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Unified Engineering
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Problem Set #14
Solutions

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UNIFIED ENGINEERING

Problem Set #14 -- SOLUTIONS

M19. $U = -\frac{A}{r^m} + \frac{B}{r^n}$ with $m=2, n=10$

This is either covalent or metallic bonding

We are also given:

- stable separation distance = $r_0 = 0.3 \text{ nm} = 0.3 \times 10^{-9} \text{ m}$
- stable energy = $U_0 = -4 \text{ eV}$

(a) To find A and B , use the values associated with the energy at the stable point ($r=r_0$):

first, $U_0 = -\frac{A}{r_0^2} + \frac{B}{r_0^{10}}$

$$\Rightarrow -4 \text{ eV} = -\frac{A}{(3 \times 10^{-10} \text{ m})^2} + \frac{B}{(3 \times 10^{-10} \text{ m})^{10}}$$

(Note: 1 Joule = 6.24×10^{18} eV)

$$\Rightarrow 1 \text{ eV} = 1.603 \times 10^{-19} \text{ J}$$

$$\Rightarrow -6.41 \times 10^{-19} \text{ J} = -\frac{A}{(3 \times 10^{-10} \text{ m})^2} + \frac{B}{(3 \times 10^{-10} \text{ m})^{10}} \quad (1)$$

This gives one equation. To get the second, we know that $\frac{dU}{dr} = 0$ at the stable point ($r=r_0$) and apply that:

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

and with the values for m and n :

$$\frac{dU}{dr} = \frac{2A}{r^3} - \frac{10B}{r^{11}}$$

this is = 0 at $r = r_0$ giving:

$$\Rightarrow 0 = \frac{2A}{(3 \times 10^{-10} \text{ m})^3} - \frac{10B}{(3 \times 10^{-10} \text{ m})^{11}}$$

yielding:

$$A = \frac{5B}{(3 \times 10^{-10} \text{ m})^8} \quad (2)$$

use this second equation (2) in the first (1) to get:

$$-6.41 \times 10^{-19} \text{ J} = \frac{-5B}{(3 \times 10^{-10} \text{ m})^{10}} + \frac{B}{(3 \times 10^{-10} \text{ m})^{10}}$$

$$\Rightarrow B = \frac{1}{4} (6.41 \times 10^{-19} \text{ J}) (3 \times 10^{-10} \text{ m})^{10}$$

giving: $B = 9.46 \times 10^{-115} \text{ J} \cdot \text{m}^{10}$

use this in (2) to determine A:

$$A = \frac{5}{4} (6.41 \times 10^{-19} \text{ J}) (3 \times 10^{-10} \text{ m})^2$$

$$\Rightarrow A = 7.21 \times 10^{-38} \text{ J} \cdot \text{m}^2$$

Summarizing:

$$B = 9.46 \times 10^{-115} \text{ J} \cdot \text{m}^{10}$$

$$A = 7.21 \times 10^{-38} \text{ J} \cdot \text{m}^2$$

(b) We know the stiffness of the bond, S_{bond} , is related to energy via:

$$S_{\text{bond}} = \frac{d^2U}{dr^2}$$

and we need to find this at r_0 to get S_0 (the stiffness at the stable point):

$$\frac{dU}{dr} = \frac{2A}{r^3} - \frac{10B}{r^{11}}$$

$$S = \frac{d^2U}{dr^2} = -\frac{6A}{r^4} + \frac{110B}{r^{12}}$$

Use the values of A , B , and r_0 in this:

$$\begin{aligned} \Rightarrow S_0 &= -\frac{6(8.01 \times 10^{-19} \text{ J})(3 \times 10^{-10} \text{ m})^2}{(3 \times 10^{-10} \text{ m})^4} + \frac{110(1.60 \times 10^{-14} \text{ J})(3 \times 10^{-10} \text{ m})^{10}}{(3 \times 10^{-10} \text{ m})^{12}} \\ &= -\frac{48.1 \times 10^{-19} \text{ J}}{(3 \times 10^{-10} \text{ m})^2} + \frac{176 \times 10^{-19} \text{ J}}{(3 \times 10^{-10} \text{ m})^2} = \frac{128 \times 10^{-19} \text{ J}}{(3 \times 10^{-10} \text{ m})^2} \end{aligned}$$

also using $1 \text{ J} = 1 \text{ N} \cdot \text{m}$ and providing:

$$\Rightarrow S_0 = 1.42 \times 10^{12} \text{ N} \cdot \text{m} / \text{m}^2 = 142 \frac{\text{N}}{\text{m}}$$

