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**FUNDAMENTAL CONCEPTS**

Solid materials may be classified according to the regularity with which atoms or ions are arranged with respect to one another. A **crystalline** material is one in which the atoms are situated in a repeating or periodic array over large atomic distances; that is, long-range order exists, such that upon solidification, the atoms will position themselves in a repetitive three-dimensional pattern, in which each atom is bonded to its nearest-neighbor atoms. All metals, many ceramic materials, and certain polymers form crystalline structures under normal solidification conditions. For those that do not crystallize, this long-range atomic order is absent; therefore solid materials found in nature in crystalline (single crystal and polycrystalline) and noncrystalline (amorphous).
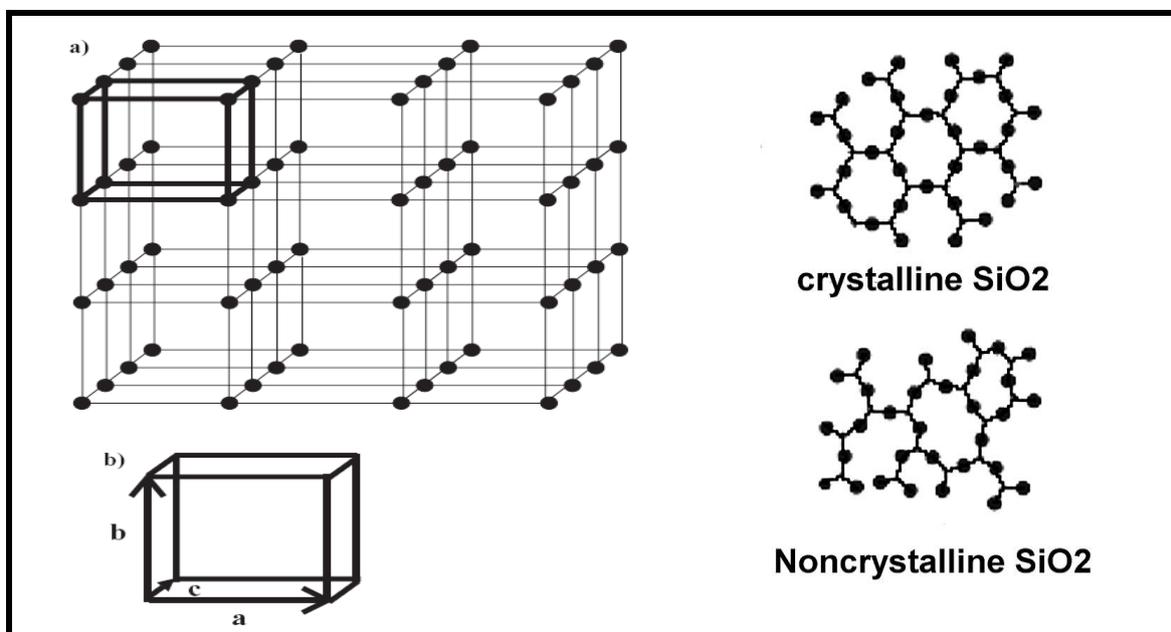
Some of the properties of crystalline solids depend on the **crystal structure** of the material, the manner in which atoms, ions, or molecules are spatially arranged. There is an extremely large number of different crystal structures all having long-range atomic order; these vary from relatively simple structures for metals to exceedingly complex ones, as displayed by some of the ceramic and polymeric materials. The present discussion deals with several common metallic crystal structures. When describing crystalline structures, atoms (or ions) are thought of as being solid spheres having well-defined diameters. This is termed the *atomic hard sphere model* in which spheres representing nearest-neighbor atoms touch one another. In this particular case all the atoms are identical. Sometimes the term **lattice** is used in the context of crystal structures; in this sense "lattice" means a three-dimensional array of points coinciding with atom positions (or sphere centers). Lattice to be an array of points in space so arranged that each point has identical surroundings. The smallest unit, or **unit cell**, can be obtained by constructing planes

