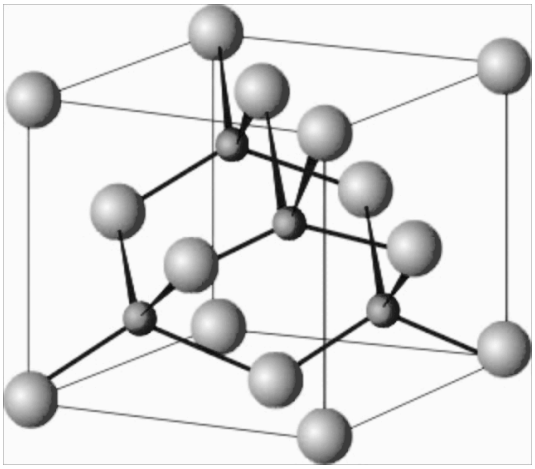
Marks 5

- 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 the nitrogen atoms and the smaller spheres represent boron atoms.



From the unit-cell shown above, determine the empirical formula of boron nitride.

Answer:

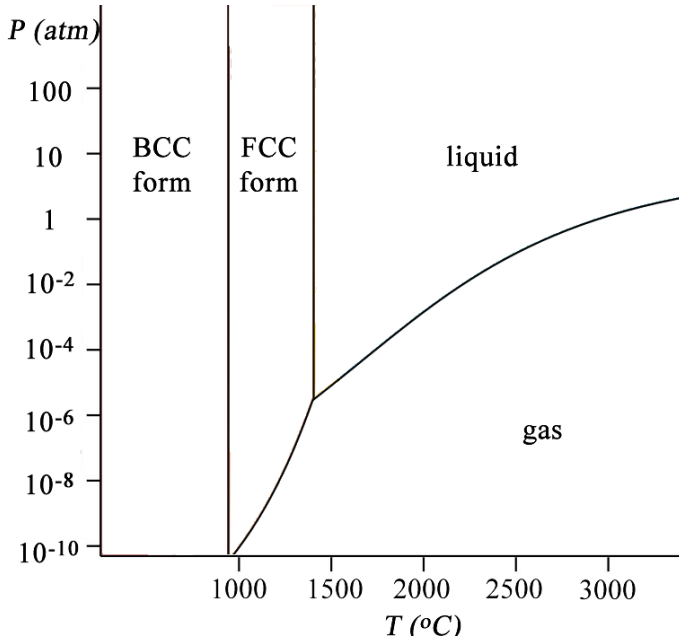
Determine the oxidation state of the boron atoms.

Answer:

The cubic form of boron nitride is more thermally stable in air than diamond. Provide a reasonable explanation for this observation.

Marks 5

- A simplified phase diagram for iron is shown below, with the solid part divided into the body-centred cubic (BCC) and face-centred cubic (FCC) phases.



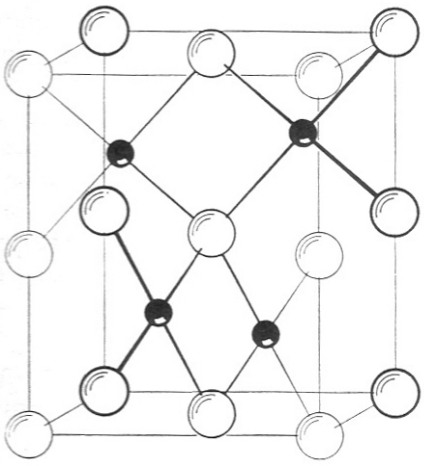
Which form of iron is stable at room temperature and pressure?

If molten iron is cooled slowly to around 1200 °C and then cooled rapidly to room temperature, the FCC form is obtained. Draw arrows on the phase diagram to indicate this process and explain why it leads to the FCC form as a metastable phase.

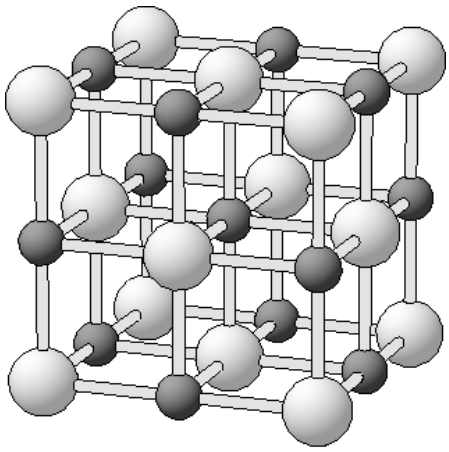
The line dividing the BCC and FCC forms is almost, but not quite vertical. Predict which way this line slopes and explain your answer.

