Skills to Develop

- Recognize a unit cell.
- Use geometry to correlate atomic radius with unit cell edge length.
- Calculate parameters relevant to crystal chemistry.

The Model for Polonium Crystal Structure

If you always consider atoms to be spherical, you certainly will consider a simple cubic structure very unstable. The unit cell of such a structure is cubic, and the origin can be the center of an atom. One such sphere is placed in the diagram here, and you may complete the diagram by placing 7 more spheres at the 7 corners. We do not encounter simple cubic structures with one atom per unit cell often. However, one phase of polonium called alpha polonium has been reported to have such a structure by Beamer and Maxwell in 1946, and they re-affirm the result in 1949.

This so called primitive or simple cubic structure in the packing of spheres contains only one atom per cubic unit. do not take these words for granted, work it out yourself from the diagram shown here or one you have completed. Since correlating atomic radius with the unit cell edge of this structure is simple, we use it as a model of teaching. We ask you to calculate some relevant crystal parameters of this model.

Example 1

The alpha polonium is primitive cubic with a cell edge of 335 pm. Show the following:

- the six neighboring \(\text{Po}\) atoms form an octahedron around the central \(\text{Po}\) atom with \(\text{Po-Po}\) distances of 335 pm.
- the radius of the \(\text{Po}\) atom is 168 pm.
- the packing fraction = 0.52.
- the density of \(\text{Po}\) is 9.23 g/cc.

SOLUTION

You are supposed to work on this problem. In case you have difficulty, some hints are given here to help you. These hints are given in such a way that you can work on them.

- Draw the unit cell as described in the problem. The diagram here is a good start, but complete it yourself.
- Mark \(R\) and and work out the cell edge length in \(R\).
- You should remember the formula for volume of spheres of radius \(R\):

\[
(V_{\text{sphere}} = \frac{4}{3} \pi R^3)
\]

- Since cell edge length \(a = 2R\), \(V_{\text{unit cell}} = (2R)^3 = 8R^3\)
- Packing fraction \(\frac{V_{\text{sphere}}}{V_{\text{unit cell}}}\)
Derive the simplified formula above, do not let your calculator do unnecessary calculations.

- Density $\left(= \frac{209}{6.023 \times 10^{23}} \text{(6)}\right)$ and convert to proper units.

**DISCUSSION**

**Packing fraction** is the fraction of space occupied by the spherical atoms in the structure.

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**Confidence Building Questions**

1. **Simple cubic packing is not common. The only example of this type of structure is polonium, Po. How many atoms per unit cell are there in this structure type?**

   Hint: Simple cubic structure has one atom per unit cell

   **Discussion**
   
   The number of atoms per unit cell for structures resulting from packing are: 1 for simple cubic, 2 for bcc type, 4 for fcc type. The unit-cell edge = 2 r for this structure type.

2. **Alpha polonium has a simple cubic packing, and its cell edge has been determined to be 336 pm. Its molar mass is 209. Calculate its density in g/cm$^3$.**

   **Avogadro’s number = 6.023e23 atoms/mol. (e23 means $10^{23}$)**

   Hint: Density = 9.1 g/mL

   **Discussion**
   
   Density = mass / volume. Use suitable formulas. Only about 52 % of the space is occupied by atoms in simple cubic packing. The density is thus not very high.

3. **Which of the following structures has the highest packing efficiency?**
   
   a. **primitive (simple) cubic packing**
   
   b. **fcc packing**
   
   c. **bcc packing**
   
   d. **diamond structure (see diagram here)**

   Hint: b.

   **Discussion**
   
   The order of packing efficiency in the list is diamond < primitive cubic < bcc < hcp = fcc
   
   The packing efficiencies of fcc and hcp are the same, 74.05%.

4. **How many atoms are there in a body centered cubic packed structure?**

   Hint: two, 2

   **Discussion**
A more general way is to say that there are two lattice points in a body centered lattice. The point is an abstract atom or group of atoms. Generalization may be hard for you. If you find this confusing, do not worry about it.

5. The \(\text{NaCl}\) structure belongs to a face centered lattice. How many \(\text{Na}^+\) ions are there in a unit cell?

Hint: Four each of sodium and chloride ions.

Discussion -
The number of \(\text{Na}^+\) or \(\text{Cl}^-\) is the same as the number of spheres in a fcc packing, \(\text{4Na}^+\) and \(\text{4Cl}^-\) ions, a total of 8 ions per unit cell.

Contributors

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