

1.Bravais Lattices

12.1. The Bravais lattices

2.2.4 Bravais Lattice detail

The Bravais lattice are the distinct lattice types which when repeated can fill the whole space. The lattice can therefore be generated by three unit vectors, a_1 , a_2 and a_3 and a set of integers k , l and m so that each lattice point, identified by a vector r , can be obtained from:

$$\vec{r} = k\vec{a}_1 + l\vec{a}_2 + m\vec{a}_3 \quad (12.1.1)$$

In two dimensions there are five distinct Bravais lattices, while in three dimensions there are fourteen. These fourteen lattices are further classified as shown in the table below where a_1 , a_2 and a_3 are the magnitudes of the unit vectors and \mathbf{a} , \mathbf{b} and \mathbf{g} are the angles between the unit vectors.

Name	Number of Bravais lattices	Conditions
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\mathbf{a} \neq \mathbf{b} \neq \mathbf{g}$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\mathbf{a} = \mathbf{b} = 90^\circ \neq \mathbf{g}$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\mathbf{a} = \mathbf{b} = \mathbf{g} = 90^\circ$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\mathbf{a} = \mathbf{b} = \mathbf{g} = 90^\circ$
Cubic	3	$a_1 = a_2 = a_3$ $\mathbf{a} = \mathbf{b} = \mathbf{g} = 90^\circ$
Trigonal	1	$a_1 = a_2 = a_3$ $\mathbf{a} = \mathbf{b} = \mathbf{g} < 120^\circ \neq 90^\circ$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\mathbf{a} = \mathbf{b} = 90^\circ, \mathbf{g} = 120^\circ$

12.2. Cubic lattices

Cubic lattices are of interest since a large number of materials have a cubic lattice. There are only three cubic Bravais lattices. All other cubic crystal structures (for instance the diamond lattice) can be formed by adding an appropriate base at each lattice point to one of those three lattices. The three cubic Bravais lattices are the simple cubic lattice, the body centered cubic lattice and the face centered cubic lattice. A summary of some properties of cubic lattices is listed in the table below:

Lattice type	Number of lattice points/atoms per unit cell	Nearest distance between lattice points	Maximum packing density	Example
Simple cubic	1/1	a	$\pi/6 = 52 \%$	Phosphor
Body centered cubic	2/2	$a\sqrt{3}/2$	$\pi\sqrt{3}/8 = 68 \%$	Tungsten
Face centered cubic	4/4	$a\sqrt{2}/2$	$\pi\sqrt{2}/3 = 74 \%$	Aluminum
Diamond	4/8	$a\sqrt{2}/2$ Nearest distance between atoms: $a\sqrt{3}/4$	$\pi\sqrt{3}/16 = 34 \%$	Silicon

Cubic lattices have the highest degree of symmetry of any Bravais lattice. They belong to the (m3m) symmetry group, which contains the following symmetry groups and operations:

Symmetry group	Symbol	Symmetry Operations
Identity	1	
Three equivalent axis of two-fold rotation	3[2]	[100], [010], [001]
Six equivalent axis of four-fold rotation	6[4]	[100], [010], [001], [-100], [0-10], [00-1]
Six equivalent axis of two-fold rotation	6[2]	[110], [101], [011], [1-10], [10-1], [01-1]
Eight equivalent axis of three-fold rotation	8[3]	[111], [11-1], [1-11], [-111], [-1-1-1], [-1-11], [-11-1], [-111]

rotation		$11-1$, $[1-1-1]$
Inversion	-1	
Three equivalent mirror planes	$3[m]$	$[100]$, $[010]$, $[001]$
Six equivalent axis of four-fold rotation with inversion	$6[-4]$	$[100]$, $[010]$, $[001]$, $[-100]$, $[0-10]$, $[00-1]$
Six equivalent mirror planes	$6[m]$	$[110]$, $[101]$, $[011]$, $[1-10]$, $[10-1]$, $[01-1]$
Eight equivalent axis of three-fold rotation with inversion	$8[-3]$	$[111]$, $[11-1]$, $[1-11]$, $[-111]$, $[-1-1-1]$, $[-1-11]$, $[-11-1]$, $[1-1-1]$

Note that the $(m\bar{3}m)$ symmetry group is the highest possible symmetry group associated with a cubic crystal. A limited symmetry of the basis (the arrangement of atoms associated with each lattice point) can yield a lower overall symmetry group of the crystal.

12.3. Simple cubic lattice

The simple cubic lattice consists of the lattice points identified by the corners of closely packed cubes.

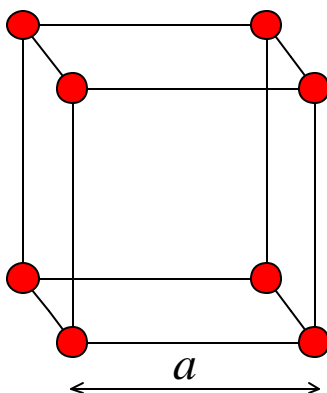


Figure A12.3.1 The simple cubic lattice.

The simple cubic lattice contains one lattice point per unit cell. The unit cell is the cube connecting the individual lattice points. The atoms in the picture are shown as an example and to indicate the location of the lattice points. The maximum packing density occurs when the atoms have a radius, which equals half of the side of the unit cell. The corresponding maximum packing density is 52 %.

