

structure of crystalline solids

30 Eylül 2024 Pazartesi 09:28

atoms are in a periodic order in a repetitive three dimensional pattern.
atomic array is over large distances, meaning a long range atomic order.
noncrystalline=amorphous

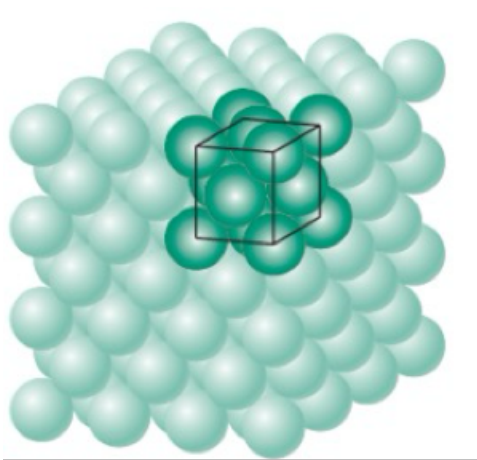
all metals, many ceramics and some polymers are in the crystalline form.

atomic hard sphere model

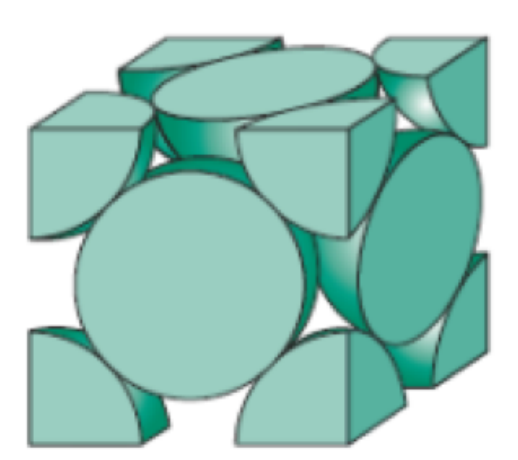
atoms or ions are considered solid spherres having well-defined diameters.
spheres represent the nearest neighbor atoms touching each other.
one cubic structure is a unit cell.
parameters of unit cell:
lengths of threesides and the angles between sides are called lattice parameters.

FACE CENTERED CUBIC STRUCTURE (FCC)

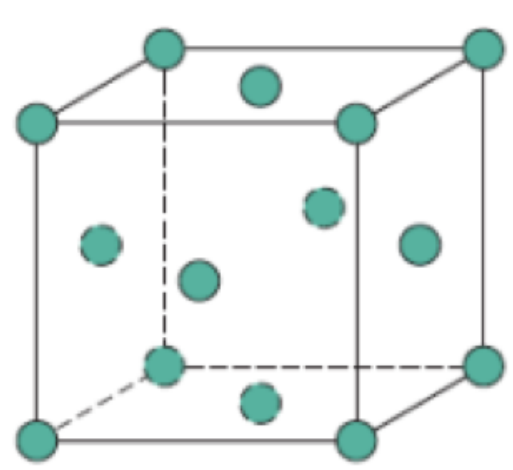
a cubic geometry with atoms located at each orner and centers of the cubes faces.



aggregate of many atoms



hard sphere unit cell



a reduced sphere unit cell

spheres or ion cores touch each other across a face diagonal. the lattice parameter is as follows,

$$a=2R\sqrt{2}$$

a total of four atoms may be assigned to a cell unit

$$6 \times (1/2 \text{ face}) + 8 \times 1/8 \text{ (corner)}$$

atoms
unit cell

4

$\frac{4}{3} \pi R^3$

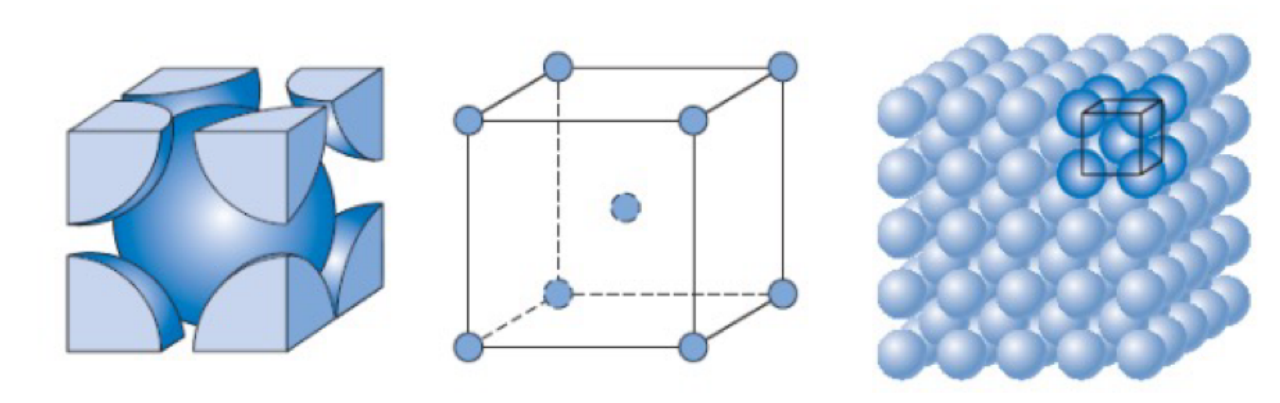
volume
atom

APF =

$\frac{16 R^3 \sqrt{2}}{16 R^3 \sqrt{2}}$

$\text{APF} = \frac{\text{Volume of atoms in unit cell}^*}{\text{Volume of unit cell}}$
*assume hard spheres

BODY CENTERED CUBIC STRUCTURE (BCC)



$$1 \text{ (body)} + 8 \times 1/8 \text{ (corner)}$$

atoms at each corner and one single atom in the center of the cube.

FCC can absorb more energy than BCC. distance between atoms in BCC are larger than FCC. Means it has weaker bonding.

$$a=4R/\sqrt{3}$$

atoms
unit cell

2

$\frac{4}{3} \pi (\sqrt{3}a/4)^3$

volume
atom

APF =

$\frac{a^3}{a^3}$

$\frac{\text{volume}}{\text{unit cell}}$

HEXAGONAL CLOSE PACKED CRYSTAL STRUCTURE (HCP)

instead of a cubic, there is also a hexagonal unit cell geometry. top and bottom surfaces form a hexagon and surround a single atom in the center.
The equivalent of six atoms is contained in each unit cell; one-sixth of each of the 12 top and bottom face corner atoms, one-half of each of the 2 center face atoms, and all 3 midplane interior atoms.

