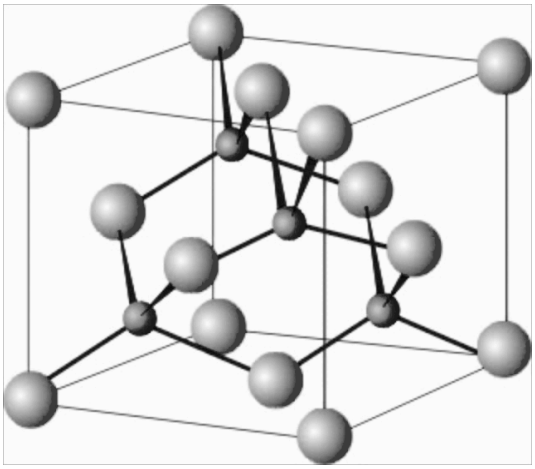
Marks
2

- The cubic form of boron nitride (borazon) is the second-hardest material after diamond and it crystallizes with the structure shown below. The large spheres represent nitrogen atoms and the smaller spheres represent boron atoms.



From the unit cell shown above, determine the empirical formula of boron nitride. Show your working.

There are N atoms on the corners and on the faces of the unit cell:

- **There are 8 N atoms on the corners. These contribute 1/8 to the unit cell giving a total of 8 × 1/8 = 1 N atom.**
- **There are 6 N atoms on the faces. These contribute 1/2 to the unit cell giving a total of 6 × 1/2 = 3 N atoms.**
- **There are a total of 1 + 3 = 4 N atoms in the unit cell.**

There are B atoms inside the unit cell:

- **There are 4 B atoms completely inside the cell. These contribute only to this unit cell giving a total of 4 × 1 = 4 B atoms.**

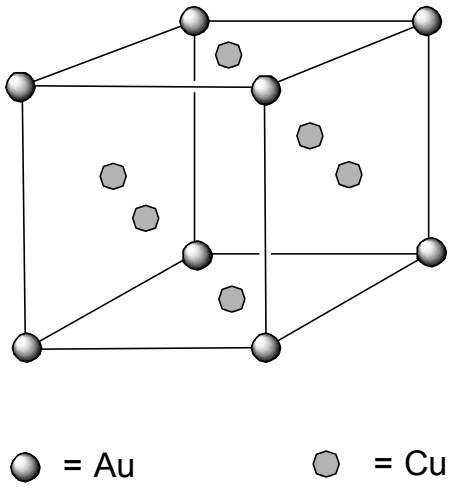
The formula is therefore B_4N_4 which simplifies to BN.

Answer: **BN**

THE REMAINDER OF THIS PAGE IS FOR ROUGH WORKING ONLY.

Marks
2

- The diagram below shows the structure of an alloy of copper and gold with a gold atom at each of the corners and a copper atom in the centre of each of the faces.



= Au = Cu

What is the chemical formula of the alloy?

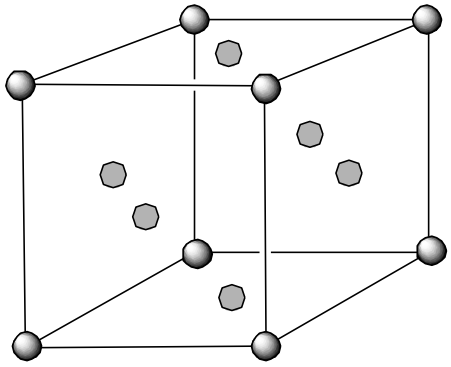
There are 8 Au atoms on the corners, each contributes 1/8 to the cell. The total number of Au atoms is 8 × 1/8 = 1.

There are 6 Cu atoms on the faces, each contributes 1/2 to the cell. The total number of Cu atoms is 6 × 1/2 = 3

Answer: **Cu_3Au (or $AuCu_3$)**

Marks 6

- The diagram below shows the structure of an alloy of copper and gold with a gold atom at each of the corners and a copper atom in the centre of each of the faces. The length of the side of the cubic unit cell is 0.36 nm.



= Au = Cu

What is the chemical formula of the alloy?

There are 8 Au atoms and each is on a corner so contributes 1/8 to the unit cell:

total number of Au atoms = 8 × 1/8 = 1

There are 6 Cu atoms and each is on a face so contributes 1/2 to the unit cell.

total number of Cu atoms = 6 × 1/2 = 3

Answer: **$AuCu_3$ or Cu_3Au**

Pure gold is 24 carat, whilst gold alloys consisting of 75 % gold by weight are termed 18 carat gold. What carat gold is this alloy?