12.4. Body centered cubic lattice

The body-centered lattice equals the simple cubic lattice with the addition of a lattice point in the center of each cube.

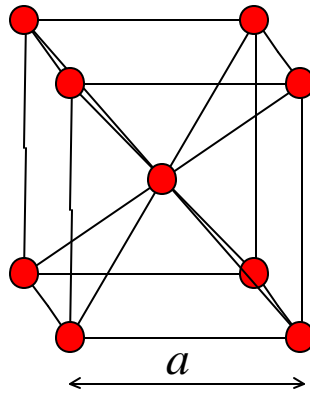


Figure 12.4.1 The body-centered cubic lattice.

The body centered cubic lattice contains two lattice point per unit cell. The maximum packing density occurs when the atoms have a radius, which equals one quarter of the body diagonal of the unit cell. The corresponding maximum packing density is 68 %.

12.5. Face centered cubic lattice

The face centered lattice equals the simple cubic lattice with the addition of a lattice point in the center of each of the six faces of each cube.

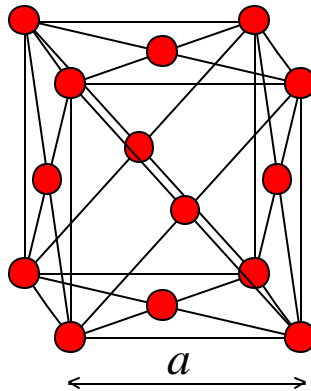


Figure 12.5.1 The face centered cubic lattice.

The face centered cubic lattice contains four lattice points per unit cell. The maximum packing density occurs when the atoms have a radius, which equals one quarter of the diagonal of one face of the unit cell. The corresponding maximum packing density is 74 %. This is the highest possible packing density of any crystal structure as calculated using the assumption that atoms can be treated as rigid spheres.

12.6. Diamond lattice

The diamond lattice consists of a face centered cubic Bravais point lattice, which contains two identical atoms per lattice point. The distance between the two atoms equals one quarter of the body diagonal of the cube. The diamond lattice represents the crystal structure of diamond, germanium and silicon.

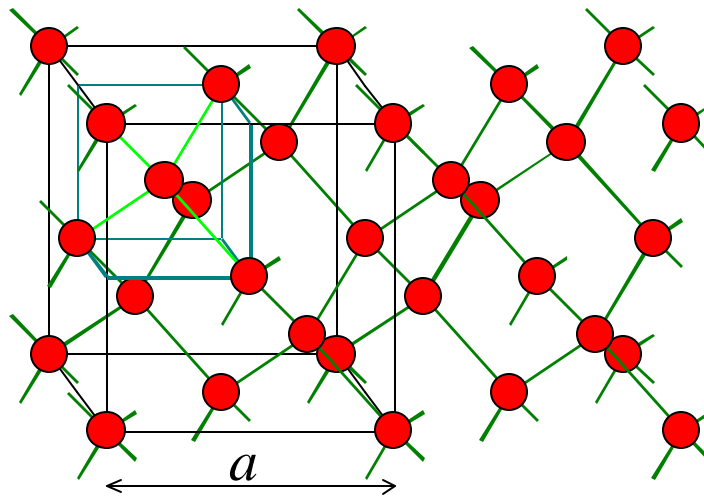


Figure A12.6.1 The diamond lattice of silicon and germanium

The diamond lattice contains also four lattice points per unit cell but contains 8 atoms per unit cell. The maximum packing density occurs when the atoms have a radius, which equals one eighth of the body diagonal of the unit cell. The corresponding maximum packing density is 34 %.

12.7. Zincblende lattice

The zincblende lattice consists of a face centered cubic Bravais point lattice, which contains two different atoms per lattice point. The distance between the two atoms equals one quarter of the body diagonal of the cube. The diamond lattice represents the crystal structure of zincblende (ZnS), gallium arsenide, indium phosphide, cubic silicon carbide and cubic gallium nitride.

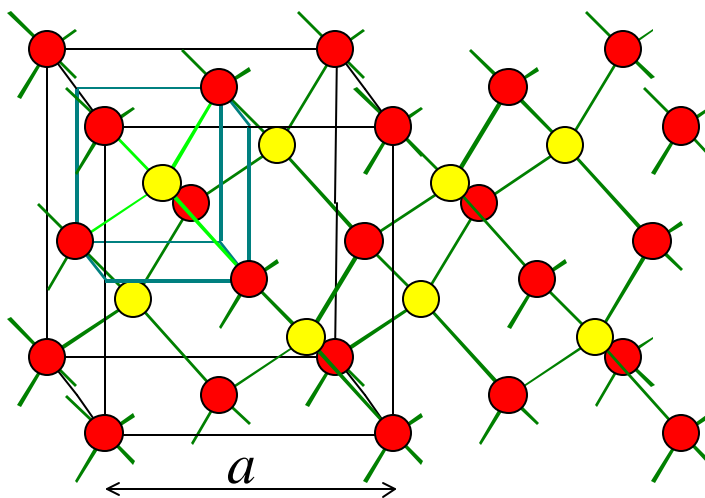


Figure A12.7.1 The zinc-blende crystal structure of GaAs and InP

12.8. Crystal models

Make your own model of a cubic crystal and a C₆₀ (carbon 60 bucky ball) molecule. Print the pdf files and follow the assembly instructions.