_0^{\ n}U_0} = r_*^{\ m-n}$$

$$\frac{m(m+1)r_0^{\ m-n}}{(n+1)} = r_*^{\ m-n}$$

$$\left(\frac{m(m+1)}{n+1}\right)^{\frac{1}{m-n}} r_0 = r_*$$

Expression for Force:

$r = r_*$

$$F_* = \frac{mA}{r^{m+1}} - \frac{nB}{r^{n+1}}$$

$$F_* = \frac{mnr_0^{\,m}U_0}{1-n\left(\left(\frac{m(m+1)}{(n+1)}\right)^{\frac{1}{m-n}} r_0\right)^{m+1}} - \frac{nU_0 r_0^{\,n}}{(1-n)\left(\left(\frac{m(m+1)}{(n+1)}\right)^{\frac{1}{m-n}} r_0\right)^{n+1}}$$

d) m = 2, n = 10, r_0 = .3nm, $U_0 = -4eV$

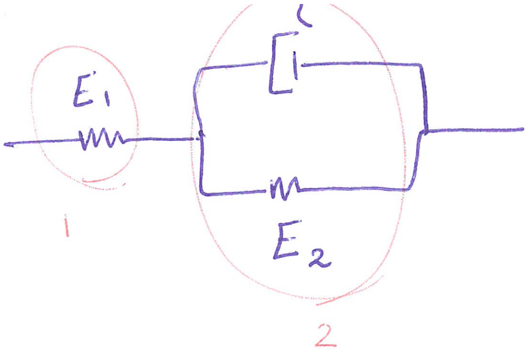
$A = 4 \times 10^{-19} m^2 eV$

$B = 2.62 \times 10^{-96} m^{10} eV$

$E_0 = S_0 = 2.55 \times 10^{11} = 255GPa$

$r^* = .323 \times 10^{-9} m$

$F^* = 2.37 \times 10^{10} - 1.47 \times 10^{10} = 8.9GPa$



$$\sigma = \sigma_1 = \sigma_2$$

$$\varepsilon = \varepsilon_1 + \varepsilon_2 \rightarrow \varepsilon_2 = \varepsilon - \varepsilon_1 \;\&\; \dot{\varepsilon}_2 = \dot{\varepsilon} - \dot{\varepsilon}$$

$$\varepsilon_1 = \frac{\sigma}{E_1}$$

$$\sigma = E_2 \varepsilon_2 + \eta \dot{\varepsilon}_2$$

$$\varepsilon = \frac{\sigma}{E_1} + (\sigma - \eta \dot{\varepsilon}_2)\frac{1}{E_2}$$

$$= \frac{\sigma}{E_1} + \frac{\sigma}{E_2} - \frac{\eta}{E_2}(\dot{\varepsilon} - \dot{\varepsilon}_1)$$

$$\varepsilon = \frac{\sigma}{E_1} + \frac{\sigma}{E_2} - \frac{\eta}{E_2}\left(\dot{\varepsilon} - \frac{\dot{\sigma}}{E_1}\right)$$

$$\varepsilon = \frac{\sigma}{E_1} + \frac{\sigma}{E_2} - \frac{\eta \dot{\varepsilon}}{E_2} - \frac{\eta \dot{\sigma}}{E_1 E_2}$$

$$E_1 E_2 \varepsilon = E_2 \sigma + E_1 \sigma - \eta E_1 \dot{\varepsilon} - \eta \dot{\sigma}$$

$$\boxed{\sigma(E_1 + \sigma_2) + \eta \dot{\sigma} = \eta E_1 \dot{\varepsilon} + E_1 E_2 \varepsilon}$$

$$f(\sigma, \dot{\sigma}, \varepsilon, \dot{\varepsilon}) = 0$$