

## PHYS1169 tut 12 answers

### Atomic structure of solids.

#### Q1.

$$U(r) = -\frac{A}{r^n} + \frac{B}{r^m} \quad \text{See C\&L p43.}$$

$$\text{For a minimum } \frac{\partial U}{\partial r}(r_0) = n \frac{A}{r_0^{n+1}} - m \frac{B}{r_0^{m+1}} = 0$$

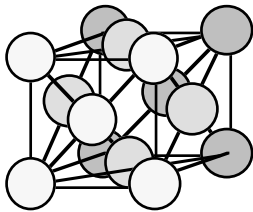
$$U(r_0) = -\frac{A}{r_0^n} + \frac{B}{r_0^m} = -r_0 \left( \frac{A}{r_0^{n+1}} - \frac{B}{r_0^{m+1}} \right) = -r_0 \left( \frac{A}{r_0^{n+1}} - \frac{n}{m} \frac{A}{r_0^{n+1}} \right)$$

$$= -\frac{A}{r_0^n} \left( 1 - \frac{n}{m} \right) \quad \text{and, taking } n = 6 \text{ and } m = 12, \quad U(r_0) = -\frac{A}{2r_0^n}$$

$$\text{rearrange gives } r_0 = \left( \frac{mB}{nA} \right)^{1/m-n}$$

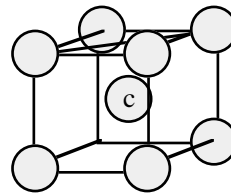
For the second part, see C&L p66 and substitute. (For those who want to derive this equation, it is a somewhat messier derivation, but looking for a maximum in  $F(r)$  ultimately gives eqn 5.2)

**Q2.** For coordination numbers and atomic packing factors and for diagrams, see C&L p30.



(darker are more distant)

For FCC, the nearest neighbours (NN) are at  $a/\sqrt{2}$  (Consider the atom at the centre of the front plane. The 4 at the corners of the front plane are NN. The two at the centres of the LH and RH sides, and the top and bottom are at this distance and so are NN. If we draw another cell in front of this one, there are another four such NN, so the coordination number is 12.



The one marked "c" is at the centre of this BCC cell. Here it is easy to count the NN

**Q3.** In an ideal glass, there are no crystals. It is an amorphous solid.

**Q4.** At the grain boundaries, the angles between nearby atoms are not in general the angles in the crystal. For strongly directional bonds, such as covalent solids, this makes for weak bonds. For metallic solids, the bonds are not strongly directional. (However, the irregular spacing and voids make it weaker than a pure crystal, of courses.)

### Elasticity and surface energy

$$\text{Q5. } \epsilon_x = \sigma_x/Y - \nu\sigma_y/Y - \nu\sigma_z/Y$$

but a hydrostatic pressure is isotropic, so (i) this is the strain in all directions, and (ii)  $\sigma_x = \sigma_y = \sigma_z = -P$

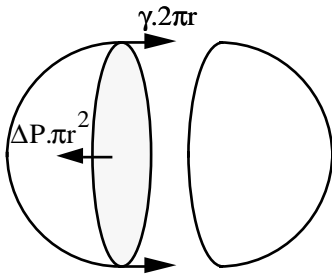
$$\epsilon = -P/Y + \nu P/Y + \nu P/Y = -(1 - 2\nu)P/Y$$

**Q6.** Elasticity:  $\sigma(\epsilon)$  is reversible, or there is no hysteresis, or when  $\sigma$  returns to zero,  $\epsilon = 0$ . Strength usually means the yield or fracture stress.

$$Y = \sigma_{\text{longitudinal}}/\epsilon_{\text{longitudinal}} = \frac{F/A}{\partial L/L} = \frac{760\text{N}/\pi(2.2\text{mm})^2}{0.2\text{m}/120\text{m}} = 30 \text{ GPa}$$

**Q7.** Surface energy is the work done per unit area in creating a new surface. Surface tension is the force per unit length in the plane of the surface against which this work is done. For the interface between two pure liquids, the two are numerically equal.

