Condensed Matter Physics: Weekly Problem 1

These problems are to be formatively self-assessed by you, the student. Students taking part in the peer-marking pilot scheme will also be required to mark one of their peer's weekly problems. A mark scheme, out of 10, will be provided with each solution to aid your assessment before your timetabled weekly workshop.

Summary: These problems review properties of solids from Level 1 and also explore different aspects of symmetry, lattices and crystal structure using material covered in Lectures 2 and 3.

a. Describe, with the aid of a simple sketch, a model of a crystalline solid which allows the molar heat capacity at constant volume to be determined. State the equipartition theorem and use it to show that $C_V = 3R$ where R is the ideal gas constant. **[3 marks]**

b. Miller Indices:
   i. For a simple cubic lattice draw a sketch illustrating planes with the Miller indices (011) and (120). **[1 mark]**
   ii. The lattice constant a is 0.5 nm. For each set of indices above determine the spacing between the planes. **[1 mark]**

c. A crystal structure is composed of a lattice and a basis, as described in lectures. The figure shows a unit cell for the salt caesium chloride (CsCl). Each Cs ion is bonded to 8 Cl ions; each Cl ion is bonded to 8 Cs ions.
   i. Determine the lattice and basis, justify your answer. **[1 mark]**
   ii. Illustrate your answer with a sketch. **[1 mark]**
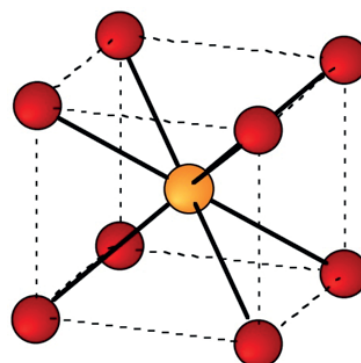
d. A lattice is a mathematical construct for filling space. Determine the maximum percentage of available space that can be filled in 3D by a face centre cubic lattice with a single atom basis. You will need to make some sensible assumptions to determine the solution. **[3 marks]**

Condensed Matter Physics: Question 1 - Solutions

When completing your assessment please enter the numerical marks for each question. Please also give information on any parts which you found difficult, as this will allow me to go over any common issues in the workshops. The workshops also provide the opportunity to individually talk to myself, and other staff members about any issues you faced when solving the problem. Information in the model solutions underlined/boxed in red is required for marks to awarded.

a. A solid is modelled as a series of underlined <u>atoms connected by bonds</u> where the atoms are <u>free to vibrate</u> about a <u>mean position</u> (but not move, <u>no translational motion</u>). **[1 mark]**

(The model allows us to predict how much energy can be absorbed by the solid and how much is required to heat the solid by one degree. In a solid we know that the atoms vibrate about a mean position but have no translational motion).
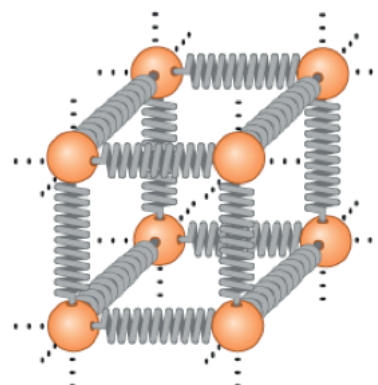
The equipartition theorem tells us the <u>thermal energy</u> for each <u>degree of freedom</u> is $\frac{1}{2}k_BT$.
There will be a <u>kinetic energy</u> and <u>potential energy</u> of vibration in each of <u>3 spatial dimensions</u> giving a total of <u>6 degrees of freedom</u>. Applying the equipartition theorem gives a <u>total energy per atom</u> of $3k_BT$. **[1 mark]**

For one mole, the Total Internal Energy U is then: $U_{\text{mole}} = 3N_A k_B T = 3RT$