Finally, get an estimate for E by recalling:

$$E = \frac{S_0}{r_0} = \frac{128 \times 10^{-19} \text{ N} \cdot \text{m} / (3 \times 10^{-10} \text{ m})^2}{(3 \times 10^{-10} \text{ m})}$$

$$\Rightarrow E = 4.74 \times 10^{11} \frac{\text{N}}{\text{m}^2}$$

$$= 474 \times 10^9 \text{ Pa}$$

$$\Rightarrow \boxed{E = 474 \text{ GPa}}$$

(c) Metals have moduli in the range of 35-200 GPa, and materials with covalent bonds (e.g. C-C) are in the vicinity of 1000 GPa. Thus, the estimate is "in the ballpark"; however, discrepancies will arise as we have considered only the forces between the atoms in isolation. We actually need to consider the influence of all the atoms in the lattice, particularly the immediate neighbors.

U20. Unidirectional composite material with:
graphite fibers with modulus of 230 GPa and
an epoxy matrix with modulus of 10 GPa

To estimate the composite modulus along
and perpendicular to the fiber direction, use
the Rule of Mixtures:

for E_L : (modulus along fiber direction)

$$E_L = E_f v_f + \bar{E}_m (1 - v_f)$$

v_f = volume fraction of fibers

for \bar{E}_T : (modulus perpendicular to fiber direction)

$$\bar{E}_T = \frac{\bar{E}_f \bar{E}_m}{\bar{E}_m v_f + \bar{E}_f (1 + v_f)}$$

use the given values of:

