## Important information needed to understand a crystal structure:

The hard sphere model is usually adopted to represent a crystal structure. Here each sphere represents an ion core. So you need to know the number of nearest-neighbor distance (coordination number), and the packing fraction.

### Nearest neighbor distance:

It is the distance between the centers of two nearest neighboring atoms. This is an important property of the lattice. The number of nearest neighbors is also another important property of lattice and sometimes is referred to as the *coordination number* of the lattice.

Examples:

| Lattice | coordination number |
|---|---|
| Sc | 6 |
| Bcc | 8 |
| Fcc | 12 |
| Diamond | 8 |

## Atomic packing factor (or filling factor or packing fraction):

It is the fraction of space occupied by atoms in a unit cell. It is termed $PF$, which is the ratio of the volume of atoms in a unit cell to the volume of that unit cell related to a given structure under study.

$PF = \frac{v_{atoms}}{V_{cell}} = \frac{n(\frac{4}{3}\pi r^3)}{V_{cell}}$, where $n$ is the number of atoms per unit cell and $V_{cell}$ is the volume of the unit cell. This is another important quantity that shows how tightly atoms are packed in a given structure.

[Note: The radius of sphere (ion core) is half the distance between nearest neighbors in a crystal of a pure element in a $sc$ lattice].

## Packing of atoms in cubic unit cells:

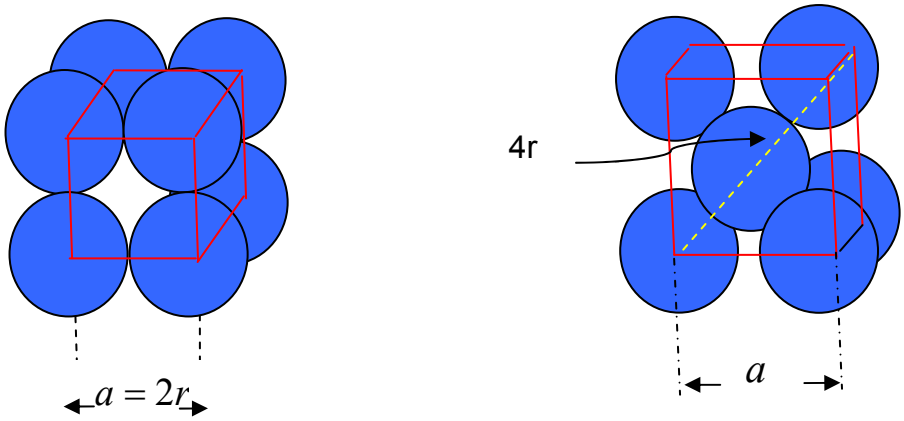


Figure 12:
a) Simple cubic unit cell b) Body-centered cubic unit cell

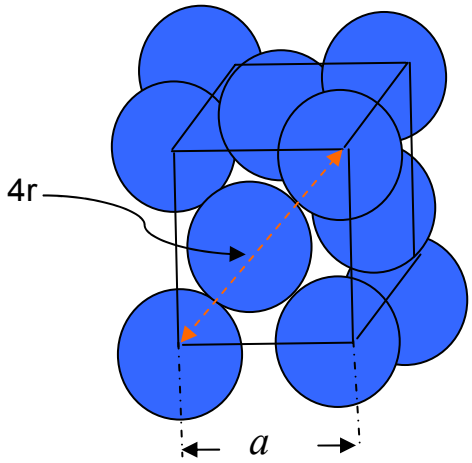


Figure 13: Face-centered cubic unit cell