Example below explores the nature of the bonds found in silica.

Examples

How Do Oxygen and Silicon Atoms Join to Form Silica?

Assuming that silica (SiO_2) has 100% covalent bonding, describe how oxygen and silicon atoms in silica (SiO_2) are joined.

SOLUTION

Silicon has a valence of four and shares electrons with four oxygen atoms, thus giving a total of eight electrons for each silicon atom. Oxygen has a valence of six and shares electrons with two silicon atoms, giving oxygen a total of eight electrons.

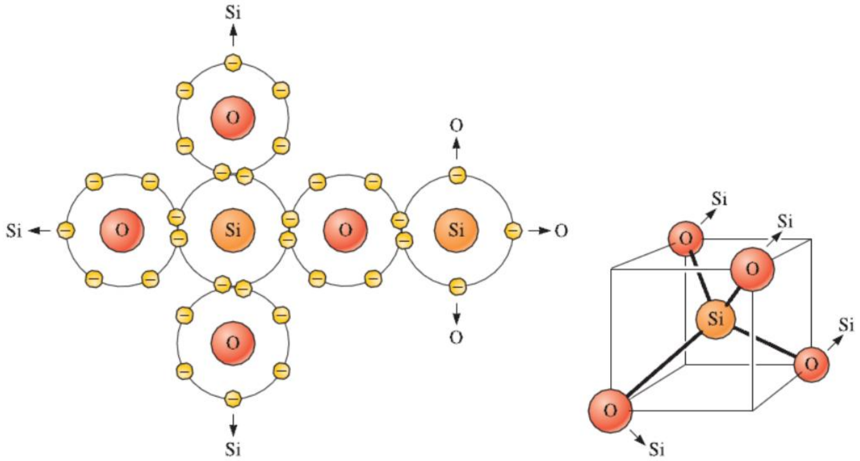


Figure: illustrates one of the possible structures. Similar to silicon (Si), a tetrahedral structure is produced.

Determining if Silica is Ionically or Covalently Bonded

In a previous example, we used silica (SiO_2) as an example of a covalently bonded material. In reality, silica exhibits ionic and covalent bonding. What fraction of the bonding is covalent? Give examples of applications in which silica is used.

SOLUTION

From Figure A, the electronegativity of silicon is 1.8 and that of oxygen is 3.5. The fraction of the bonding that is covalent is

$$\text{Fraction covalent} = \exp[-0.25(3.5 - 1.8)^2] = 0.486$$

Although the covalent bonding represents only about half of the bonding, the directional nature of these bonds still plays an important role in the eventual structure of SiO_2.

Silica has many applications. Silica is used for making glasses and optical fibers. We add nanoparticles of silica to tires to enhance the stiffness of the rubber.

High-purity silicon (Si) crystals are made by reducing silica to silicon.

Ionic and ionic arrangements

The term **defect** refers to a lack of perfection in atomic or ionic order of crystals and not to any flaw or quality of an engineered material. these atomic level defects actually enable the development of formable, strong steels used in cars and buildings, aluminum alloys for aircraft, solar cells and photovoltaic modules for satellites, and many other technologies.

Short range order versus long rang order

In different states of matter, we can find four types of atomic or ionic arrangements (see figure below).