Marks 8

- PdO is used as a hydrogenation catalyst and it crystallizes with the tetragonal structure shown below. NiO has a variety of uses and crystallizes with the rocksalt structure. The large spheres represent the oxygen atoms and the smaller spheres represent palladium or nickel atoms.



palladium(II) oxide, PdO



nickel(II) oxide, NiO

Show the structure on the left is consistent with the formula PdO.

What is the coordination number about each metal atom?

Pd:	Ni:

The radius of the Pd^{2+} ion is 86 pm, that of the Ni^{2+} ion is 69 pm. Give a reason why the larger ion has a smaller coordination number.

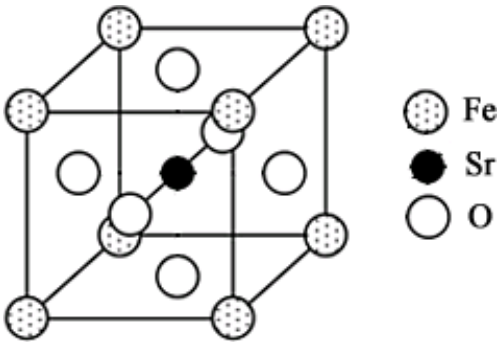
Does either structure contain a close-packed arrangement of O^{2-} ions?

PdO: YES / NO	NiO: YES / NO

If YES, indicate the layers on the unit cell(s) above.

Marks
9

- $SrFeO_3$ crystallises with the perovskite structure, shown below. The structure is cubic with iron atoms on each corner, oxygen atoms at the centre of each face and a strontium atom at the centre of the cube. Mixed metal oxides such as this are of current research interest because of their magnetic and possible superconducting properties.



Show the structure is consistent with the formula $SrFeO_3$ and give the coordination numbers of the Sr, Fe and O atoms.

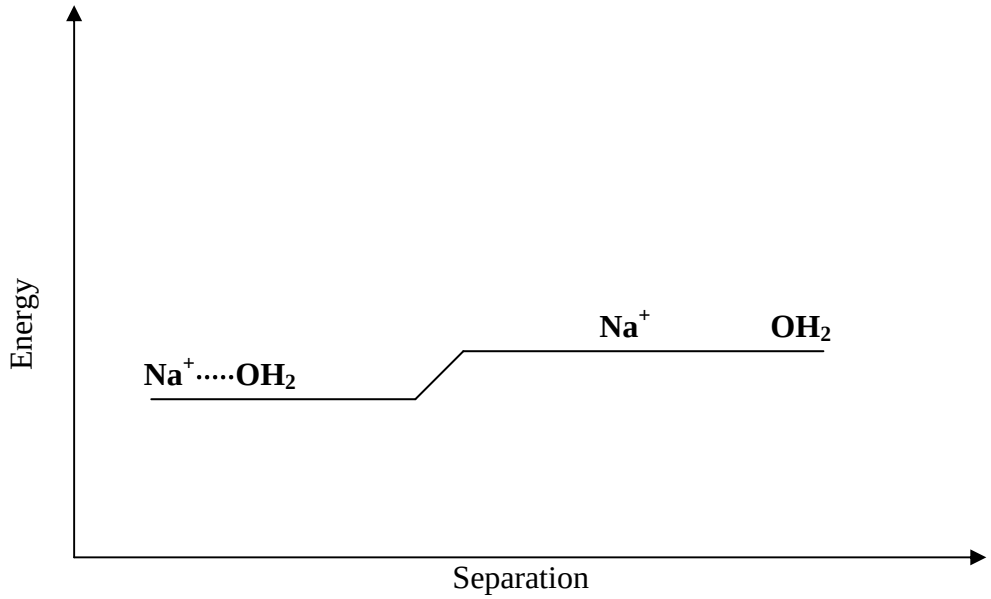
Using the box notation to represent atomic orbitals, work out how many unpaired electrons are present on the iron cation in this compound.

It is possible to substitute the Sr^{2+} ions at the centre of the unit cell by La^{3+} ions to make a series of compounds with the formula $La_{1-x}Sr_xFeO_3$ with $0 \leq x \leq 1$. Suggest why this substitution is achieved without significant change to the unit cell dimensions and describe how charge balance is achieved in these compounds.

Page Total:

Marks 6

- Shown below is the energy profile for the separation of Na^+ from H_2O. Draw energy profiles for the separation of Mg^{2+} from Cl^- and for the breaking of the C–C bond in ethane to the same scales (approximately).