The molar mass of Cu_3Au is:

molar mass = (3 × 63.55 (Cu) + 196.97 (Au)) g mol^{-1} = 387.62 g mol^{-1}

The percentage gold is therefore:

percentage gold = 196.97 / 387.82 ×100% = 50%

As 100% gold is 24 carat and 75% gold is 18 carat, this corresponds to 12 carat.

Answer: **12 carat**

What is the volume (in cm^3) of the unit cell?

The length of the side of the unit cell is 0.36 nm. This corresponds to 0.36 × 10^{-9} m or 0.36 × 10^{-7} cm. As the unit cell is cubic, its volume, *V*, is given by:

$V = (0.36 \times 10^{-7})^3\ cm^3 = 4.7 \times 10^{-23}\ cm^3$

Answer: **$4.7 \times 10^{-23}\ cm^3$**

ANSWER CONTINUES ON THE NEXT PAGE

What is the density (in g cm^{-3}) of the alloy?

From above, the mass of a mole of Cu_3Au is 387.62 g mol^{-1}. As this corresponds to Avogadro's number of formula units, the mass of the unit cell is:

mass of unit cell = (387.62 g mol^{-1}) / (6.022×10^{23} mol^{-1}) = 6.43673×10^{-22} g

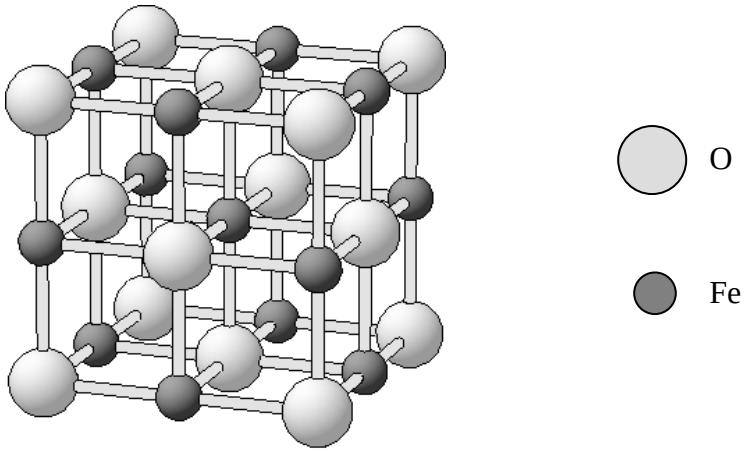
The density of the unit cell is therefore:

density = mass / volume
= (6.43673×10^{-22} g) / (4.7×10^{-23} cm^3)
= 14 g cm^{-1}

Answer: **14 g cm^{-1}**

Marks 8

- Iron forms three common oxides, FeO, Fe_3O_4 and Fe_2O_3. The unit cell for one of these oxides is shown below.



Explain which oxide the structure represents and describe the nature of the packing of the ions and their coordination numbers.

The structure contains 1 Fe atom at the centre and 12 Fe atoms on the edges. The atoms on the edges are shared between 4 cells and so contribute 1/4 to each:

number of Fe atoms = 1 (centre) + 12 × 1/4 (edges) = 4

The structure contains 8 O atoms on the corners and 6 O atoms on the faces. The atoms on the corners are shared between 8 cells and so contribute 1/8 to each and the atoms on the faces are shared between 2 cells and so contribute 1/2 to each:

number of O atoms = 8 × 1/8 (corners) + 6 × 1/2 = 4

There are 4 Fe atoms and 4 O atoms in the unit cell: the stoichimetry is Fe_4O_4 or FeO.

The coordination number is 6 for both Fe and O. The structure can be described as the cubic close packed arrangement of O atoms, with Fe in all of the octahedral holes.

The mineral magnetite, Fe_3O_4, is found in the beaks of homing pigeons. It contains a mixture of Fe^{2+} and Fe^{3+} ions. What is the ratio of Fe^{2+} to Fe^{3+} in Fe_3O_4?

As each O has an oxidation number of -2 and there are 4 of them in the formula, the 3 Fe atoms must together have a charge of +8. This is consistent with their being two Fe^{3+} ions and one Fe^{2+} per formula unit.

The ratio of Fe^{3+} to Fe^{2+} is 2 to 1.

ANSWER CONTINUES ON THE NEXT PAGE

How many unpaired electrons are there in an Fe^{2+} ion and in an Fe^{3+} ion? Explain your answer using the box notation.

Fe is in Group 8 so Fe^{2+} has a d^6 configuration and Fe^{3+} has a d^5 configuration. These electrons arrange in the five *d*-orbitals to minimise the repulsion between them by maximising the number of unpaired electrons:

Fe^{2+} 

Fe^{3+} 

Fe^{2+} has 4 unpaired electrons and Fe^{3+} has 5 unpaired electrons.

Fe^{2+}: **4**	Fe^{3+}: **5**