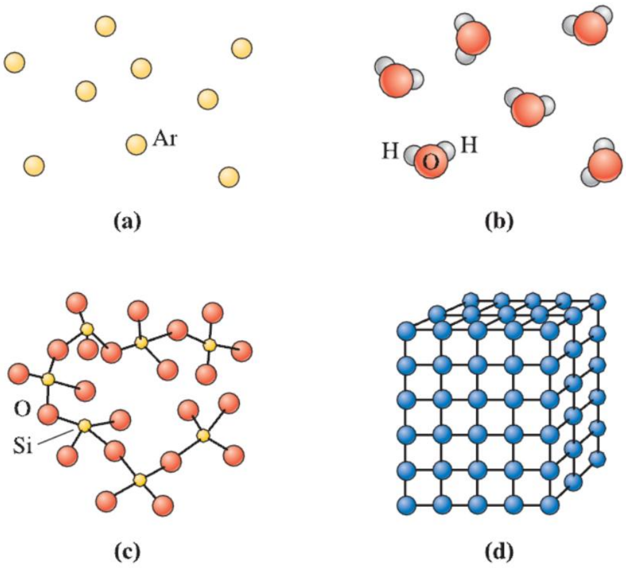


Figure :Levels of atomic arrangements in materials: (a) Inert monoatomic gases have no regular ordering of atoms. (b,c) Some materials, including water vapor, nitrogen gas, amorphous silicon, and silicate glass, have short-range order. (d) Metals, alloys, many ceramics and some polymers have regular ordering of atoms ions that extends through the material.

Short-Range Order (SRO) A material displays short-range order (SRO) if the special arrangement of the atoms extends only to the atom’s nearest neighbors.

Each water molecule in steam has short-range order due to the covalent bonds between the hydrogen and oxygen atoms; that is, each oxygen atom is joined to two hydrogen atoms, forming an angle of 104.5° between the bonds. There is no long-range order, however, because the water molecules in steam have no special arrangement with respect to each other’s position.

Many polymers also display short-range atomic arrangements that closely resemble the silicate glass structure. Polyethylene is composed of chains of carbon atoms, with two hydrogen atoms attached to each carbon. Because carbon has a valence of four and the carbon and hydrogen atoms are bonded covalently, a tetrahedral structure is again produced [Figure below]. Tetrahedral units can be joined in a random manner to produce polymer chains.

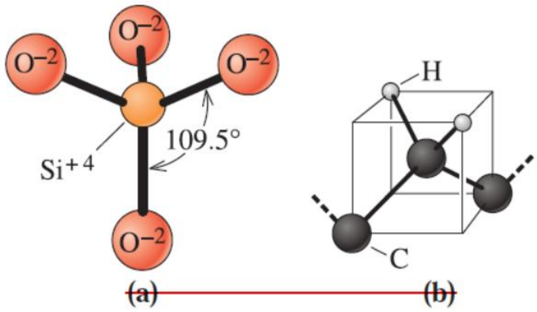


Figure : Basic Si-O tetrahedron in silicate glass. (b) Tetrahedral arrangement of C-H bonds in polyethylene.

Long-Range Order (LRO) Most metals and alloys, semiconductors, ceramics, and some polymers have a crystalline structure in which the atoms or ions display **long-range order (LRO)**; the special atomic arrangement extends over much larger length scales ~ 7100 nm. The atoms or ions in these materials form a regular repetitive, grid-like pattern, in three dimensions. We refer to these materials as **crystalline materials**.

If a crystalline material consists of only one large crystal, we refer to it as a *single crystal*. Single crystals are useful in many electronic and optical applications.

For example, computer chips are made from silicon in the form of large (up to 12 inch diameter) single crystals [Figure below].

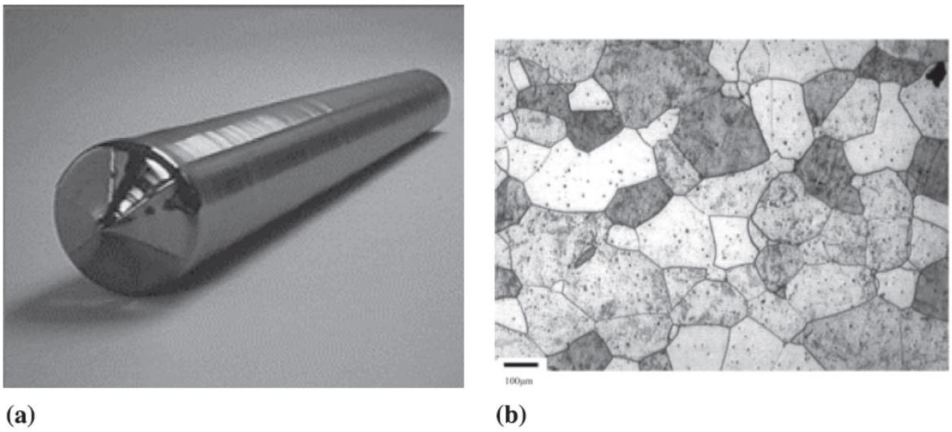


Figure:(a) Photograph of a silicon single crystal. (b) Micrograph of a polycrystalline stainless steel showing grains and grain boundaries