$$E_f = 230 \text{ GPa}$$

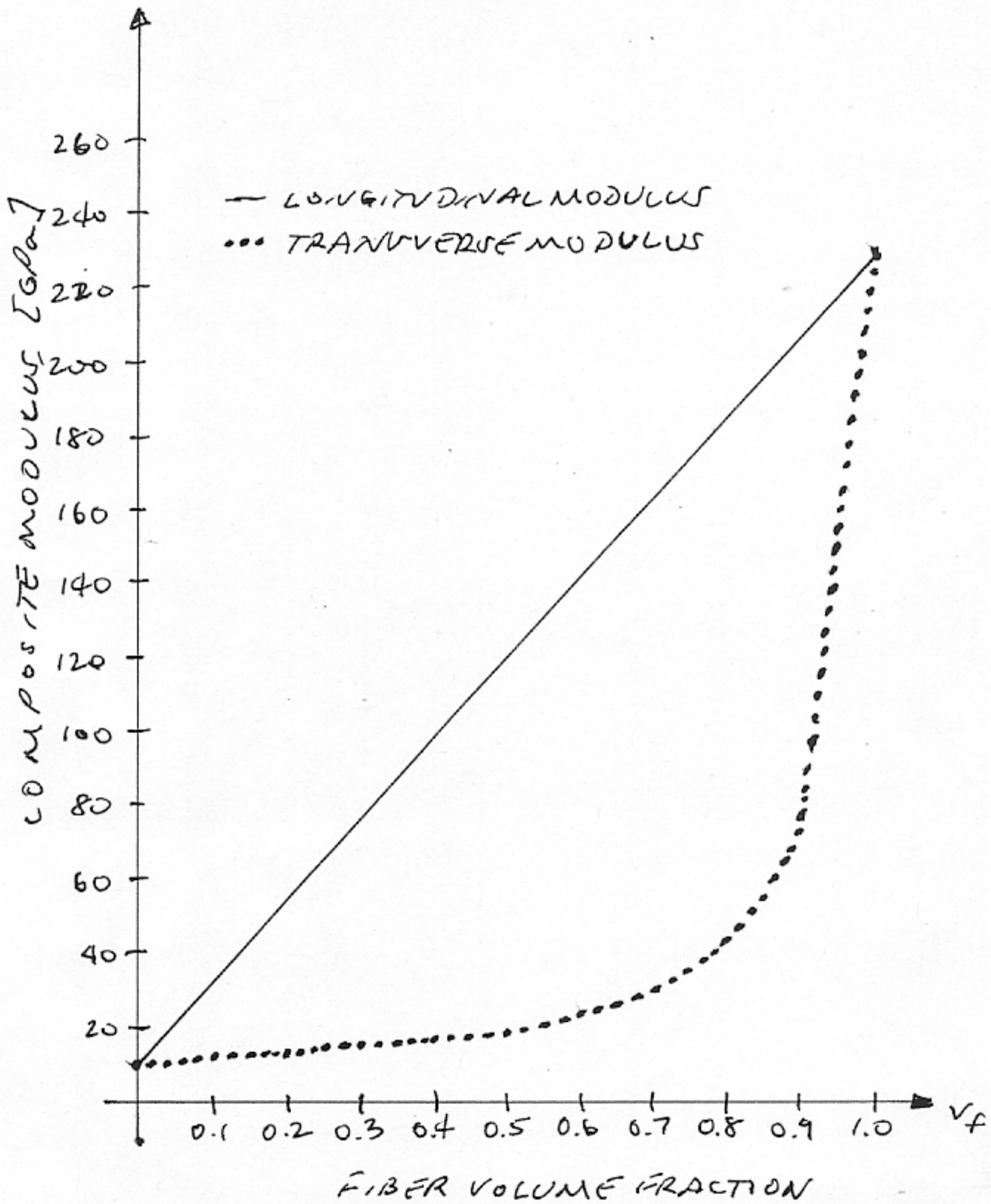
$$E_m = 10 \text{ GPa}$$

Make a table and calculate values for 0.1 increments in V_f :

V_f	E_L [GPa]	E_T [GPa]
0	10	10
0.1	32	11.1
0.2	54	12.4
0.3	76	14.0
0.4	98	16.2
0.5	120	14.2
0.6	142	23.5
0.7	164	30.3
0.8	186	42.6
0.9	208	71.9
1.0	230	230

This is plotted in the figure on the next page

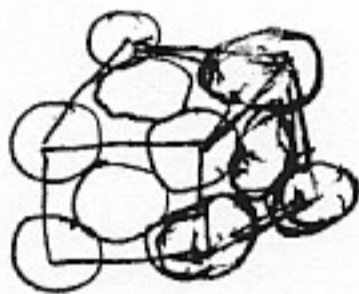
COMPOSITE PLY MODULUS ESTIMATED FROM CONSTITUENT VALUES



m 21. Aluminium - face-centered cubic
 Titanium - close-packed hexagonal

(a) To get the percentages of the volume occupied by the atoms, put a "hard sphere" (the assumption for the representation of the atom) at each point in the packing so that they just touch.

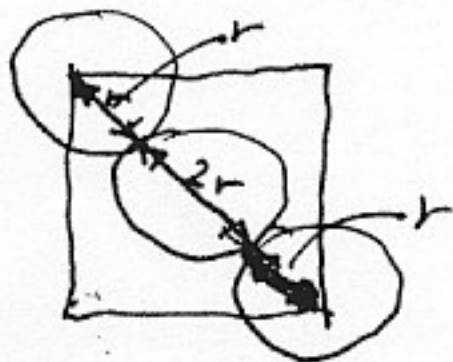
For the face-centered cubic (FCC) crystal



Each unit cell has:

- 8 corners each with $\frac{1}{8}$ of an atom in them = 1 atom
 - 6 faces each with $\frac{1}{2}$ of an atom in them = 3 atoms
- Total = 4 atoms

We can see the diagonal of a cell has length $4r$ where r is the sphere radius:



(8)

Thus, a side has length: $\frac{4r}{\sqrt{2}} = \sqrt{2}(2r)$

So calculate the volumes:

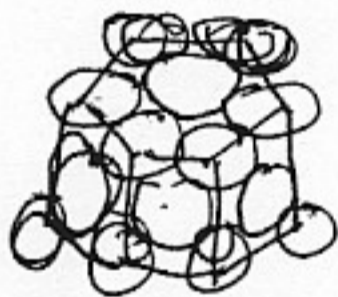
$$\text{Cube volume} = [\sqrt{2}(2r)]^3 = \sqrt{2}(2)(8r^3) = \sqrt{2}16r^3$$

$$\text{Atom volume} \times 4 = 4 \times \frac{4}{3}\pi r^3 = \frac{16}{3}\pi r^3$$

$$\% \text{ occupied by atoms} = \frac{\frac{16}{3}\pi r^3}{\sqrt{2}16r^3} = \frac{\pi}{\sqrt{2}3}$$

$$\Rightarrow \boxed{\% \text{ volume} = 0.74} \quad \text{for Aluminum}$$

Do the same for the close-packed hexagonal (HCP) crystal:



