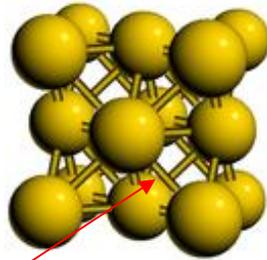


Face-Centered Cubic Lattice

Crystalline solids are those solids, unlike amorphous solids, that have a regular and repeating arrangement of atoms. Each of these crystalline solids consists of a unit cell which is a small group of atoms that contain unique features. When a large number of these unit cells are stacked together, they form a macroscopic crystal. The three cubic crystal types are the simple cubic lattice (primitive cubic), body-centered cubic, and the face-centered cubic. The face-centered cubic unit cell is shown below.



An atom has been added at the center of each face of the unit cell.

The line joining opposing face corner atoms are called face diagonals.

The length of a side of the unit cell, a , is called the lattice constant. An important feature of a crystal structure is the nearest distance between atomic centers (nearest-neighbor distance) and for the face-centered cubic this distance is $a/\sqrt{2}$.

A face-centered cubic lattice has eight lattice points where a lattice point is defined as a point of intersection of two or more grid lines. Each lattice point, eight in the diagram above, is a "site" for an atom to reside. **However, the unit cell above does not contain 8 atoms but only 1.** When considering cubic lattices, one must always think in terms of 3-D. Atoms at the corners of any cube are shared by 8 contiguous units cells, so only $1/8$ of an atom is attributed to a single lattice point. Therefore,

$$1/8 \text{ atom/lattice point} \times 8 \text{ lattice points} = 1 \text{ atom}$$

Each face of the unit cell contains an atom at its center and the atom is shared between two adjacent cells meaning that only $1/2$ of an atom is attributed to a unit cell. Therefore,

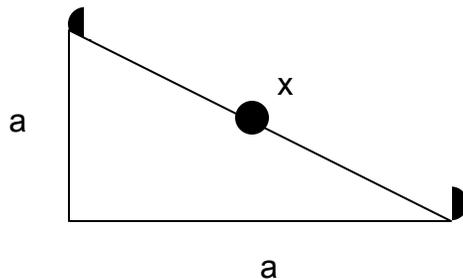
$$1/8 \text{ atom/lattice point} \times 8 \text{ lattice points} + 1/2 \text{ atom/face} \times 6 \text{ faces} = 4 \text{ atoms}$$

An interesting property of a face-centered cubic is that of packing efficiency where

$$PE = V_a/V_{uc} \times 100\%$$

and V_a is the volume of the atoms occupying the interior of the cell and V_{uc} is the volume of the unit cell.

To determine the volume of the atoms contained within the interior of the cells, first start with the diagram of a diagonal which passes through the atom at the center of the face.



$$x^2 = a^2 + a^2 = 2a^2$$

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

$$x = 4r$$

$$4r = \sqrt{2} a$$

$$r = \sqrt{2} a/4$$

Now substituting for r in the formula for the volume of a sphere gives:

$$V_a = 4/3 \cdot \pi \cdot r^3 \cdot Z$$

$$V_a = 4/3 \cdot \pi \cdot (\sqrt{2} a/4)^3 \cdot 4 = 0.74a^3$$

$$V_r = a \cdot a \cdot a = a^3$$

$PE = 0.74a^3/a^3 \times 100\% = 74\%$ which applies to all face centered cubic cells.

An interesting application for crystal lattices is that if you know the atomic radius of an element along with its unit cell structure, then it is possible to calculate the density of that element. For example:

Determine the density of lead given that it has a face centered cubic structure and an atomic radius of 175 pm.

$$D = m/V$$

$$m = 4 \text{ Pb-atoms} \times 207.20 \text{ g Pb}/1 \text{ mol-Pb} \times 1 \text{ mol-Pb} / (6.02 \times 10^{23} \text{ Pb-atoms})$$

$$m = 1.38 \times 10^{-21} \text{ g Pb}$$

$$r = \sqrt{2} a/4$$

$$a = 4 \times 175 \text{ pm} \times 10^{-10} \text{ cm/pm} / \sqrt{2} = 4.95 \times 10^{-8} \text{ cm}$$

$$D = (1.38 \times 10^{-21} \text{ g}) / (4.95 \times 10^{-8} \text{ cm})^3 = 11.4 \text{ g/cm}^3$$

This is in excellent agreement with the listed density of lead.

The graphic used in this tutorial was taken from the Crystal Lattice Structures Web page, <http://cst-www.nrl.navy.mil/lattice/> provided by the Center for Computational Materials Science of the United States Naval Research Laboratory.