Certain types of turbine blades may also be made from single crystals of nickel-based superalloys. **A polycrystalline material** is composed of many small crystals with varying orientations in space. These smaller crystals are known as **grains**. The borders between crystals, where the crystals are in misalignment, are known as **grain boundaries** Figure b above shows the microstructure of a polycrystalline stainless steel material.

Many crystalline materials we deal with in engineering applications are polycrystalline (e.g., steels used in construction, aluminum alloys for aircrafts, etc.).

Liquid crystals (LCs) are polymeric materials that have a special type of order. Liquid crystal polymers behave as amorphous materials (liquid-like) in one state. When an external stimulus (such as an electric field or a temperature change) is provided, some polymer molecules undergo alignment and form small regions that are crystalline, hence the name “liquid crystals.” These materials have many commercial applications in liquid crystal display (LCD) technology.

CRYSTAL STRUCTURES

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,

Crystal structure of the material, the manner in which atoms, ions, or molecules are spatially arranged.

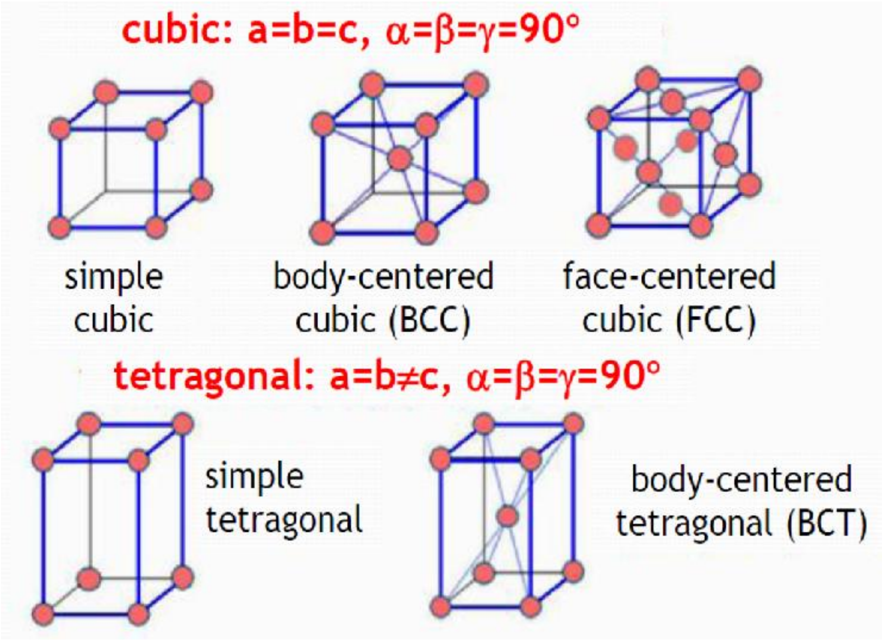
Unit cell: is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within. Convenience usually dictates that parallelepiped corners coincide with centers of the hard sphere atoms. we generally use the unit cell having the highest level of geometrical symmetry.

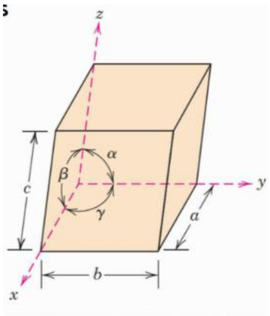
Non-crystalline or Amorphous : random arrangement of atoms

Crystal Systems

The unit vectors *a*, *b* and *c* are called lattice parameters (Figures, below).

Based on their length equality or inequality and their orientation (the angles between them, α, β and γ) a total of 7 crystal systems (cubic, tetragonal, hexagonal, orthorhombic, rhombohedral, monoclinic, triclinic) can be defined. With the centering (face, base and body centering) added to these, 14 kinds of 3D lattices, known as ***Bravais lattices***, can be generated.