The molar heat capacity at constant volume is thus: $C_V = \frac{dU_{\text{mole}}}{dT} = 3R$ **[1 mark]**

b. i. Figures show sketch of 011 and 120 family of planes (3 planes in each sketch). For 011, sketch should have planes <u>parallel to the x axis</u> and <u>intersect y and z at a</u>. For 120, sketch should have planes <u>parallel to the z axis</u> and <u>intersect x at and y at $a/2$</u>. **[1 mark]**
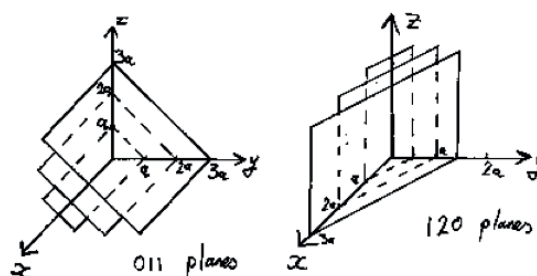
ii. Using relationship given in lectures the separation between planes is given by:

$$d = \frac{1}{\sqrt{h^2/a_1^2 + k^2/a_2^2 + l^2/a_3^2}}$$

For a cube, this reduces to: $d = a/\sqrt{h^2 + k^2 + l^2}$.
This gives <u>0.35 nm for 011 planes</u> and <u>0.22 nm for 120 planes</u>. **[1 mark]**

c. From lectures, we know that Crystal = Lattice + Basis.

The lattice is the <u>primitive cubic lattice</u> (not body centred cubic). **[1 mark]**

The basis is a <u>two-atom basis</u> with one Cs and one Cl atom <u>connected by a half body diagonal</u> (see figure). **[1 mark]**

To convince yourself of this think about replicating this basis at each corner of a simple cubic lattice and hopefully you will see that it produces the correct crystal structure.

(A common view is that this is a face centred cubic lattice. To show that this is not the case consider arranging atoms in a fcc lattice with the same basis at each lattice point. You will not be able to correctly replicate the crystal structure. The key point is that the central atom is different from the others, therefore the corner of the cube and the centre of the cube cannot be equivalent lattice points).

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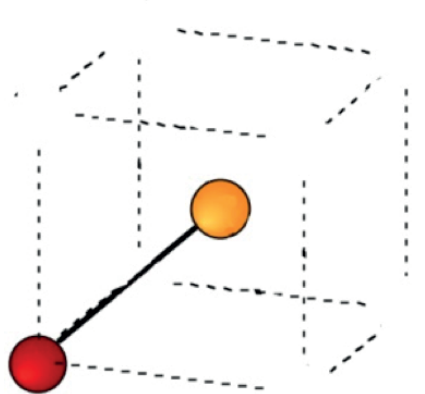
d. The fcc structure has one atom at each corner and one atom at the centre of each face. <u>Assume the</u> atoms are <u>spheres,</u> centred at each lattice point. The radius of the spheres is determined when the first two spheres touch somewhere in the crystal structure. When occupying the maximum volume, the atoms at the corners and the centre of each face touch, filling the face of the cube. The length of the face diagonal is then $4r$ where r is the diameter of each atom (assumed to be the same).
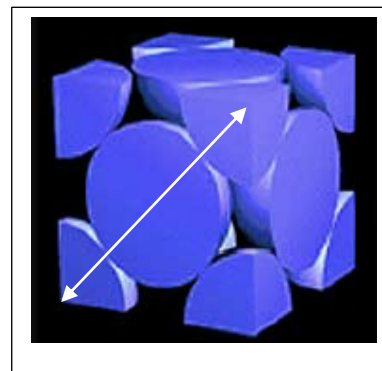
(This assumption gives the relationship between a and r).

From simple geometry, the <u>length of the side of the face is $a = \sqrt{8}r = 2\sqrt{2}r$.</u> **[1 mark]**

The <u>volume of the cube unit cell is $= a^3 = 16\sqrt{2}r^3$</u> .

Each unit cell contains <u>one atom at each corner shared between 8 unit cells</u> and <u>one atom in the centre of each face shared between two unit cells</u>, giving <u>4 atoms per unit cell</u>. **[1 mark]**

The <u>volume occupied by atoms in a unit cell</u> is: $$V_{atoms} = 4 \times \left(\frac{4}{3}\pi r^3\right) = \frac{16}{3}\pi r^3$$

The maximum packing density is the <u>ratio the volume of atoms to the volume of the unit cell</u>:

$$\text{Ratio} = \frac{V_{atoms}}{V} = \frac{\frac{16}{3}\pi r^3}{16\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}} = 0.74$$

[1 mark]

(Different structures have different packing ratios and therefore different densities).