Each unit cell contains:

12 corners each with $\frac{1}{6}$ atom in them = 2 atoms

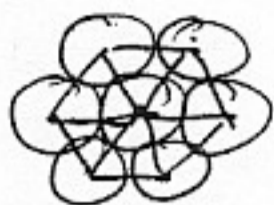
2 faces each with $\frac{1}{2}$ atom in them = 1 atom

3 center atoms = 3 atoms

TOTAL = 6 atoms

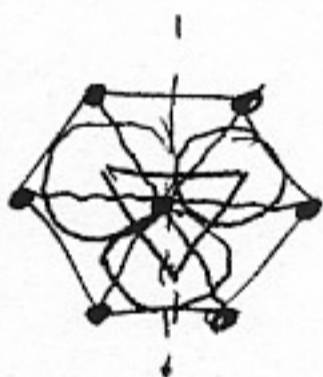
we now need to find the side length of the hexagon and the height. Consider:

In the close-packed plane, the atoms touch:

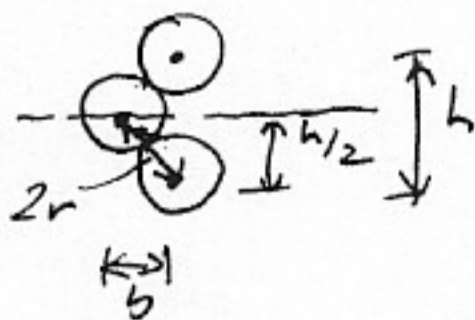


Thus, $a = 2r$ where $r = \text{radius of atom}$
 $a = \text{side of hexagon}$

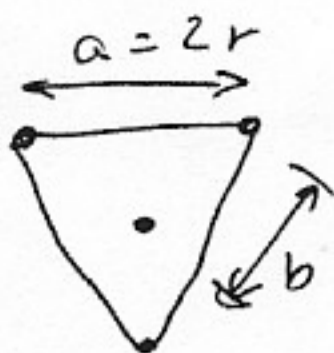
Now consider the height of this arrangement. If we think about the next close-packed plane above the first, these atoms fit in the "pockets". Represent the first plane by dots, the second by circles:



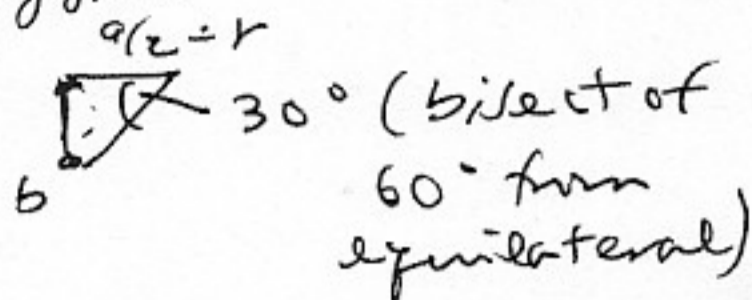
Now look at a plane cut at the dotted line:



We need the distance "b" from the center of the atom in one plane to the center of the neighbor in the next plane. Looking down, we see this atom sits at the midpoint of the equilateral triangle of the first plane:



geometry gives:



$$\Rightarrow \frac{a}{2} = b \cos 30^\circ$$

$$\Rightarrow b = \frac{2r}{\sqrt{3}}$$

Returning to the previous diagram:

$$(2r)^2 = b^2 + (h/2)^2$$

$$\Rightarrow h^2 = 4 \left[4r^2 - \frac{4r^2}{3} \right]$$

$$= \frac{32r^2}{3}$$

$$\Rightarrow h = 4 \sqrt{\frac{2}{3}} r$$

The area of the hexagon is 6 equilateral triangles of side length $2r$. The height of such a triangle is $\sqrt{3}r$.