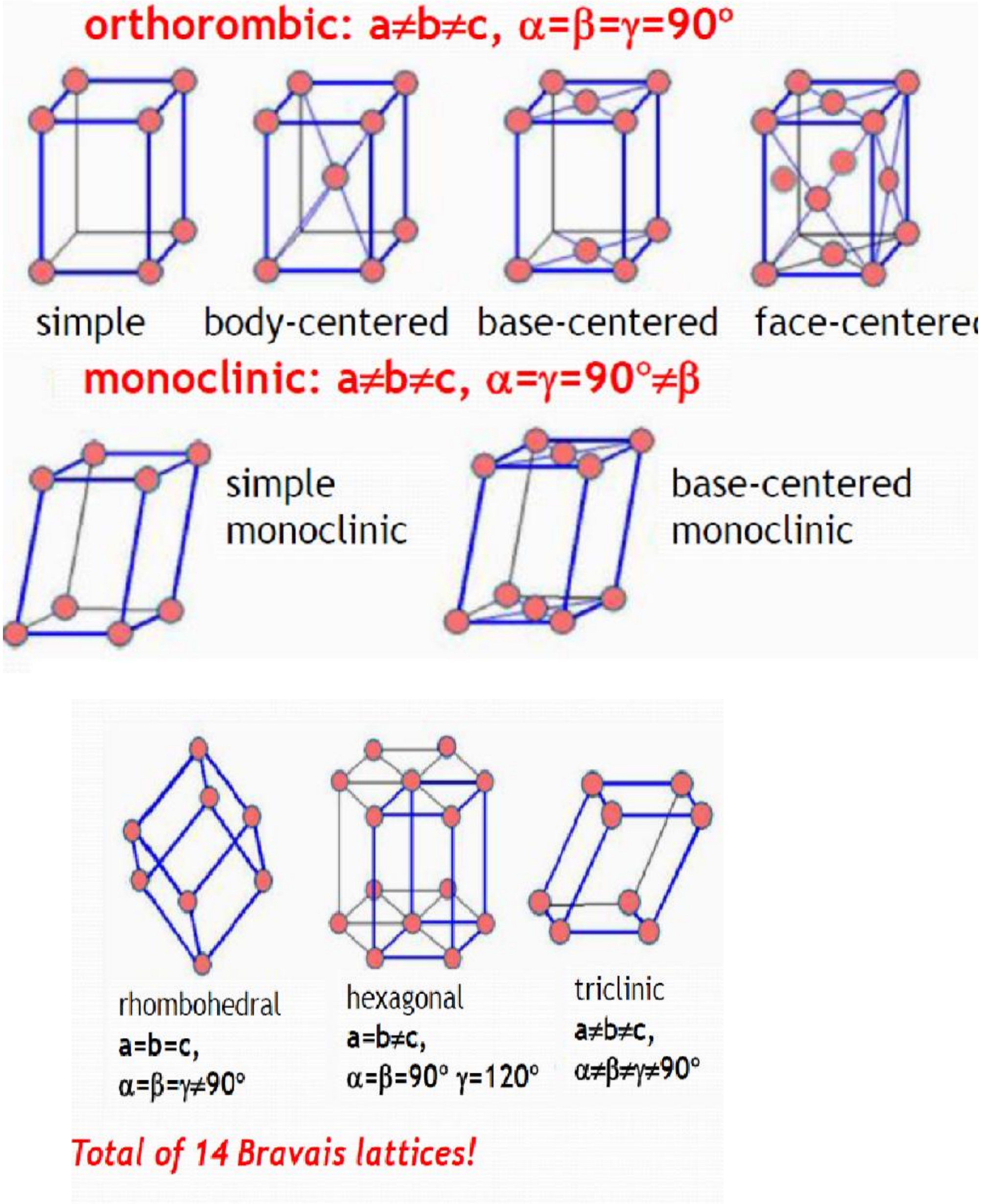


Figure : crystal systems