**Q8.**



The easiest way to demonstrate the required equation is by considering a bubble in equilibrium. The forces on one hemisphere add to zero. So the pressure excess inside is balanced by the surface tension acting at the perimeter.

$$\Delta P \cdot \pi r^2 = \gamma \cdot 2\pi r$$

$$\Delta P = \gamma \frac{2}{r} \quad (\text{the Young-Laplace equation})$$

For the work done in expansion, see the next problem.

**Q9.**  $U_T = \frac{4\pi r^3}{3} Q + 4\pi r^2 \sigma$

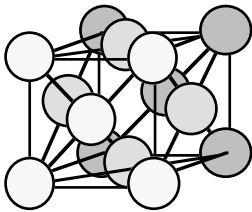
Setting these two terms equal gives the radius at which the volumetric energy first exceeds that of the surface term:  $r = 3\sigma/Q$ .

However, what is often important (eg in cavitation or nucleation or in other cases where  $Q < 0$ ) is what happens if  $r$  changes. Does  $U$  increase (stable) or decrease (unstable)? To find the critical radius for such processes, set

$$dU = 4\pi r^2 Q \cdot dr + 8\pi r \sigma \cdot dr$$

This is zero ( $U$  is a maximum) when  $r = -2\sigma/Q$

**E1.**



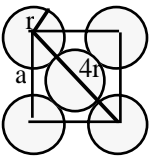
In the upper diagram, gaps are left between the spheres so that we can 'see in'. In the lower, the spheres touch.

$$\text{Face diagonal} = 4r, \text{ side of unit cube} = 4r/\sin 45^\circ = 2\sqrt{2}r$$

$$\text{p.f.} \equiv \frac{\text{Volume of spheres in unit cube}}{\text{Volume of unit cube}} = \frac{8 \text{ corners} + 6 \text{ faces}}{(2\sqrt{2}r)^3}$$

$$= \frac{(8 \times \frac{1}{8} + 6 \times \frac{1}{2}) \frac{4}{3}\pi r^3}{(2\sqrt{2}r)^3} = 0.74$$

$$\rho = \frac{(8 \times \frac{1}{8} + 6 \times \frac{1}{2}) \text{ atomic mass}}{a^3} = \frac{4m}{a^3} = \frac{4m}{(2\sqrt{2}r)^3} = 2.8 \text{ t/m}^3$$



**E2.**  $\epsilon_x = \sigma_x/Y - \nu\sigma_y/Y - \nu\sigma_z/Y$

$$\epsilon_y = -\nu\sigma_x/Y + \sigma_y/Y - \nu\sigma_z/Y$$

$$\epsilon_z = -\nu\sigma_x/Y - \nu\sigma_y/Y + \sigma_z/Y$$

$$\epsilon_{\text{vol}} = \epsilon_x + \epsilon_y + \epsilon_z = (1 - 2\nu)\sigma_x/Y + (1 - 2\nu)\sigma_y/Y + (1 - 2\nu)\sigma_z/Y$$

$$\Delta V = V\epsilon_{\text{vol}} = V \frac{1 - 2\nu}{Y} (\sigma_x + \sigma_y + \sigma_z)$$

$$= (10 \times 20 \times 100 \text{ mm}^3) \frac{1 - 2\nu}{Y} \left( \frac{10^4 \text{ N}}{10 \times 20 \text{ mm}^2} - \frac{10^5 \text{ N}}{100 \times 20 \text{ mm}^2} + \frac{10^5 \text{ N}}{100 \times 10 \text{ mm}^2} \right) = 4.6 \text{ mm}^3.$$

For no change in volume,  $\left( \frac{10^4 \text{ N}}{10 \times 20 \text{ mm}^2} - \frac{F_{\text{comp}}}{100 \times 20 \text{ mm}^2} + \frac{10^5 \text{ N}}{100 \times 10 \text{ mm}^2} \right) = 0$ , so  $F_{\text{comp}} = 300 \text{ kN}$

**E3.**

Surface tension acts on perimeters ( $\propto$  length), whereas weight is proportional to volume ( $\propto$  length<sup>3</sup>). So a doubling of the linear size increases weight by \*8, and surface forces only by \*2.