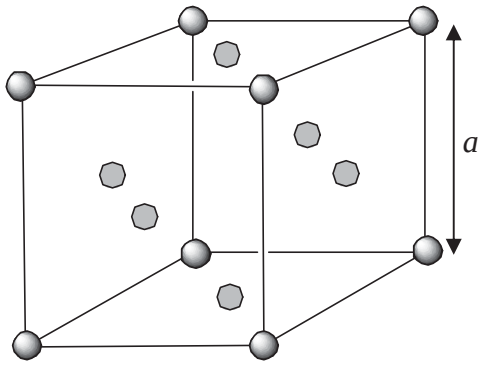
Name the inter- or intra-molecular forces involved in each of these three interactions.

Na^+ OH_2	
Mg^{2+} Cl^-	
C C	

Explain why bonds such as C–C are generally considered to be stronger than interactions such as that between Mg^{2+} and Cl^-.

Marks 5

- 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 unit cell dimension (edge length, *a*) for this alloy is 0.36 nm.



= Au = Cu

What is the chemical formula of the alloy?

Answer:

Given that pure gold is 24 carat and gold alloyed with 25% by weight of another metal is termed 18 carat gold, what carat gold is this alloy?

Answer:

What is the volume of the unit cell?

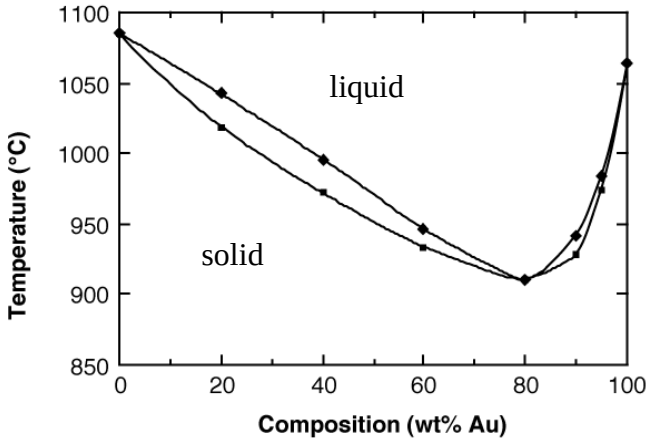
Answer:

What is the density of the alloy?

Answer:

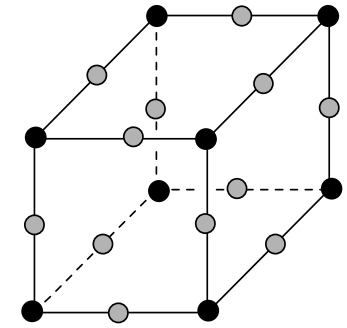
Shown below is the phase diagram for the Cu/Au system. Describe what would be seen as a sample of the alloy is heated from 900 to 1100 ^{o}C.

Marks 3



Marks 5

- The diagram below shows the structure of an oxide of rhenium. The unit cell is cubic with rhenium at each of the corners and oxygen in the centre of each of the edges.



● = Re ○ = O

What is the chemical formula of this oxide?

Answer:

What are the coordination numbers of rhenium and oxygen in this compound?

Re:	O:

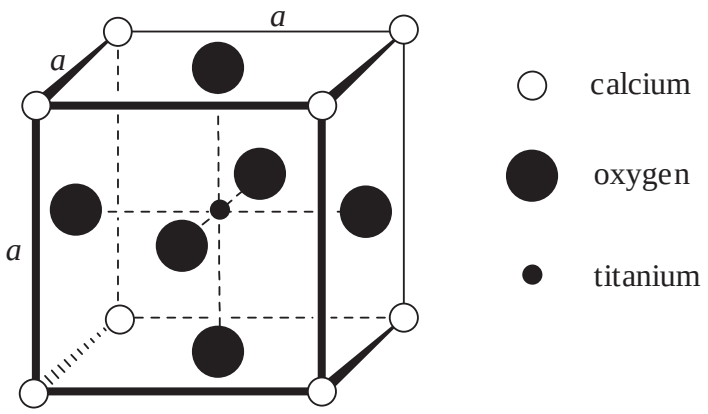
There is a large hole at the centre of the cell that in some compounds is occupied by a cation. What is the coordination number of a cation occupying this site?

Given that the density of this oxide is 7.1 g cm^{-3}, calculate the length of the cell edge. (The structure is cubic.)

Answer:

Marks 5

- The diagram below shows the structure of perovskite, a mineral made up of calcium (at each of the corners), oxygen (in the centre of each of the faces), and titanium (at the centre of the cube). The unit cell dimension (edge length, *a*) for perovskite is 0.38 nm.



What is the chemical formula of perovskite?

Answer:

What is the volume of the unit cell?

Answer:

What is the density of perovskite? Give your answer in g cm^{-3}.

Answer:

	Marks
• Many elemental metals crystallise in one of three cubic forms, either with a face-centred cubic, a body-centred cubic or a simple cubic unit cell. Explain the main differences and similarities between these different crystalline forms.	**3**