through points, and the lines resulting from the intersection of the planes at lattice points define the unit cell. Figure above shows a unit cell in darker outline and defined by the **cell** parameters **a**, **b**, **c** and angles (not shown) α, β, γ called **lattice** parameters. The angles are defined where α is the angle between vectors **a** and **b**, β the angle between **a** and **c**, and γ is the angle between **b** and **c**. It should be noticed that the unit cell so defined embodies the symmetry of the entire lattice. The entire lattice can be generated by simply translating the unit cell by |**a**| in the **a** direction, by |**b**| in the **b** direction, and by |**c**| in the **c** direction.
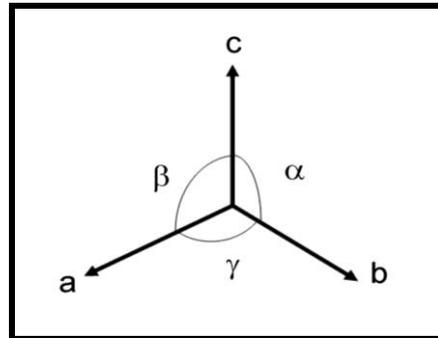

Thus translation becomes an important operation in understanding the long-range ordering represented by the lattice. The question as to how many different kinds of unit cells are necessary to fill all space by translation and how to accomplish this for all possible symmetries is a solved mathematical question for which we herein accept the solution without proof. The lattices that accomplish this task are called **Bravais lattices**, and there are **14** such Bravais lattices, as shown in Figure. These (14) Bravais lattices are organized into**7** crystal systems according to the basic symmetry that the lattice possesses: **cubic, trigonal, hexagonal, orthorhombic, rhombohedral, monoclinic, and triclinic.** Some of these systems can have different lattices: simple or primitive (**P**), body centered (**BC**), and face centered (**FC**). The number of lattice points for a unit cell, **N**, is calculated by counting the points that bound and are interior to the cell and then considering the sharing of points by adjacent cells. For example, the eight lattice points at the cell corners in the unit cell in Figure above are each shared by eight adjacent cells (**Nc**), the points on the face of a cell by two cells (**Nf**), and of course, the interior points (**Ni**) belong solely to the cell in question. Hence the following relationship summarizes this:

