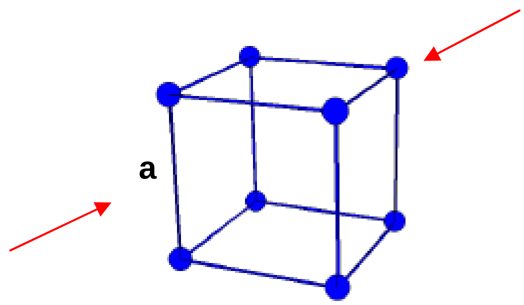
<u>Simple Cubic Lattice</u>

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 simple cubic unit cell is shown below.

lattice point



The length of each side is **a** (2r) where r is the radius of the atom at the lattice point.

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 primitive cubic this distance is **a**.

A simple 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 atom/~~lattice point~~ × 8 ~~lattice points~~ = 1 atom

An interesting property of primitive cubic cells 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.

$V_a = 4/3 \bullet \pi \bullet r^3 \bullet Z$ where r is the atomic radius and Z the number of atoms contained within the unit cell.

$V_r = l \bullet w \bullet h = w \bullet w \bullet w = (2r)^3 = 8r^3$

$PE = 4/3 \bullet \pi \bullet \cancel{r^3} \bullet Z/8\cancel{r^3} \times 100\% = 52\%$ which applies to <u>all</u> primitive cubic cells.

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.