$$\Rightarrow \text{Area} = 6 \left(\frac{2r}{2} \right) (\sqrt{3}r)$$

$$= 6\sqrt{3}r^2$$

So the volume is area \times height

$$\Rightarrow \text{Volume} = 24\sqrt{2}r^3$$

6 atoms are in this volume, so atom volume is:

$$6 \times \frac{4}{3}\pi r^3 = \frac{24}{3}\pi r^3$$

(11)

$$\text{Finally, \% volume occupied by atoms} = \frac{\frac{24}{3} \pi r^3}{24\sqrt{2} r^3}$$

$$= \frac{\pi}{3\sqrt{2}}$$

$$\Rightarrow \boxed{\% \text{ volume} = 0.74} \quad \text{Titanium}$$

Note: Same as FCC (they are basically the same)

(b) For a material, we know the density. We can also look up the atomic mass and this gives us the mass of an atom in AMU (atomic mass units) where:

$$1 \text{ AMU} = 1.661 \times 10^{-24} \text{ g}$$

Al

$$\rho_{\text{Al}} = 2.7 \text{ Mg/m}^3 \quad \text{Atomic mass} = 26.98$$

$$\rho = \text{density} = \frac{\text{mass/unit cell}}{\text{volume/unit cell}}$$

In (a), we found the volume/unit cell = $\sqrt{2} 16 r^3$;
 or the a side of the cube is: $a = 2\sqrt{2} r$, or
 better yet the volume is a^3

$$\text{Now, mass/unit cell} = \frac{\text{mass}}{\text{atom}} \times \text{number of atoms}$$

Again in (a), we found 4 atoms, so:

$$\text{mass/unit cell} = (26.98 \text{ AMU}) (1.661 \times 10^{-24} \text{ g/AMU}) (4)$$

giving: $\text{mass/unit cell} = 1.793 \times 10^{-22} \text{ g}$

This yields:

$$\rho = 2.7 \times 10^6 \text{ g/m}^3 = \frac{1.793 \times 10^{-22} \text{ g}}{a^3}$$

$$\Rightarrow \boxed{a = 4.14 \times 10^{-10} \text{ m}} \text{ side of Al cube} \\ = 41.4 \text{ nm}$$

Ti

$\rho_{\text{Ti}} = 4.5 \text{ Mg/m}^3$ Atomic mass = 47.90

from (a), the height, h , of the cell is $4\sqrt{\frac{2}{3}}r$
and the side of the hexagon is $a = 2r$
in terms of a and h : $h = 2a\sqrt{\frac{2}{3}}$

$$\text{Volume} = \frac{3}{2} \sqrt{3} a^2 h \\ = 3\sqrt{2} a^3$$

Solve for a as before:

Number of atoms in unit cell is 6. So:

$$\text{mass/unit cell} = (47.90 \text{ AMU}) (1.661 \times 10^{-24} \text{ g/AMU}) (6) \\ = 4.774 \times 10^{-22} \text{ g}$$

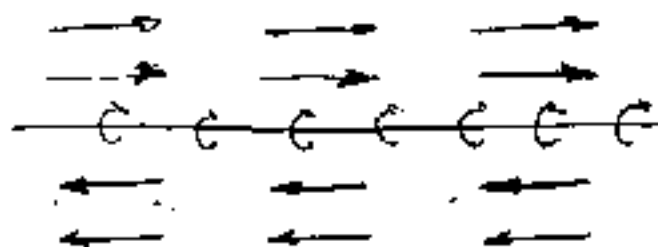
This gives: $\rho = 4.5 \times 10^6 \text{ g/m}^3 = \frac{4.774 \times 10^{-22} \text{ g}}{3\sqrt{2} a^3}$

$$\Rightarrow \boxed{\begin{matrix} a = 2.93 \times 10^{-10} \text{ m} & = 29.3 \text{ nm} \\ h = 4.78 \times 10^{-10} \text{ m} & = 47.8 \text{ nm} \end{matrix}}$$