$$N = Ni + \frac{Nf}{2} + \frac{Nc}{8}$$

Therefore **N** for **SC, FCC** and **BCC** are: **1**, **4**, and **2** respectively.
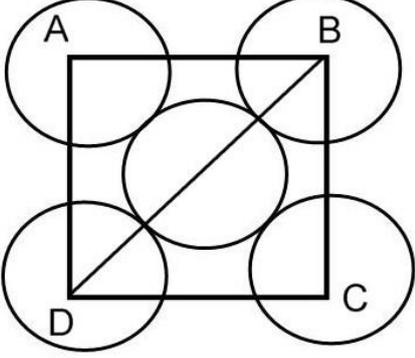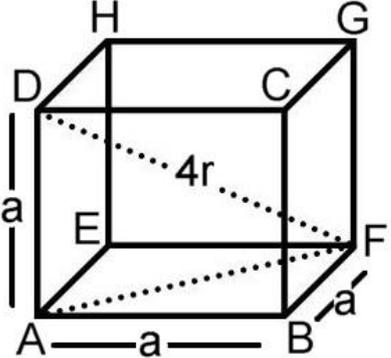
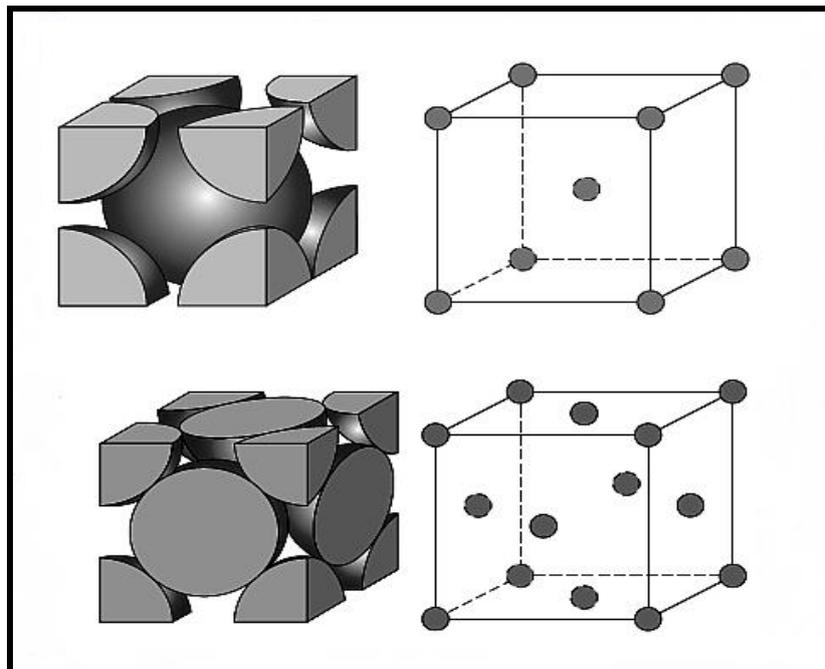| Crystal System	Unit Cell Vectors	Unit Cell Angles
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$
Hexagonal (trigonal)	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$
Monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90° \neq \gamma$
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$
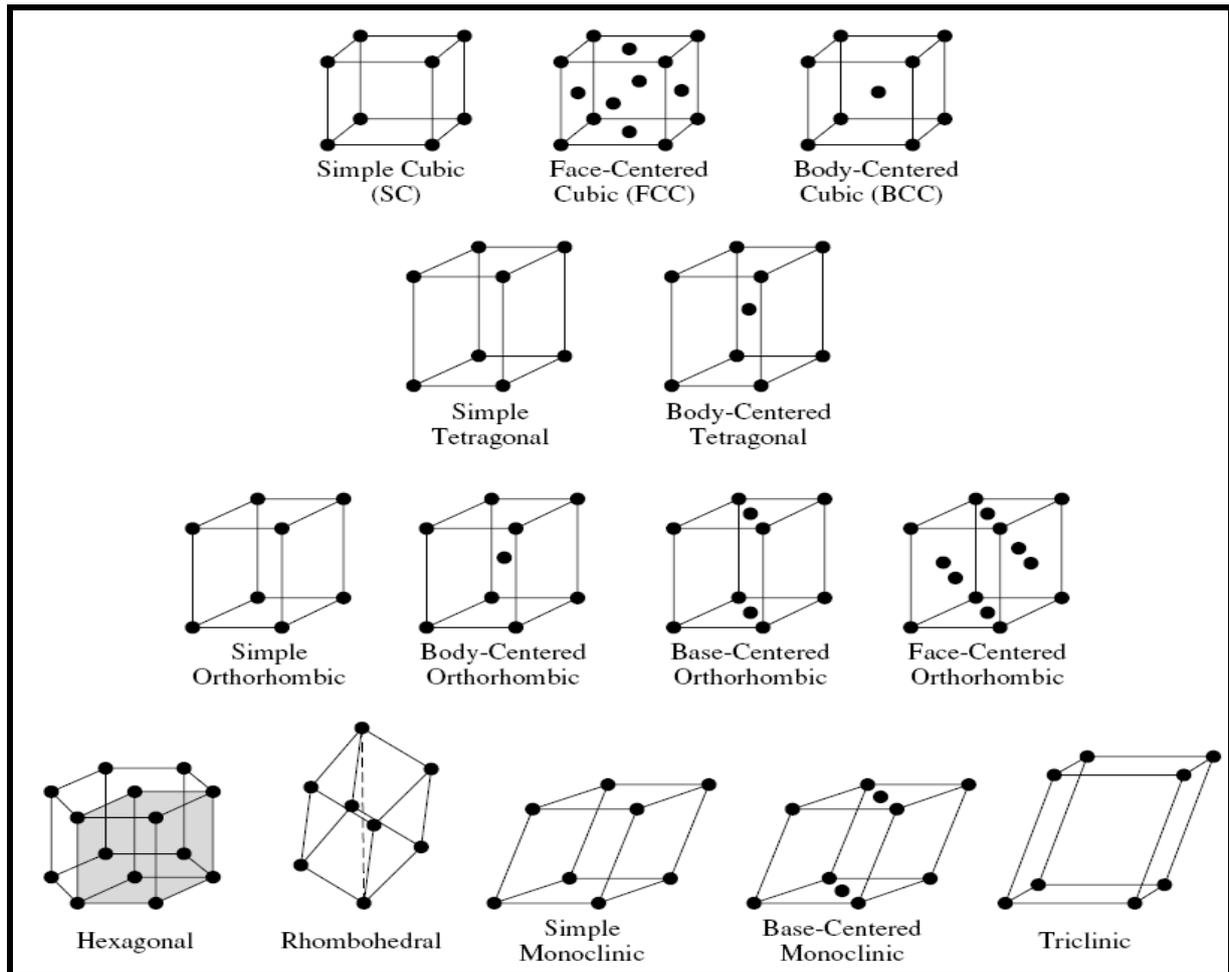
Calculation the volume of the unit cell