Velocity field of top sheet:

$$u = \frac{y}{2} = +1$$

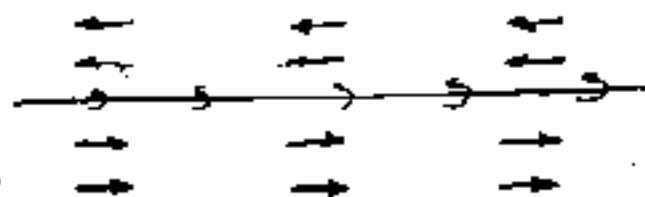
$$u = -\frac{y}{2} = -1$$



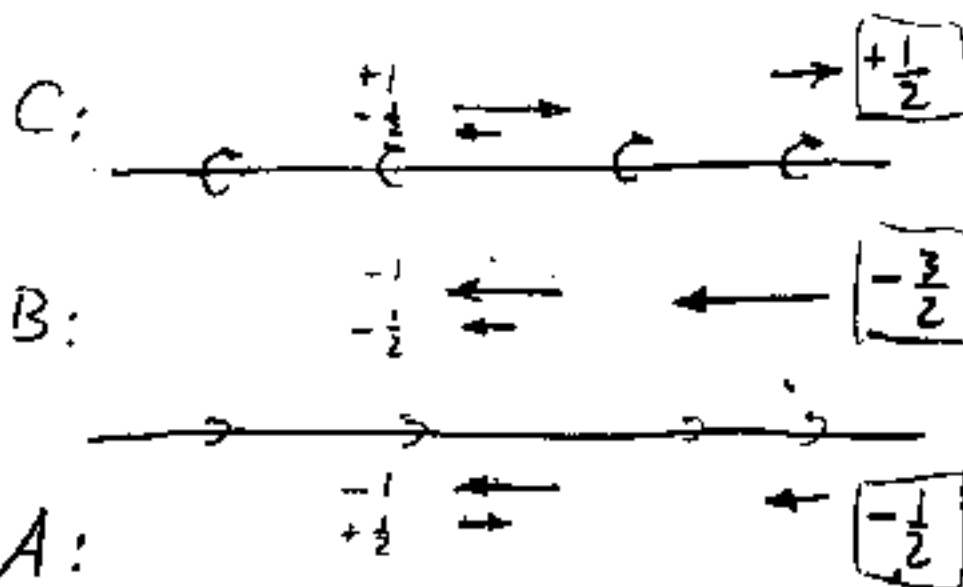
Velocity field of bot. sheet

$$u = \frac{y}{2} = -\frac{1}{2}$$

$$u = -\frac{y}{2} = +\frac{1}{2}$$



Superimpose:



$$L = \int_{-b/2}^{b/2} L' dy$$

$$= \int_{-b/2}^{b/2} \frac{1}{2} \rho V_\infty^2 c c_l dy$$

$$= \frac{1}{2} \rho V_\infty^2 \int_{-b/2}^{b/2} c c_l dy$$

$$D = \int_{-b/2}^{b/2} D' dy$$

$$= \int_{-b/2}^{b/2} \frac{1}{2} \rho V_\infty^2 c c_d dy$$

$$= \frac{1}{2} \rho V_\infty^2 \int_{-b/2}^{b/2} c c_d dy$$

If $c = \text{constant}$:

$$L = \frac{1}{2} \rho V_\infty^2 c \int_{-b/2}^{b/2} c_l dy$$

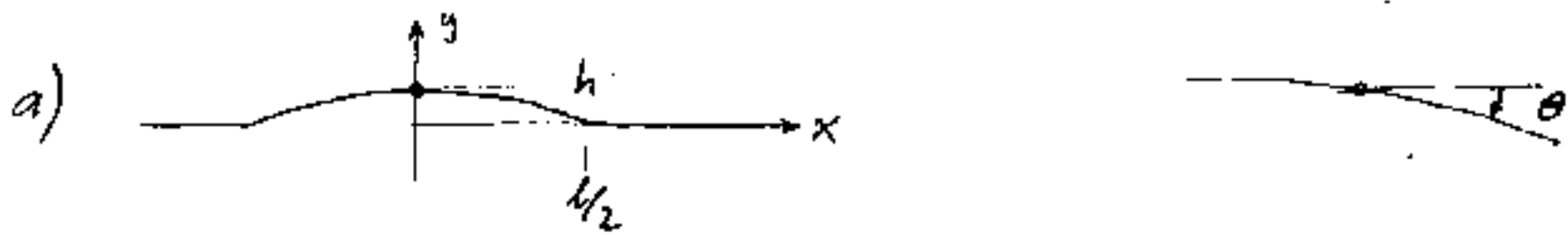
$$D = \frac{1}{2} \rho V_\infty^2 c \int_{-b/2}^{b/2} c_d dy$$

$$C_L \equiv \frac{L}{\frac{1}{2} \rho V_\infty^2 b c} = \frac{1}{b} \int_{-b/2}^{b/2} c_l dy$$

$$C_D \equiv \frac{D}{\frac{1}{2} \rho V_\infty^2 b c} = \frac{1}{b} \int_{-b/2}^{b/2} c_d dy$$

span-averaged $c_l(y)$

span-averaged $c_d(y)$



$$y = h - h \left(\frac{x}{l/2} \right)^2 \quad \text{parabolic bump}$$

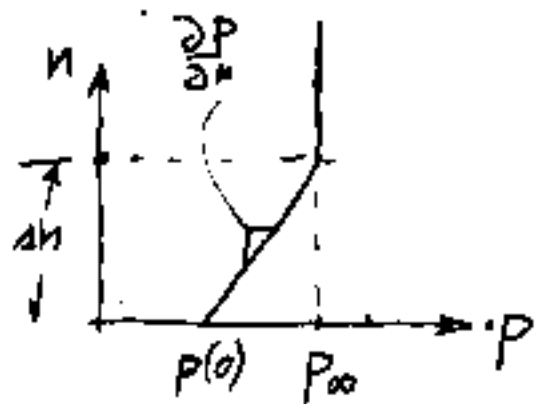
$$\theta = \frac{dy}{dx} = -2h \frac{x}{(l/2)^2} = -8h \frac{x}{l^2}$$

$$\boxed{\kappa = \frac{d\theta}{dx} = -8 \frac{h}{l^2}}$$

$$\boxed{\frac{\partial p}{\partial n} = -\rho V_\infty^2 \kappa = 8\rho V_\infty^2 \frac{h}{l^2}}$$

$$b). \quad p(n) = p_\infty + \frac{\partial p}{\partial n} (n - \Delta n)$$

$$p(n) = p_\infty + 8\rho V_\infty^2 \frac{h}{l^2} (n - \Delta n)$$



$$\boxed{\Delta p \equiv p(0) - p_\infty = -8\rho V_\infty^2 \frac{h}{l^2} \Delta n}$$

$$\boxed{\Delta p < 0 \quad \text{for bump}}$$

c) Experiment shows $\Delta p \sim \frac{h}{l}$ or $\frac{\Delta p}{h/l} = \phi$

$$\frac{\Delta p}{h/l} = -8\rho V_\infty^2 \frac{\Delta n}{l} = \phi$$

indicates that $\frac{\Delta n}{l} = \phi$ for any bump

$$\text{or } \Delta n \sim l$$



Pressure field extends vertically a distance $\leftarrow l \rightarrow$ proportional to the bump length l

$$a) P = V_{\infty} D = \frac{1}{2} \rho V_{\infty}^3 S C_D \quad \left(\text{since } D = \frac{1}{2} \rho V_{\infty}^2 S C_D \right)$$

In level flight, $L = W$

$$\text{or } \frac{1}{2} \rho V_{\infty}^2 S C_L = W$$

$$\text{or } V_{\infty} = \sqrt{\frac{2W/S}{\rho C_L}}$$

$$\rightarrow P = \frac{1}{2} \rho \left(\frac{2W/S}{\rho C_L} \right)^{3/2} S C_D$$

$$P = \left(\frac{2W^3}{\rho S} \right)^{1/2} \frac{C_D}{C_L^{3/2}}$$

$$b) P \sim \frac{1}{\rho^{1/2}} \quad \text{as } \rho \downarrow, P \uparrow \quad \text{power increases with lower density (higher altitude)}$$

$$\text{We can write } P = V_{\infty} D = V_{\infty} W \frac{D}{L} = V_{\infty} W \frac{C_D}{C_L}$$

Reducing ρ will increase V_{∞} — \uparrow

$$c) P \sim C_D$$

$$P = \phi \cdot C_D$$

$$\ln P = \ln \phi + \ln C_D$$

$$\frac{dP}{P} = \frac{dC_D}{C_D}$$

$$\frac{\Delta P}{P} \approx \frac{\Delta C_D}{C_D} \rightarrow 1\% C_D \text{ decrease gives } 1\% P \text{ decrease}$$

$$d) P \sim W^{3/2}$$

$$\ln P = \ln \phi + \frac{3}{2} \ln W$$

$$\frac{\Delta P}{P} = \frac{3}{2} \frac{\Delta W}{W} \rightarrow 1\% W \text{ decrease gives } 1.5\% P \text{ decrease}$$