The calculation of volume of unit cell depending in facts that the atoms considered as sphere geometry also we consider the side of cubic system **a** there for the cubic side of **FCC** and **BCC** structure drive as the following:

$(BD)^2 = (DC)^2 + (CB)^2$	$(DF)^2=(DA)^2+(AF)^2$
$(4r)^2 = a^2 + a^2$	$(4r)^2=a^2+2a^2$
$4r = \sqrt{2}\, a$	$4r = \sqrt{3}\, a$
$a = \dfrac{4r}{\sqrt{2}}$	$a = \dfrac{4r}{\sqrt{3}}$
(FCC)	*(BCC)*

Two other important characteristics of a crystal structure are the **coordination number** and the **atomic packing factor (APF).** For metals, each atom has the same number of nearest-neighbor or touching atoms, which is the coordination number. For **face-centered cubic**, the coordination number is **12** and for **body centered cubic 8** and **simple cubic 6**. This may be confirmed by examination of Figure above for FCC; the front face atom has four corner nearest-neighbor atoms surrounding it, four face atoms that are in contact from behind, and four other equivalent face atoms residing in the next unit cell to the front, which is not shown. The APF is the sum of the sphere volumes of all atoms within a unit cell (assuming the atomic hard sphere model) divided by the unit cell volume—that is:

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$$APF = \frac{vol.\,of\,atoms\,per\,unit\,cell}{vol.\,of\,unit\,cell}$$

$$APF = \frac{No.\,of\,atoms \times Volume\,of\,one\,atom}{vol.\,of\,unit\,cell}$$

As an example the APF for FCC structure calculated as follow:

Vol. of atoms per unit cell= $(4) \times \frac{4}{3}\pi r^3$

Vol. of unit cell = $(a)^3 = 16\,r^3\sqrt{2}$
Therefore the APF for FCC =0.74   and for BCC is 0.68, SC is 0.52 (prove)

Depending on crystal structure we can simply calculated theoretical density as:

$$\sigma = \frac{n \times A}{Vc \times Na}$$

Where **n** is the no. of atoms per unit cell, **A** atomic weight, **Vc** vol. of unite cell and **Na** Avogadro's no.

As an example calculate the density of copper with an atomic radius **0.128 nm**, atomic weight **63.5 g/mol** and with FCC structure.

$$\sigma = \frac{n \times A}{Vc \times Na} \ldots = \frac{(4\,atoms/unit\,cell \times 63.5g/mol)}{[16\sqrt{2} \times (1.28 \times 10^{-8}\,cm)^3/unit\,cell] \times (6.023 \times 10^{23}\,atoms/mol)} = 8.89 g/cm^3$$

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